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SANTA CRUZ

STRONG CORRELATIONS IN LATTICE MODELS

A dissertation submitted in partial satisfaction of the
requirements for the degree of

DOCTOR OF PHILOSOPHY

in

PHYSICS

by

Daniel Hansen

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The Dissertation of Daniel Hansen
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Table of Contents

List of Figures	v
Abstract	xvi
Dedication	xvii
Acknowledgments	xviii
1 Introduction	1
Bibliography	4
2 1D Hubbard with Mott Transition	5
2.1 Introduction	5
2.2 Mean Field	9
2.3 An Integrable Model of Mott Transitions	15
2.3.1 U-independent Symmetries	16
2.3.2 Diagonalization and Phase Diagram	19
2.3.3 Double Occupancy	30
2.3.4 New Ground States	30
2.4 Summary	35
Bibliography	36
3 Level Statistics in Ansatz Matrices	39
3.1 Introduction	39
3.2 Defining quantum integrable models	43
3.2.1 The Ansatz Matrices	45
3.2.2 The maximal case and the connection with Gaudin/BCS	49
3.3 Numerical Results	51
3.3.1 Spectral Observables	53
3.3.2 Three Crossovers	59

3.3.3	Placing the results in a single framework	75
3.3.4	Type dependence of the basis operator statistics	76
3.4	Analytical results	76
3.4.1	Analytic unfolding	77
3.4.2	α	79
3.4.3	Statistics of $E_m^{(i)}$ in Type 1	80
3.4.4	Type $M > 1$	85
3.4.5	How a linear superposition quickly leads to Poisson statistics . .	87
3.4.6	Crossover scaling by perturbation	89
3.5	Summary	91
Bibliography		93
4	Split Hubbard Bands at Low Density	94
4.1	Motivation and Introduction	94
4.2	Ladder Scheme Equations at Low Density	97
4.2.1	Low density limit and self energy sum rule	99
4.2.2	The Atomic Limit	102
4.2.3	Emergence and structure of the Split bands of Hubbard	102
4.2.4	Frequency Dependent Self energy	106
4.2.5	Momentum occupancy	112
4.3	Doublons and their dynamics	114
4.3.1	Doublon Decay in the low density limit	114
4.3.2	Exact Solution of the Doublon Decay Problem for Two Particles.	116
4.4	Conclusions	122
4.A	Exact correlation functions for the two particle Hubbard Model	122
Bibliography		127
5	Spectral Functions of the t-J model by ECFL Formalism	130
5.1	Motivation	130
5.2	The Model	132
5.3	Explicit equations and the Zero source limit in Fourier space	136
5.3.1	Exact equations: reduced vertex function	137
5.3.2	To $O(\lambda^2)$ Theory	138
5.4	Computation of Spectral Functions	142
5.4.1	GGG-type Convolutions	144
5.4.2	FFT Hilbert Transform	149
5.5	Results	149
5.5.1	ARPES: Dispersion and Lineshapes	153
5.5.2	Electron pocket and a possible source of quantum oscillations . .	162
5.5.3	Optics	164
Bibliography		174

List of Figures

2.1	This figure relates to the perturbation J_2 within MFT. The zero field order parameter persists independent of the field strength until a critical value is reached. The curve through the transition points was obtained independently of the magnetization curves by plotting the zero field x of a given U against the λ where the bands first touch for that U and $x(U)$. That is, the transition occurs precisely when the field causes the bands to touch.	12
2.2	These curves relate to the perturbation J_3 in MFT. They are smooth functions of λ and U , showing no critical behavior in contrast to those shown above. Also, for weak interaction, the field strengths which maximize the density of states at the Fermi level result in sharp peaks in the order parameter.	14
2.3	As the field strength of H_{I_3} is increased at $U=0$, the simple Hubbard band is distorted until the Fermi line is finally broken into three Fermi segments when $\lambda = 1/3$. This also occurs when $\lambda = -1$	21
2.4	Above some critical field the Fermi line is broken at half filling.	22
2.5	As the field strength of H_{I_2} is increased at $U=0$, the simple Hubbard band is distorted until the Fermi line is finally broken into two Fermi segments.	23
2.6	Above some critical field the Fermi line is broken at half filling.	24
2.7	For finite rings the Lifshitz transition occurs at a slightly higher field than that predicted in the thermodynamic limit. This plot shows that for the case of $N_s = 6$, adjacent single particle states do not become degenerate until well after the thermodynamic dispersion curve has developed new minima.	25
2.8	Here we have a phase diagram in λ and U which shows that we can transition away from the Mott insulating ground state as we move away from the U -axis. Dashed contours represent transitions without any change of symmetry. The $U < 0$ half of the diagram can be obtained by a $\hat{Z}_\uparrow$ transformation of the top half. Unless otherwise indicated in the diagram the symmetry is that of the Mott state: $p=S=L=0$	26

2.9	Comparing with the equivalent diagram for the 6 sited ring we see that although there is a higher complexity here, the same general structure persists. Namely, we still observe a central phase which exists above the Lifshitz transition point. However, since the range of the L and S quantum is increased by the added sites and particles, we see a greater number of states. It is particularly interesting the transition on the left side of the Lifshitz zone which had no change of symmetry for the case of $N_s = 6$, is now broadened into an entirely new phase which does have a different symmetry.	28
2.10	As in the previous diagram, the $U < 0$ region can be obtained by $\hat{Z}_\uparrow$ transformation but here we can obtain the negative λ by a reflection transformation(Reflection is not a symmetry because of the field's odd parity). In this diagram, there is no general trend toward a particular order. The spin and charge orders are in competition so neither prevails over the entire quadrant. The quantum numbers of each region are given here: A=($p = 1, S = 0, L = 1$), B=($p = 3, S = 0, L = 1$), C=($p = 2, S = 0, L = 0$), D=($p = 0, S = 1, L = 0$), Mott=($p = S = L = 0$).	29
2.11	The integrability of the model allows level crossings between states of the same symmetry. This is seen here as a discontinuity in the expectation value of the Hubbard Hamiltonian as the field strength is increased. Adding a small perturbation which breaks no symmetries but does break the integrability we find that certain discontinuities become smooth. This indicates that a level crossing has become an avoided crossing. Only those transitions without change of symmetry can become smooth.	30
2.12	The plot on the left is typical of the system for large U: as the field strength is increased, the doublon expectation will also increase. Furthermore, this increase is accompanied by an increase in the L quantum number. The plot on the right shows the doublon expectation for U=1. We see that the transition actually reduces the charge order. This transition is one of those with no change in symmetry.	31
2.13	Although the Mott insulator and Lifshitz zone share the same symmetry, the two states respond quite differently to changes in the interaction. In the Mott state, double occupancy decreases monotonically as U is increases. The Lifshitz phase exhibits a qualitatively different behavior.	33

- 2.14 For a 8 sited ring, the phase diagram has a small sliver of a third ground state between the classic Mott insulator and the Lifshitz phase. This sliver has the quantum number $L=1$, while the other two states have $L=0$. This change in the charge ordering between the Mott insulator and the sliver explains the existence of a doublon persisting to high U in the sliver phase. Thus, we can say that the sliver phase is actually another Mott insulator which has a different symmetry than the first but the same general behavior. The Lifshitz phase exhibits behavior very similar to that seen in the same phase of the 6 sited ring. Namely, it shows doublons persisting to high U without the protection of charge ordering. 34
- 3.1 The Brody function $P(s)$ and the rigidity $\Delta(L)$ as computed for an uncorrelated spectrum (Red) which exhibits Poisson behavior and a correlated spectrum which comes from the eigenvalues of a real symmetric matrix. In each panel the red curves (points) show the GOE behavior while the blue curves (points) show the Poisson behavior. The error bars show typical variances of the function. The Brody parameter ω_B and α will interpolate smoothly between these functions providing a means of measuring intermediate spectral statistics. 60
- 3.2 With constant γ and both ε_m and d_m chosen from the GOE we can observe x dependent crossovers in the level repulsion. At very small x , the level repulsion of H and $h^{(i)}$ will match the statistics of the input parameters, d_m and ε_m respectively. As x is increased, the generic behavior of Type 1 matrices takes over, the level repulsion of H drops to zero. At a higher value of x the level repulsion of $h^{(i)}$ increases through a similar monotonic crossover. The crossovers occur at different values of x . The N dependence of the crossover scale is plotted in Fig. (3.4). 61
- 3.3 For type 1 matrices with ε_m and d_m of GOE, impact of the choice of constant vs random γ is displayed for $N=500$. For an arbitrary H , the spectral statistics are unchanged whereas the statistics of the basis operators become more repulsive at large x when the γ_k 's are chosen as a constant value. Whatever mechanism is working to increase level repulsion in the basis operators has no impact on the general matrix which is Poisson in any case for large x 62

- 3.4 The position of the crossover has a smooth dependence on the dimension N . The red squares show the crossover position extracted from the logarithmic tanh fits for the basis operator statistics. The blue circle show the Brody parameter averaged over generic matrices. In all cases the matrices were built using ε_i and d_i from the GOE with constant γ . The position of the $h^{(i)}$ crossover has no dependence on the matrix dimension. It is very well fit as a constant, $x_0 = 1.01$. The position of the crossover for a general Ansatz matrix, H , is well fit by $1.47N^{-1}$. These fits are shown as the superposed curves. From the scaling we learn that the region where a generic type 1 matrix is non-Poisson vanishes as N goes to infinity. In this sense, we can call the non-Poisson regions a finite size effect. Each point represents averaging over 10 instances. 63
- 3.5 When d_k are chosen to be some power of ε_k the spacing statistics will not be Poisson in general. They inherit the level repulsion of ε_k . There are many points where d_k 's and ε_k 's are correlated. We perturb around one such point with a finite delta which blurs the correlation between the d 's and ε 's. Consequently the statistics of T eventually return to the generic Poissonian case. The crossover has the same logarithmic tanh function form that was seen in the x dependent crossover of Fig. (3.2). In Fig. (3.6) the crossover scale is plotted against the matrix dimension. The scaling indicates that the non-Poisson regions vanish in the thermodynamic limit. 68
- 3.6 The δ -crossover is fit with a tanh function and the scale of the crossover is extracted. The fit shows that the crossover occurs at $\delta \sim O(N^{-1})$. This is the same scaling which was observed for the x -dependent crossover. 69
- 3.7 We plot the Brody parameter for basis operators in the limit of large x . The matrices were constructed with constant γ_m and ε_m of the GOE. As we have seen in earlier figures, the level repulsion of the basis operators is bounded below by the repulsion of ε_m . For constant γ we see that at low types the Brody parameter is greater (about 2 as compared to 1 which we would normally expect of the GOE) than that of ε but it decays (roughly exponentially) with increasing type. 72

- 3.8 Above we plot the Brody parameter parameter for high type matrices as a function of L where L is the dimension of the subspace within which the linear combination is taken. In each case $N=500$. The curves are types 1 (Red Circle), 480 (Blue Square), and 497 (Brown Triangle). Besides the dimension and type noted in the figure, all other parameters are chosen in the same way. For each value of L we compute 50 instances and average the results. In each case, ω_B appears to decay roughly exponentially at low L . Consequently, the statistics have nearly fallen to the Poisson limit by $L \approx 10$. The type $M=497$ case shares this decay but never reaches Poisson statistics because it runs out of basis operators at $L=3$. We also include a set of Empty Red Circles which are from type 1 matrices where the basis operators included in the superposition are built from the lowest L ε_i . Because of this choice, the statistics do not decay as in the case where the L operators are chosen at random. In this case it will require $L \sim O(N)$ to achieve Poisson statistics. Note however that the error bars of the filled red circles overlap with those of the empty circles. 73
- 3.9 Above we plot the rigidity parameter α for high type matrices as a function of L where L is the dimension of the subspace within which the linear combination is taken. In each case $N=500$. The curves are types 1 (Red Circle), 480 (Blue Square), and 497 (Brown Triangle). Besides the dimension and type noted in the figure, all other parameters are chosen in the same way. For each value of L we compute 50 instances and average the results. In each case, α appears to decay roughly exponentially at low L . Consequently, the statistics have nearly fallen to the Poisson limit by $L \approx 10$. The type $M=497$ case shares this decay but never reaches Poisson statistics because it runs out of basis operators at $L=3$. As compared to Fig. (3.8) the error bars are much wider and there is 74
- 3.10 Comparison of α with constant and random γ for a type 1 matrix with $N=500$ and ε_m of the GOE. On the Right is the case of constant γ . There is clear trend from low to high in the α dependence. The difference between neighboring α is $\ll 1$. With random γ this trend is still present to some extent but the scatter is $O(1)$ 80

- 3.11 This plot shows the eigenvalues of a type 1 matrix for $L=1,2,3$. The ε are GOE, constant γ , and x is large. In the $L=1$ case, there is a wide smooth region where the E_m is simultaneously ordered with m . This implies that the level repulsion of E_m will be comparable to that of λ . As L is increased, the spectrum gets chopped up into a series of branches by the various singularities. There is now no guarantee that into large segment of the E_m spectrum will be simultaneously ordered with m . Ordering E_m requires a complicated shuffling of the index m . Consequently any short range correlations in λ will be significantly diminished in E_m . As L increases, the shuffling step becomes more severe because there are ever more branches being shuffled together to reach an ordered E_m . This will inevitably randomize the spectrum leading to Poisson spacing statistics. Surprisingly, this process occurs very fast ($L \approx 10$ assuming the singularities are well spread out). There is no dependence on type in this behavior. 89
- 4.1 The zeroth moment of the self energy versus the density normalized to the exact value $U^2 \times \frac{n(2-n)}{4}$. This data is in 2-dimensions with $U=10, W=2$. The inset shows the k independence of the sum rule along the (11) direction for the case $n=.04$, with variations in the sixth significant figure. . . 101
- 4.2 High frequency (UHB) DOS in 2D, $U=10, n=1/20$; As the hopping is decreased, the UHB feature does not become narrow, but rather maintains a width of $O(U)$. The sharp k -dependent features narrow as the hopping decreases. The broad continuum is essentially k -independent, showing very little dependence on the hopping in the limit of strong coupling. In this limit, the UHB becomes completely independent of the bandstructure. In Fig. (4.3) the broad UHB of the full band can be seen with the Hubbard-1-like G_1 superimposed. In G_1 , the UHB feature is broadened only by η and the LHB is suppressed for clarity. 103
- 4.3 2D, $U=10, W=2.5, n=1/20$; The spectral function at three values of the wave vector $(0,0)$, $(\frac{\pi}{2}, \frac{\pi}{2})$, (π, π) , in blue, red and gold colors. Besides the quasiparticles we observe three features emerging in each spectral function. Most obvious is the UHB feature which lies at a $\omega \approx O(U)$ and integrates to a weight of $n/2 + O(n^2)$. This feature is dramatically broadened in the self consistent G also becoming less k -dependent. On each edge of the quasiparticle band we observe small dispersing features. Ref.([15]) have previously identified the negative frequency feature as a 2-hole antibound state while Ref.([22]) has discussed a particle-hole antibound state just above the quasiparticle band. These features are essentially unchanged in going from G_1 to the exact G 105

4.4	2D, $U=.25$, $U=10$, $W=2$, $n=.049$. The local $\rho_\Sigma(\omega)$ divided by U versus ω . The two chosen values of U are in the weak coupling (blue $U = .25$) and strong coupling (red $U = 10$) ranges respectively. We see at the lowest temperatures that the the self energy curves overlap when scaled by U displaying a characteristic quadratic dip at the chemical potential.	107
4.5	The local self energy spectrum in 2D, $U=10$, $W=2$, $n=.05$ The log scale plot shows the full scale of the UHB. The inset highlights the quadratic minimum at low energies. The quadratic minimum drops below the scale of η so it can be said to represent an infinite lifetime.	108
4.6	The 2D DOS i.e. the momentum averaged spectral function $\rho_G(\vec{k}, \nu)$ and the momentum averaged $\rho_\Sigma(\vec{k}, \nu)$. The LHB feature is the sharp peak near $\omega \sim 0$. The UHB feature in the DOS is nearly invisible here but lies just below the feature in ρ_Σ scaled down by a factor of ω^2 . The real part of the self energy for $\omega \geq 0$ initially drops linearly with frequency over a range $W \ll \omega \sim \frac{U}{2}$, as required in the limit of extreme correlations [24, 26]. It then flips at the threshold of the UHB, rising across the range of the UHB until at the highest energy it begins to decay down towards the Hartree term at infinite energy.	109
4.7	The integrated spectral weight over the UHB is called $m_3(k)$. It is plotted here for $\frac{W}{U} = 1.6, .56, .196, .0686, .024, .0085$. In this case $n=.15$. We observe that the weight of the UHB exceeds $n/2$ and becomes flat as U/W tends to infinity.	110
4.8	From the convolution structure of $\rho_\Sigma(k, \omega)$ we see that the local objects of Σ and Γ are related by the ratio $n/2$ when $\omega > W$ for all values of W/U . In the strong coupling limit where the upper band is essentially independent of k , this relationship will be approximately true for each wavevector. On the negative frequency side, the thermal function act differently such that the ratio for $\omega < -W$ is approximately $(1 + \frac{n}{2})$.	111
4.9	1D $U=10$ $W=.56$ (dashed), $W=.196$ (solid), $n=.15$ 1d $T=.005$. Here m_1 is essentially the zero temperature quasiparticle occupation, while m_2 accounts for the LHB particle addition spectrum, The sharp step in occupation occurs precisely at the Luttinger Fermi surface which satisfies the Luttinger Ward sum rule. The sum of m_1 and m_2 is less than one due to the weight transferred to the upper band. The total lower band weight approaches $1-n/2$ as U/W goes to infinity.	113
4.10	The doublon dynamics breaks into two regimes: a sharp decay at early times followed by a long exponential tail. The magnitude of the initial decay depends strongly on the density. In the limit $n \rightarrow 0$ the initial decay disappears, indicating that the UHB is comprised of sharp features only in the limit of vanishing density. In the right panel, the U dependence of the long time decay is shown, it slows down and is finally limited by the level broadening η assumed in our numerics.	115

4.11	The inset shows that $\gamma(1, t_r)$ goes to zero at early times since there is no mechanism to hop at small times. On a longer time scale we see the development of an exponential decay. The small magnitude of the correlation is due to fact that the UHB is largely k-independent.	116
4.12	Doublon decay on a cubic lattice with $U = 15$ and $W = 12$. The shape of $ \gamma_U(Ut_r) ^2$ (red curve) initially deviates slightly from the exact numerical result (blue curve) due to the neglect of the γ_L term, which decays much more quickly than the UHB contribution.	119
4.13	Doublon decay on a cubic lattice with $U = 5$ and $W = 12$. In the case $U < W$, it is much more difficult to find an exact analytical form, so only the numerical result is displayed.	120
4.14	Two theoretical calculations, from ladder diagrams of Eq. (4.19) in 2-dimensions (blue) and the exact 2 particle solution from Eq. (4.21) and Eq. (4.33) in 2- and 3- dimensions (red and gold). These are compared to the experiment Eq. (4.22) in 3-dimensions (green), scaled to coincide at weak coupling by a factor 26.4. The theory and experiment are in very different limits of physical parameters, but have a similar shape except at large U/t	121
5.1	In scheme A, we find that the ECFL equations are already nearly selfconsistent over a wide range of densities. At low densities $ Q /(n/2) < 1/15$ indicating that the error in the particle sumrule is on the order of 5%. Beyond $n \approx .6$ the ratio $ Q /(n/2)$ grows steadily so that we can identify $n = .6$ as the upper limit for the validity of the $O(\lambda^2)$ ECFL equations.	151
5.2	In scheme B, γ is used as a free parameter to fix the second level particle sumrule, Eq. (5.37). The figure shows γ for the case $J = 0, t' = -.4$ at low temperature on 1D, 2D, and 3D square lattices. In all three cases γ rises linearly from zero before falling back toward zero at $n = 1$. For comparison note that the exact γ is $n/2$ (straight line) while to $O(\lambda)$ $\gamma = n/2 - \lambda(n/2)^2$ (curve). The inset shows the ratio of lower Hubbard band spectral weight to the exact value. It is found that at low densities the spectral function has nearly the correct weight. At densities greater than $n=.65$ the violation becomes greater than 20% and thus places a limit on the range of validity of scheme B.	152

5.3	The dispersion $x_0\varepsilon_k$ at $n = .3$ is very narrow compared to the bare bandwidth, 8t. $x_0 = .43$ and $.44$ for the low (T=104K) and high (T=288K) temperature, respectively. The solid curves depict T=104K and the dashed depict 288K. However, the QP peaks actually lie on a much smaller bandwidth due to the action of $\bar{\Phi}$ which dynamically renormalizes the dispersion $x_0\varepsilon_k$. The location of the peaks, E_k , has its own temperature dependence which arises from the temperature dependence of $\text{Re}\bar{\Phi}$. While x_0 is a k-independent rescaling of the bandwidth, the reduction due to $\text{Re}\bar{\Phi}$ is not. This causes the bandwidth to shrink and change shape. A minimum appears near (π, π) . The bandwidth of E_k is approximately 1/5 of the bare bandwidth, 8t.	155
5.4	As in Eq. (5.3) we plot the dispersion $x_0\varepsilon_k$ and E_k in this case for a density of $n=.6$. While x_0 is similar to $n = .3$, E_k is significantly more narrow at this higher density due to differences in the $\text{Re}\bar{\Phi}$ between the two densities. Furthermore the nascent pocket near $k = (\pi, \pi)$ is more prominent with respect at this density as compared to the total bandwidth of E_k	156
5.5	We plot the location of the peak of the physical spectral function, $\rho_{\mathcal{G}}$ (Black) and the location of the two half maxima (Blue Dotted), as well as the energy E_k from Eq. (5.63) (Red Dashed). The skew in the lineshapes translates to the nonsymmetric location of the black line relative to the blue dotted lines. This is more clear in Fig. (5.9) where we plot the computed lineshapes.	157
5.6	The linewidths of the QP peaks change very little in the presence of a finite J . The Fermi surface does not move and the linewidths are nearly the same as in the case where $J = 0$. This plot has all of the same parameters as Fig. (5.8) except for J	158
5.7	This plot compares the $J = 0$ and $J = .3$ cases for a single wavevector outside of the Fermi surface at T=480K and $n=.6$ with a next neighbor hopping $t'=-.4t$. The QP is not shifted or significantly broadened. However, a fraction of the background spectral weight has been shifted to higher frequencies. This result is typical for wavevectors outside the Fermi surface. Close to the Fermi surface, the effect of J is less.	159
5.8	We plot the location of the peak of the auxiliary spectral function, $\rho_{\mathbf{g}}$ (Black) and the location of the two half maxima (Blue Dotted), as well as the energy E_k from Eq. (5.63) (Red Dashed). The skew in the lineshapes translates to the nonsymmetric location of the black line relative to the blue dotted lines. This is more clear in Fig. (5.9) where we plot the computed lineshapes.	161
5.9	The lineshapes of the auxiliary and physical spectral functions are shown together for $k = k_f$ and $k = (\pi, \pi)$. For the smaller magnitude of k the caparison factor shifts the background spectral weight toward negative frequency. Near $k = (\pi, \pi)$ the background spectral is transfered toward positive frequencies.	162

- 5.10 The renormalized dispersion E_k which denotes the vanishing of the real part of the $\mathcal{G}$ is shown to evolve as a function of density. With increased density the bandwidth becomes quite narrow and an electron pocket forms near the (π, π) point at a density near $n=1/2$. This crossing is accompanied by a rise in the occupation n_k near (π, π) . Similar pockets form in 1D at $k = \pi$ and in 3D at $k = (\pi, \pi, \pi)$. Variants of scheme A have been explored for which this crossing is moved toward higher density by decreasing γ . At a low enough value of γ the pocket will cross back over the chemical potential and be unoccupied. 166
- 5.11 In scheme B γ is used as a selfconsistency parameter to fix the sumrule Eq. (5.37). Consequently, the dispersion renormalization factor (x_0) and the static part of $\mu(k)$ are both different than in scheme A. Here we plot the dispersion E_k for scheme B. As in scheme A, the dispersion near the X-point bends downward. However, in this case it does not cross the chemical potential even at the highest densities. Nonetheless at finite temperature, there will be a heightened occupation n_k near $k = (\pi, \pi)$ which would be absent if not for this reshaping of the dispersion. . . . 167
- 5.12 In scheme A the point $k = (\pi, \pi)$ drops downward from the top of the band. Near the point $n=.5$ it crosses the chemical potential forming an electron pocket which then grows as a function of density. The figure depicts the fractional of the BZ which is filled by the pocket. A quantum oscillation frequency can be computed for this area through the equation $f = \frac{h}{ea^2} \frac{A}{(2\pi)^2}$ where h is Planck's constant, e is the electron charge and a is the lattice parameter for the Cuprates. This predicts a frequency in the range of $2 * 10^4$ Tesla at the highest densities. The oscillations seen in Cuprates are much smaller and suggest a pocket which occupies only about 2.5% of the Brillouin zone at densities around $n=.9$. The pocket seen in scheme A is an order of magnitude larger. The scheme we call A' adjusts the gamma expansion by some $O(1)$ change and places the critical density of pocket formation at $n=.85$. This results in a much smaller pocket which more accurately predicts the QO frequency near 660T. 168

5.13	In scheme A the dispersion becomes deformed by $\bar{\Phi}$ and a pocket forms near (π, π) . The panel shows the Fermi surface for a series of densities at low temperature (60K) and with a next neighbor hopping $t' = -.4t$ and $J = 0$. The pocket forms at $n=.55$ and grows monotonically with increased density. Note that at $n=.9$ the Fermi volume is quite low. This occurs because at this density the bandwidth has decreased to the extent that this is effectively high temperature. Thus the volume theorem is not strictly satisfied. By altering the density dependence of γ this pocket can be enhanced or diminished. For instance, it is completely absent in scheme B. As noted elsewhere, the highest densities (i.e. $n = .9$) are not as accurate as densities $n < .6$. They are included in this panel to tell a complete story of the evolution of the pocket within scheme A.	169
5.14	In scheme A the point $k = (\pi, \pi)$ drops downward from the top of the band. As a result, the QP occupation has a maximum in this region of the BZ. A feature much like this was found in Ref. ([3]).	170
5.15	In scheme B the dispersion E_k near does dip below the chemical potential to form a Fermi pocket. Nonetheless it has a minimum near (π, π) . Consequently, the QP occupation has a peak in that region because increased portion of the tail of the spectral function will sit at negative frequencies.	171
5.16	The inverse lifetimes for k_f QP's in plotted as a function of temperature for the ECFL along with the momentum averaged inverse lifetime obtained from the optical conductivity. The ECFL has higher k_f scattering rates along the (11) direction than the (10). The temperature dependence is essentially linear until very low temperatures where a quadratic dependence typical of a Fermi liquid takes over. The crossover temperature is at approximately $.02t$ which corresponds to 60K if we take $t=3000K$. In this plot the density is $n = .3$ At higher densities the crossover temperature decreases below our temperature range.	172
5.17	The low frequency dependence of the optical conductivity is Lorentzian-like. From the normalized curve we can extract an effective scattering rate from the width of the Lorentzian. In this case there is negligible temperature dependence over nearly the entire temperature range studied. The slight curvature at low kT is caused by the finite η which is intrinsic to the calculation.	173

Abstract

Strong Correlations in Lattice Models

by

Daniel Hansen

The primary aim of this thesis is to understand the effects of electronic frustration generated by local interactions of the Hubbard U type on a lattice. Specifically we attempt to study the strongly interacting liquid phase of the Hubbard model and the so called extremely correlated phase of the t - J model without any broken symmetries. Of particular interest is the fate of the Fermi Liquid state under the influence of a large U . Exact solutions in solvable limits inform most of the physical intuition. Perturbative methods such as an infinite order calculation in the particle-particle channel ladder expansion yield fruitful results. Finally the non-perturbative field theory of Schwinger is used to generate a calculation scheme for the Green's function of the non-canonical Fermions of the t - J model. Numerical results are compared with important experimental results from the high- T_c Cuprate compounds.

To my parents, David and Ellen,
who were my first teachers,
and my first friends.

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Chapter 1

Introduction

Since the earliest days of Quantum theory it has been observed that periodic structures give rise to behaviors which can be quite different from those seen in continuum models [1]. The phenomenal success of the band theory of solids emerges from the simplest application of periodicity to the electronic wavefunction. To this day however, it is not clear in general what can arise when the atomistic character of the crystalline lattice is passed on to the wavefunction. The essence of the competition between a fluid-like phase and simultaneous atomistic properties is captured by the famous Hubbard Hamiltonian[2]. While this model was originally put forward as a means of explaining Ferromagnetic tendencies in Transition metals it since found wide application.

The discovery of the so called high- T_c Cuprate superconductors by Bednorz and Muller [3] set off a particularly large experimental and theoretical effort in condensed matter physics. It is now commonly held that the normal state of the Cuprate family can be described by a $t-J$ or Hubbard Hamiltonian on a square lattice[4, 5]. Thus, the

theoretical challenge of the Cuprate superconductors lends an immediacy to the general problem of strong correlations on lattices. This document is, more or less, a response to that challenge. Two general strategies are pursued.

The first strategy is to build intuition of strongly correlated states by studying integrable models. The integrable 1-D Hubbard model is particularly appropriate for this kind of study. In chapter 2, I present an exact diagonalization calculation of this model on a finite lattice. Leib and Wu [6] were the first to show that the half filled case is gapped for any finite values of the on-site repulsion U . This occurs in the absence of any broken symmetry and has been termed a Mott Insulator. I demonstrate that a “Mott Transition” can be induced without disturbing integrability by coupling the Hamiltonian to its own dynamical conservation laws which were first constructed by Shastry [7].

In chapter 3, I discuss integrable models at a broader level. Specifically, it has been observed that integrable models differ from non-integrable models in certain correlations within their eigenvalue spectra. The integrable spectra appear to be completely uncorrelated. This behavior can be explained (for a certain subclass of models) due to an explicit parameteriation of prototypically “quantum integrable” blocks which is due to [8] and Owusu et al [9]. Numerical and Analytic results will be presented.

The final chapters present calculations which are more direct in their applicability to real experimental results. In chapter 4 for instance I present a calculation of the single particle Green’s function of the Hubbard model on a square lattice. This calculation incorporates all lowest order diagrams in a low density expansion. It is therefore

accurate at low densities regardless of the value of U . The resultant spectral function shows the development of an “Upper Hubbard Band” at high energies which coexists with the Fermi liquid phase. Furthermore, this spectral function is used to compute the lifetime of “Doublon” excitations which have recently been measured experimentally in gases of cold Fermions.

Finally in chapter 5, I present a calculation of the spectral function of the t - J model on a square lattice. This calculation follows Shastry’s ECFL formalism [10]. While the formalism technically preserves the Fermi liquid state it nonetheless results some interesting renormalizations as compared to bare G . The spectral function is examined in light of Cuprate experiments such as ARPES and recent Quantum Oscillation results.

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Chapter 2

1D Hubbard with Mott Transition

2.1 Introduction

A comprehensive understanding of the Mott Transition has long been a central concern of the Condensed Matter community. Not only is it a highly relevant problem for the physics it describes, it also bears the status of being a prototypical quantum critical point. In recent decades, the realization that a Mott Insulator lies adjacent to the superconducting state in the phase diagram of the cuprates has pushed the question to an even higher level of immediacy.

Recent work has started to examine interesting issues arising from the proximity of Mott insulators to other states, possibly also Mott insulators[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13]. The surface reconstruction of two non-magnetic insulators leads to novel conducting as well as magnetic states, where new quantum states of matter are expected to be realizable. These studies further motivate us to investigate the possible

metalization routes of Mott insulators. The 1D Hubbard model at half-filling ($n=1$) serves as a unique laboratory for the study of Mott Insulators as it is our only non-controversial example of such a state. Our certainty of it's Mottness[14] stems from the 1968 solution by Lieb and Wu[15] by Bethe's method which showed a gapped system for all finite U without *any broken symmetry*. In the intervening years, a vast literature has sprung out of this early solution including a characterization of excited states and a more explicit understanding of the algebraic structure underlying the Hamiltonian including its integrability[16, 17, 18, 19]. The term integrability is used to denote the existence of several (in fact infinite for large systems) conservation laws for the model, which make it solvable by special techniques, such as the Bethe Ansatz. There has been considerable work in exploring the details of these conservation laws in literature[20, 21, 23, 22, 24].

Much theoretical work has been done on the development of the Mott gap under doping (i.e. going away from half filling). This is mainly due to the immediate experimental practicability of chemical doping. Until recently, however, far less attention has been paid to the effect of perturbing fields on gapped correlated systems. We wish to pursue the possibility of a Mott transition in a half-filled Hubbard band where an applied field drives the Mott gap to zero in much the same way a semiconductor may become conducting through Zener breakdown in the presence of a sufficiently strong field. While a straightforward application of an electric field does produce a metallic state, as our preliminary studies indicate, we lose the integrability by this perturbation. One way of retaining integrability is to study the model under twisted boundary conditions[25, 26, 27, 28]. However, this involves the difficult task of solving a time

dependent Schrodinger equation. In this work, we present a time independent perturbation that achieves metalization without destroying the integrability.

The main thrust of this work is to foster an understanding of the perturbed Hubbard model in 1-d, with a special set of perturbing fields (the “smart fields” below). Since these are quite complex in their structure, we first present a very simple version of the perturbations treated within the mean field theory, in order to set the stage for the exact results. In section II, we present a simple mean field calculation where antiferromagnetic order is built into the Hubbard model by hand in order to create a gap at the Fermi surface. This is *not* the Mott gap, but is a caricature of it since we create it through the imposition of broken symmetry. We study the effects on this gap on two added hopping fields which are prototypes of more specialized fields which appear in later sections. In section III we use the dynamically conserved operators of the 1D Hubbard model discovered by Shastry[16, 17, 18] as “smart fields” which can cause only first order transitions. These Hamiltonians are solved exactly on finite rings for $L \leq 8$ after extracting all constants of motion, following Heilmann and Lieb[29] and Yuzbashyan et al[30]. We show a wide variety of ground states in the full parameter space labeling various quantum numbers. In section IV we draw out some connections between the two methods employed, in particular, the role of a Lifshitz transition in the non-interacting limit as the parent of phase transitions in interacting systems.

The method of exact diagonalization succeeds in initiating an understanding of this special family of integrable Hamiltonians in the context of the relevant space-time symmetries. Furthermore, it does so in a transparent manner. We are able to look at

exact phase diagrams with a complete set of quantum numbers. This result requires the diagonalization of all symmetry matrices which is already computationally expensive for $L=10$ where the Hilbert space of a single k -sector is $O(10^4)$. The workhorses of 1-D physics (DMRG, Bosonization) which commonly permit the study of larger systems are for various reasons not well suited to this Hamiltonian.

DMRG has one particularly fatal limitation: it requires open boundary conditions. The 1D Hubbard Model is known to be integrable regardless of its boundary conditions so it is conceivable that a similar search for first order MIT's could be done on an open, perturbed Hubbard chain. However, the explicit form of the conservation laws of the Hubbard model has not been found for the case of the open chain. Therefore, we are confined to the case of periodic boundary conditions. Furthermore, we would like an exact solution.

The use of Bosonization techniques is possible but fails exactly where this system becomes most interesting. Bosonization requires a well-defined Fermi momentum around which low energy bosonic excitations can be described. More explicitly, it is a small U expansion of the Hamiltonian where U must be small compared with the slope of the dispersion at the Fermi momentum. As the Lifshitz transition is approached in the non-interacting limit, the slope of the dispersion goes to zero precisely at the Fermi momentum. Since the small U requirement of this method is made with respect to that value it is not hard to see that Bosonization is untenable. Of course, it may be possible to concoct several different Bosonization schemes to describe the small U behavior for states which appear in different regimes of the smart field coupling strength

(far from the Lifshitz point), but that is exactly the point which makes this Hamiltonian compelling. Bosonization also gives no information about the behavior of the system for intermediate or large U .

2.2 Mean Field

We start from the Hubbard Hamiltonian where we have added an extra coupling constant λ , times a current $\hat{J}_2$.

$$\hat{H} = T \sum_{j=1,\sigma}^L (c_{j\sigma}^\dagger c_{j+1\sigma} + h.c.) + U \sum_{j=1}^L n_{j\uparrow} n_{j\downarrow} + \lambda \hat{J}_2, \quad (2.1)$$

where

$$\hat{J}_2 = -i \sum_{j=1,\sigma}^L (c_{j\sigma}^\dagger c_{j+2\sigma} - h.c.). \quad (2.2)$$

The Hermitian operator $\hat{J}_2$ is similar to the charge current except that the hopping is to next-nearest neighbors only¹. With this form, the added term is analogous to the paramagnetic current term under minimal coupling between the charged system and an electromagnetic field[28]. It biases the system and encourages a flow of charge in one direction over the other.

We know the Hubbard Hamiltonian to have AFM correlations at half filling. To explore the effect of the applied field on these correlations we will simplify the Hubbard interaction term using a mean field description based on this magnetic character of the

¹ $\hat{J}_2$ is later generalized to include a U dependent term so that the new operator is an exact conservation law of the Hamiltonian. This is the consideration that motivates the form of $\hat{J}_2$.

Hubbard ground state. With x as the staggered magnetization order parameter, let us assume

$$\langle n_{j\sigma} \rangle = \frac{1}{2} + \sigma(-1)^j x \quad (2.3)$$

leads to a state that is qualitatively unlike the Mott state in that it breaks a translational symmetry, but it is as close as we can achieve in its average behavior. Using this description of the interaction we apply a Bogoliubov-like transformation to diagonalize the Hamiltonian in a reduced Brillouin zone, $|k| < \pi/2$ which is halved due to the reduced translational symmetry of the doubled unit cell. We write the energy of a bare particle with wave vector k as

$$\epsilon_k = 2 \cos k + 2\lambda \sin 2k, \quad (2.4)$$

where we have set $T=1$. In this reduced zone we find that there are two quasiparticle bands with dispersions given by,

$$E_{k\pm} = \frac{\epsilon_k + \epsilon_{k+\pi}}{2} \pm \sqrt{(xU)^2 + \left(\frac{\epsilon_k - \epsilon_{k+\pi}}{2} \right)^2}. \quad (2.5)$$

Solving for the normalized eigenvectors of this transformation we get

$$\alpha_{k\sigma\pm} = \begin{pmatrix} \frac{c_{k\sigma}}{\sqrt{2\rho(\rho \pm y)}} \\ \frac{c_{k+\pi\sigma}}{\sqrt{2\rho(\rho \mp y)}} \end{pmatrix} \quad (2.6)$$

where we have used the following definitions:

$$\begin{aligned} \chi_k &= \frac{\epsilon_k - \epsilon_{k+\pi}}{2} \\ y &= \frac{\chi_k}{xU} \\ \rho &= \sqrt{1 + y^2} \end{aligned} \quad (2.7)$$

Finally, our diagonalized Hamiltonian is

$$H_{MFT} = UL \left(\frac{1}{4} + x^2 \right) + \sum_{k_r, \sigma, \eta} E_{k\eta} \alpha_{k\sigma\eta}^\dagger \alpha_{k\sigma\eta}. \quad (2.8)$$

Using the standard variational principle to find the self-consistent x , we write

$$\frac{\partial \langle H_{MFT} \rangle}{\partial x} = 0 = 2ULx - \sum_{k_r, \sigma, \eta} \frac{2xU^2}{2\sqrt{(xU)^2 + \chi_k^2}} (n_{k\sigma 1} - n_{k\sigma 2}). \quad (2.9)$$

Simplifying and ignoring the trivial solution $x=0$, we can reduce this triple sum to a single sum over k which has limits determined by the difference of the occupancy of the two bands. We also remove the spin sum for which we get a factor of 2.

$$L = \sum_{k_r} \frac{n_{k\uparrow 1} - n_{k\uparrow 2}}{\sqrt{x^2 + \left(\frac{2\cos(k)}{U} \right)^2}}. \quad (2.10)$$

To simplify our treatment of this equation we notice that for any values of U , λ and x there are two categories into which the band structure can fall: gapped and ungapped. Because we are dealing with non-interacting quasiparticles, as long as the gap persists the lower band is full and the upper band empty. In this light, the consistency equation becomes very simple because it is independent of the field strength up to the point of band overlap. Therefore, the zero field order parameter will be constant with increasing field until some critical value is reached at which particles move from the top of the lower band into the bottom of the upper band. This will reduce the value of x which will result in a still greater occupancy of the upper band. In this way, the band overlap results in a complete redistribution of filling such that the bands become degenerate, i.e. the order is destroyed. This tells us that there will be a first order

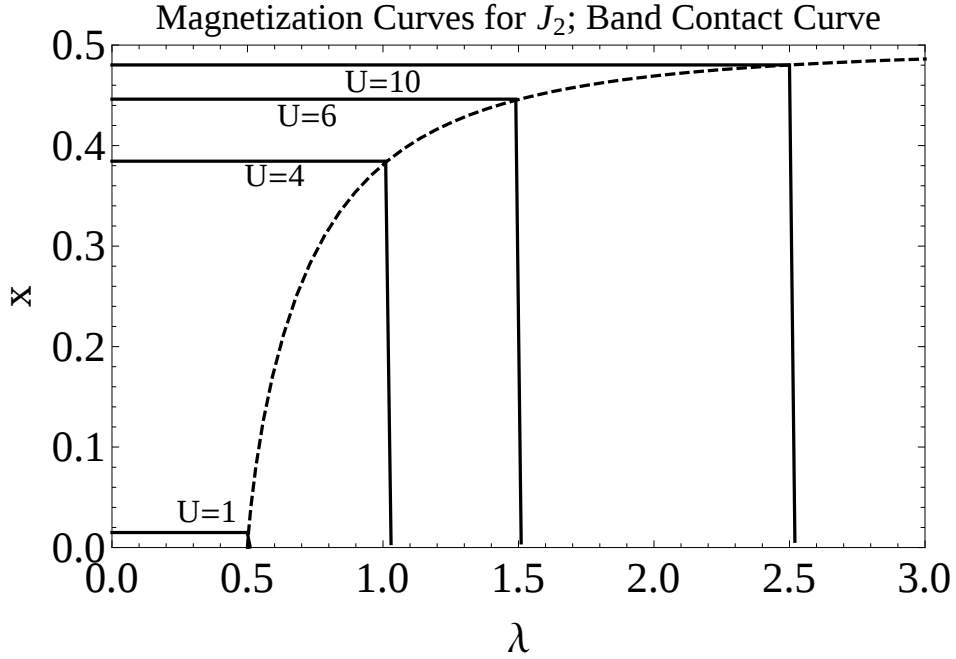


Figure 2.1: This figure relates to the perturbation J_2 within MFT. The zero field order parameter persists independent of the field strength until a critical value is reached. The curve through the transition points was obtained independently of the magnetization curves by plotting the zero field x of a given U against the λ where the bands first touch for that U and $x(U)$. That is, the transition occurs precisely when the field causes the bands to touch.

phase transition at the field strength which causes the bands to touch. In Fig. (2.1) we show magnetization curves for a wide range of U . They clearly exhibit a transition to a non-magnetic state. These magnetization curves are plotted on top of a parametric curve which indicates the point at which the bands touch. For all U , the discontinuity in the order parameter as a function of λ occurs where it meets this band contact curve.

We next consider Eq. (2) with J_2 replaced by J_3 defined as

$$J_3 = \sum_{j=1, \sigma}^L (c_{j\sigma}^\dagger c_{j+3\sigma} + h.c.). \quad (2.11)$$

This object has even parity and may be regarded as a third neighbor hopping. It perturbs the band structure in a symmetrical fashion, and for a large enough strength, can cause a Lifshitz transition where the number of Fermi points jumps from 2 to 6, as detailed below.

For the most part, we can use the same formalism as with J_2 . Now χ_k becomes a function of λ . On the other hand, the quantity

$$\frac{\epsilon_k + \epsilon_{k+\pi}}{2} \quad (2.12)$$

is equal to zero, meaning that the lower band is always negative and the upper band is always positive. Therefore we know that for all values of U , λ and x our lower band will always be full and our upper band empty. As a consequence we expect that as λ is varied there should be no discontinuities in x because a band overlap can never occur. Instead, because χ_k is a function of λ we expect smooth, continuous change in the magnetization with applied field. This is shown in Fig. (2.2).

$$L = \sum_{k_r} \frac{1}{\sqrt{x^2 + \left(\frac{2\cos(k) + 2\lambda\cos(3k)}{U}\right)^2}} \quad (2.13)$$

It warrants mention that although there is no notion of a critical field strength for J_3 , there are two unique field strengths which cause the magnetization to vary anomalously for small U . This arises from a sharp peak in the Fermi energy density of states at these values of λ . Inspection of the form of the dispersion reveals that it is states nearest the Fermi energy that are most effected by the value of the order

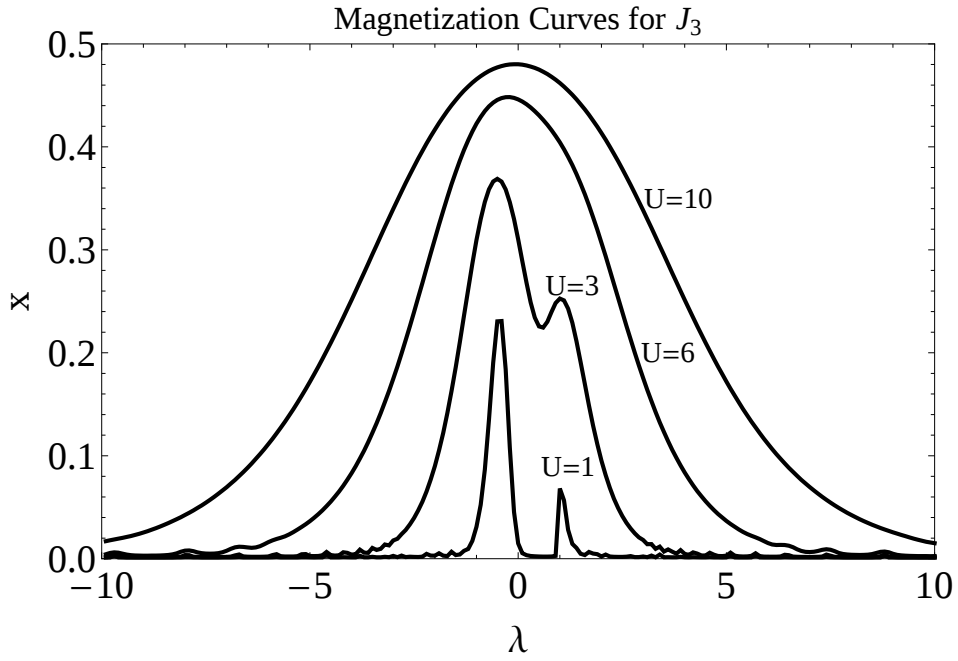


Figure 2.2: These curves relate to the perturbation J_3 in MFT. They are smooth functions of λ and U , showing no critical behavior in contrast to those shown above. Also, for weak interaction, the field strengths which maximize the density of states at the Fermi level result in sharp peaks in the order parameter.

parameter, x , particularly for small U . Thus, these peaks should be no surprise. Later, we will see these critical values of λ reappear in a slightly different context.

2.3 An Integrable Model of Mott Transitions

The nature of the U -independent symmetries of the Hubbard Hamiltonian were detailed by Lieb and Heilmann[29]. For the case of a Benzene ring ($N_s = 6$) they showed the existence of level crossings between states of the same symmetry, thereby violating the Wigner-Von Neumann non crossing rule. Their work pointed to the existence of U dependent symmetries which were found much later[16, 17, 18]. Later, this work was extended by Yuzbashyan et al[30], who applied the same method to the first few higher conserved charges of Shastry in a work which drew a causal connection between the existence of dynamical conservation laws and the observed level crossing of the model. We will be using this same diagonalization scheme on a new Hamiltonian which is the tunable sum of the Hubbard Hamiltonian and it's conserved charges.

$$H_{I_n} = H_0(U) + \lambda I_n(U) \quad (2.14)$$

In this case, we will use the particle hole symmetrized version of the Hubbard model:

$$H_0 = T \sum_{j=1}^{N_s} \sum_{s=\uparrow\downarrow} (c_{j+1s}^\dagger c_{js} + c_{js}^\dagger c_{j+1s}) + U \sum_{j=1}^{N_s} (n_{j\uparrow} - \frac{1}{2})(n_{j\downarrow} - \frac{1}{2}) \quad (2.15)$$

By construction, I_n commutes with H_0 for all U so we know that they must share eigenstates. Therefore, the addition of I_n to H_0 as a perturbing field may continuously change the eigenvalues but not the eigenstates. Due to the integrability of

the model, level crossings within blocks of the same space-time symmetry are admitted, violating the Wigner Von-Neumann rule. Thus, transitions in finite systems will always be first order. This opens up the interesting possibility of the ground state changing abruptly with λ , a quantum phase transition that retains integrability. Until now this has not been possible since the only parameter involved was U which was shown not to result in any transitions. We expect that we can find some λ_c where the eigenvalue of H_{I_n} of some excited state of the Hubbard model crosses the eigenvalue of the Mott Insulating ground state creating a new ground state.

As we seek the new ground states under the influence of these fields, the block diagonalization procedure of Heilmann and Lieb will prove useful in two respects. First, it provides a numerical expedience. Second, we can use the symmetry quantum numbers of the ground state to develop an understanding of how the Mott Insulator is changing.

2.3.1 U-independent Symmetries

It is worth laying out briefly the spacetime and internal space symmetries of the model. We will follow exactly the notation of Yuzbashyan et al[30]. Firstly, we consider the symmetries of the polygon including translation and reflection. If we begin our analysis from k -space, many-body states made of Bloch waves are already diagonal under the translation operator. The reflection operator only commutes with the Hubbard Hamiltonian for $p = 0, \pi$ so we must be careful only to apply this symmetry in the appropriate sectors.

Next we have the particle-hole and spin symmetries. The simplest is to flip all

spins. We call this operation J_s . However, this symmetry only exists when $S_z = 0$, so again, we must be careful to apply it only in the appropriate sectors. There is also a particle hole symmetry which exists only at half filling called $I^{(o)}$.

We will write down a basis which is a superposition of Bloch waves using the following notation

$$|r\rangle = |p; q\rangle = d_{p_1\uparrow}^\dagger \dots d_{p_{N_\uparrow}\uparrow}^\dagger d_{q_1\downarrow}^\dagger \dots d_{q_{N_\downarrow}\downarrow}^\dagger |vac\rangle \quad (2.16)$$

and the fermionic ordering conventions

$$p_1 < p_2 < \dots < p_{N_\uparrow} \quad (2.17)$$

and

$$q_1 < q_2 < \dots < q_{N_\downarrow}. \quad (2.18)$$

Using this notation we can write down the effect of the various symmetry operators on our many-body basis states by which we can generate matrix elements of these symmetries.

$$\begin{aligned} \hat{R}|r\rangle &= |-r\rangle \\ \hat{J}_s|p, q\rangle &= |q, p\rangle \\ \hat{I}^{(o)}|r\rangle &= \rho |-(r + ne)\rangle \end{aligned} \quad (2.19)$$

The sign factor ρ which appears in the operation of $I^{(o)}$ is needed to make this operator commute with H_0 for arbitrary system size, N_s . It has the form

$$\rho = \langle -(r + ne) | LO * (-1)^P | -(r + ne) \rangle \quad (2.20)$$

The LO operator determines the signature of the ordering of the ket upon which it operates. For the case where $N_s = 6$ (Benzene), this sign factor simplifies considerably to look like the expression given in references [29] and [30].

Finally, we know that there is an $SU(2)$ spin symmetry of our spin $\frac{1}{2}$ fermions. We can also construct a second $SU(2)$ symmetry through a partial particle-hole transformation of the spin symmetry operators. This operator, called $\hat{Z}_\uparrow$ by Yuzbashyan et al, anticommutes with the Hamiltonian such that

$$\left[\hat{Z}_\uparrow S^2 \hat{Z}_\uparrow^\dagger, H_0 \right] = 0. \quad (2.21)$$

The generators of these symmetries are:

$$\begin{aligned} S_+ &= \sum_{j=1}^{N_S} c_{j\uparrow}^\dagger c_{j\downarrow} = (S_-)^\dagger \\ S_z &= \sum_{j=1}^{N_S} \frac{n_{j\uparrow} - n_{j\downarrow}}{2} \\ S^2 &= S_+ S_- + S_z^2 - S_z \end{aligned} \quad (2.22)$$

and

$$\begin{aligned} L_+ &= \sum_{j=1}^{N_S} (-1)^j c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger = (L_-)^\dagger \\ L_z &= \sum_{j=1}^{N_S} \frac{n_{j\uparrow} + n_{j\downarrow}}{2} - \frac{N_S}{2} \\ L^2 &= L_+ L_- + L_z^2 - L_z. \end{aligned} \quad (2.23)$$

A quick glance at the L_+ operator will convince the reader that this symmetry is, in essence, a measure of charge ordering in the form of double occupancy of lattice sites.

The L^2 quantum number will therefore serve as a measure of the metallicity of our ground state. The $SO(4)$ symmetry discussed by Yang and Zhang[19] consists of these two $SU(2)$ groups.

For a detailed development of the construction of these operators from single particle creation and annihilation operators see reference [29]

2.3.2 Diagonalization and Phase Diagram

As mentioned, we will be using Shastry's conserved currents as our applied fields. They were generated by taking logarithmic derivatives of a transfer matrix which was shown to commute with H_0 for all values of some spectral parameter [18]. These currents fall into one of two groups. One group has precisely the symmetry of H_0 while the other lacks the reflection symmetry. We will employ one of each.

$$\begin{aligned}
\hat{I}_2 = & -iT \sum_{j=1}^N \sum_{s=\uparrow\downarrow} (c_{j+2s}^\dagger c_{js} - c_{js}^\dagger c_{j+2s}) \\
& -iU \sum_{j=1, s}^N (c_{j+1s}^\dagger c_{js} - h.c.) (\hat{n}_{j+1\bar{s}} + \hat{n}_{j\bar{s}} - 1)
\end{aligned} \tag{2.24}$$

$$\begin{aligned}
\hat{I}_3 = & T^3 \sum_{j=1}^N \sum_{s=\uparrow\downarrow} (c_{j+3s}^\dagger c_{js} + c_{js}^\dagger c_{j+3s}) \\
& + T^2 U \sum_{j=1}^N \sum_{s=\uparrow\downarrow} \left(c_{j+1s}^\dagger c_{j-1s} + h.c. \right) \left(\hat{n}_{j+1\bar{s}} + \hat{n}_{j\bar{s}} + \hat{n}_{j-1\bar{s}} - \frac{3}{2} \right) \\
& + T^2 U \sum_{j=1}^N \sum_{s=\uparrow\downarrow} \left[\left(c_{j+1s}^\dagger c_{js} - h.c. \right) \left(c_{j\bar{s}}^\dagger c_{j-1\bar{s}} - h.c. \right) - \left(\hat{n}_{j+1s} - \frac{1}{2} \right) \left(\hat{n}_{j\bar{s}} - \frac{1}{2} \right) \right] \\
& + T^2 U \sum_{j=1}^N \left[\left(c_{j+1\uparrow}^\dagger c_{j\uparrow} - h.c. \right) \left(c_{j+1\downarrow}^\dagger c_{j\downarrow} - h.c. \right) - \left(\hat{n}_{j\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{j\downarrow} - \frac{1}{2} \right) \right] \\
& - T U^2 \sum_{j=1}^N \sum_{s=\uparrow\downarrow} \left(c_{j+1s}^\dagger c_{js} + h.c. \right) \left(\hat{n}_{j+1\bar{s}} - \frac{1}{2} \right) \left(\hat{n}_{j\bar{s}} - \frac{1}{2} \right) \\
& - \frac{U^3}{4} \sum_{j=1}^N \left(\hat{n}_{j\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{j\downarrow} - \frac{1}{2} \right)
\end{aligned} \tag{2.25}$$

[20, 21, 30]. Notice that the leading (U independent) terms of these operators are equal to the currents used in section II. The U-dependent parts ensure proper commutation for all values of U but are not easily interpreted as any physical quantity or correlation. We deal with them in their full form simply to preserve the integrability of the Hubbard model while seeking a field induced transition.

To initiate our understanding of these new models we look at the behavior of the ground state in the non-interacting limit (U=0) where the Hamiltonian can be described by a simple one band picture where the field dependence simply distorts the dispersion. By filling in the lower half of the band we find that as the field strength

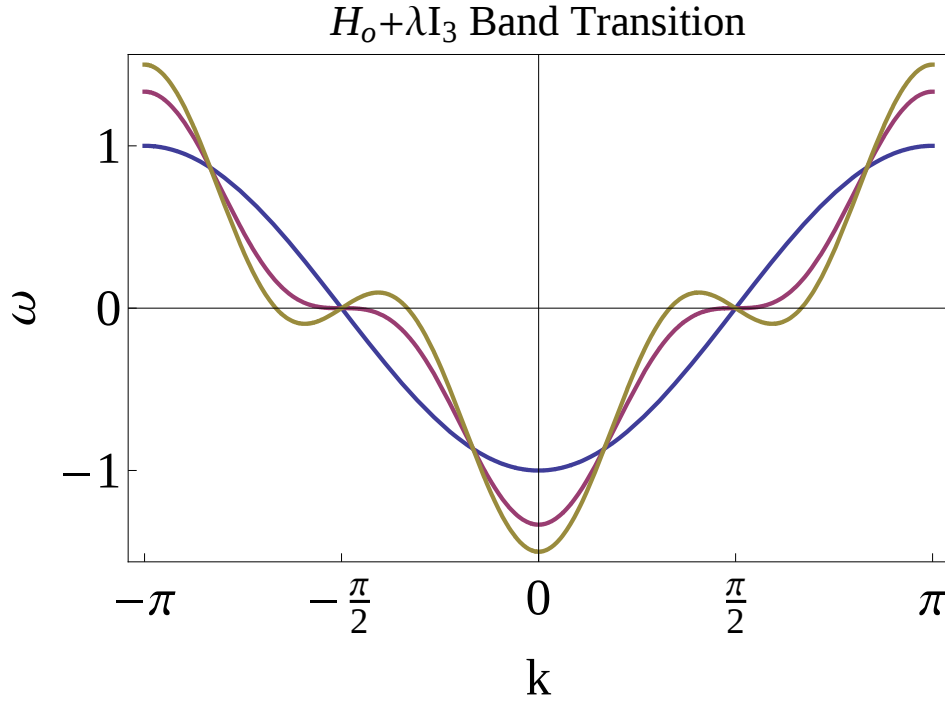


Figure 2.3: As the field strength of H_{I_3} is increased at $U=0$, the simple Hubbard band is distorted until the Fermi line is finally broken into three Fermi segments when $\lambda = 1/3$. This also occurs when $\lambda = -1$.

is varied, the Fermi surface can undergo what is called a Lifshitz transition, whereby the number of Fermi points increases and the Fermi surface is split apart, ceasing to be simply connected. For the case of H_{I_3} observe in Fig. (2.3) the band structure for three values of λ . Fig. (2.4) shows explicitly how the deformation of this Hubbard band results in the formation of two occupied side bands at half filling.

Similar results occur for the case where I_2 is applied to the Hubbard model. In this case, however, the dispersion loses its reflection symmetry; one direction is preferred energetically. Still, we see a Lifshitz transition resulting in two Fermi segments.

Finite size effects are easy to compute for $U=0$. We know that the Lifshitz

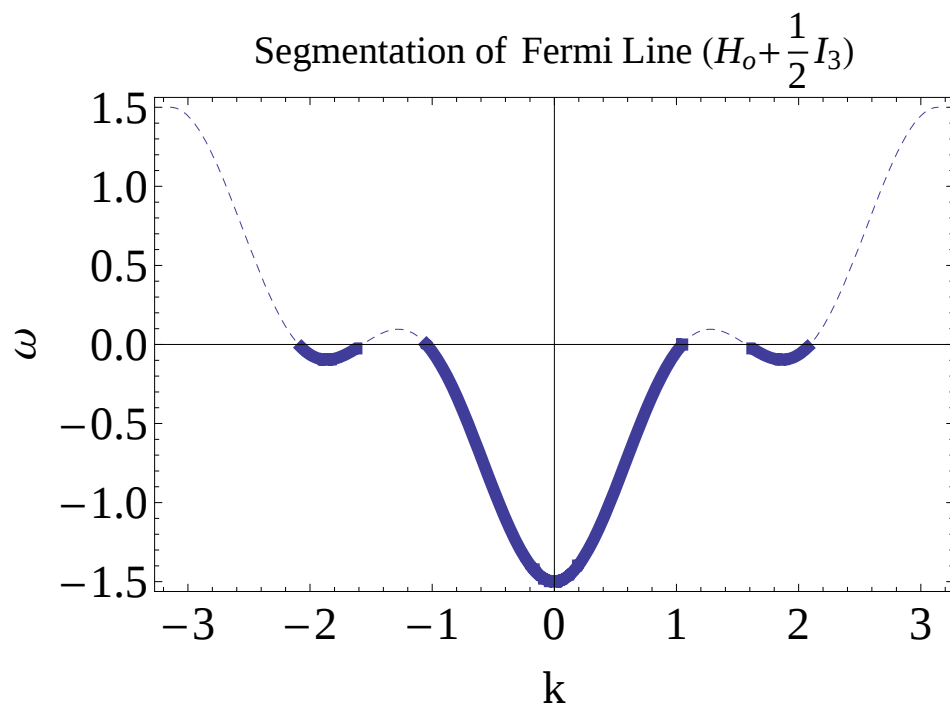


Figure 2.4: Above some critical field the Fermi line is broken at half filling.

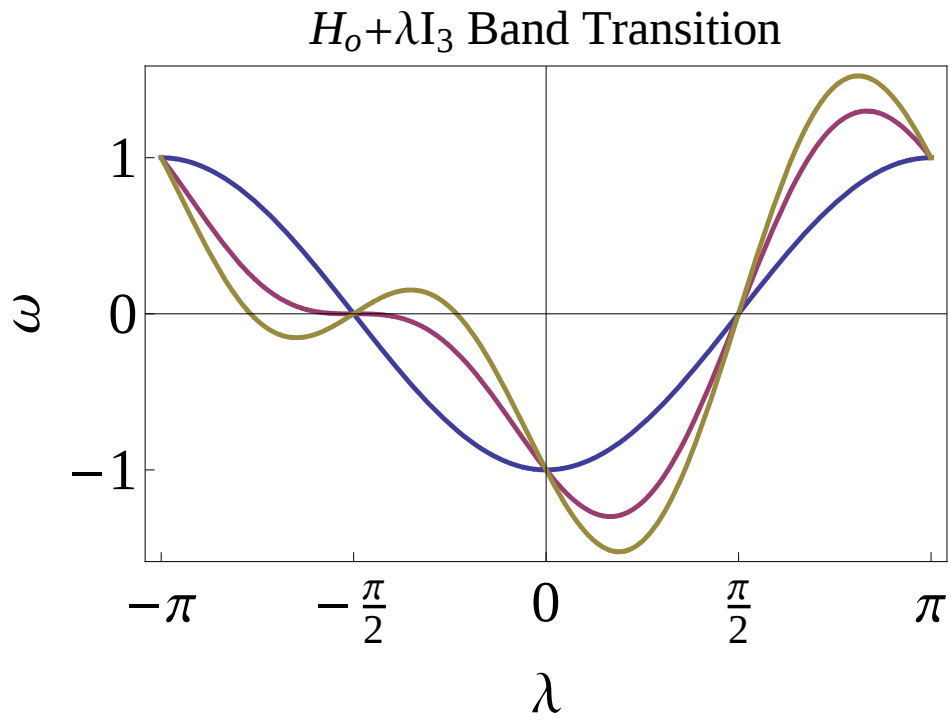


Figure 2.5: As the field strength of H_{I_2} is increased at $U=0$, the simple Hubbard band is distorted until the Fermi line is finally broken into two Fermi segments.

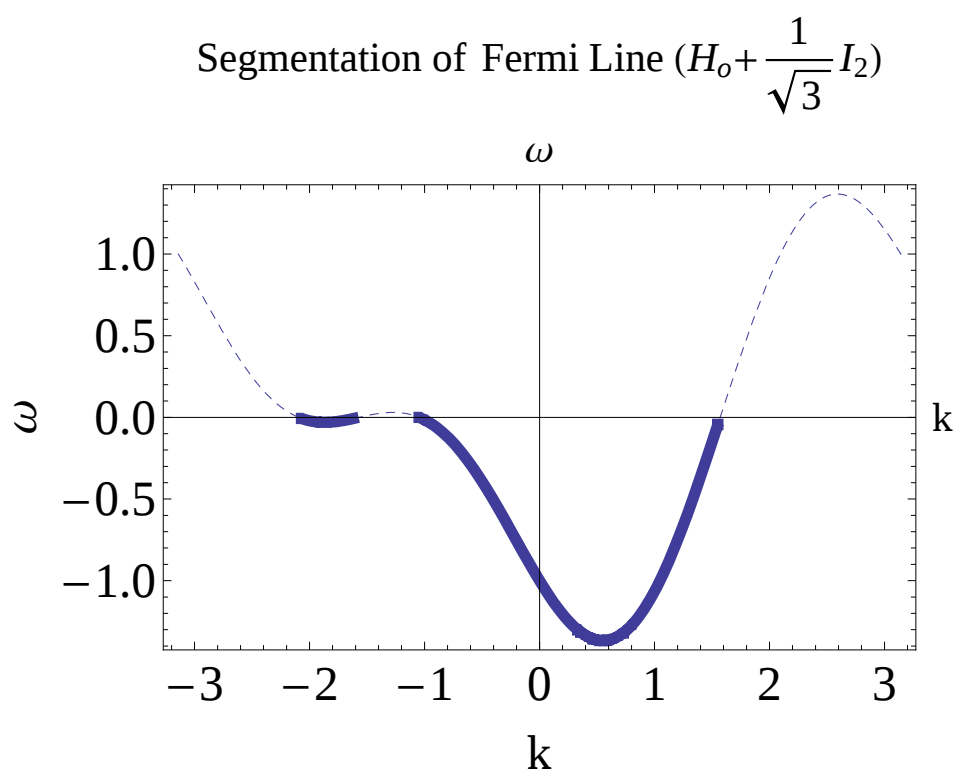


Figure 2.6: Above some critical field the Fermi line is broken at half filling.

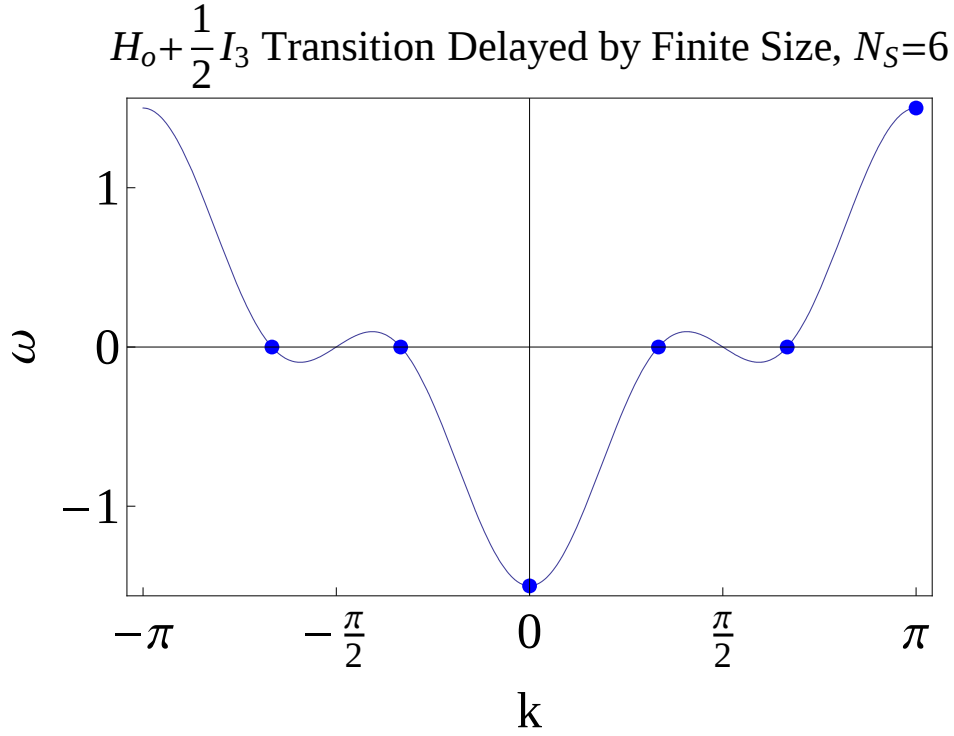


Figure 2.7: For finite rings the Lifshitz transition occurs at a slightly higher field than that predicted in the thermodynamic limit. This plot shows that for the case of $N_s = 6$, adjacent single particle states do not become degenerate until well after the thermodynamic dispersion curve has developed new minima.

transition occurs when k-points just beyond the Fermi surface fall to an energy lower than those just inside the Fermi surface. For an infinite system we can find exactly the field strengths at which this occurs, namely, the one at which the group velocity at the Fermi surface passes through zero. On a finite lattice however, the finite separation of allowed k values complicates that simple description. The critical field becomes dependent upon the system size for small N_s with λ_c being always slightly larger than it would be in the thermodynamic limit.

To discover the effects of these fields at finite U requires exact diagonalization.

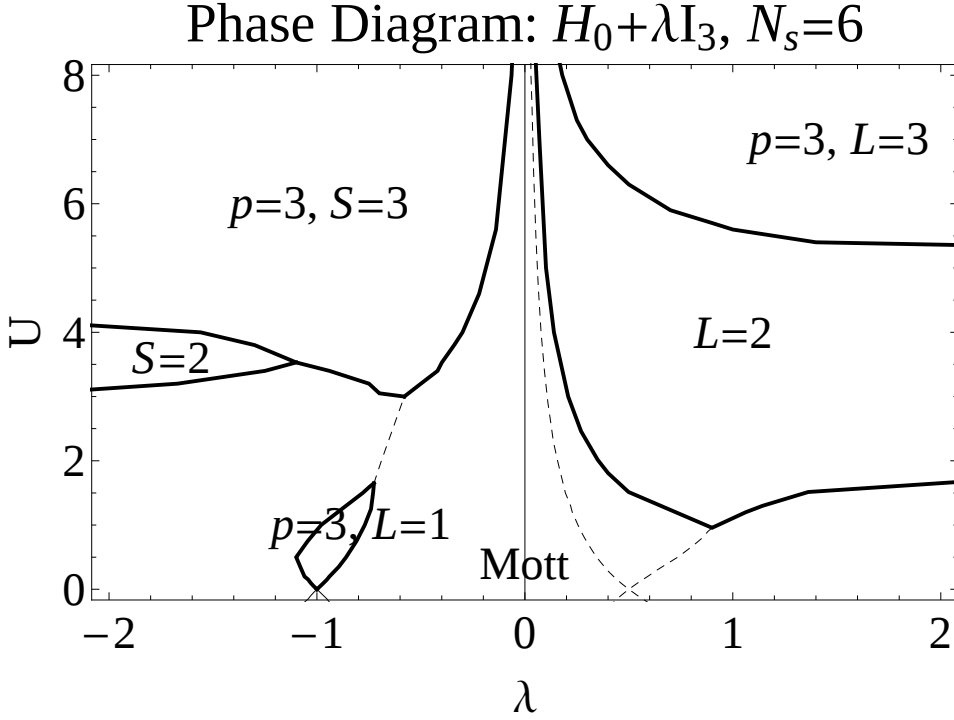


Figure 2.8: Here we have a phase diagram in λ and U which shows that we can transition away from the Mott insulating ground state as we move away from the U -axis. Dashed contours represent transitions without any change of symmetry. The $U < 0$ half of the diagram can be obtained by a $\hat{Z}_\uparrow$ transformation of the top half. Unless otherwise indicated in the diagram the symmetry is that of the Mott state: $p=S=L=0$.

We show a phase diagram of H_{I_3} with some interesting quantum numbers of the ground state in Fig. (2.8). Of greatest importance are L and S which tell us the extent of charge and spin ordering respectively. The Lifshitz transition spoken of previously is a prominent feature in this diagram. On the positive λ side of the $U=0$ axis there are two phase contours which emanate from the point of the Lifshitz transition and define two boundaries of a new phase which does not exist in the Hubbard model or in I_3 . We will call this central phase the Lifshitz zone. It should also be noted that these two contours are first order yet have no change of symmetry.

Fig. (2.9) shows just the first quadrant of the equivalent diagram for H_{I_3} on an 8 sited ring as opposed to just 6 in the previous figure. For simplicity, we denote only the L quantum numbers. The general structure of the diagram is unchanged but there is a greater degree of complexity in that the L quantum number now has a wider range. One interesting difference is that dashed transition on the left side of the Lifshitz zone has become an entirely new phase which lies between the Mott insulator and the Lifshitz zone. Later we will attempt to understand this state by comparing it to its two neighbors.

Finally, we show in Fig. (2.10), the phase diagram for H_{I_2} on a 6 sited ring. Whereas in the case of H_{I_3} we saw one or the other of the L and S quantum numbers going to its maximum as U and λ were increased, here we see a sort of competition between the two, in which neither wins.

Perhaps the greatest consequence of the integrability of these Hamiltonians is that we observe only 1^{st} order transitions, even when the transition has no change of symmetry. This occurs because as the field strength is changed, the eigenvalues change but not the eigenvectors. Thus the only change possible in the ground state is for it to switch to an orthogonal state, i.e undergo a level crossing. This situation can be changed by adding a small integrability-breaking perturbation into the Hamiltonian. At transitions without change of symmetry, the perturbation will round off discontinuities and cause crossing states to repel each other. Fig. (2.11) shows how an integrability breaking terms turns a 1^{st} order transition to 2^{nd} order

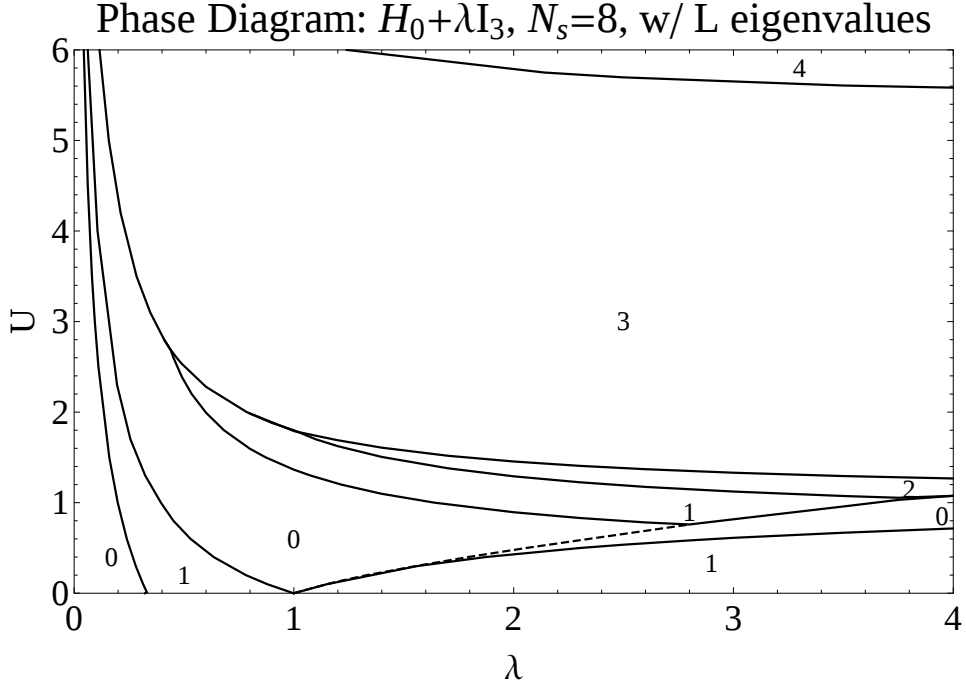


Figure 2.9: Comparing with the equivalent diagram for the 6 sited ring we see that although there is a higher complexity here, the same general structure persists. Namely, we still observe a central phase which exists above the Lifshitz transition point. However, since the range of the L and S quantum is increased by the added sites and particles, we see a greater number of states. It is particularly interesting the transition on the left side of the Lifshitz zone which had no change of symmetry for the case of $N_s = 6$, is now broadened into an entirely new phase which does have a different symmetry.

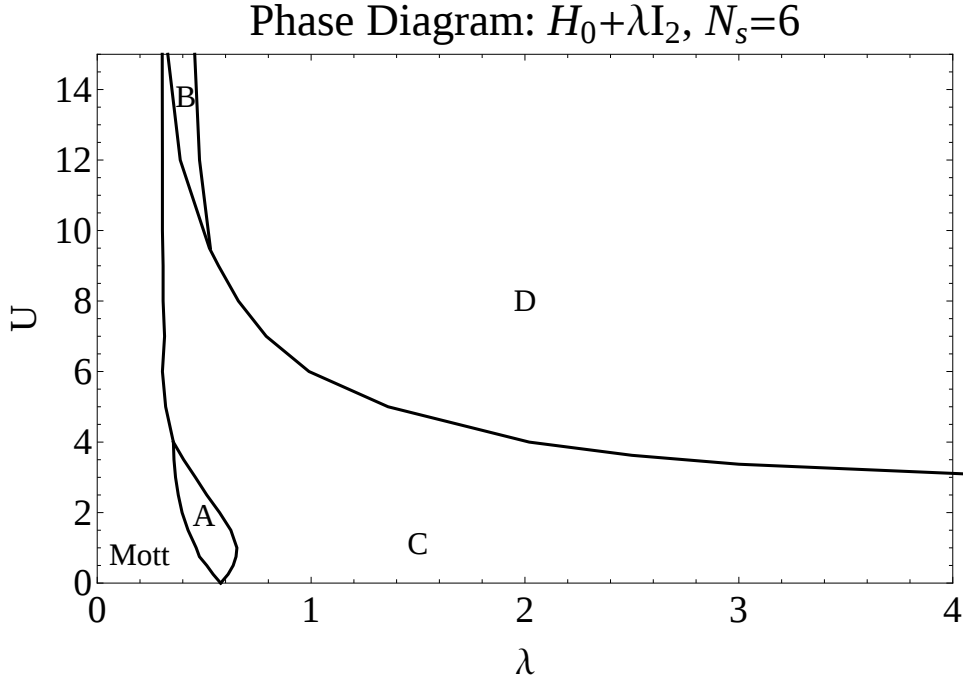


Figure 2.10: As in the previous diagram, the $U < 0$ region can be obtained by $\hat{Z}_\uparrow$ transformation but here we can obtain the negative λ by a reflection transformation (Reflection is not a symmetry because of the field's odd parity). In this diagram, there is no general trend toward a particular order. The spin and charge orders are in competition so neither prevails over the entire quadrant. The quantum numbers of each region are given here: $A=(p=1, S=0, L=1)$, $B=(p=3, S=0, L=1)$, $C=(p=2, S=0, L=0)$, $D=(p=0, S=1, L=0)$, $\text{Mott}=(p=S=L=0)$.

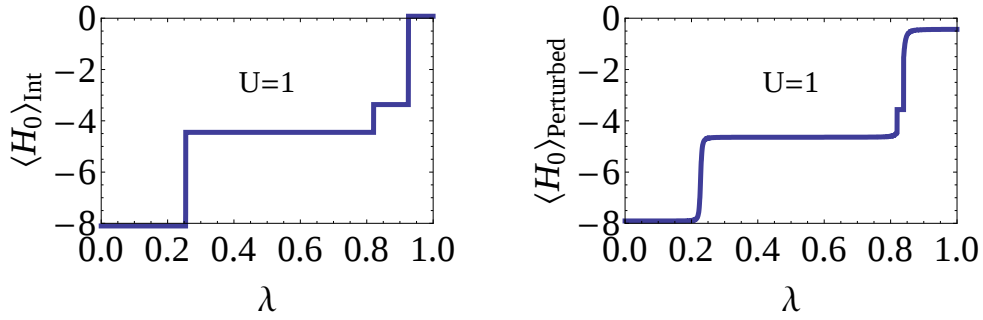


Figure 2.11: The integrability of the model allows level crossings between states of the same symmetry. This is seen here as a discontinuity in the expectation value of the Hubbard Hamiltonian as the field strength is increased. Adding a small perturbation which breaks no symmetries but does break the integrability we find that certain discontinuities become smooth. This indicates that a level crossing has become an avoided crossing. Only those transitions without change of symmetry can become smooth.

2.3.3 Double Occupancy

In addition to tracking the total L quantum number we can also find the expectation value of double occupancy in the ground state. There is a large degree of overlap in these two forms of information but it is also good to see the differences. As a general rule, greater L equates to a greater doublon expectation. However, since we have 1^{st} order transitions between states of the same quantum numbers we must be content with there being no general rule about how $\langle \sum n_{j\uparrow} n_{j\downarrow} \rangle$ will change at these would-be 2^{nd} order transitions. Below we display some examples drawn from H_{I_3} on the 6 site ring.

2.3.4 New Ground States

An interesting theme here is the occurrence of band transitions in the $U=0$ limit. In section II we saw two points of interest in the magnetization curves of H_{j_3}

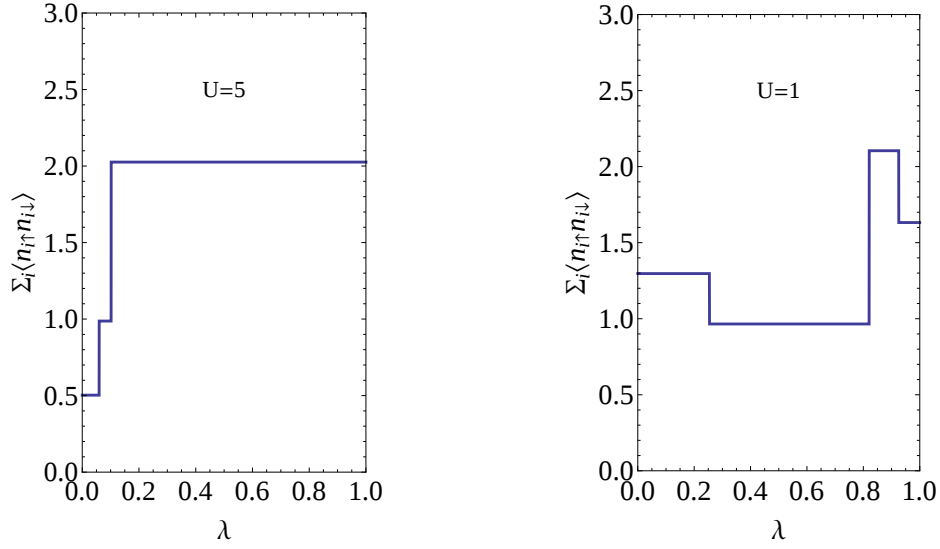


Figure 2.12: The plot on the left is typical of the system for large U : as the field strength is increased, the doublet expectation will also increase. Furthermore, this increase is accompanied by an increase in the L quantum number. The plot on the right shows the doublet expectation for $U=1$. We see that the transition actually reduces the charge order. This transition is one of those with no change in symmetry.

as the interaction integral was decreased. These points reveal themselves again in the H_{I_3} as the λ intercepts of phase transition contours, the Lifshitz transitions described earlier. We note that all other transitions in the plane seem to emanate from these points. The question is: what is changing at this point? We know that there is no change of symmetry. Also, if we take an infinitesimal step away from $U=0$, we observe a spike in the antiferromagnetic order at the transition (at least in the mean field). It would be interesting to uncover the details of how this simple band transition distorts into a more subtle many-body phase transition for large U , and furthermore, to see how various correlations evolve along these phase contours. Unfortunately, due to the small size of the systems studied here, correlation functions fail to exhibit even the standard

signatures of Mott insulating or conducting behavior.

Although we cannot name our new ground states with absolute certainty it is possible to demonstrate that these ground states behave in a way that is altogether unlike the Mott insulator. We do this by identifying a state and looking at the way its double occupancy changes as a function of U . This may involve looking at the behavior of that state in a region where it is not the ground state. We understand that as U is increased, the double occupancy of a Mott insulator should decrease monotonically. In fact this is observed of the ground state on the U -axis of our diagram. The Lifshitz zone does not display this sort of behavior. Fig. (2.13) compares the two curves.

We do not show unequivocally that the Lifshitz phase is metallic, but it is reasonable to say the boundary between it and the Mott insulator is a Mott transition because it clearly does not behave like a Mott insulator. However, in the case where $N_s=8$ this boundary has been widened into an entire phase which is charge ordered (has a different symmetry) so that now there are two transition each with a change of symmetry. If we look at the double occupancy of all three of these states as a function of U we find that the charge ordered sliver behaves much like the Mott insulator except that it maintains a single doublon to infinite U . This doublon is actually protected by the charge ordering. Since the double occupancy, monotonically decreases to its high- U limit we can say that this state is actually a partially charge ordered Mott Insulator. Again we see that the Lifshitz phase sustains doublons without any charge ordering, indicating something like metallic behavior.

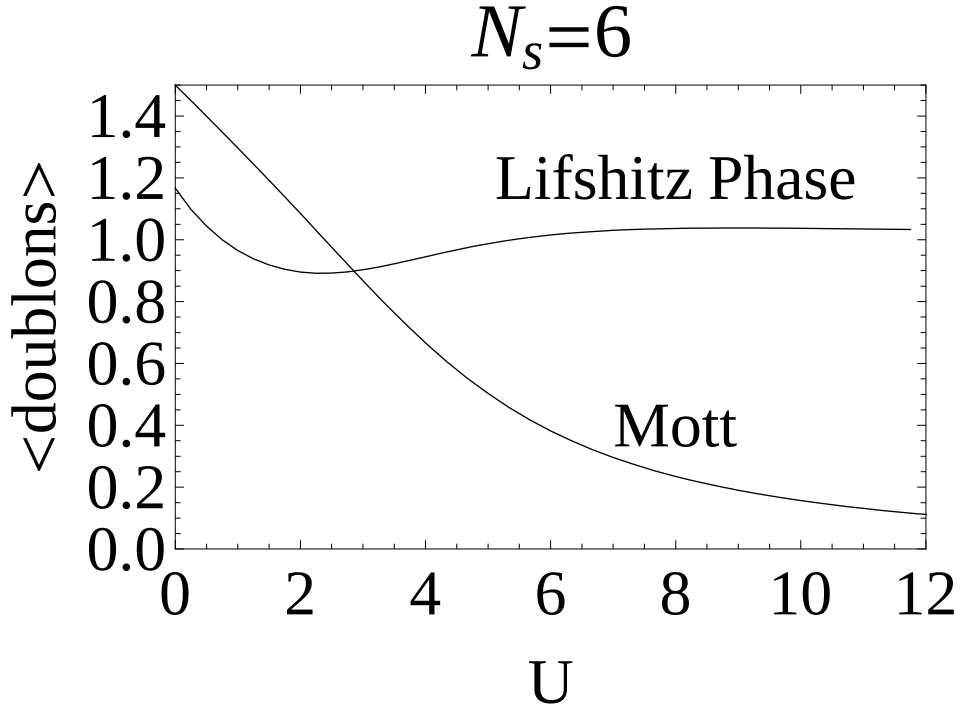


Figure 2.13: Although the Mott insulator and Lifshitz zone share the same symmetry, the two states respond quite differently to changes in the interaction. In the Mott state, double occupancy decreases monotonically as U is increases. The Lifshitz phase exhibits a qualitatively different behavior.

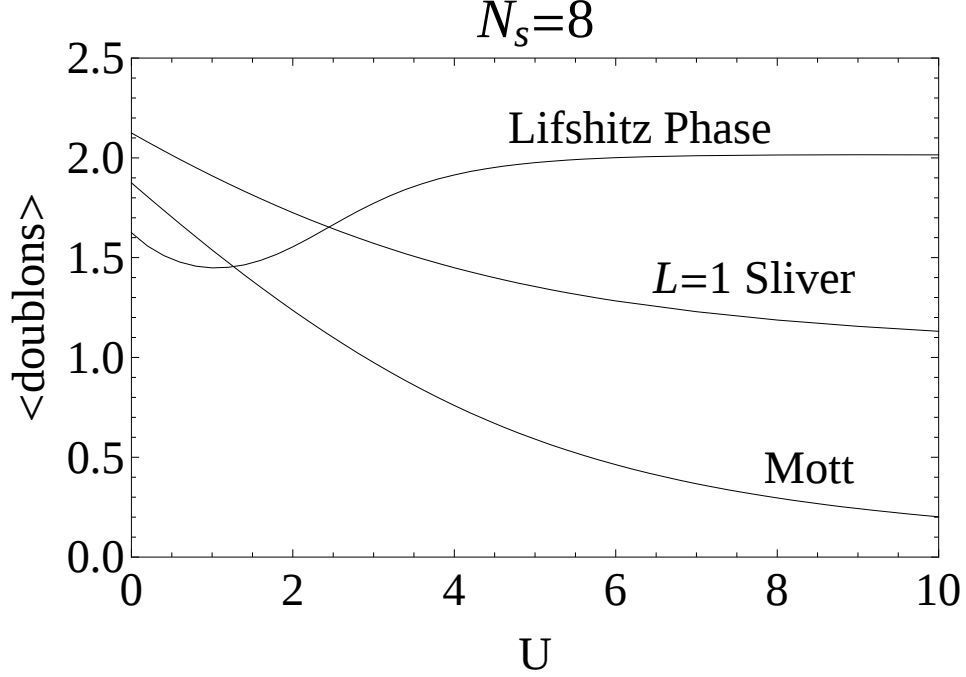


Figure 2.14: For a 8 sited ring, the phase diagram has a small sliver of a third ground state between the classic Mott insulator and the Lifshitz phase. This sliver has the quantum number $L=1$, while the other two states have $L=0$. This change in the charge ordering between the Mott insulator and the sliver explains the existence of a doublon persisting to high U in the sliver phase. Thus, we can say that the sliver phase is actually another Mott insulator which has a different symmetry than the first but the same general behavior. The Lifshitz phase exhibits behavior very similar to that seen in the same phase of the 6 sited ring. Namely, it shows doublons persisting to high U without the protection of charge ordering.

2.4 Summary

We have shown a simple mean field calculation which teaches us to expect field induced Mott transitions for fields of a certain type. Furthermore, fields which do not produce a transition, such as J_3 may yet exhibit interesting behavior. We also demonstrated the existence of 1^{st} order Mott transitions in a family of integrable Hamiltonians. The existence of phase transitions between states of the same symmetry is a curious phenomenon that deserves further study. We have presented numerical work for fairly small systems $L \leq 8$. We hope to return to the exact Bethe Ansatz wave functions with the correct quantum numbers, which would solve the integrable models discussed here. Indeed the very same Bethe Ansatz that solves the Hubbard model in 1-d should solve these extended models too. The difficulty is in finding the quantum numbers which produce the correct ground state. For the Hubbard model there are simple rules for identifying the groundstate quantum numbers of H_0 . The extended models discussed in this paper have novel groundstates which correspond to excited states of the Hubbard spectrum. These states are describes with the Bethe's Ansatz equations as $k - \Lambda$ strings but they are very hard to treat numerically, even for small systems.

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Chapter 3

Level Statistics in Ansatz Matrices

3.1 Introduction

The spectral statistics of generic quantum Hamiltonians are well described by the results of Random Matrix Theory, specifically by analytic results regarding the Gaussian ensembles. This accounts for the level repulsion and spectral rigidity which are the rule for generic models. However, it is widely observed that the eigenvalues of typical quantum integrable models (such as the Hubbard, Heisenberg, XXZ and Gaudin Hamiltonians, etc.) are uncorrelated, in direct opposition to the exact results obtained from the Gaussian Ensembles. This notable exception is believed to be caused by the existence of a large number (infinite for thermodynamic sizes) of conserved quantities. This exception is so reliable that spectral statistics are now used extensively as indicators of the transition from integrability to chaos.

Berry and Tabor attempted to understand the occurrence of Poisson statistics

by quantizing classically integrable systems. They were able to prove that the spectrum of these models were all uncorrelated with level spacing distributions which follow the Poisson form

$$P(s) = e^{-s} \quad (3.1)$$

where s is the normalized separation between levels defined everywhere in this paper as

$$s = \frac{S}{\langle S \rangle} \quad (3.2)$$

with S being the actual spacing and $\langle S \rangle$ is the mean level spacing. Unexpectedly, the harmonic oscillator, the poster child for integrability, is the exception to this rule. For instance, the spectrum of a high dimensional oscillator with incommensurate frequencies exhibits a distribution $P(s)$ which can be peaked at some finite values of “ s ”. Stranger still, in the case that the frequencies are commensurate the distribution $P(s)$ does not exist at all. This work provided the first exact results on the statistics of integrable systems. However, it is a semi-classical result made possible by a well-defined notion of classical integrability. It does not begin from an independent notion of quantum integrability. Nonetheless, it demonstrates that generic models have Poisson like spectra but exceptions can be found in special cases.

Subsequently, crossovers in the spectral statistics have been studied for a variety of quantum models. For example, Millis et al studied the level repulsion (and other spectral observables) of the XXZ model under the influence of a finite coupling to some integrability breaking term. It was found that a variety of observables do crossover from Poisson-like behavior to the Wigner-Dyson behavior which is appropri-

ate for generic real symmetric matrices. However, the exact scaling of the crossover was hard to extract given that the size of the matrices was limited numerically. Furthermore, the claims made therein are typical of such studies in that they apply to a single model. Perhaps the biggest weakness of such studies is that they are unable to predict the Poisson statistics based on some generic form of the matrices. These studies tend to be descriptive, beginning and ending with numerics. It would be preferable to begin from some generic notion of integrability and make statements on the statistics based upon that foundation. In classical mechanics, for instance, there are numerous frameworks for understanding integrability: action-angle variables, invariant tori, etc. Through these paradigms it is possible to deal with general properties of classically integrable systems. For quantum systems there is the Yang-Baxter equation (quantum inverse scattering method) but no general solutions are known and it is hard to see how one can say anything about level statistics from this starting point.

Recently Shastri considered the constraints placed on the elements of a matrix by the existence of some mutually commuting operators. The form of the commuting partner is essential to the problem since it is clear that any two diagonal matrices will commute trivially. The constraints placed on the matrix elements become nontrivial only when some non-diagonal structure is imposed. Taking a cue from the Heisenberg and Hubbard models Shastri considered a pair of matrices which each have a linear parameter. They must commute at all values of that parameter. This serves as a working definition of quantum integrability which allows for explicit construction of matrices in any dimension which may be regarded as being quantum integrable. Following on

this framework, Owusu et al were able to explicitly parameterize a further subset of solutions for H . These solutions, called Ansatz matrices, are rare in the sense that they comprise a measure-zero set of all real symmetric matrices. For $N \gg 1$ they generically exhibit Poisson statistics to high accuracy. Furthermore, these matrices have an exact solution which allows us to explore their statistics analytically. Thus it is shown that the existence of conservation laws linear in some parameter results in matrices which have an exact solution and Poisson statistics, arguably the two primary signatures of integrability.

Interestingly, it is found that only a relatively small number of conserved operators are required to ensure Poisson-like behavior. Specifically, the Ansatz matrices are defined as some Type M where $M=N-K+1$, with N being the dimension of the matrix and K being the number of linearly independent commuting operators. From such a family, one may build a matrix from a linear superposition of L of those operators. We find that the requisite for Poisson statistics is that $L \gtrsim 10$ regardless of the size of N (provided $N > L$ of course). In many other respects the Poisson statistics of Ansatz matrices are found to be robust. Even when we deliberately choose parameters which promote non-Poisson behavior, the spectrum remains uncorrelated except in rare domains of the parameter space. We show that these domains vanish with increasing dimension.

The layout of this chapter is as follows. In section II we will briefly recount the Ansatz parameterization and the “typology” of integrable matrices, i.e. we explain the meaning of “M” in general type-M matrices. The maximal case and its connection

with the Gaudin magnets will be highlighted. In section III we will discuss the level repulsion and rigidity as indicators of spectral correlation. Numerical results from a variety of Ansatz matrices will be displayed in terms of these observables, including examples of exceptions to the predominant Poisson behavior. The domain of such non-Poisson regions is shown to vanish in the limit of large matrices dimension, N . In section IV the Poisson statistics will be explained in terms of an explicit calculation of spectral fluctuations in the basis operators. The crossover scales seen in the numerics are then explained through a perturbative argument. In section V we summarize our findings and discuss loose ends.

3.2 Defining quantum integrable models

A definition of quantum integrability in finite systems was initiated by Shastry. He noted that the existence of an exact solution and Poisson statistics arise as a consequence of the existence of certain parameter dependent conservation laws. Specifically he studied matrices which obey the commutation rule

$$\left[H(u), \tilde{H}(u) \right] = 0 \quad (3.3)$$

where

$$\begin{aligned} H(u) &= T + uV \\ \tilde{H}(u) &= \tilde{T} + u\tilde{V} \end{aligned} \quad (3.4)$$

and H (and $\tilde{H}$) are real symmetric matrices and none of the four matrices, T , $\tilde{T}$, V or $\tilde{V}$ are identically zero. It is important to be explicit about the functional form of

the parameter dependence in this way because for any generic $H(u)$ there are always N linearly independent conserved operators with some high order polynomial dependence on u . The linear parameter dependence for *both operators* turns out to be a sufficient constraint to generate solutions for H which are reminiscent of, and occasionally even parameterize irreducible blocks of known integrable models.

The commutation relation, Eq. (3.3) can be resolved into powers of u .

$$\left[T, \tilde{T}\right] = \left[V, \tilde{V}\right] = 0 \quad (3.5)$$

and

$$\left[T, \tilde{V}\right] + \left[V, \tilde{T}\right] = 0 \quad (3.6)$$

These commutation relations imply the existence of an antisymmetric matrix S which is characteristic of a family of linearly independent, mutually commuting matrices

$$h_i(u) = uV_i + [V_i, S] \quad (3.7)$$

where V_i must be linearly independent. Generic matrices can now be built as linear combinations of these basis matrices in the form

$$H(u) = \sum_i d_i h_i \quad (3.8)$$

The problem is now to solve for S given two commuting matrices V^i . It is found that these solutions can be categorized by the number of linearly independent commuting operators in the family. For any matrix family of dimension N there are at most N linearly independent operators of the form of $H(u)$ and one of them must be proportional to the identity matrix. This maximal family is called type 1. Families with $N-M$ linearly

independent members are called type M. The smallest possible non-trivial commuting family is that which has only two members and the identity. This is called type N-2. These high types are in some sense ‘less integrable’ than the low types near the maximal limit. However, as we will see in the next sections, the high types can exhibit Poisson statistics nearly as readily as the low.

3.2.1 The Ansatz Matrices

Beginning in [3] and continuing in [5], a subset of solutions for S have been solved for and explicitly parameterized. These are called Ansatz solutions and describe commuting families of arbitrary type. The most general parameterization is as follows. First we choose N numbers γ_m and N numbers ε_m arbitrarily. To obtain a proper large N limit one has to make sure that the scaling of parameters ε_m , and γ_m with N is such that the eigenvalues of V and T scale in the same way for large N . This is accomplished by imposing the constraints

$$\langle \gamma_m^2 \rangle \sim O(1/N) \quad (3.9)$$

and

$$\langle \varepsilon_{i+1} - \varepsilon_i \rangle \sim O(1/N) \quad (3.10)$$

where ε_i are ordered such that $\varepsilon_{i+1} > \varepsilon_i$ for all i .

We choose a parameter B which determines an auxiliary spectrum of N numbers λ_m according to the equation

$$B = \sum_k \frac{\gamma_k^2}{\lambda_m - \varepsilon_k}. \quad (3.11)$$

The roots, λ_m , fall nicely in the interstices of the ε spectrum so they retain many of the properties of ε although slightly shifted. They have an interesting dependence on B. It is useful to describe the λ_m spectrum in terms of another set of numbers α_m where

$$\alpha_m = \frac{\lambda_m - \varepsilon_m}{\varepsilon_{m+1} - \varepsilon_m} \quad (3.12)$$

such that α_m is always between 0 and 1 and accounts for all the B dependence of λ_m ¹. For $B \gg O(1)$ the λ 's draw close to a single ε . It can be shown that the roots of Eq. (3.11) coincide with the eigenspectrum of a matrix Λ whose elements are given by

$$[\Lambda]_{ij} = \frac{\gamma_i \gamma_j}{B} + \delta_{ij} \varepsilon_i \quad (3.13)$$

where δ_{ij} is the standard Kronecker- δ function. This allows for the perturbative result

$$\lambda_m = \varepsilon_m + \frac{\gamma_m^2}{B} \quad (3.14)$$

when B is large. Equivalently,

$$\alpha_m = \frac{1}{B} \frac{\gamma_m^2}{\varepsilon_{m+1} - \varepsilon_m} \quad (3.15)$$

which indicates that all α_m are positive numbers of $O(B^{-1})$. Each root λ_m is determined (to first order) by its difference with a single ε_m and the summation in Eq. (3.11) makes a negligible contribution except for a single term.

$$\begin{aligned} B &= \sum_k \frac{\gamma_k^2}{\lambda_m - \varepsilon_k} \\ &= \sum_{k \neq m} + \frac{\gamma_m^2}{\varepsilon_m + \frac{\gamma_m^2}{B} - \varepsilon_m + O(B^{-2})} \end{aligned} \quad (3.16)$$

¹The definition given for α_m is appropriate for positive B. A slightly different definition is required for negative values of B. There is also a single root, λ_1 (λ_N) which goes as $1/B$ when $|B| \ll 1$ for negative (positive) B and is therefore not described in terms of the α_m spectrum. In the remainder of the document I consider only positive B.

which implies that

$$\frac{\gamma_k^2}{\lambda_m - \varepsilon_k} \sim O(B^{-1}). \quad (3.17)$$

For $B \lesssim 1$ this is not the case. The entire ε_m spectrum is involved in the determination of each λ_m . Later we will see that this results in a λ spectrum which is more correlated (i.e stronger level repulsion) than the ε spectrum upon which it is built. Also, α_m is $O(1/2)$.

Next choose M residues P_l , where M is the type of the commuting family. These residues are used to construct the function Γ which is given by

$$\Gamma(y) = \delta \sqrt{1 + \sum_l \frac{P_l}{\lambda_l - y}} \quad (3.18)$$

where $\delta = \pm 1$. The freedom in choosing the P_l 's is two-fold. We must choose their magnitude as well as M λ_l 's with which to associate them. Using the definition

$$\Gamma_m = \Gamma(\varepsilon_m) \quad (3.19)$$

we can write down the elements of the S matrix as

$$[S]_{mn} = \frac{\gamma_m \gamma_n}{\varepsilon_m - \varepsilon_n} \left(\frac{\Gamma_m + \Gamma_n}{2} \right); \quad m \neq n \quad (3.20)$$

The matrix elements of the the Ansatz matrices are then

$$\begin{aligned} [H]_{ij} &= \gamma_i \gamma_j \frac{d_i - d_j}{\varepsilon_i - \varepsilon_j} \left(\frac{\Gamma_i + \Gamma_j}{2} \right); \quad i \neq j \\ [H]_{jj} &= u d_j - \sum_{m \neq j} \gamma_m^2 \frac{d_j - d_m}{\varepsilon_j - \varepsilon_m} \frac{1}{2} \frac{(\Gamma_m + \Gamma_j)(\Gamma_m + 1)}{\Gamma_j + 1} \end{aligned} \quad (3.21)$$

where d_m are the eigenvalues of the matrix V and can be written as

$$d_m = g_0 + \sum_j^{N-M} \frac{g_j}{\lambda_j - \varepsilon_m}. \quad (3.22)$$

The g_j 's are free parameters, the number of which coincides with the number of linearly independent operators within the commuting family, $K=N-M+1$. Choosing g_j to be a Kronecker delta is a natural choice for basis operators within the K dimensional space of matrices.

This matrix has an exact solution. The j^{th} component of the eigenvector labeled by σ is

$$[v^\sigma(u)]_j = \frac{\gamma_j}{\sigma - \varepsilon_j} \frac{\Gamma(\sigma) + \Gamma_j}{2} \quad (3.23)$$

with the u dependence contained in σ . These eigenvectors are shared by every member of the commuting family. The eigenvalues of the i^{th} member of that family are

$$E_\sigma^i(u) = \sum_m \frac{1}{\lambda_i - \varepsilon_m} \frac{\gamma_m^2}{\sigma - \varepsilon_m} \frac{\Gamma(\sigma) + \Gamma_m}{2} \quad (3.24)$$

where σ are solutions of the equation

$$\sum_k \frac{\gamma_k^2}{\sigma - \varepsilon_k} \frac{\Gamma(\sigma) + \Gamma_k}{2} + \frac{B}{2}(\Gamma(\sigma) - 1) = u. \quad (3.25)$$

The solutions to this equation become like those of λ in the limit that all of the residues P_l go to zero. All three spectra, ε_k , λ_k , and σ_k have roughly the same density of states but differ in their short range fluctuations. On this basis we define

$$\beta_m = \frac{\sigma_m - \varepsilon_m}{\varepsilon_{m+1} + \varepsilon_m}. \quad (3.26)$$

The β_m are not perfectly bounded by 0 and 1 like α_m . However, in the limit of low type they approach this same behavior.

3.2.2 The maximal case and the connection with Gaudin/BCS

For type M=1, the Ansatz parameterization generates a family of commuting operators which is maximal in the sense that it has the highest possible number of linearly independent commuting partners. In this case the parameterization simplifies significantly, and the S matrix depends on only 2N parameters. As before we choose γ and ε which fully describe S.

$$[S]_{ij} = \frac{\gamma_i \gamma_j}{\varepsilon_i - \varepsilon_j} \quad (3.27)$$

The matrix elements simplify in a similar manner

$$\begin{aligned} [H]_{ij} &= \gamma_i \gamma_j \frac{d_i - d_j}{\varepsilon_i - \varepsilon_j}; \quad i \neq j \\ [H]_{jj} &= u d_j - \sum_{m \neq j} \gamma_m^2 \frac{d_j - d_m}{\varepsilon_j - \varepsilon_m} \end{aligned} \quad (3.28)$$

resulting in an eigenvalue solution

$$E_m(u) = \sum_k \frac{d_k \gamma_k^2}{\lambda_m - \varepsilon_k} \quad (3.29)$$

where in this case the numbers d_k are free parameters. For type 1 we have the auxiliary equation

$$u = \sum_k \frac{\gamma_k^2}{\lambda_m - \varepsilon_k} \quad (3.30)$$

which has N solutions for λ and is a simplification of Eq. (3.25) which applies for arbitrary type. Note that it has the same form as Eq. (3.11) with B replaced with u. We can therefore apply our description of λ_m (in terms of α_m) to the M=1 case as well as the case of general M. The eigenvalues of the basis operators are given by

$$E_m^{(i)}(u) = \frac{\gamma_i^2}{\lambda_m - \varepsilon_i} \quad (3.31)$$

As mentioned above, the d_m 's are eigenvalues of an arbitrary Hermitian matrix V by design, where $H = uV + T$. Thus, for any arbitrary choice of d_m there exists some T such that $H(u)$ will be a member of a type 1 family. Indeed, Eqs. (3.28) is written in the eigenbasis of V . Both the basis and the eigenvalues of V (the parameters d_m) can be chosen arbitrarily. By symmetry one can similarly choose T at will, though this is not apparent from Eqs. (3.28). As soon as V is fixed, T is severely constrained; one is left with only $2N$ parameters γ_i, ε_i to specify its matrix elements. This ability to choose either V or T arbitrarily means in particular that any u -independent Hamiltonian can be 'embedded' into a type 1 family in many different ways. For example, one can choose V to be the Haldane-Shastry model and find T so that $T + uV$ belongs to a given type 1 family. Such a freedom does not exist, in general, for the higher types.

Type 1 integrable families are closely related[3] to the Gaudin magnets[6] for which $\hat{h}_i = B\hat{s}_i^z + \sum_{j \neq i} \hat{\mathbf{s}}_i \hat{\mathbf{s}}_j (\varepsilon_i - \varepsilon_j)^{-1}$, where $\hat{\mathbf{s}}_j$ are quantum spins of arbitrary length s_j . In the sector with (conserved) $\hat{S}^z = \sum_j \hat{s}_i^z$ equal to its maximum (minimum) possible value less (plus) one, $\hat{h}_i$ are N commuting $N \times N$ matrices which form a type 1 family with $u = B$ and $\gamma_j^2 = s_j$. The BCS model is obtained[9] as $\sum_j \varepsilon_j \hat{h}_j$ for $\gamma_j^2 = s_j = 1/2$ and a replacement $u = B \rightarrow 1/g$, where g is the dimensionful BCS coupling constant.

Some blocks of the 1D Hubbard model characterized by a complete set of u -independent symmetry quantum numbers are type 1 matrices, though most blocks are type $M > 1$ [3]. A similar typology can be developed for e.g. the 1D XXZ Hamiltonian and other sectors of Gaudin and BCS models using the method of[3] for determining the type of parameter-dependent matrices.

One can also construct fermionic (bosonic) Hamiltonians[4] out of type 1 matrices as $\hat{H} = \sum_{mn} [H(u)]_{mn} a_m^\dagger a_n$, where a_n are the usual fermionic (bosonic) destruction operators. $[\hat{H}_1, \hat{H}_2] = 0$ as long as the corresponding matrices $H_1(u)$ and $H_2(u)$ commute, i.e. belong to the same family.

3.3 Numerical Results

We have performed an extensive numerical study of level statistics of type $M = 1$ as well as higher type matrices for various choices of the parameters. In a vast majority of cases the statistics are Poisson for $N \gg 1$ with high accuracy, even when we deliberately choose parameters which enhance non-Poisson statistics. In this section we present these results in terms of some scalar observables which crossover to non-Poisson behavior in certain limits. The basic strategy is to show that Poisson statistics are the rule by demonstrating that the non-Poisson limits become vanishingly small in the limit of large N . This strategy is made possible by the freedom of having an explicit parameterization of the Ansatz matrices. We can intentionally promote non-Poisson behavior and then see how the correlations persist when perturbed. In all cases, the non-Poisson behavior is found to be fragile. We show this for three identified non-Poisson limits: 1) large u in Type 1 where $E_m \approx u d_m$, 2) again in type 1, the case where d_m can be expressed as some simple smooth function of ε_m and 3) somewhat related to case 2, the situation where E_m is made up of a superposition of only a small number of the basis operators.

The parameter space of the Ansatz matrices is huge yet we will show that the majority of these parameters have very little impact upon the level statistics. Regardless of our choices the statistics turn out to be Poisson in most cases. For example, while different choices of Γ_i may effect the eigenspectrum to some extent, they do not play a central role in determining the average level repulsion as measured by Brody function fits. Another example, γ_i has no effect upon the statistics except in the some rare case that the statistics are non-Poisson for another reason. In such a case, the choice of constant γ will maximize the non-Poisson behavior whereas uncorrelated γ will result in a middling amount of level repulsion as is illustrated in Fig. (3.3). By experience it has become clear that the most relevant parameters are the ε_i 's which form the backbone of the spectrum. Second to ε_i are the d_i 's which have an interesting relationship with ε . Namely, if the two sets of numbers are uncorrelated the Ansatz matrices have Poisson statistics. Any smooth functional dependence between them results in the development of level repulsion. This interplay between d_i and ε_i will be a focus of the numerics which follow. Other details will be highlighted where relevant.

We have also learned that the statistics of the Ansatz matrices can not be predicted perfectly from the statistics of the input matrices. There is a finite variance in the output statistics, the origin of which is quite complicated. Furthermore, even exact results of the Gaussian ensembles have an intrinsic variance. Therefore we should not be surprised that some finite variance crops up in the Ansatz. For this reason we present data which are averaged over many instances of Ansatz matrices and include error bars to indicate the variance. These error bars are not from any lack of precision in

our calculation. They represent an intrinsic variation which is a consequence of dealing with randomly generated matrices. The variance itself has an interesting dependence on the parameter choices. Of course there is some natural uncertainty in the fits which lead to ω_B . However, this uncertainty is much less than the intrinsic variance of the statistics.

3.3.1 Spectral Observables

Before getting to the numerical results we must discuss the spectral observables which we employ as measures of the spectral statistics. Two particularly common and simple spectral observables are the nearest neighbor spacing distribution and the number variance. These quantities are well-studied and have exact results for the Gaussian random matrix ensembles. These exact results apply to random matrices which by definition have no internal symmetries. When dealing with Integrable models it has been necessary to construct symmetry-reduced blocks of the Hamiltonian. Treatment of symmetries has therefore been a central matter in previous discussions of statistics and/or crossings. In our case, this issue is circumvented in that we construct these matrices without any internal symmetries. The matrices studied here should therefore be seen as examples, not of some integrable Hamiltonian at large, but of some subspace thereof in an irreducible representation.

3.3.1.1 Level Repulsion and the Brody Parameter

The Gaussian Ensembles are known to exhibit level repulsion. That is, if we define a distribution $P(s)$ for the nearest neighbor level spacing s measured in units of the average spacing, it is found that for small s the spacing distribution vanishes according to $P(s) \propto s^\beta$. The famous Wigner surmise assumes $\beta = 1$ and predicts that the spacing statistics of random, real symmetric matrices follow the Wigner-Dyson distribution

$$P_{WD}(s) = \frac{\pi s}{2} e^{-\pi s^2/4} \quad (3.32)$$

while random Hermitian and Symplectic matrices have $\beta = 2$ and $\beta = 4$, respectively, with Gaussian tails at large s . This is in contrast to the Poisson form expected of uncorrelated levels

$$P_{Poisson}(s) = e^{-s} \quad (3.33)$$

where there is a finite probability of adjacent levels being arbitrarily close to each other since the limit of $P(s)$ is finite as $s \rightarrow 0$.

These distributions from Random Matrix Theory form a discrete set of benchmarks for level repulsion. However, the statistics of any given matrix may exhibit some $P(s)$ which is quite unlike any known exact result. For this reason it is useful to define a function which interpolates between the exact solutions as a function of some parameter. In this way we can smoothly quantify the amount of level repulsion/clustering which appears in some spectrum. Such a function has been introduced by Brody.

$$P_{Brody}(\omega; s) = a s^\omega e^{-b s^{\omega+1}} \quad (3.34)$$

The parameters a and b can be uniquely fixed by the requirement that the distribution be properly normalized according to

$$\begin{aligned}\int_0^\infty P(s)ds &= 1 \\ \int_0^\infty sP(s)ds &= 1.\end{aligned}\tag{3.35}$$

When ω is zero (one) the Brody function coincides with the Poisson (Wigner-Dyson) distribution and it interpolates smoothly between them. This interpolating function is not unique; there are many possible interpolating functions. The Brody function is designed to be a particularly good interpolation between the Poisson and Wigner-Dyson limits. We will attempt to choose our parameters to make the most use of this optimized range of ω_B . I note however, that the two sumrules in Eq. (3.35) heavily constrain the allowed forms of $P(s)$. Consequently the Brody function can successfully fit distributions which have $\omega_B > 1$ or $\omega_B < 0$ where, for instance, the exponential decay of the tail of the distribution may have the wrong shape. The fit will not be perfect but ω_B remains a decent measure of the level repulsion.

The evaluation of $P(s)$ involves a complication which has come to be known as “unfolding.” The universal behavior of $P(s)$ appears only when “ s ” is measured in units of the mean level spacing. However, the mean level spacing is not, in general, nor even commonly, a constant across an entire spectrum. The Gaussian Ensembles, for instance, have a density of states which has a semi-circular shape. The variation of the density of states must be unfolded from the spectrum in such a manner that short range fluctuations remain. Only after the unfolding can the nearest neighbor spacings

be compiled into a histogram which may be expected to show some universal result.

The unfolding procedure is simple. To understand the method we must first define the cumulative density of states as

$$N(E) = \sum_i \Theta(E - E_i) \quad (3.36)$$

where E_i is the i^{th} level sorted such that

$$E_{i+1} > E_i \quad (3.37)$$

for all i . $N(E)$ is called a staircase function because it is a monotonically rising series of unit steps. The staircase function can be thought of as the sum of two parts: $N_{smooth}(E)$ which captures the broad features of the density of states, and $N_{fluc}(E)$ which captures small scale local fluctuations. N_{fluc} contains the information which will be expressed in $P(s)$. The running density of states is therefore

$$\rho_{DOS}(E) = \frac{dN_{smooth}(E)}{dE}. \quad (3.38)$$

An unfolded spectrum must have the form

$$\xi_i = i + \delta_i \quad (3.39)$$

where δ_i are numbers of $O(1)$ which are equally likely to be positive or negative. The spacings of this spectrum become

$$\begin{aligned} \rho_i &= \xi_{i+1} - \xi_i \\ &= 1 + \delta_{i+1} - \delta_i. \end{aligned} \quad (3.40)$$

These numbers ρ_i are those which follow the distribution $P(s)$ and its form is determined by correlations among the short range fluctuations, δ_i .

One way to obtain a spectrum of the form of Eq. (3.39) is to note that $N(E_i) = i$. Therefore

$$\begin{aligned} N_{smooth}(E_i) &= N(E_i) - N_{fluc}(E_i) \\ &= i - N_{fluc}(E_i). \end{aligned} \tag{3.41}$$

Thus it is appropriate to define the unfolded spectrum by the mapping

$$\xi_i = N_{sm}(E_i). \tag{3.42}$$

The average spacing should always be unity over any handful of levels, but the local fluctuation spectrum are preserved. Finally, $P(s)$ can be computed by forming a histogram out of all of the level spacings of ξ . In practice we fit the spectrum with a 25th order polynomial. We find numerically that this is a high enough order to capture all smooth features of the staircase function for the types of matrices we have studied. Furthermore, near the edges of the spectrum the density of states changes more rapidly, i.e. over shorter scales. It is therefore more likely that the unfolding procedure described above does not properly disentangle the variations of the density of the states from the local fluctuations. Thus, it is prudent to use only the middle 50% of the spectrum to avoid the influence of edge effects.

3.3.1.2 Spectral Rigidity

Another useful statistic is called the spectral rigidity. It measures the constancy of the density of states over a finite length scale. Technically, it is defined as the variance of the density of states and can be written as

$$\begin{aligned}\Delta(L) &= \langle (n(L) - \langle n(L) \rangle)^2 \rangle \\ &= \langle n(L)^2 \rangle - \langle n(L) \rangle^2\end{aligned}\tag{3.43}$$

where $n(L)$ is the number of levels which occur over some stretch of the spectrum which has length L in units of the local average level separation. If the density of states is constant then we say it is rigid as compared to a spectrum with a varying DOS. Note that the former has a straight line for the staircase function while the latter has a staricase function which is more curvy and meandering. A rigid spectrum is one for which an energy range L is very likely to contain a number of levels close to L . Equivalently, if the spectrum is rigid we can expect that large sections of it will be well fit by straight lines. In practice this statistic can be calculated by first computing

$$\Delta(E, L) = \frac{1}{L} \int_{E-L/2}^{E+L/2} (N(E') - N_{fit}(E'))^2 dE' \tag{3.44}$$

where $N(E)$ is the staircase function defined above and $N_{fit}(E)$ is the best linear fit of $N(E)$ over the region being integrated. This is subsequently averaged over the spectrum as

$$\Delta(L) = \langle \Delta(E, L) \rangle_E. \tag{3.45}$$

As with $P(s)$, exact results for $\Delta(L)$ are known in the Gaussian ensembles and for uncorrelated spectrum. Once again we will construct a function which interpolates between the Poisson limit,

$$\Delta_{Poisson}(L) = \frac{L}{15}, \quad (3.46)$$

and the Wigner-Dyson limit,

$$\Delta_{WD}(L) = \frac{1}{\pi^2} \left(\ln(2\pi L) + \gamma - \frac{5}{4} - \frac{\pi^2}{8} \right), \quad (3.47)$$

as a function of a single parameter where, in this case, γ is the Euler-Mascheroni constant. The simplest way to accomplish this interpolation is

$$\Delta_{Interp}(L) = (1 - \alpha)\Delta_{Poisson}(L) + \alpha\Delta_{WD}(L) \quad (3.48)$$

where α is the fit parameter going from 0 to 1 as Δ goes from a Poisson to a Wigner-Dyson form. Again, we note that this interpolation is not unique and is in fact inadequate to capture every possible form of $\Delta(L)$. Nonetheless it is an effective measure of the rigidity crossover in that region which interpolates from Poisson to Wigner-Dyson. Some examples of our $P(s)$ and $\Delta(L)$ are given in Fig. (3.1).

3.3.2 Three Crossovers

3.3.2.1 x-dependent crossover in Type 1

As noted earlier, the Type 1 parameterization places no constraints on the parameters d_k . Therefore, we can choose them to be the eigenvalues of a real symmetric matrix thus embedding level repulsion into the spectrum. For here on we find it useful

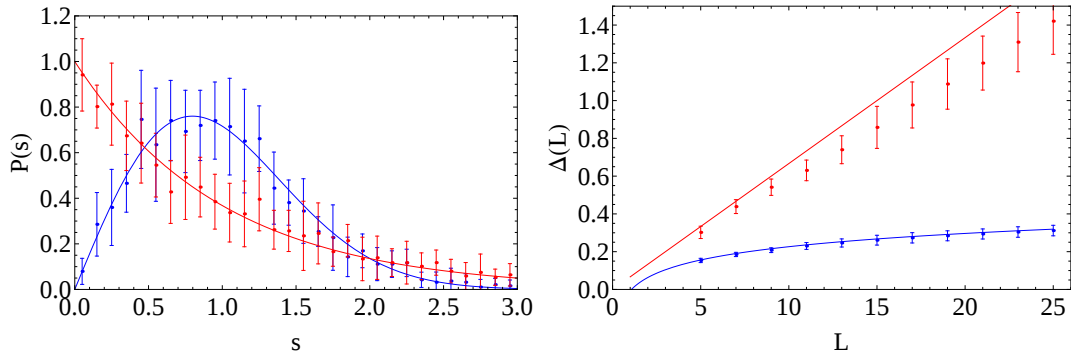


Figure 3.1: The Brody function $P(s)$ and the rigidity $\Delta(L)$ as computed for an uncorrelated spectrum (Red) which exhibits Poisson behavior and a correlated spectrum which comes from the eigenvalues of a real symmetric matrix. In each panel the red curves (points) show the GOE behavior while the blue curves (points) show the Poisson behavior. The error bars show typical variances of the function. The Brody parameter ω_B and α will interpolate smoothly between these functions providing a means of measuring intermediate spectral statistics.

to define $x = 1/u$ and work with the Hamiltonian $V + xT$ rather than $T + uV$. In the limit of large u ($x = 0$) the statistics of a generic type 1 matrix coincide with those of the d_k 's. For good measure we can pick the ε 's in the same fashion and take γ to be constant. These choices are made with the intention of promoting level repulsion. In Fig. (3.2) this intercept at small x is clearly visible. However, the Brody parameter crosses over to the Poisson limit at some value of $x = x_0$. The rigidity shows a similar crossing at the same scale x_0 . Both observables remain Poisson-like up to the limit of large x . The shapes of these crossings are well fit by a hyperbolic tangent function on the logarithmic scale.

$$\omega_B(x) = a_1 + a_2 \tanh\left(\frac{1}{W} \ln \left| \frac{x}{x_0} \right| \right) \quad (3.49)$$

where x_0 is the crossover scale, and W is it's width on the log scale. Using this fit we can obtain information about the crossovers and determine how they scale with the

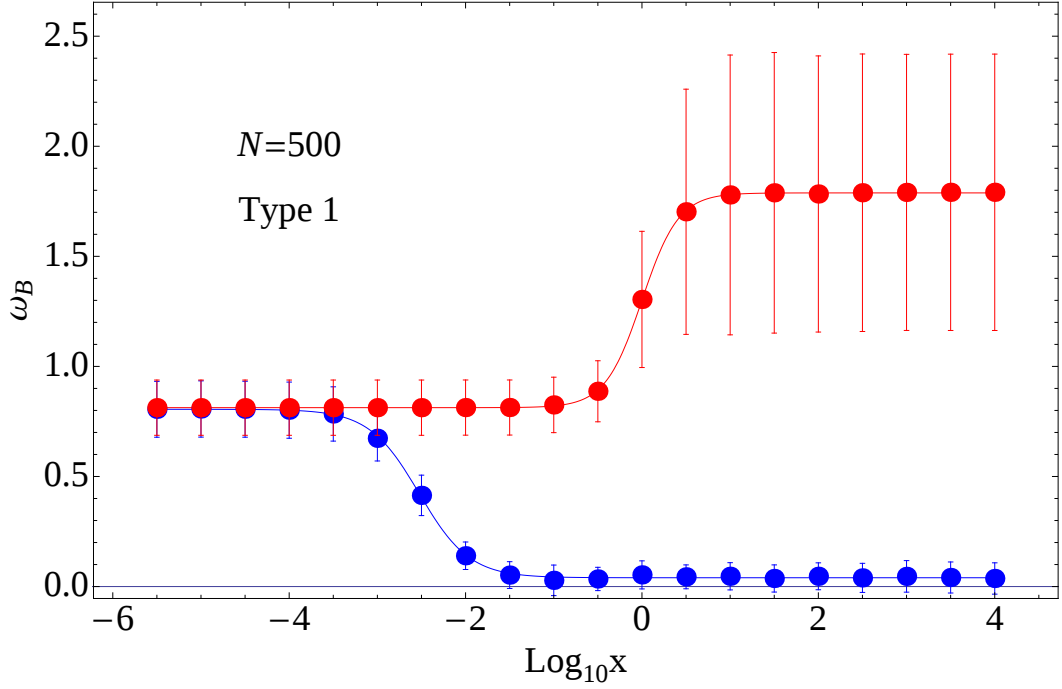


Figure 3.2: With constant γ and both ε_m and d_m chosen from the GOE we can observe x dependent crossovers in the level repulsion. At very small x , the level repulsion of H and $h^{(i)}$ will match the statistics of the input parameters, d_m and ε_m respectively. As x is increased, the generic behavior of Type 1 matrices takes over, the level repulsion of H drops to zero. At a higher value of x the level repulsion of $h^{(i)}$ increases through a similar monotonic crossover. The crossovers occur at different values of x . The N dependence of the crossover scale is plotted in Fig. (3.4).

dimension of the matrix. It is found that the crossover scale goes as $x_0 \sim \frac{1}{N}$. Thus the influence of d_k at low x is a finite size effect which has a vanishing significance as the matrix dimension is increased. Fig. (3.4) shows the extracted crossover scale as a function of N .

The crossover from low to high x has been performed with different choices for the statistics of d_m , such as Poisson and even negative Brody parameter. In every case the crossover proceeds as above. Specifically, at low x , the statistics of H are those

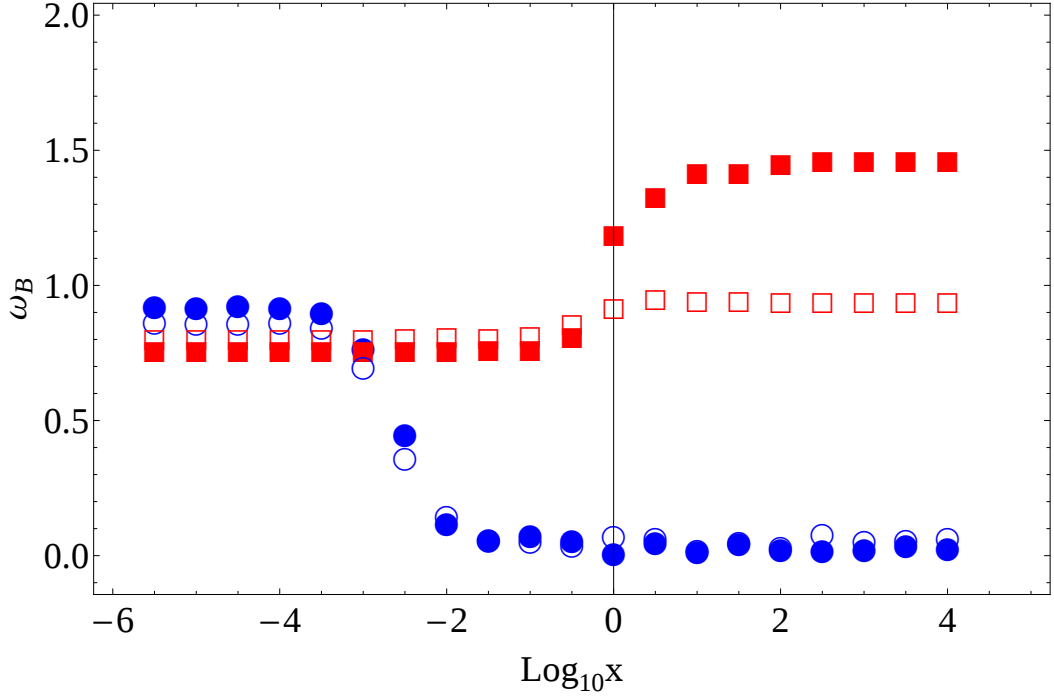


Figure 3.3: For type 1 matrices with ε_m and d_m of GOE, impact of the choice of constant vs random γ is displayed for $N=500$. For an arbitrary H , the spectral statistics are unchanged whereas the statistics of the basis operators become more repulsive at large x when the γ_k 's are chosen as a constant value. Whatever mechanism is working to increase level repulsion in the basis operators has no impact on the general matrix which is Poisson in any case for large x .

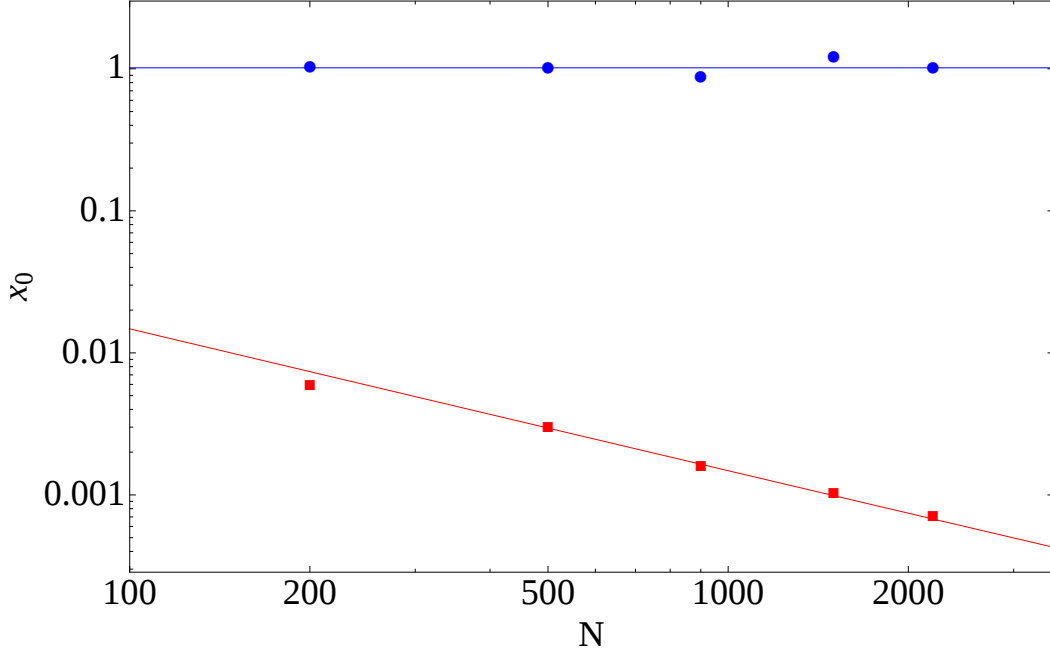


Figure 3.4: The position of the crossover has a smooth dependence on the dimension N . The red squares show the crossover position extracted from the logarithmic tanh fits for the basis operator statistics. The blue circles show the Brody parameter averaged over generic matrices. In all cases the matrices were built using ε_i and d_i from the GOE with constant γ . The position of the $h^{(i)}$ crossover has no dependence on the matrix dimension. It is very well fit as a constant, $x_0 = 1.01$. The position of the crossover for a general Ansatz matrix, H , is well fit by $1.47N^{-1}$. These fits are shown as the superposed curves. From the scaling we learn that the region where a generic type 1 matrix is non-Poisson vanishes as N goes to infinity. In this sense, we can call the non-Poisson regions a finite size effect. Each point represents averaging over 10 instances.

of the d_m while the statistics of any $h^{(i)}$ are those of the ε_m . At large x , the statistics of H crossover to Poisson but $h^{(i)}$ actually becomes more correlated. The increase in the level repulsion depends on the choice of γ . The associated increase in the Brody parameter is greatest when γ is a constant. If γ are random numbers, the increase in the level repulsion will be quite small.

For general M it is difficult to perform this same test because the d_k are not all free parameters. They are controlled by the parameters g_k . However, for a large range of types greater than 1 but not too close to N (“too close” will be defined later) we see Poisson statistics. Since we cannot force d_k to have some level repulsion for $M > 1$ we have only partial control of the stats at low x . Consequently the crossover seen in Type 1 is unsure for higher M . In the following section we give an argument that, although unseen, it is still present and scales as in the case $M=1$.

3.3.2.2 Correlated d_m and ε_m

In the preceding section the d_k ’s and ε_k ’s were chosen independently of each other. We now examine the consequences of imposing a functional relationship between them. It is known from the BCS literature and further noted by Shastry Ref. ([4]) that the choice $d_k = \varepsilon_k$ results in non-Poisson statistics. Shastry’s argument compares the level repulsion of $\lambda_m(x)$ and $E_m(x)$ (called $\omega_m(x)$ and $\alpha_m(x)$ respectively in that work). It is observed that λ_m displays avoided crossings while α_m has true crossings. This is explained as α_m being a “smeared” version of the λ_m eigenspectrum which does not need to follow the Wigner-von Neumann noncrossing rule so strictly as generic Hamiltonians.

The BCS case is an exception to this rule in the sense that no crossings of $E_m(x)$ occur at finite x . It is the position of Ref. ([3]) that all of the crossings may be viewed as occurring simultaneously at $x = \pm\infty$. This exception can actually be made simpler by noting the following:

$$\begin{aligned}
E_m^{(BCS)}(x) &= \sum_k \frac{\varepsilon_k \gamma_k^2}{\lambda_m - \varepsilon_k} \\
&= \sum_k \gamma_k^2 \left(\frac{\lambda_m}{\lambda_m - \varepsilon_k} - 1 \right) \\
&= \frac{\lambda_m(x)}{x} - \sum_k \gamma_k^2.
\end{aligned} \tag{3.50}$$

Thus, for the BCS problem, E_m and λ_m are related in a simple way which changes no relevant spectral statistics. They are effectively the same spectrum in the sense that they are related by some “gauge” transformations of the Ansatz parameters. Later we will see that all basis operators $h^{(i)}(x)$ have the same statistics as λ_m . Only by choosing some d_k ’s which mix several $h^{(i)}(x)$ will the level statistics become uncorrelated and the crossing happen at finite x . However, the BCS d ’s mix the $h^{(i)}(x)$ in a special way which reproduces the spectral statistics of λ_m .

While the BCS hamiltonian has no crossings presumably some perturbation of the d_k ’s would create crossings at finite x . What is the scale of the perturbation needed to create such a crossing when x is $O(1)$? We consider the crossings which occur for a BCS-like Hamiltonian where a single d_k is modified according to

$$d_k = \varepsilon_k + \sigma \delta_{(i,k)} \tag{3.51}$$

where $\delta_{(i,k)}$ is a Kronecker- δ function. We can write out the E_m explicitly as

$$E_m = \frac{\lambda_m}{x} - \sum_k \gamma_k^2 + \sigma \frac{\gamma_i^2}{\lambda_m - \varepsilon_i} \quad (3.52)$$

and after a few steps of algebra we find that

$$E_{m+1} - E_m = (\lambda_{m+1} - \lambda_m) \left(1/x - \frac{\sigma \gamma_i^2}{(\lambda_{m+1} - \varepsilon_i)(\lambda_m - \varepsilon_i)} \right). \quad (3.53)$$

Since there are no crossings in the λ spectrum we can say that the condition for a crossing of E_m is

$$1/x = \frac{\sigma \gamma_i^2}{(\lambda_{m+1} - \varepsilon_i)(\lambda_m - \varepsilon_i)}. \quad (3.54)$$

We can extract the scale of σ by recalling that the scale of each factor of Eq. (3.54) is determined by Eq. (3.9) and Eq. (3.10). We must also note that each λ_m is pinned to the associated ε_m so that we may say $(\lambda_m - \varepsilon_i) \approx (\varepsilon_m - \varepsilon_i) \approx (m - i)/N$. Finally, for the case $1/x \sim O(1)$ we find

$$\sigma \sim \frac{(m - i)^2}{N} \quad (3.55)$$

So a perturbation of d_i in the BCS problem need only be $O(N^{-1})$ to draw a crossing from $x = \pm\infty$ down to $x = 1$. Furthermore we see that the difference $(m - i)$ is relevant. This occurs because the smearing effect created by the perturbation is strongest for the eigenvalues closest to E_i . Thus it takes a larger perturbation to cause crossing between levels which are far away from E_i .

In fact it is not difficult to find many other functional relationships between d_k and ε_k which exhibit non-Poisson statistics. For example, $d_k = \varepsilon_k^p$ where p is an integer will cause level repulsion. For $p > 1$ there are level crossing at finite x but the spacing

statistics are non-Poisson. Such non-Poisson choices are numerous in parameter space. It is therefore interesting to determine their size. Do they fill a large fraction of the space? For this reason we examine the statistics of E_m when d_m are given by

$$d_k = \varepsilon_k^4(1 + \delta\eta_k) \quad (3.56)$$

where η_k is a random number of order one and δ sets the scale of the random perturbation. The fourth power of ε_k is an arbitrary choice of a known oscillator solution. Again we choose the ε 's to be eigenvalues of a real symmetric matrix and γ are constant. The level repulsion is quite strong in the limit of small δ but the Poisson statistics return for $\delta_0 \sim O(N^{-1})$. This crossover is reminiscent of that seen in the previous section. The common scaling suggests a shared mechanism.

As in the previous example, it is difficult to perform this test for arbitrary type because of the complex constraints on d_m for $M > 1$.

3.3.2.3 Statistics of a single Basis operator

We have seen two examples of the statistics approaching Poisson as a function of some continuous variable. Now we examine a discrete approach to Poisson statistics. To begin we note that each of the basis operators which comprise a commuting family will have statistics which are determined primarily by ε_k and are therefore not necessarily Poisson (ε being free to be chosen with repulsion). However, we have already seen that (at least for large x) the generic Type 1 matrices have robust Poisson statistics. Therefore it is interesting to ask how many basis operators H^i need to be superposed before the statistics become Poisson. Furthermore, are all superpositions equivalent?

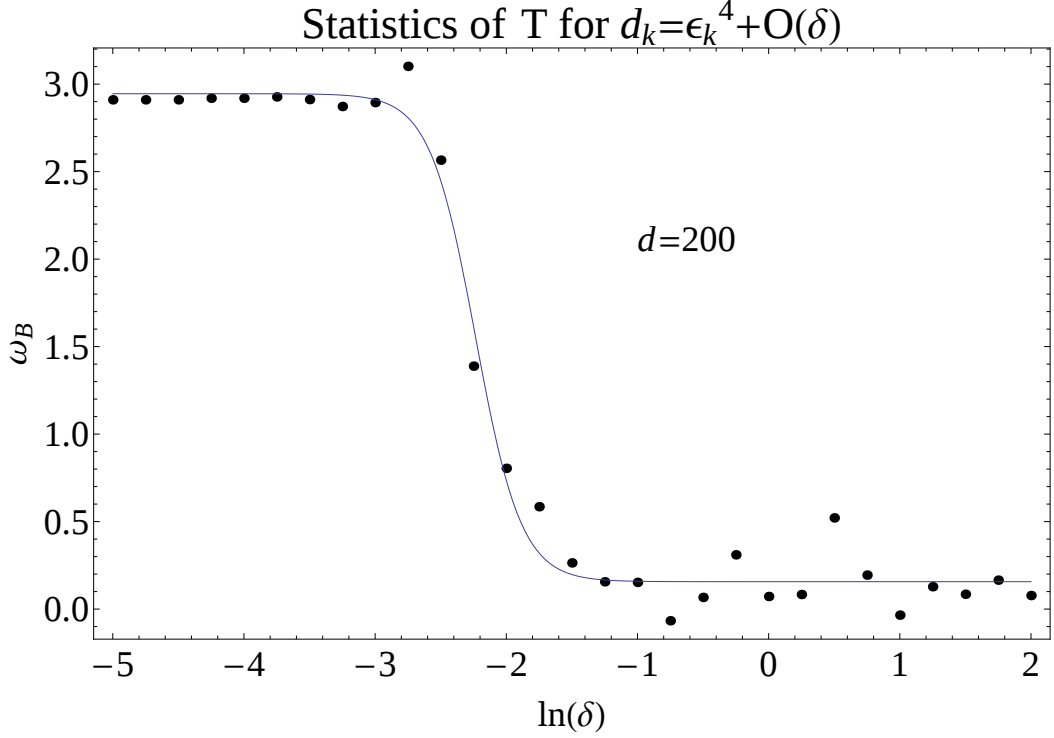


Figure 3.5: When d_k are chosen to be some power of ϵ_k the spacing statistics will not be Poisson in general. They inherit the level repulsion of ϵ_k . There are many points where d_k 's and ϵ_k 's are correlated. We perturb around one such point with a finite delta which blurs the correlation between the d 's and ϵ 's. Consequently the statistics of T eventually return to the generic Poissonian case. The crossover has the same logarithmic tanh function form that was seen in the x dependent crossover of Fig. (3.2). In Fig. (3.6) the crossover scale is plotted against the matrix dimension. The scaling indicates that the non-Poisson regions vanish in the thermodynamic limit.

Radius of Non-Poisson region of parameter space, δ_0

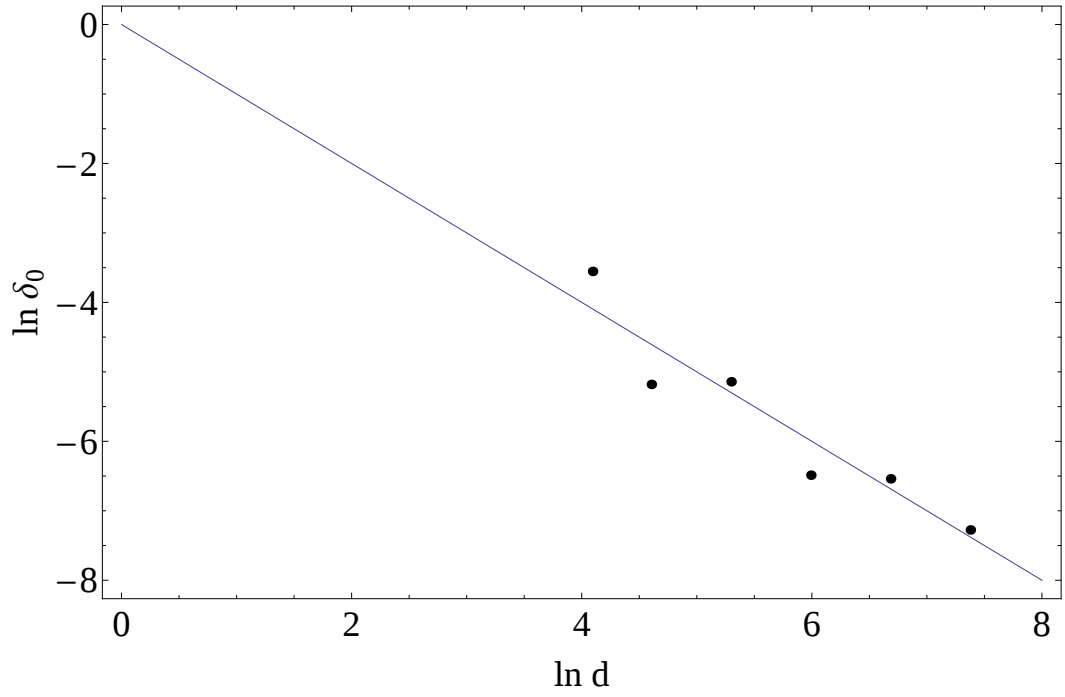


Figure 3.6: The δ -crossover is fit with a tanh function and the scale of the crossover is extracted. The fit shows that the crossover occurs at $\delta \sim O(N^{-1})$. This is the same scaling which was observed for the x-dependent crossover.

We define a number L to go along with N and M . L is the number of superposed basis operators that go into the matrix H . For example the most general example of a type M matrix would have $L=K=N-M+1$ while $L=1$ corresponds to the limit of the basis operators. Decreasing L from K should eventually lead to a crossover to non-Poisson statistics. In Fig. (3.7) we show the high x limit of statistics in the basis matrices as a function of type to demonstrate that in the limit $L=1$ the Poisson stats break down for all types.

Recall that the eigenvalues of a type 1 basis operator H^i are given by $E_m^i(u) = \frac{\gamma_i}{\lambda_m - \varepsilon_i}$. These spectra all have a single singularity as λ_m nears ε_i . Otherwise the spectrum is smooth. With each new operator added to the superposition, a new singularity will enter the spectrum. It is found that when these singularities lie near each other the statistics are very much like the individual basis operator. However, if the singularities are spread across the spectrum, the level repulsion quickly fades to Poisson. Grouping the singularities preserves a large smooth part of the spectrum. This is one source of the large variances observed in the data.

When we looked at the x -dependent crossovers we had no recourse to show the equivalent plots for high Types because the d_m 's are much harder to control away from type 1. In this case it is simple to add in more basis operators regardless of the type. We can therefore compare the discrete crossover scale for type 1 with that of other types. For $M > 1$ we see again that the eigenvalue spectrum of a single basis operator

has a single singularity

$$E_{\sigma}^i = \frac{u - \tilde{u}_i}{\lambda_i - \sigma} \quad (3.57)$$

where the roots σ are close to λ_i . It is found that, the behavior is essentially unchanged across all of the types. It only takes a few well dispersed basis operators to create Poisson statistics. This process occurs even in the limit of very high type, like $M = N - 2$. However, in this case the family runs out of members before the statistics can fully decay to Poisson. L is bounded by K . Nonetheless, it appears that this low L crossover behavior applies to all types with essentially the same rate of decay. In Fig. (3.8) we plot this L dependent decay towards Poisson behavior. We show the statistics for the case $(N,M)=(500,480), (N,M)=(500,497)$ and $(N,M)=(500,1)$. In each case it is found that the decay in the Brody parameter is well fit by an exponential. The exponent has a prefactor of ≈ -0.2 in all cases. This value is comparable to what is seen for type 1 (although type 1 has a larger intercept as can be seen in Fig. (3.7)). This indicates that a linear combination of about 10 basis operators is sufficient to wipe out the majority of spectral correlations. This assumes of course that the singularities are spread across the spectrum. Fig. (3.8) also demonstrates the case where the basis matrices are not truly chosen at random. For the type 1 case we show that a certain biased choice of the basis operators included in the superposition can result in statistics which do not decay with L . In such cases one may take $L \sim O(N/2)$ to get to the Poisson limit rather than merely $L \sim 10$.

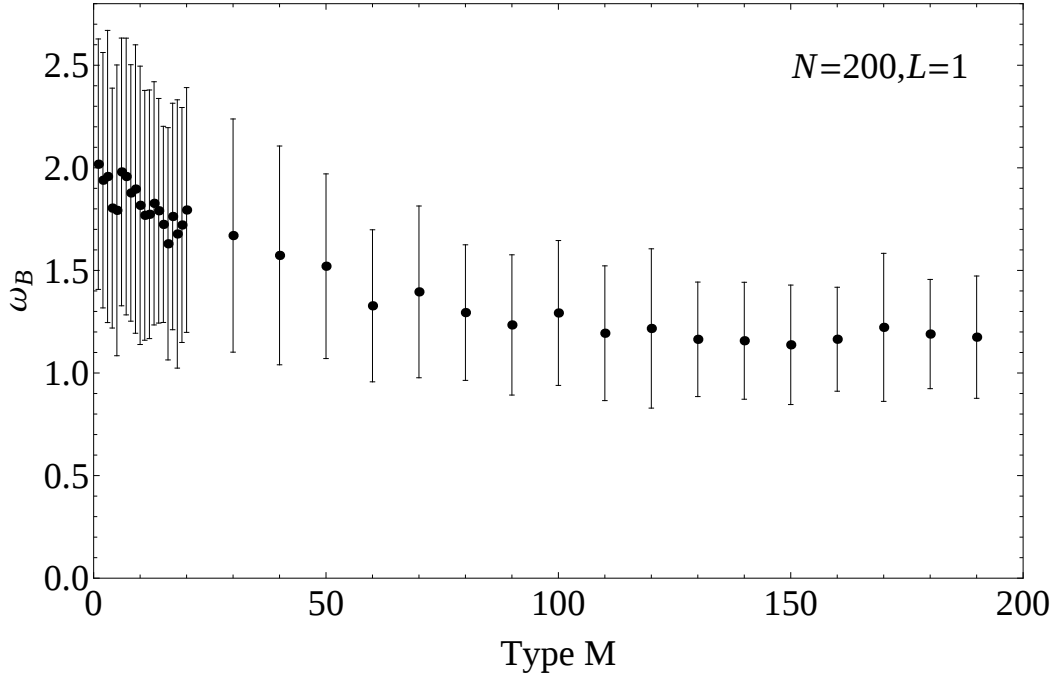


Figure 3.7: We plot the Brody parameter for basis operators in the limit of large x . The matrices were constructed with constant γ_m and ε_m of the GOE. As we have seen in earlier figures, the level repulsion of the basis operators is bounded below by the repulsion of ε_m . For constant γ we see that at low types the Brody parameter is greater (about 2 as compared to 1 which we would normally expect of the GOE) than that of ε but it decays (roughly exponentially) with increasing type.

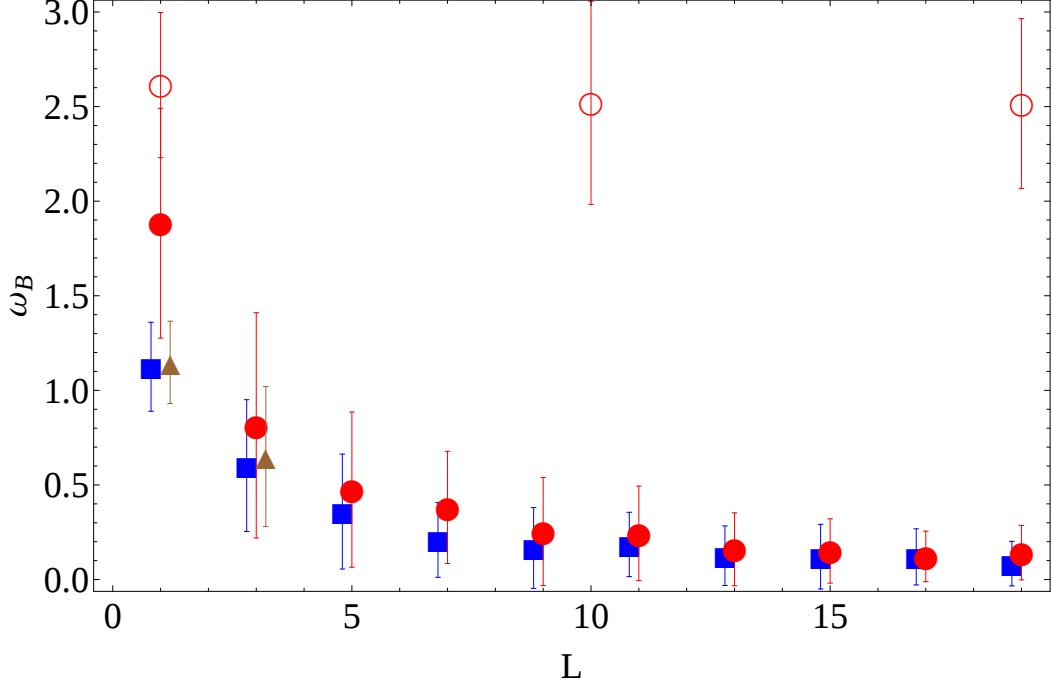


Figure 3.8: Above we plot the Brody parameter parameter for high type matrices as a function of L where L is the dimension of the subspace within which the linear combination is taken. In each case $N=500$. The curves are types 1 (Red Circle), 480 (Blue Square), and 497 (Brown Triangle). Besides the dimension and type noted in the figure, all other parameters are chosen in the same way. For each value of L we compute 50 instances and average the results. In each case, ω_B appears to decay roughly exponentially at low L . Consequently, the statistics have nearly fallen to the Poisson limit by $L \approx 10$. The type $M=497$ case shares this decay but never reaches Poisson statistics because it runs out of basis operators at $L=3$. We also include a set of Empty Red Circles which are from type 1 matrices where the basis operators included in the superposition are built from the lowest $L \varepsilon_i$. Because of this choice, the statistics do not decay as in the case where the L operators are chosen at random. In this case it will require $L \sim O(N)$ to achieve Poisson statistics. Note however that the error bars of the filled red circles overlap with those of the empty circles.

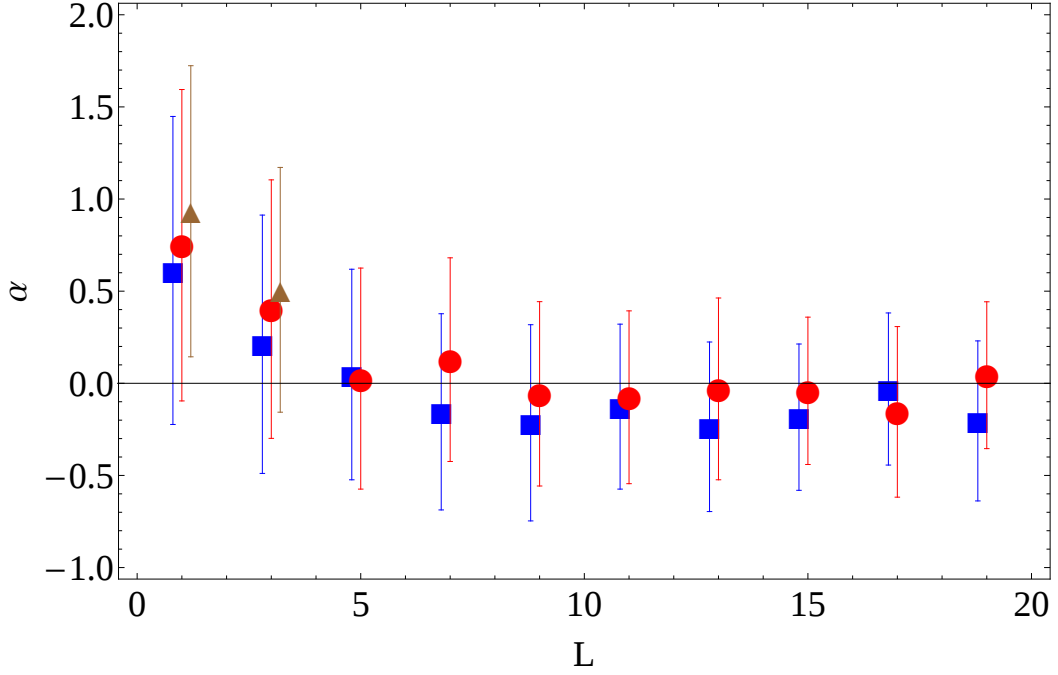


Figure 3.9: Above we plot the rigidity parameter α for high type matrices as a function of L where L is the dimension of the subspace within which the linear combination is taken. In each case $N=500$. The curves are types 1 (Red Circle), 480 (Blue Square), and 497 (Brown Triangle). Besides the dimension and type noted in the figure, all other parameters are chosen in the same way. For each value of L we compute 50 instances and average the results. In each case, α appears to decay roughly exponentially at low L . Consequently, the statistics have nearly fallen to the Poisson limit by $L \approx 10$. The type $M=497$ case shares this decay but never reaches Poisson statistics because it runs out of basis operators at $L=3$. As compared to Fig. (3.8) the error bars are much wider and there is

3.3.3 Placing the results in a single framework

The only exception to Poisson statistics we were able to identify which is true for arbitrary x occurs when parameters d_k and ε_k are correlated, so that $d_k = f(\varepsilon_k)$, where $f(\varepsilon)$ is a piecewise differentiable function of ε . This is the case in e.g. the BCS model where $d_k = \varepsilon_k$ (see above). In such cases the statistics is distinctly non-Poissonian and, moreover, in case (a) above, for example, $P(s)$ crosses over at $x = O(N^0) \equiv O(1)$ from the Wigner-Dyson $P_{WD}(s)$ to a more repulsive distribution $P(s) \propto s^\omega$ for small s with $\omega \approx 2$. The repulsion is softened by randomizing γ_k . More importantly, the statistics quickly becomes Poissonian when the correlation between d_k and ε_k is destroyed, $d_k = f(\varepsilon_k)(1 + \eta_k)$, where η_k are random. We find Poisson distribution already for $\eta_k = O(1/N)$ at $x = O(1)$, see also [8] for a similar study of Gaudin model. $d_k = f(\varepsilon_k)$ define exceptional ‘surfaces’ of certain measure zero in parameter space. This seems analogous to the harmonic oscillator exceptions to the Poisson distribution in classical integrable systems[1]. There too one finds increased level repulsion for oscillators instead of Poisson $P(s)$.

This viewpoint also explains level repulsion of the basis operators for which it can be said that $d_k = f(\varepsilon_k)$ when there are only a few finite g_j ’s. Adding in several more finite g_j ’s will make the function $f(\varepsilon)$ considerably less smooth because each basis operator adds a new singularity.

3.3.4 Type dependence of the basis operator statistics

We have seen that for all types built with repulsive ε_k there is repulsion in the basis operators. At high u (low x) the statistics of the basis operators are those of the ε_m which we have briefly discussed. At low u (high x) this repulsion is increased in a way which depends on type with the lowest types having the most repulsive behavior. This is depicted in Fig. (3.7). The effect of increasing type therefore seems similar to the effect of randomizing γ_m . This makes sense in light of the fact that increasing for low types Γ_m is essentially a smooth function of m . Increasing the type will randomize the Γ_m which should have the same effect as random γ_m .

3.4 Analytical results

In this section we attempt to explain the key features of the numerical results. To begin we present some notation which makes some sense of the unfolding process and sheds light on the observed statistics of the Basis operators, namely, that the level repulsion is greater than or equal to that of ε depending on the value of u . This understanding of the fluctuation spectrum for one basis operator lends itself to a particularly simple argument for Poisson statistics as the general result. Finally we present a simple perturbative argument to explain the position of the x -dependent crossover.

3.4.1 Analytic unfolding

A clean definition of spacing statistics involves a decomposition of local fluctuations from more slowly-varying features. The unfolding process used in the numerics has obscured the details of this decomposition to the effect that analytical treatments of fluctuation spectrum are difficult to achieve. In this section we describe a notation which gets around this problem. The basic idea is to express any spectrum as a product of the density of states and the normalized fluctuations such that the unfolding process can be performed in an intuitive symbolic manner. Specifically, we should find answers which have a slowly varying factor multiplying a factor which is fluctuates locally. Then unfolding proceeds simply by dropping the slowly varying factors.

The first step is to define a local mean level spacing for the ε spectrum.

$$\langle s_m \rangle = \frac{\varepsilon_{m+r} - \varepsilon_{m-r}}{2r} \quad (3.58)$$

where r is taken to be some number $\sim O(50)$. For this quantity to be meaningful it is important that it be of the slowly varying type. Specifically, we say that at large r ,

$$\langle s_{m+1} \rangle - \langle s_m \rangle \sim O\left(\frac{1}{r}\right). \quad (3.59)$$

The quality of this approach depends crucially on this smoothness of $\langle s_m \rangle$ as well as it's fidelity to the actual variation in the density of states. Thus, we require that r is big enough that a large number of states are being averaged over, and that r is still much less than N such that actual features in the density of states are not washed out. Thus we wish to choose r such that

$$1 \ll r \ll N. \quad (3.60)$$

Next, we present the notion of an unfolded spectrum where the local mean level spacing is a constant equal to unity. Such a spectrum can be written as

$$\varepsilon_m^{(unfolded)} = m + \delta_m^{(\varepsilon)}. \quad (3.61)$$

Thus, in an unfolded spectrum there is a regular grid of equally spaced points m where numbers $\delta_m^{(\varepsilon)}$ (which are always of $\leq O(1)$) represent the deviation of the m^{th} level from the m^{th} grid point. The m^{th} spacing in this unfolded spectrum is

$$\begin{aligned} \rho_m^{(\varepsilon)} &= \varepsilon_{m+1}^{(unfolded)} - \varepsilon_m^{(unfolded)} \\ &= (m + 1 + \delta_{m+1}^{(\varepsilon)}) - (m + \delta_m^{(\varepsilon)}) \\ &= 1 + \delta_{m+1}^{(\varepsilon)} - \delta_m^{(\varepsilon)}, \end{aligned} \quad (3.62)$$

the difference of two neighboring deviations plus one unit step on the grid. These numbers, $\rho_m^{(\varepsilon)}$, are the same numbers commonly dealt with in the study of fluctuation statistics, i.e. they are the numbers which follow a properly normalized distribution $P(s)$.

The natural spectrum (meaning “un-unfolded”) can now be written as

$$\varepsilon_m = \varepsilon_0 + \sum_{j=1}^m \langle s_j \rangle \rho_j^{(\varepsilon)} \quad (3.63)$$

I have introduced a number ε_0 which holds the place of the bottom of the spectrum. The second term integrates the local mean spacing from the bottom up to the m^{th} level. It is necessary to include a factor of $\langle s_m \rangle$ which is the effective spacing unit in the normal spectrum. Now the spectrum is conveniently written in terms of the density of

states and a normalized fluctuation. This will facilitate a convenient treatment of the unfolding process.

If we consider the m^{th} spacing of the normal spectrum and use the fact that

$$\langle s_{m+1} \rangle \approx \langle s_m \rangle \quad (3.64)$$

we find

$$\varepsilon_{m+1} - \varepsilon_m = \langle s_m \rangle \rho_m^{(\varepsilon)} \quad (3.65)$$

In this notation it is clear that the local unfolding process is a simple division by the local mean level spacing.

3.4.2 α

It is now useful to recall our definition of α which describes the difference between the λ_m and ε_m spectra

$$\alpha_m = \frac{\lambda_m - \varepsilon_m}{\varepsilon_{m+1} - \varepsilon_m}. \quad (3.66)$$

With this definition we can write

$$\begin{aligned} \lambda_m &= \varepsilon_m + \alpha_m (\varepsilon_{m+1} - \varepsilon_m) \\ &= \varepsilon_m + \alpha_m \langle s_m \rangle \rho_m^{(\varepsilon)}, \end{aligned} \quad (3.67)$$

so that the λ 's are now written in simple symbolic terms and all of the u dependence has been captured in α which is nicely bounded between 0 and 1. In this form it becomes important to understand the behavior of α . In the case where γ is chosen

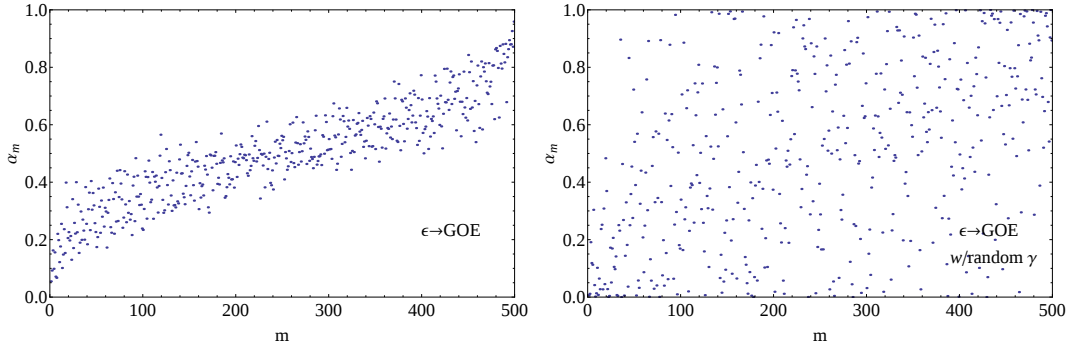


Figure 3.10: Comparison of α with constant and random γ for a type 1 matrix with $N=500$ and ε_m of the GOE. On the Right is the case of constant γ . There is clear trend from low to high in the α dependence. The difference between neighboring α is $\ll 1$. With random γ this trend is still present to some extent but the scatter is $O(1)$.

to be constant and the ε spectrum taken from some Gaussian ensemble, α becomes approximately smooth.

$$\alpha_{m+1} = \alpha_m + O\left(\frac{1}{\text{Log}N}\right) \quad (3.68)$$

The error in this approximation is actually appreciable even for $N \sim O(10^3)$ because the leading correction is logarithmic. However, it is instructive to see how the fluctuation spectrum simplifies in the limit that α becomes smooth as compared to the random limit. In Fig. (3.10) we plot the m dependence of α for the case of constant and random γ_m with ε_m of the GOE.

3.4.3 Statistics of $E_m^{(i)}$ in Type 1

The eigenvalues of a general type 1 matrix are given by

$$E_m = \sum_k \frac{d_k \gamma_k^2}{\lambda_m - \varepsilon_k}. \quad (3.69)$$

This eigenvalue is a linear combination of the N different eigenvalues

$$\begin{aligned}
E_m^{(i)} &= \frac{\gamma_i^2}{\lambda_m - \varepsilon_i} \\
&= \frac{\gamma_i^2}{\varepsilon_m - \varepsilon_i + \alpha_m \langle s_m \rangle \rho_m^{(\varepsilon)}}.
\end{aligned} \tag{3.70}$$

For a general choice of d_k the eigenvalues will always be uncorrelated. Here we consider the level statistics of a single canonical member of the family.

The $E_m^{(i)}$ spectrum is mostly smooth except for a singularity which occurs when the roots λ_m cross ε_i . If we ignore the region of the singularity then we can Taylor expand in the limit $|\varepsilon_m - \varepsilon_i| \gg \langle s_m \rangle$, or equivalently, $|m - i| \gg 1$.

$$\begin{aligned}
E_{m+1}^{(i)} - E_m^{(i)} &= \frac{\gamma_i^2}{(\varepsilon_m - \varepsilon_i) + \langle s_m \rangle (\rho_m^{(\varepsilon)} + \alpha_{m+1} \rho_{m+1}^{(\varepsilon)})} - \frac{\gamma_i^2}{(\varepsilon_m - \varepsilon_i) + \langle s_m \rangle \rho_m^{(\varepsilon)} \alpha_m} \\
&= \frac{\gamma_i^2}{\varepsilon_m - \varepsilon_i} \left(1 - \frac{\langle s_m \rangle}{\varepsilon_m - \varepsilon_i} \left(\rho_m^{(\varepsilon)} + \alpha_{m+1} \rho_{m+1}^{(\varepsilon)} \right) - 1 + \frac{\langle s_m \rangle}{\varepsilon_m - \varepsilon_i} \alpha_m \rho_m^{(\varepsilon)} \right) \\
&= -\frac{\gamma_i^2 \langle s_m \rangle}{(\varepsilon_m - \varepsilon_i)^2} \left(\rho_m^{(\varepsilon)} (1 - \alpha_m) + \rho_{m+1}^{(\varepsilon)} \alpha_{m+1} \right)
\end{aligned} \tag{3.71}$$

$$\begin{aligned}
E_{m+1}^{(i)} - E_m^{(i)} &= \frac{\gamma_i^2}{(\varepsilon_m - \varepsilon_i) + \langle s_m \rangle (\rho_m^{(\varepsilon)} + \alpha_{m+1} \rho_{m+1}^{(\varepsilon)})} - \frac{\gamma_i^2}{(\varepsilon_m - \varepsilon_i) + \langle s_m \rangle \rho_m^{(\varepsilon)} \alpha_m} \\
&= \frac{\gamma_i^2}{\varepsilon_m - \varepsilon_i} \left(1 - \frac{\langle s_m \rangle}{\varepsilon_m - \varepsilon_i} \left(\rho_m^{(\varepsilon)} + \alpha_{m+1} \rho_{m+1}^{(\varepsilon)} \right) - 1 + \frac{\langle s_m \rangle}{\varepsilon_m - \varepsilon_i} \alpha_m \rho_m^{(\varepsilon)} \right) \\
&= -\frac{\gamma_i^2 \langle s_m \rangle}{(\varepsilon_m - \varepsilon_i)^2} \left(\rho_m^{(\varepsilon)} (1 - \alpha_m) + \rho_{m+1}^{(\varepsilon)} \alpha_{m+1} \right)
\end{aligned} \tag{3.72}$$

The unfolding procedure here amounts to division by the prefactor, $-\frac{\gamma_i^2 \langle s_m \rangle}{(\varepsilon_m - \varepsilon_i)^2}$.

I argue that this is true based on the observation that, far from the singularity, this prefactor varies slowly with respect to the index m. On the other hand, terms in the parentheses all fluctuate locally. This treatment of the unfolding will become less

successful as ε_m approaches ε_i where the prefactor will display a stronger m dependence. However, the singular region of the spectrum has already been neglected. The levels which lie near the singularity will end up being near the band edge so they are also being dropped in the numerics. Hence we have

$$\rho_m^{(E^{(i)})} = \rho_m^{(\varepsilon)}(1 - \alpha_m) + \rho_{m+1}^{(\varepsilon)}\alpha_{m+1}. \quad (3.73)$$

Incidentally it is also possible to show that

$$\rho_m^{(\lambda)} = \rho_m^{(\varepsilon)}(1 - \alpha_m) + \rho_{m+1}^{(\varepsilon)}\alpha_{m+1} \quad (3.74)$$

which indicates that for type 1 matrices, the λ -spectrum and all of the basis operators have the same statistics.

3.4.3.1 Smooth α

If we use the approximation that α is smooth we end up with.

$$\rho_m^{(E^{(i)})} = \left(\rho_m^{(\varepsilon)} + \alpha_m(\rho_{m+1}^{(\varepsilon)} - \rho_m^{(\varepsilon)}) \right) \quad (3.75)$$

The numbers $\rho_m^{(\varepsilon)}$ follow from a distribution $P^{(\varepsilon)}(s)$ which is doubly normalized by the constraints

$$1 = \int P(s)ds \quad (3.76)$$

$$1 = \int sP(s)ds. \quad (3.77)$$

These same constraints will also be satisfied by a distribution $P^{(E^{(i)})}(s)$. Speaking broadly about these distributions, the more weight which lies near 1, the higher will be

the Brody parameter. The relationship Eq. (3.75) implies that the $E^{(i)}$ spectrum will have a larger Brody parameter than ε . I will now argue that this is the case.

It is useful to think of the high s and low s limits of $P(s)$ separately. First I will address the difference between $P(s)$ of ε_i and $E^{(i)}$ at high s . Specifically, the high s tail of the spacing distribution is populated by levels m for which $\rho_m^{(\varepsilon)} > 1$, we can reason by the normalizations given above that it is more likely than not, that $\rho_m^{(\varepsilon)}$ will be larger than it's neighbors. Therefore, the quantity

$$\alpha_m(\rho_{m+1}^{(\varepsilon)} - \rho_m^{(\varepsilon)}) \quad (3.78)$$

is likely to be negative (α is always positive). Thus, the situation

$$\rho_m^{(E^{(i)})} < \rho_m^{(\varepsilon)} \quad (3.79)$$

will occur more frequently than

$$\rho_m^{(\varepsilon)} < \rho_m^{(E^{(i)})} \quad (3.80)$$

the net effect being that spectral weight from the tail of $P(s)$ will decay more quickly for the $E^{(i)}$ spectrum than for the ε spectrum. A similar effect occurs on small spacing side of the spectrum. If we have $\rho_m^{(\varepsilon)} < 1$, it is more likely than not, that it will be smaller than it's neighbors. Thus the situation

$$\rho_m^{(\varepsilon)} < \rho_m^{(E^{(i)})} \quad (3.81)$$

will occur more frequently than

$$\rho_m^{(E^{(i)})} < \rho_m^{(\varepsilon)}. \quad (3.82)$$

This indicates that at low s $P(s)$ is smaller for $E^{(i)}$ than for ε .

Both the high s and low s limits indicate that $P(s)$ of $E^{(i)}$ spectrum will have more weight near $s=1$ than $P(s)$ of ε . This manifests as an increase in the measured Brody parameter.

$$\omega_B^{(E^{(i)})} > \omega_B^{(\varepsilon)} \quad (3.83)$$

The argument given above is not mathematically rigorous but it is reasonable considering that the distributions observed tend to be very smooth with only one peak at $s=1$. Furthermore it explains the numerically observed behavior. Particularly, we can immediately see why the randomization of α through the choice of random γ will have such a pronounced effect on the statistics of the basis operators. The preceding argument assumed smooth α dependence. Let us now consider α which are randomly distributed between 0 and 1.

3.4.3.2 Random α

If we do not make the approximation that α is smooth we have

$$E_{m+1}^{(i)} - E_m^{(i)} = \langle s_m \rangle \left(\rho_m^{(\varepsilon)} + \alpha_{m+1} \rho_{m+1}^{(\varepsilon)} - \alpha_m \rho_m^{(\varepsilon)} \right) \quad (3.84)$$

Noting that α and ρ^ε are positive, independent variables, we should expect $E^{(i)}$ to exhibit fluctuation statistics which are similar to those of ε . So we claim that

$$P^{(\varepsilon)}(s) \approx P^{(E^{(i)})}(s). \quad (3.85)$$

Of course the numbers α_m will never be completely random just as it is never completely smooth. However, the limits considered here correspond roughly to the conditions that

obtain when γ is chosen to be constant or not, respectively. At any rate we reason that the level repulsion of ε is a lower bound on the level repulsion of any basis operator.

3.4.4 Type $M > 1$

For type M matrices, the eigenvalues are related to the roots σ_k which satisfy the equation,

$$\sum_m \frac{\gamma_m^2}{\sigma - \varepsilon_m} \frac{\Gamma(\sigma) + \Gamma_m}{2} - B \frac{\Gamma(\sigma) - 1}{2} = u. \quad (3.86)$$

Empirically, we have found that there are N solutions to this equation and that they are spread across the spectrum with approximately the same density as ε . Although this spectrum does not fall nicely into the interstices of ε it is nonetheless convenient to describe this spectrum in terms of some normalized numbers, much like we did with λ , as

$$\beta_m = \frac{\sigma_m - \varepsilon_m}{\varepsilon_{m+1} - \varepsilon_m} \quad (3.87)$$

where σ_m is the m^{th} solution to Eq. (3.86) when the solutions are ordered such that $\sigma_{m+1} > \sigma_m$. The difference between α and β is that β_m does not necessarily lie between 0 and 1, yet we can expect it to be of $O(1)$ because the density of states of σ is like that of ε . Because, it is not so constrained as λ , we might assume that the level repulsion of σ falls in a middle ground that of ε and λ .

The eigenvalues of the canonical type M operators are given in two forms. The first,

$$E_{\sigma_k}^{(i)} = \sum_m \frac{1}{\lambda_i - \varepsilon_m} \frac{\gamma_m^2}{\sigma_k - \varepsilon_m} \frac{\Gamma(\sigma) + \Gamma_m}{2} \quad (3.88)$$

is rather cumbersome and difficult to work with in general. A second form mentioned in the Owusu paper [3] which is much more convenient can be written as

$$E_{\sigma_k}^{(i)} = \frac{u - \tilde{u}_i}{\lambda_i - \sigma_k} \quad (3.89)$$

where

$$\tilde{u}_i = \sum_m \frac{\gamma_m^2}{\lambda_i - \varepsilon_m} \frac{1 + \Gamma_m}{2} \quad (3.90)$$

and it is important to note that $\tilde{u}_i$ does not depend on σ . Thus all of the σ dependence is in the denominator of a single term and it is clear that there is only one singularity near λ_i (as well as a large scale degeneracy at $u = \tilde{u}_i$). Thus, we can proceed expanding in terms of α and β far from the singularity, and using the same tools as we did in the Type 1 problem.

$$\begin{aligned} E_{\sigma_{k+1}}^{(i)} - E_{\sigma_k}^{(i)} &= (u - \tilde{u}_i) \left(\frac{1}{\lambda_i - \sigma_{k+1}} - \frac{1}{\lambda_i - \sigma_k} \right) \\ &= (u - \tilde{u}_i) \left(\frac{1}{\lambda_i - \varepsilon_k - \langle s_k \rangle \rho_k^{(\varepsilon)} - \langle s_{k+1} \rangle \rho_{k+1}^{(\varepsilon)} \beta_{k+1}} - \frac{1}{\lambda_i - \varepsilon_k - \langle s_k \rangle \rho_k^{(\varepsilon)} \beta_k} \right) \\ &= \frac{u - \tilde{u}_i}{\lambda_i - \varepsilon_k} \left(\frac{1}{1 - \frac{\langle s_k \rangle \rho_k^{(\varepsilon)} + \langle s_{k+1} \rangle \rho_{k+1}^{(\varepsilon)} \beta_{k+1}}{\lambda_i - \varepsilon_k}} - \frac{1}{1 - \frac{\langle s_k \rangle \rho_k^{(\varepsilon)} \beta_k}{\lambda_i - \varepsilon_k}} \right) \\ &= \frac{u - \tilde{u}_i}{\lambda_i - \varepsilon_k} \left(\left(1 + \frac{\langle s_k \rangle \rho_k^{(\varepsilon)} + \langle s_{k+1} \rangle \rho_{k+1}^{(\varepsilon)} \beta_{k+1}}{\lambda_i - \varepsilon_k} \right) - \left(1 + \frac{\langle s_k \rangle \rho_k^{(\varepsilon)} \beta_k}{\lambda_i - \varepsilon_k} \right) \right) \\ &= \frac{-(u - \tilde{u}_i) \langle s_k \rangle}{(\lambda_i - \varepsilon_k)^2} \left(\rho_k^{(\varepsilon)} (1 - \beta_k) + \rho_{k+1}^{(\varepsilon)} \beta_{k+1} \right) \end{aligned} \quad (3.91)$$

This result is familiar from Type 1, and we can observe the factorization of slowly varying functions from the local fluctuations. Thus we make the claim that the unfolded spectrum has spacings

$$\rho_k^{(E^{(i)})} = \rho_k^{(\varepsilon)} (1 - \beta_k) + \rho_{k+1}^{(\varepsilon)} \beta_{k+1}, \quad (3.92)$$

in the limit that

$$|i - k| \gg 1. \quad (3.93)$$

This result is actually identical to the result from type 1 except that the α 's have been replaced by β 's which have a slightly different nature. However, the smoothness of β_m is related to the choice of γ as it was with α in the case $M=1$.

3.4.5 How a linear superposition quickly leads to Poisson statistics

In the previous section, we found an analytic expression relating the spacing fluctuations of E_m^i to the local fluctuations of ε_m . This allows for the basis operators of any Ansatz family to have non-Poisson statistics. What happens if we imagine the fluctuation spectrum of a linear combination of 2 basis operators? For simplicity we work with the Type 1 case (but the argument is the same for all M) with $L=2$ so

$$\begin{aligned} H(u) &= d_{l_1} H^{(l_1)} + d_{l_2} H^{(l_2)} \\ E_m &= \frac{d_{l_1} \gamma_{l_1}^2}{\lambda_m - \varepsilon_{l_1}} + \frac{d_{l_2} \gamma_{l_2}^2}{\lambda_m - \varepsilon_{l_2}}. \end{aligned} \quad (3.94)$$

In this case we cannot proceed as before because we do not actually know which eigenvalue is adjacent to E_m as when did for the basis operator. With the basis operators we used the fact that the ordering of λ_m was inherited by the eigenvalues $E_m^{(i)}$ such that index m was ordered for both spectra. Therefore we knew which eigenvalues were neighbors and could write their difference in terms of the indices of the input parameters. For $L > 1$ there is no way to know this if we allow the numbers d_{l_1} and d_{l_2} to be free. This is easy to see in Fig. (3.11). Each additional finite d_l will create another

singularity in the curve E_m . Because of this E_m and m are not simultaneously ordered. Thus in the notation where ε (and λ) are ordered, each additional singularity reduces the probability that adjacent eigenvalues E_{m_1} and E_{m_2} will have $|m_1 - m_2| = 1$. In fact, it becomes increasingly likely that neighboring levels come from very different values of m so that we should not expect them to be correlated even if the input parameters ε have short range level repulsion as in the GOE case.

The correlated fluctuations of the input parameters will show up in E_m to the extent that E_m and m are simultaneously ordered. Therefore, the emergence of Poisson statistics can be likened to a shuffling process. While this picture may be physically intuitive it does not leave much more room for analytic process. To give an example of the type of complication involved we note the importance of the rigidity to the shuffling process. If λ is very rigid, the shuffling will be more complete and therefore correlations will become mixed more quickly. If the rigidity is low the shuffling may be clumpy so that the correlations of the input parameters last to larger L . At any rate, the number of matrices needed to wash out the correlations is rather small, being on the order of 10 regardless of the dimension or type of the matrix.

This shuffling picture also explains the lack of crossover when the singularities are grouped together. When there is room between the singularities a branch of eigenvalues extends across the range of the spectrum. If there are very few eigenvalues between the singularities the shuffle will be very asymmetric, placing just a few eigenvalues out of order. Like breaking a deck of 52 cards in 4 and 48 and shuffling the two stacks back together. Thus, the fluctuation spectrum of E_m will still look like that of λ

Superposition of Basis Operators

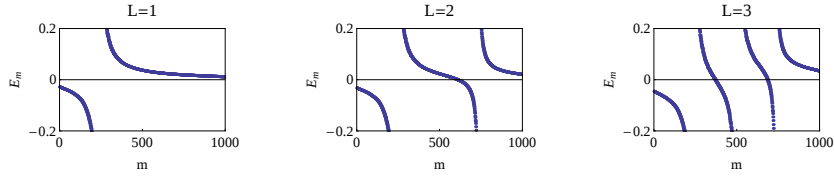


Figure 3.11: This plot shows the eigenvalues of a type 1 matrix for $L=1,2,3$. The ε are GOE, constant γ , and x is large. In the $L=1$ case, there is a wide smooth region where the E_m is simultaneously ordered with m . This implies that the level repulsion of E_m will be comparable to that of λ . As L is increased, the spectrum gets chopped up into a series of branches by the various singularities. There is now no guarantee that into large segment of the E_m spectrum will be simultaneously ordered with m . Ordering E_m requires a complicated shuffling of the index m . Consequently any short range correlations in λ will be significantly diminished in E_m . As L increases, the shuffling step becomes more severe because there are ever more branches being shuffled together to reach an ordered E_m . This will inevitably randomize the spectrum leading to Poisson spacing statistics. Surprisingly, this process occurs very fast ($L \approx 10$ assuming the singularities are well spread out). There is no dependence on type in this behavior.

but with a few impurities. This process will eventually lead to Poisson statistics but it will require L to be of the order of N .

3.4.6 Crossover scaling by perturbation

Some of these numerical observations can be understood using perturbation theory. Energies to the first order in x are given by the second equation in Eq. (3.28), where we set $|\gamma_j|^2 = 1/N$ to achieve proper scaling for large N as discussed above[7]. We have

$$E_m(x) \approx d_m - \frac{x}{N} \sum_{j \neq m} \left(\frac{d_m - d_j}{\varepsilon_m - \varepsilon_j} \right). \quad (3.95)$$

The first term comes from V , which we take to have Wigner-Dyson $P(s)$, the second – from T , which is determined by the integrability condition and whose level statistics

we do not control. Let us estimate x at which the two terms in Eq. (3.95) become comparable. Without loss of generality we can take $d_k = O(N^0) = O(1)$ and we must also take $\varepsilon_k = O(1)$ so that T and xV scale in the same way for large N . Suppose ε_k are ordered as $\varepsilon_1 < \varepsilon_2 < \dots < \varepsilon_N$. When d_k and ε_k are uncorrelated $d_m - d_j$ is $O(1)$ when j is close to m , i.e. when $(\varepsilon_m - \varepsilon_j) = O(1/N)$. The second term in Eq. (3.95) is then $xc_m \ln N$, where $c_m = O(1)$ is a random number only weakly correlated with d_m .

If we now order d_m , c_m in general will not be ordered, i.e. if $d_{m+1} > d_m$ is the closest level to d_m and therefore $(d_{m+1} - d_m) = O(1/N)$, the corresponding difference $(c_{m+1} - c_m) = O(1)$. The contributions to level-spacings from the two terms in Eq. (3.95) become comparable for $x = x_c \approx 1/(N \ln N)$. It makes sense that the second term introduces a trend towards Poisson distribution because it is a (nonlinear) superposition of ε_k and d_k – eigenvalues of two uncorrelated random matrices. Thus, we expect a crossover from Wigner-Dyson to Poisson distribution at $x = x_c$.

This argument breaks down when $d_k = f(\varepsilon_k)$, since in this case $(d_m - d_j) = O(1/N)$ when $(\varepsilon_m - \varepsilon_j) = O(1/N)$. The two terms in Eq. (3.95) become comparable only at $x = O(1)$ in agreement with the numerics for this case. Moreover, the second term no longer trends towards Poisson statistics. Relaxing the correlation between d_k and ε_k with $d_k = f(\varepsilon_k)(1 + \eta_k)$ and going through the same argument, one expects a Wigner-Dyson to Poisson crossover at $x = O(1)$ for $\eta_k = O(1/N)$.

3.5 Summary

In summary, we study the Ansatz matrices, previously shown to exhibit a prototypical form of quantum integrability for which we have an explicit parameterization. While a broader class of quantum integrable matrices are known to exist, we do not have access to workable parameterization which would allow for a detailed study of spectral statistics. The properties of the Ansatz matrices are considered herein to be typical of all quantum integrable blocks (though further study will be necessary to verify this assumption). We find that Ansatz matrices generically exhibit Poisson spectral statistics in the limit $N \gg 1$. This situation is stable against a variety of attempts to construct counter examples. For example, choosing the eigenvalues of V to have level repulsion, choosing γ 's to be constant, choosing the d 's and ε to be correlated, or building matrices within a small subspace of the family do not hinder the Poisson statistics except in some small window of the parameter space. These results are given a qualitative explanation in terms of a reshuffling of the local fluctuations of λ which inevitably leads to Poisson statistics when they become completely randomized. Finally, the crossover scales are understood in terms of a perturbative argument.

Our understanding of spectral properties of integrable models is far from complete. Here we present a list of open question and possible extensions of this work.

1. The Ansatz matrices studies here are a subset of the space of matrices which satisfy Eq. (3.3). Without explicit general solutions for the solutions of Eq. (3.3) it is difficult to make completely general claims about the statistics of integrable

Hamiltonians.

2. The Wigner von Neumann non-crossing rule is generically violated by Ansatz matrices. This is associated with a lack of level repulsion in the spectrum. However, we can construct matrices which have strong level repulsion and yet the crossings remain. This indicates that the association of non-crossing rule and level repulsion are not so simply related. A more coherent understanding of crossings in light of the Poisson statistics might now be possible.
3. The Ansatz matrices studied in this work have been constructed to have real spectra. The Ansatz matrices are more general than this and we can imagine that the spectral statistics have some interesting generalization in the case that we allow complex eigenvalues. This question would require a new conception of the spectral statistics.

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Chapter 4

Split Hubbard Bands at Low Density

4.1 Motivation and Introduction

Hubbard's introduction of split bands in [1], i.e. the so called upper Hubbard band (UHB) and the lower Hubbard band (LHB), is one of the most important qualitative ideas in the theory of correlated electrons. Their origin is the idea that since the energy levels of the atomic limit show two sets of states, one at $\omega \sim 0$ and another at $\omega \sim U$ as in Eq. (4.8) below, the formation of a crystal would broaden these levels into two sets of sub-bands. These sub-bands were originally discussed by Hubbard using a non perturbative technique, that has the advantage of being exact in the limit of vanishing bandwidth $W \rightarrow 0$, i.e. the atomic limit. However, the technique failed to produce a Fermi liquid for weak couplings, as one expects physically. This failure led to severe early criticism of Hubbard's work[2]. The problem of reconciling Fermi liquids with the local picture developed by Hubbard, leading to the split bands, is of great importance

in the physics of strong correlations. The one exception is the dynamical mean field theory that gives a good account of the sub-band formation, especially in the proximity of half filling[3, 4]. However, away from half filling, the picture is obscure and remains largely unresolved. It is this task that we address in the present work. We study the ladder diagrams that are argued to be exact at low densities, sharpen the argument for their validity in terms of the self energy, and show that at least in this limit, the concept of the split bands is completely consistent with the Fermi liquid picture. The numerical solution of the ladder diagrams is carried out in a self consistent way and shows the emergence of the Hubbard split bands for large enough U/W . These merge for weak couplings and our results give a vivid picture of the crossover from weak to intermediate to strong coupling.

The self energy is momentum and also frequency dependent in the ladder scheme, and for low densities provides a full picture of the renormalization processes that occur at arbitrarily large interaction scale U . In particular we see that the spectral function shows a low lying feature and a high energy $\sim O(U)$ feature, with spectral weights that are equal to $1 - \frac{n}{2}$ and $\frac{n}{2}$ respectively. It is seen that every single added particle thus depletes the weight of the LHB and adds to the UHB, thereby accomplishing a “long range spectral transfer” - that has been described in literature as “Motttness”[5, 6].

The momentum space occupancy $m(k) = \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle$ is computed and it is usefully broken up into three parts Eq. (4.16). The occupied part $m_1(k)$ in Eq. (4.16), corresponding to occupied states that are automatically inside the LHB, the unoccupied LHB part $m_2(k)$ corresponding to unoccupied LHB states, and the unoccupied

UHB part $m_3(k)$. In the limit of $U \rightarrow \infty$, only m_1 and m_2 survive, and this projection gives an exact view of the physics of the t - J model as well in the low density limit. At low densities we find that the ladder diagrams lead to a Luttinger Ward compliant Fermi surface, and this Fermi surface survives the limit $U \rightarrow \infty$. Thus even in this limit of extreme correlations $U \rightarrow \infty$, adiabatic continuity to the Fermi gas holds. Therefore we have a useful and concrete alternative to the extreme coupling ideas proposed in work by one us [24], where a different Fermi volume emerges at *all densities*, including the lowest ones.

One contemporary context for the Hubbard split bands is the problem of high T_c superconductors, here Anderson[7] has eloquently argued that for large U , one can confine attention to carriers in the LHB, with the UHB pushed out of the range of relevant states. Given this projection to the LHB, the charge carriers inherit exotic properties such as spin charge separation, and also a new interaction, namely the super exchange that comes with a scale of t^2/U . We see that at least at low densities where the ladder scheme is valid, the LHB does separate out cleanly for $U \geq W$, but the carriers are yet subject to Fermi liquid behavior.

Another recent context for motivating this work is the study of the Hubbard model far away from equilibrium with cold atom realization[8, 9], where the carriers in the UHB are optically excited, and their lifetime studied by measuring the overlap of the excited state with the initial state. We find that a calculation of a related correlation function is possible in the Fermi liquid at low densities, albeit in a close to equilibrium situation unlike the experiments. We are also able to exhibit the correlation function

exactly for a pair of particles in the Hubbard band. Interestingly, the resulting life times show some similarity in functional dependence to those found in experiment, although with a very different time scale.

4.2 Ladder Scheme Equations at Low Density

The ladder scheme for the Greens function Refs.[[10, 11, 12, 14, 15]] corresponds to convoluting a particle-particle ladder scattering amplitude $\Gamma(Q)$ with a single Greens function $G(k)$ to form the self energy $\Sigma(k)$ as follows:

$$\begin{aligned}\Gamma(Q) &= \frac{U}{1 + U\Pi(Q)}, \\ \Pi(Q) &= \frac{1}{\beta N_s} \sum_p G(p)G(Q - p), \\ \Sigma(k) &= \frac{1}{\beta N_s} \sum_p G(p)\Gamma(k + p).\end{aligned}\tag{4.1}$$

Here N_s, N_e are the number of sites and electrons, $n = N_e/N_s$ is the electron number density, and we use the notation $k = (\vec{k}, i\omega_k)$ with imaginary odd frequencies $\omega_k = \pi\frac{1}{\beta}(2k + 1)$ of the finite temperature field theory[16] for Fermions, and reserve the capital letters for Bosonic frequencies, e.g. $Q = (\vec{Q}, i\Omega_\nu)$ and $\Omega_\nu = 2\pi\frac{1}{\beta}\nu$. Here the summation over p represents a sum over the vector component and also the imaginary frequency. A paramagnetic state is assumed and the spin label is suppressed for brevity. In addition to Eq. (4.1), we have the Dyson equation $G^{-1}(k) = G_0^{-1}(k) - \Sigma(k)$ with the usual non interacting Greens function $G_0^{-1}(k) = i\omega_k - \varepsilon_k + \mu$. Thus the ladder scheme is a self consistent non linear scheme that needs to be solved numerically for the various objects $G(k)$, $\Sigma(k)$, $\Pi(K)$. We can solve for the Dyson equation in the ladder scheme

iteratively:

$$G^{-1}(k) = G_0^{-1}(k) - \frac{1}{\beta N_s} \sum_p G(p) \frac{U}{1 + \frac{U}{\beta N_s} \sum_q G(q) G(k+p-q)}. \quad (4.2)$$

For example in the first step we can calculate the scattering amplitude (and self energy) using G_0 and use Dyson's eqn to obtain a new Green's function we call G_1 :

$$G_1^{-1}(k) = G_0^{-1}(k) - \frac{1}{\beta N_s} \sum_p G_0(p) \frac{U}{1 + \frac{U}{\beta N_s} \sum_q G_0(q) G_0(k+p-q)}. \quad (4.3)$$

We may continue and compute $G_2(k)$ using $G_1(k)$ to recompute the self energy (i.e. the second term in Eq. (4.3)), and repeat this process iteratively to obtain $G(k) = \lim_{n \rightarrow \infty} G_n(k)$. The difference between $G_1(k)$ and the fully self consistent $G(k)$ arises from the repeated renormalizations implicit in the full equations, and this brings about the self consistent broadening of several sharp features that arise in $G_1(k)$. In Fig. (4.3) we discuss the difference in the spectral functions from these two theories as an illustration of this phenomenon.

Alternatively we start by introducing spectral representations for the various quantities of physical interest[16, 17]:

$$\begin{aligned} G(\vec{k}, i\omega_k) &= \int d\nu \frac{\rho_G(\vec{k}, \nu)}{i\omega_k - \nu}, \\ \Sigma(\vec{k}, i\omega_k) &= U \frac{n}{2} + \int d\nu \frac{\rho_\Sigma(\vec{k}, \nu)}{i\omega_k - \nu}, \\ \Gamma(\vec{Q}, i\Omega_Q) &= U + \int d\nu \frac{\rho_\Gamma(\vec{Q}, \nu)}{i\Omega_Q - \nu}. \end{aligned} \quad (4.4)$$

The spectral functions $\rho_\Gamma(\vec{Q}, \nu)$ etc have a compact support and are therefore convenient for numerical integration on a suitably discretized grid of frequencies. The numerical solution is performed after using a spectral representation for various physical quantities.

We first turn the Dyson equation Eq. (4.2) into a non linear integral equation for the spectral function from Eq. (4.4) as follows:

$$\begin{aligned}
\rho_\Sigma(\vec{k}, \omega) &= \frac{1}{N_s} \sum_{\vec{p}} \int d\nu \rho_G(p, \nu) \rho_\Gamma(\vec{p} + \vec{k}, \nu + \omega) (f(\omega) + n_B(\omega + \nu)), \\
\rho_\Pi(\vec{Q}, \Omega) &= \sum_{\vec{q}} \int d\nu \rho_G(q, \nu) \rho_G(Q - q, \Omega - \nu) (f(\nu) + f(\Omega - \nu) - 1), \\
\rho_\Gamma(\vec{Q}, \Omega) &= \frac{-U^2 \rho_\Pi(\vec{Q}, \Omega)}{(1 + U \text{Re } \Pi(\vec{Q}, \Omega))^2 + (\pi U \rho_\Pi(\vec{Q}, \Omega))^2},
\end{aligned} \tag{4.5}$$

with $f(\omega)$ and $n_B(\omega)$ as the Fermi and Bose distribution functions $[\exp \beta\omega \pm 1]^{-1}$, and $\text{Re } \Pi(\vec{Q}, \Omega)$ defined as the Hilbert transform of $\rho_\Pi(\vec{Q}, \nu)$, i.e.

$$\text{Re } \Pi(\vec{Q}, \Omega) = P.V. \int d\nu \frac{\rho_\Pi(\vec{Q}, \nu)}{\Omega - \nu}.$$

4.2.1 Low density limit and self energy sum rule

The original argument for the ladder scheme[11, 10] is that it is exact in the low density limit. This argument is borrowed from the theory of nuclear matter, where Brueckner[18] originally argued that at any order n of perturbation theory for the ground state energy (i.e. the Goldstone diagrams), the dominant diagrams are those with the smallest number of downward lines of holes. Topologically there need to be at least two such hole lines in the free energy diagrams. The particle particle ladder diagrams have only two hole lines at any order. Thus the ladder diagrams dominate all others at each order in perturbation theory. Importantly for nuclear matter, this logic shows that the large (divergent) two body interaction is not a problem, it is cut off by these ladders, giving in the end an expansion in a dimensionless parameter

obtained by combining the two body scattering length with the average inter particle separation. A parallel argument for bosons was provided by Lee, Huang and Yang [19]. The Kanamori- Galitskii papers implement this idea for the Feynman diagrams, where one has additionally hole hole scattering, in addition to particle particle ladders- for structural reasons that distinguish the Feynman diagrams from the Goldstone ones. However these extra terms do not detract from the particle particle ladders that cohabit the Feynman series and provide a particular $O(n^2)$ correction term.

The reader would note that the above argument is rather indirect, in particular it gives us no clue to why we should accept the self energy that emerges from this scheme as exact. In this context, it is useful to note that the self energy satisfies an exact series of sum rules[20, 6, 21], of which the lowest is

$$s_0(k) \equiv \int d\nu \rho_\Sigma(\vec{k}, \nu) = U^2 \times \frac{n(2-n)}{4}, \quad (4.6)$$

where the RHS is *independent of $\vec{k}$* . Note that this sum rule is valid for arbitrarily large U and at all densities. We can use this as a check of our calculation by testing for the $\vec{k}$ independence of the computed LHS, and also monitor its weight relative to the RHS. The self consistent solution of the ladder diagrams contain the low density limit and also provide some uncontrolled results at higher densities, and it is important to know the limit on density to which we can trust these results. Fig. (4.1) gives details of this test for the ladder diagrams. For higher densities the ladder diagram theory is systematically wrong for the $O(n^2)$ term, since we can show analytically that at large U and low density $s_0(k) = U^2 \times \frac{n(1-n)}{2} + O(U)$ in contrast to Eq. (4.6).

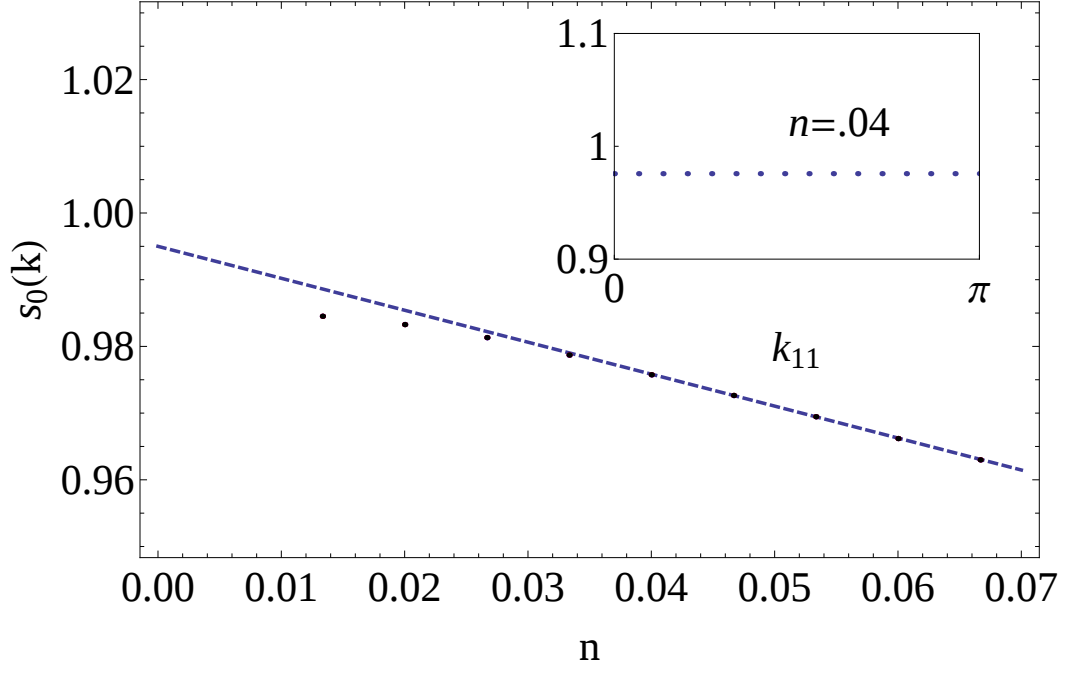


Figure 4.1: The zeroth moment of the self energy versus the density normalized to the exact value $U^2 \times \frac{n(2-n)}{4}$. This data is in 2-dimensions with $U=10, W=2$. The inset shows the k independence of the sum rule along the (11) direction for the case $n=0.04$, with variations in the sixth significant figure.

4.2.2 The Atomic Limit

We discuss briefly the atomic limit, i.e. a limit where U remains finite but the band width $W \rightarrow 0$, this is the limit where one can solve for the Greens function exactly quite simply.

$$\Sigma_{Atomic} = U \times \frac{n}{2} + U^2 \times \frac{\frac{n}{2}(1 - \frac{n}{2})}{i\omega + \mu - U(1 - \frac{n}{2})} \quad (4.7)$$

$$G_{Atomic} = \frac{1 - \frac{n}{2}}{i\omega + \mu} + \frac{\frac{n}{2}}{i\omega + \mu - U} \quad (4.8)$$

The breakup of the Greens function into two parts, with energies ~ 0 or $\sim U$ and weights $1 - n/2$ and $n/2$ is of course the fundamental factor that leads one to the picture of upper and lower Hubbard bands. Hubbard's contribution[1] was to provide a Greens function for finite hopping W using an equation of motion method that extended the Atomic limit, although the details of his treatment came in for severe criticism [2] due to the failure of his scheme to ever yield a Fermi liquid with the Luttinger Ward[23] ordained Fermi surface. The present scheme of ladder diagrams achieves this interpolation smoothly and exactly, if only in the limit of low densities. From Fig. (4.2), we see that the sharp feature is accompanied by a broad background of width $O(U)$ that presumably arises from the uncontrolled $O(n^2)$ corrections to the ladder diagram self energy sum rule Eq. (4.6).

4.2.3 Emergence and structure of the Split bands of Hubbard

In the ladder diagrams, it is straightforward to identify the origin of the upper Hubbard band: the scattering amplitude $\Gamma(Q)$ at frequencies $\Omega_Q \sim U$, has a pole in the

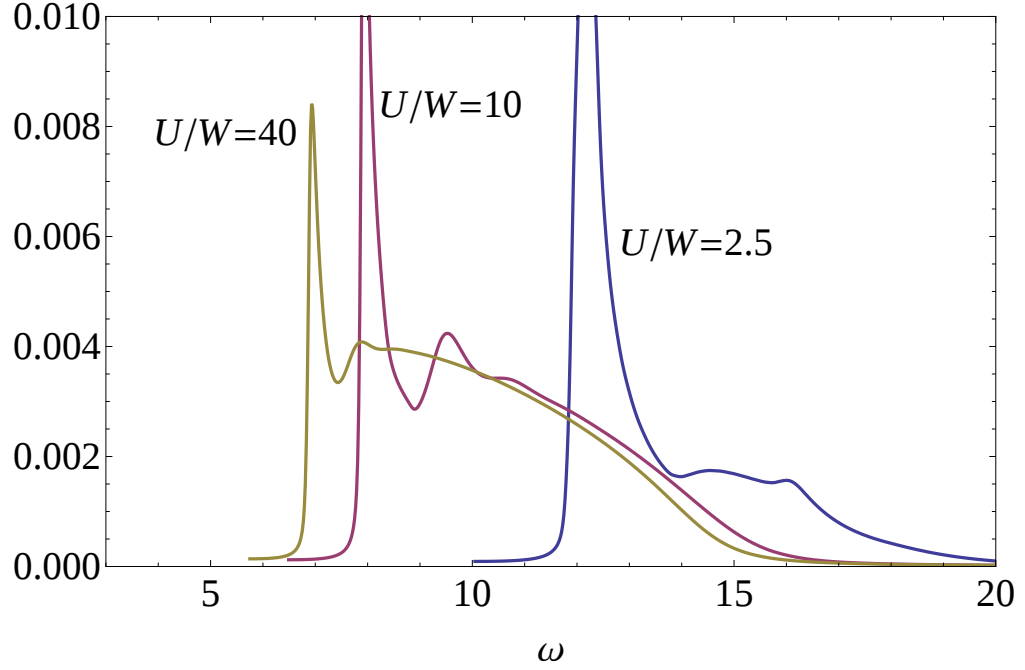


Figure 4.2: High frequency (UHB) DOS in 2D, $U=10$, $n=1/20$; As the hopping is decreased, the UHB feature does not become narrow, but rather maintains a width of $O(U)$. The sharp k -dependent features narrow as the hopping decreases. The broad continuum is essentially k -independent, showing very little dependence on the hopping in the limit of strong coupling. In this limit, the UHB becomes completely independent of the bandstructure. In Fig. (4.3) the broad UHB of the full band can be seen with the Hubbard-1-like G_1 superimposed. In G_1 , the UHB feature is broadened only by η and the LHB is suppressed for clarity.

first iteration, i.e. at the level of G_1 with

$$\Gamma_1(Q) \equiv \Gamma(Q; [G_0]) \sim \frac{U^2(1-n)}{i\Omega - U(1-n)}. \quad (4.9)$$

This pole was noted very early in works [12, 13] who identified this pole as the origin of strong correlations and Gutzwiller type factors. In Fig. (4.3), we see that the spectral function obtained from the first iteration i.e. G_1 shows a sharp feature at a higher energy of $O(U)$ that arises from this pole. This peak disperses and may be viewed as a “baby version” of the upper Hubbard band. Next a self consistent treatment of this theory with $\Gamma(Q; [G])$ evaluated with G (rather than G_0) broadens the upper band substantially as seen in Fig. (4.3). It is interesting that the lower Hubbard band, i.e. the structure at energies below U are stable with respect to the iterations, and are hardly different between the first iteration scheme and the final one.

We also see in Fig. (4.3), the existence of two features that have been commented upon in literature. The feature near the band bottom that disperses, is the so called hole-hole bound state noted by Randeria and Englebrecht [15], whereas the hump near the leading edge is a particle hole bound state feature noted by Anderson [22]. These features coexist with the other, dominant ones, namely the quasiparticle peak of the Fermi liquid and the broadened upper Hubbard band peak. If we replace the log linear scale in Fig. (4.3) with a linear linear scale as in Fig. (4.6), the UHB becomes almost negligible compared to the LHB feature.

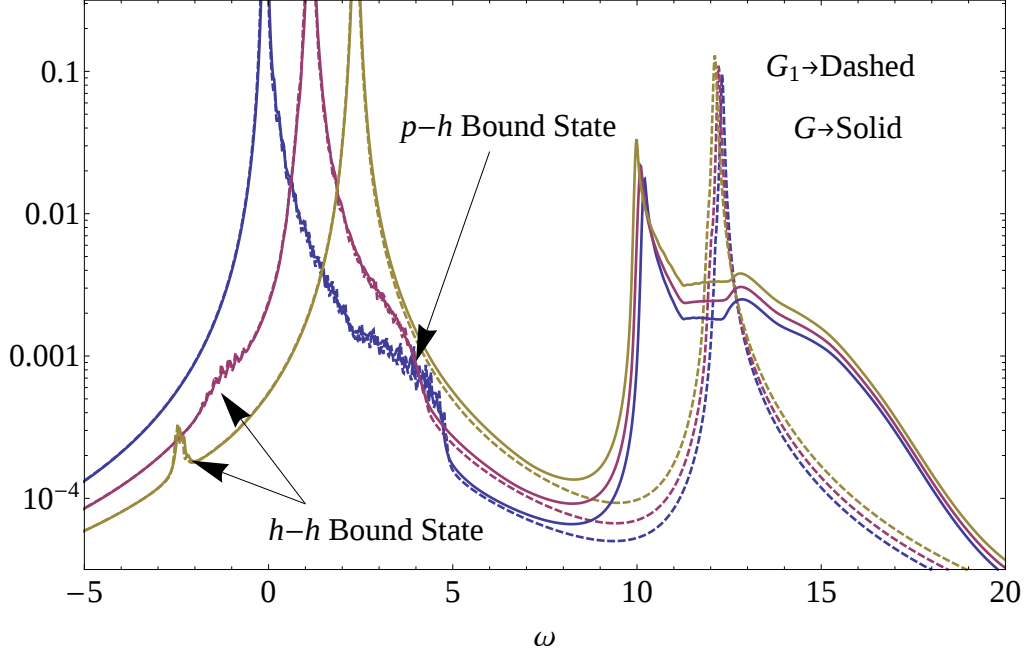


Figure 4.3: 2D, $U=10, W=2.5, n=1/20$; The spectral function at three values of the wave vector $(0, 0)$, $(\frac{\pi}{2}, \frac{\pi}{2})$, (π, π) , in blue, red and gold colors. Besides the quasiparticles we observe three features emerging in each spectral function. Most obvious is the UHB feature which lies at a $\omega \approx O(U)$ and integrates to a weight of $n/2 + O(n^2)$. This feature is dramatically broadened in the self consistent G also becoming less k -dependent. On each edge of the quasiparticle band we observe small dispersing features. Ref.([15]) have previously identified the negative frequency feature as a 2-hole antibound state while Ref.([22]) has discussed a particle-hole antibound state just above the quasiparticle band. These features are essentially unchanged in going from G_1 to the exact G .

4.2.4 Frequency Dependent Self energy

We next display the self energy in the ladder scheme. The spectral density for the self energy is given in Eq. (4.5), and it is possible to obtain an equation for its momentum sum, i.e. a local self energy density

$$\frac{1}{N_s} \sum_k \rho_\Sigma(k, \omega) = \int d\nu \rho_{G,loc}(\nu) \rho_{\Gamma,loc}(\nu + \omega) (f(\omega) + n_B(\omega + \nu)). \quad (4.10)$$

For comparison, we note that the local self energy in the atomic limit considered in Section 4.2.2 is given by a single delta function centered at $U(1 - \frac{n}{2}) - \mu$ as:

$$\rho_{Atomic}(\omega) = U^2 \frac{n}{2} (1 - \frac{n}{2}) \delta[\omega + \mu - U(1 - \frac{n}{2})]. \quad (4.11)$$

We also note the form of this object for a Fermi liquid at finite T

$$\rho_{Local}^{FermiLiquid}(\omega) = a \omega^2 + f_{Background}(\omega), \quad (4.12)$$

a simple second order self consistent theory (corresponding to truncating the ladders at the first rung) gives the picture of this in a Fermi liquid Fig. (4.4).

We see in Fig. (4.5) that the ladder scheme inherits both a quadratic minimum at $\omega = 0$ from the Fermi liquid and a large and broad feature near $\omega \sim U$ from the emergent Hubbard upper band. The inset emphasizes the Fermi liquid aspect, and the reader will observe that the absolute scale of this function is dominated by the UHB feature. In Fig. (4.6) the density of states of the Greens function $\rho_G(\vec{k}, \nu)$ is illustrated, along with the real and imaginary parts of the self energy. The small feature in the DOS at the energy scale U is the UHB. We see that the real and imaginary parts of the self energy reflect its presence in a profound fashion, that would be hard to guess from

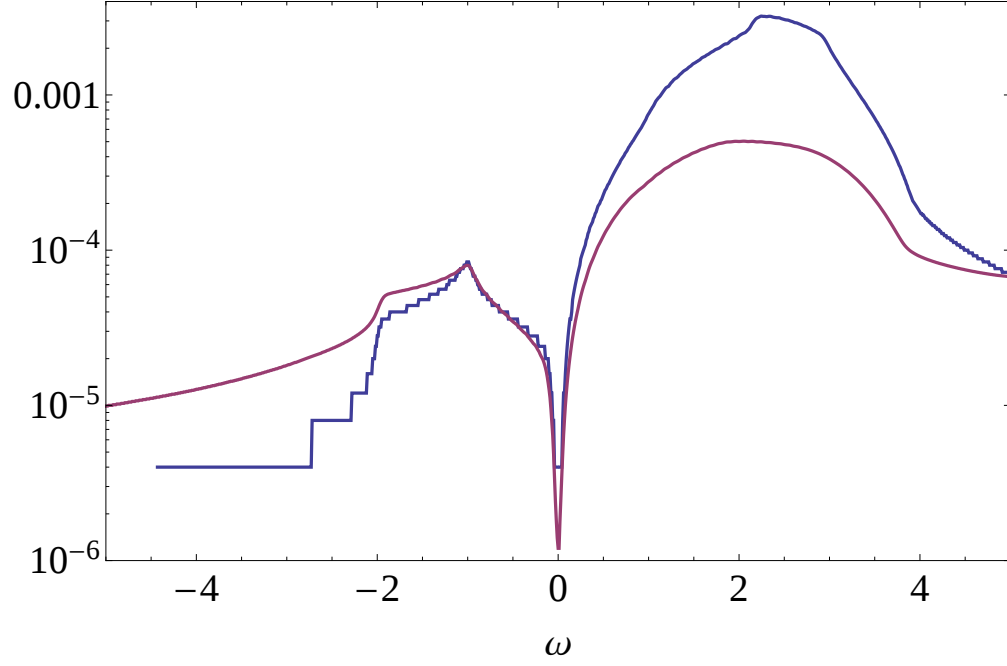


Figure 4.4: 2D, $U=.25$, $U=10$, $W=2$, $n=.049$. The local $\rho_{\Sigma}(\omega)$ divided by U versus ω . The two chosen values of U are in the weak coupling (blue $U = .25$) and strong coupling (red $U = 10$) ranges respectively. We see at the lowest temperatures that the self energy curves overlap when scaled by U displaying a characteristic quadratic dip at the chemical potential.

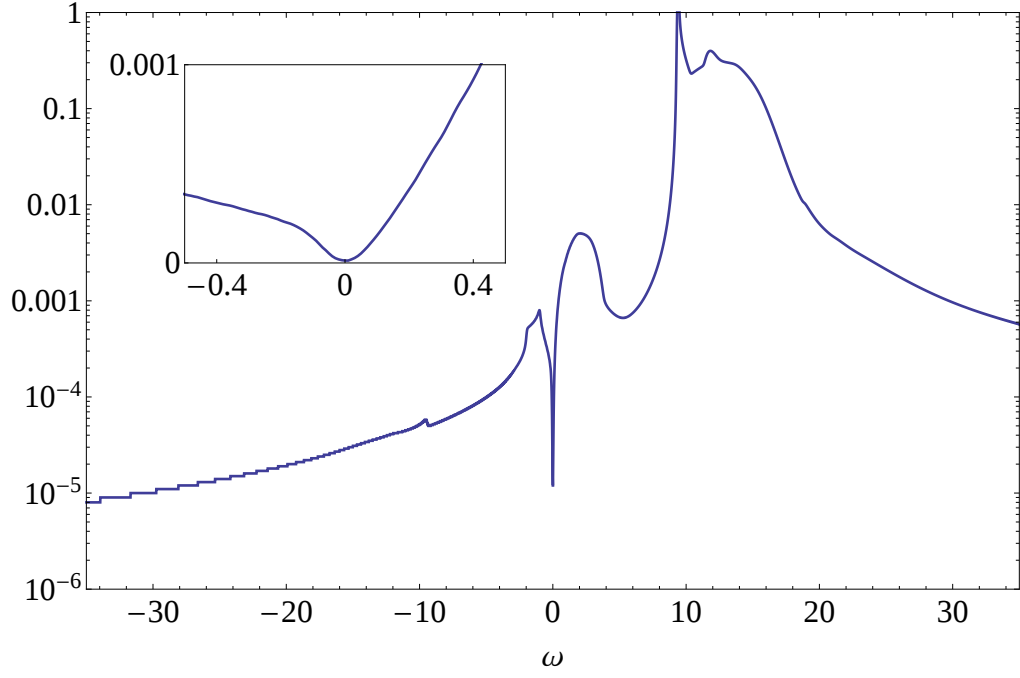


Figure 4.5: The local self energy spectrum in 2D, $U=10$, $W=2$, $n=.05$. The log scale plot shows the full scale of the UHB. The inset highlights the quadratic minimum at low energies. The quadratic minimum drops below the scale of η so it can be said to represent an infinite lifetime.

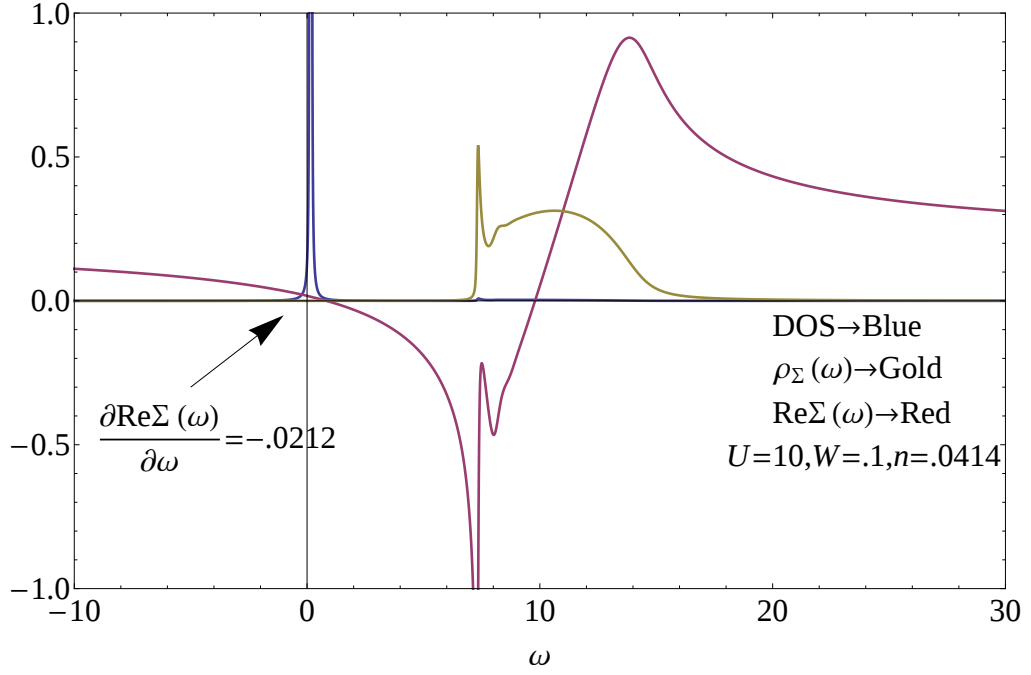


Figure 4.6: The 2D DOS i.e. the momentum averaged spectral function $\rho_G(\vec{k}, \nu)$ and the momentum averaged $\rho_\Sigma(\vec{k}, \nu)$. The LHB feature is the sharp peak near $\omega \sim 0$. The UHB feature in the DOS is nearly invisible here but lies just below the feature in ρ_Σ scaled down by a factor of ω^2 . The real part of the self energy for $\omega \geq 0$ initially drops linearly with frequency over a range $W \ll \omega \sim \frac{U}{2}$, as required in the limit of extreme correlations [24, 26]. It then flips at the threshold of the UHB, rising across the range of the UHB until at the highest energy it begins to decay down towards the Hartree term at infinite energy.

the size of the peak. In detail, it is interesting that the real part of the self energy does display a linear behavior in ω with a known slope as one expects in the intermediate frequency range $0 \ll \omega \ll U$ from the theory of extremely correlated electronic systems in Ref. ([24, 26]).

When $W = 0$ the UHB has a weight which is independent of momentum. However, for finite W , momenta near the top of the band will transfer weight more readily to the UHB. Fig. (4.7) illustrates this progression. We show in Fig. (4.8) that

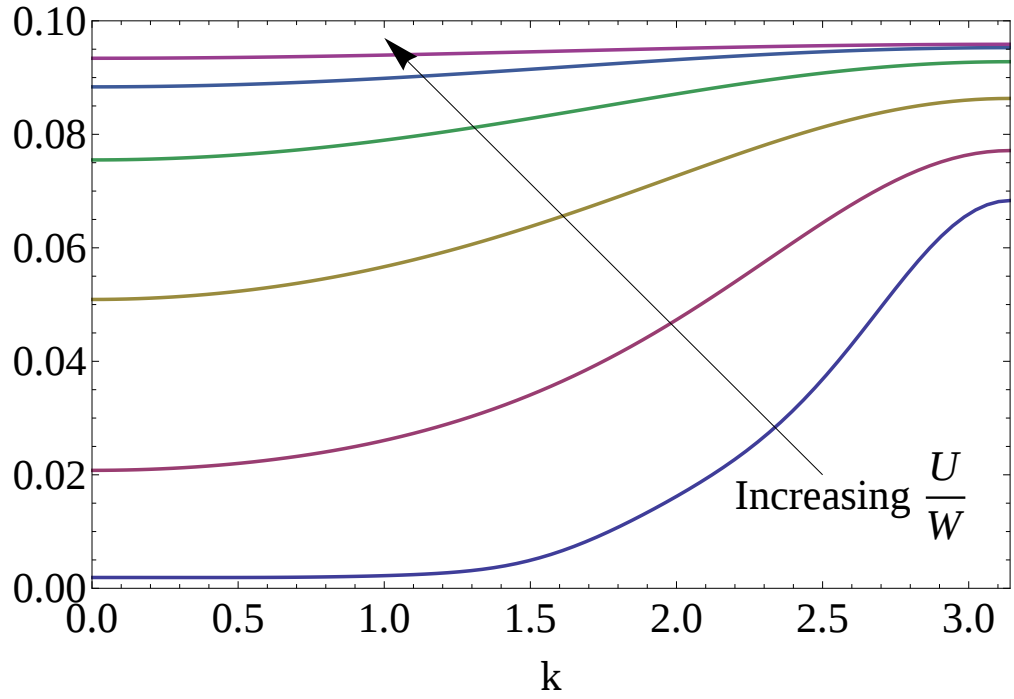


Figure 4.7: The integrated spectral weight over the UHB is called $m_3(k)$. It is plotted here for $\frac{W}{U} = 1.6, .56, .196, .0686, .024, .0085$. In this case $n=15$. We observe that the weight of the UHB exceeds $n/2$ and becomes flat as U/W tends to infinity.

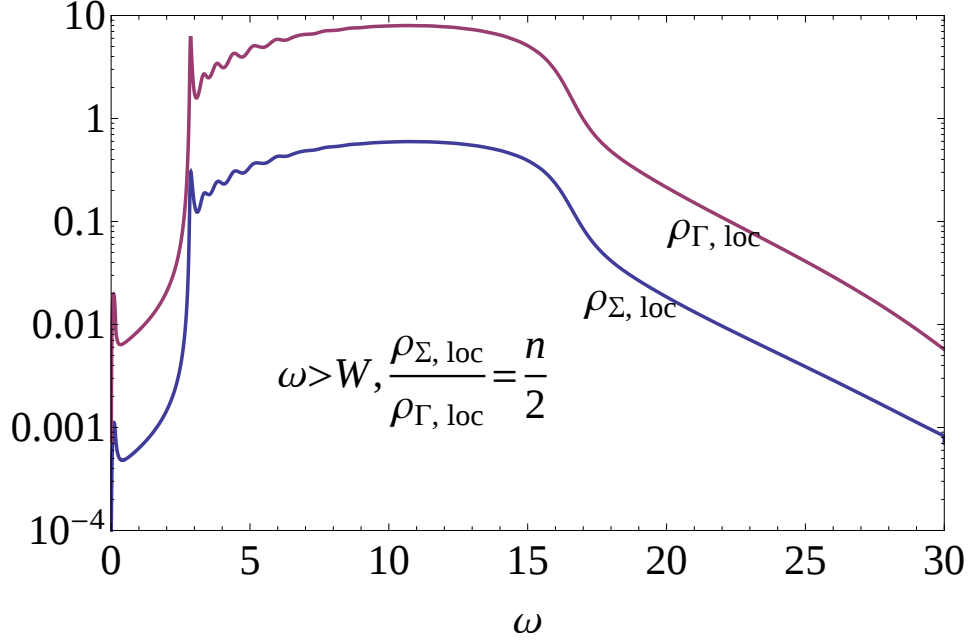


Figure 4.8: From the convolution structure of $\rho_\Sigma(k, \omega)$ we see that the local objects of Σ and Γ are related by the ratio $n/2$ when $\omega > W$ for all values of W/U . In the strong coupling limit where the upper band is essentially independent of k , this relationship will be approximately true for each wavevector. On the negative frequency side, the thermal function act differently such that the ratio for $\omega < -W$ is approximately $(1 + \frac{n}{2})$.

the behavior of the local spectral function $\langle \rho_\Gamma(\vec{Q}, \nu) \rangle_Q$ closely follows that of the local self energy $\rho_\Sigma(\nu)$. If we look at large ω such that we can make the approximation $\omega + \nu \approx \omega$, the integral for $\rho_\Sigma(k, \omega)$ in Eq. (4.5) reduces to

$$\frac{1}{N_s} \sum_k \rho_\Sigma(k, \omega) \sim \frac{n}{2} \rho_{\Gamma, loc}(\omega), \quad (4.13)$$

accounting for the similarity of these in Fig. 4.8.

4.2.5 Momentum occupancy

We next turn to the momentum occupancy $m_k = \langle c^\dagger(k)c(k) \rangle$; this can be obtained from the Greens function or $\rho_G(k, \nu)$ by integration over the frequencies. In order to understand and illustrate the nature of the LHB and UHB breakup of this important object, we carry out the integration up to the Hubbard-Mott gap energy ω_g . This energy scale is well defined when $W \ll U$, and in case of smaller $U \sim W$ it requires a definition. In our work, it is operationally defined as the energy where the spectral density $\langle \rho_G(k, \nu) \rangle_k$ is minimum. Thus we define three objects $m_j(k)$ with $j = 1, 2, 3$

$$m_1(k) = \int_{-\infty}^0 d\omega \rho_G(k, \omega) \quad (4.14)$$

$$m_2(k) = \int_0^{\omega_g} d\omega \rho_G(k, \omega) \quad (4.15)$$

$$m_3(k) = \int_{\omega_g}^{\infty} d\omega \rho_G(k, \omega). \quad (4.16)$$

Here $m_1(k)$ represents the momentum space occupancy of the occupied states that lie below the chemical potential. These are automatically in the LHB for energetic reasons, and satisfy the sum rule $\sum_k m_1(k) = n/2 \times N_s$ with a sum over the entire Brillouin zone (BZ). Next $m_2(k)$ represents the LHB contribution to the unoccupied states, since the chemical potential lies within the LHB. If we send $U \rightarrow \infty$ then we are left with only the LHB, and in that limit, we expect the sum $m_1(k) + m_2(k) = 1 - \frac{n}{2}$ pointwise at each k . However for finite but large U this sum differs from $1 - \frac{n}{2}$ by terms of $O(t/U)$, and the UHB comes into play. Indeed $m_3(k)$ refers to precisely the UHB contribution to the momentum occupation, and its momentum average over the BZ is $\frac{n}{2}$. These are displayed for typical parameters in Fig. (4.9). The sum of all three m functions should

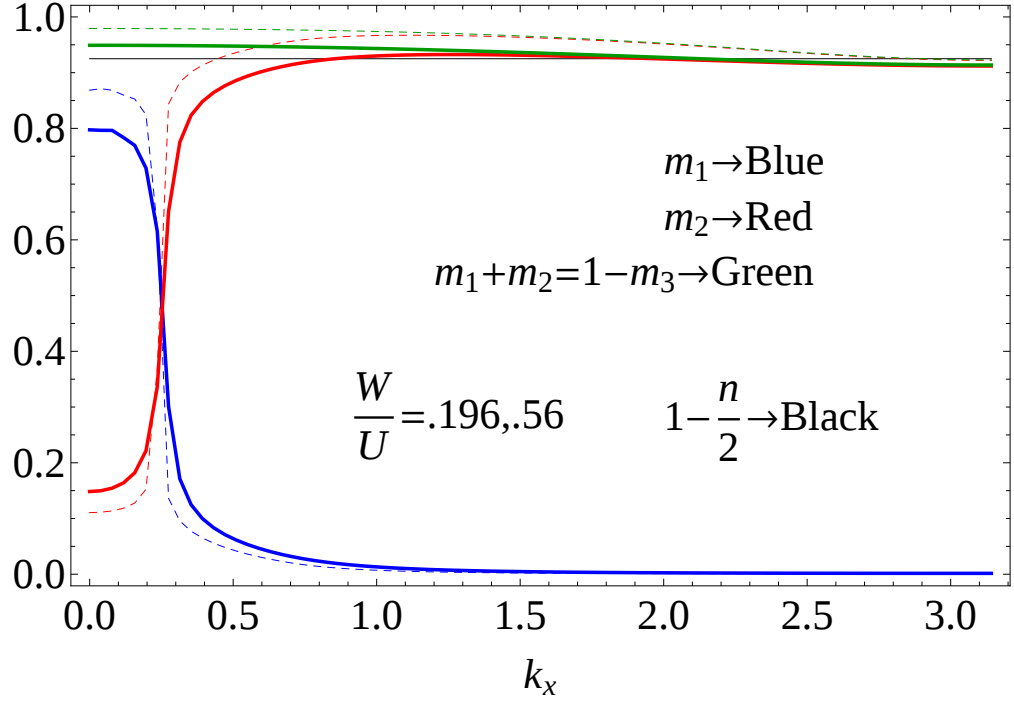


Figure 4.9: 1D $U=10$ $W=.56$ (dashed), $W=.196$ (solid), $n=.15$ 1d $T=.005$. Here m_1 is essentially the zero temperature quasiparticle occupation, while m_2 accounts for the LHB particle addition spectrum, The sharp step in occupation occurs precisely at the Luttinger Fermi surface which satisfies the Luttinger Ward sum rule. The sum of m_1 and m_2 is less than one due to the weight transferred to the upper band. The total lower band weight approaches $1-n/2$ as U/W goes to infinity.

add to unity for each wave vector. However, due to the finite frequency resolution of our numerics this sumrule is only approximately satisfied. We limit the error to $< 1\%$ by reducing our frequency step $d\omega$. The error is concentrated near k_f where the spectral function is sharpest.

In Fig. (4.9), we display the k dependence of the three occupancy functions for a typical set of parameters. It is clear that the Luttinger Ward Fermi surface controls the variations of the functions m_1 and m_2 , which complement each other so that the sum is almost a constant.

4.3 Doublons and their dynamics

4.3.1 Doublon Decay in the low density limit

In the recent experiments[8, 9] the lifetime of doublons created by optical excitation of the trapped atoms has been carried out, providing us with an added impetus for this study. The experiments actually study the decay of a highly non equilibrium initial state $|\psi_{Initial}\rangle$ with *a finite fraction of excited doublons*, i.e. $\langle\psi_{Initial}|\hat{D}|\psi_{Initial}\rangle \propto N_s$, where the doublon number $\hat{D} = \sum_i n_{i\uparrow}n_{i\downarrow}$. The object studied is the time evolution of such a state followed by a measurement of D and then a projection on to the evolved state i.e.

$$\xi(t_r) = \langle\psi_{Initial}| \exp\{it_r H\} \hat{D} \exp\{-it_r H\} |\psi_{Initial}\rangle. \quad (4.17)$$

Here and below we use the symbol t_r to denote real (Schrödinger) time, thus distinguishing it from the band hopping parameter t . Such a correlation function is not usually amenable to study near equilibrium type situations studied in many body physics. The initial state is itself quite far from being an equilibrium (ground) state. However, in the limit of very low densities, one can approximately view the initial state as the vacuum or few particle state with a few doublon excitations- and within this picture we may ask how a single doublon decays. This is roughly the question of the lifetime of a state in the upper Hubbard band, and thus related to our general theme in this work.

We are able to calculate the lifetime of a doublon within the ladder scheme, and hence presumably an exact answer at low densities as argued here. We next provide a discussion of the function γ in a low density Fermi liquid. We start with the corre-

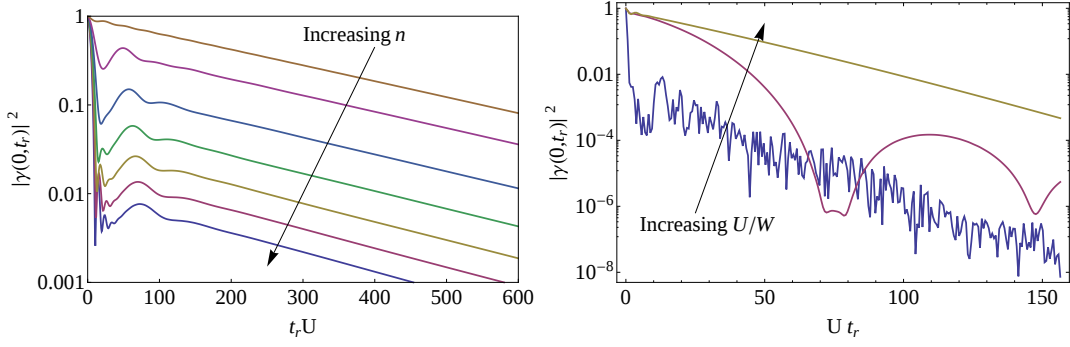


Figure 4.10: The doublon dynamics breaks into two regimes: a sharp decay at early times followed by a long exponential tail. The magnitude of the initial decay depends strongly on the density. In the limit $n \rightarrow 0$ the initial decay disappears, indicating that the UHB is comprised of sharp features only in the limit of vanishing density. In the right panel, the U dependence of the long time decay is shown, it slows down and is finally limited by the level broadening η assumed in our numerics.

lation function defined for Matsubara time $\tau \geq 0$ in terms of the two particle Greens function[16]

$$\gamma(r, \tau) \equiv G_{\uparrow, \downarrow, \uparrow}^{II}(r\tau, r\tau; 0, 0) = \langle c_{r, \uparrow}(\tau) c_{r, \downarrow}(\tau) c_{0, \downarrow}^\dagger(0) c_{0, \uparrow}^\dagger(0) \rangle, \quad (4.18)$$

and an analogous expression for real times $\gamma(r, t_r)$. This object can be expressed in terms of the scattering amplitude[27] as

$$\gamma(r, t_r) = \sum_Q \int d\Omega \rho_\Gamma(Q, \nu) (1 + n_B(\nu)) e^{-iQr - i\nu t_r}. \quad (4.19)$$

In Fig. 4.10, we display $\gamma(0, t_r)$ within the ladder scheme. As the density is increased, the UHB becomes broader and less k -dependent, however sharp k -dependent features persist with weight which decreases as n goes to zero. The k -dependent pieces remain sharp and determine the rate of the long time exponential decay. On the other hand the k -independent pieces, being broad, determine the short time decay. Due to our finite frequency resolution these numerics do not see the long time exponential decay

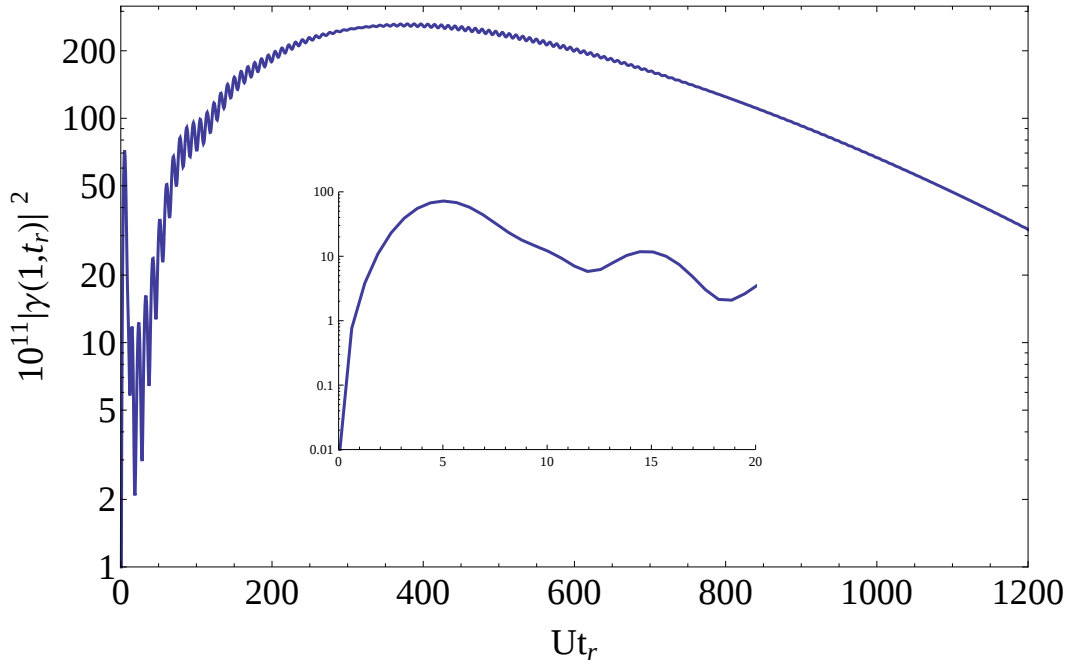


Figure 4.11: The inset shows that $\gamma(1, t_r)$ goes to zero at early times since there is no mechanism to hop at small times. On a longer time scale we see the development of an exponential decay. The small magnitude of the correlation is due to fact that the UHB is largely k -independent.

becoming infinitely long once $t < \eta$.

We have also computed the off site correlation function $\gamma(1, t_r > 0)$, Fig. 4.11 shows that even the site directly adjacent the created doublon has a very small amplitude.

4.3.2 Exact Solution of the Doublon Decay Problem for Two Particles.

In addition to the discussion of the low density case, we are able to solve exactly the admittedly simple problem of the dynamics a single doublon in the Hubbard model,

and from this study provide some feeling for the validity of the ladder scheme. The single doublon problem is solvable since for two particles of opposite spin, we have a total momentum quantum number and in each sector of this, we have a single particle type Schrodinger equation to solve. Let us first outline this problem and its solution with regard to the correlation function

$$\gamma(r, t_r) = \langle 0 | c_{r,\uparrow}(t_r) c_{r,\downarrow}(t_r) c_{0,\downarrow}^\dagger(0) c_{0,\uparrow}^\dagger(0) | 0 \rangle. \quad (4.20)$$

Here the average is with respect to the vacuum state with no particles, although below we will use the average over the thermal distribution function for a low density Fermi liquid. In the case of two particles, it is in fact possible to show that $\gamma(r, t_r)$ is related to the correlator $\xi(t_r)$ in Eq. (4.17) exactly through

$$\xi(t_r) = \sum_r |\gamma(r, t_r)|^2. \quad (4.21)$$

This follows upon using the fact that with only two particles in the system, the destruction operator $c_{r,\uparrow}(t_r) c_{r,\downarrow}(t_r)$ can only connect to the vacuum state. We expect this relation to be only approximately true for a dense Fermi system but useful since it can be computed with relative ease by one of several techniques. It is also dominated by the term $r = 0$ as shown explicitly below in Fig. (4.11), and hence it is useful to regard $|\gamma(0, t_r)|^2$ as an estimator of $\xi(t_r)$.

In Ref. ([9]), Demler et. al. estimate $\gamma(0, t_r)$ by an argument that is appropriate in an incoherent Fermi system, and estimate that this function decays on a time scale that is given as

$$\frac{h}{\tau} = A t \exp \left\{ -B \frac{U}{W} \right\}. \quad (4.22)$$

The vanishing of the rate as $W \rightarrow 0$ is expected in view of the conservation of the doublon number in the absence of electron hopping, the coefficients are estimated from experiments on the 3-d cubic lattice ($W = 12t$) as $A \sim .9 \pm 0.5$, and $B \sim 1.6 \pm 0.16$.

For the two particle problem, we have exact analytical and numerical solutions. In the interesting case of $U > W$ in d dimensional hypercubes with nearest neighbor hopping, we can write

$$\begin{aligned}\gamma(0, t_r) &= \gamma_L(0, t_r) + \gamma_U(0, t_r), \\ \gamma_U(0, t_r) &\sim e^{-i(U+4d\frac{t^2}{U})t_r} J_0^d(\frac{4t^2}{U} t_r),\end{aligned}\tag{4.23}$$

where the LHB contribution $\gamma_L \sim O((W/U)^2)$ and negligible. The second term arises from the UHB, and for intermediate $W \ll U$ is related to the Bessel function J_0 whereby it decays as a power law rather than as an exponential. This is understandable since the two body problem is an integrable system, and we expect that in the low density limit, this power law would be replaced by an exponential type decay. The function $|\gamma|^2$ can be found easily (see Appendix) by numerical means and Figs.4.12 and 4.13 give us a picture of the decay.

In Fig. 4.14, we show that the Half Width at Half Max (HWHM) of the computed $\gamma(0, t_r)$ leads to a rate $\frac{\hbar}{\tau_{HWHM}}$ which has a behavior that is similar to that in the experiments Eq. (4.22).

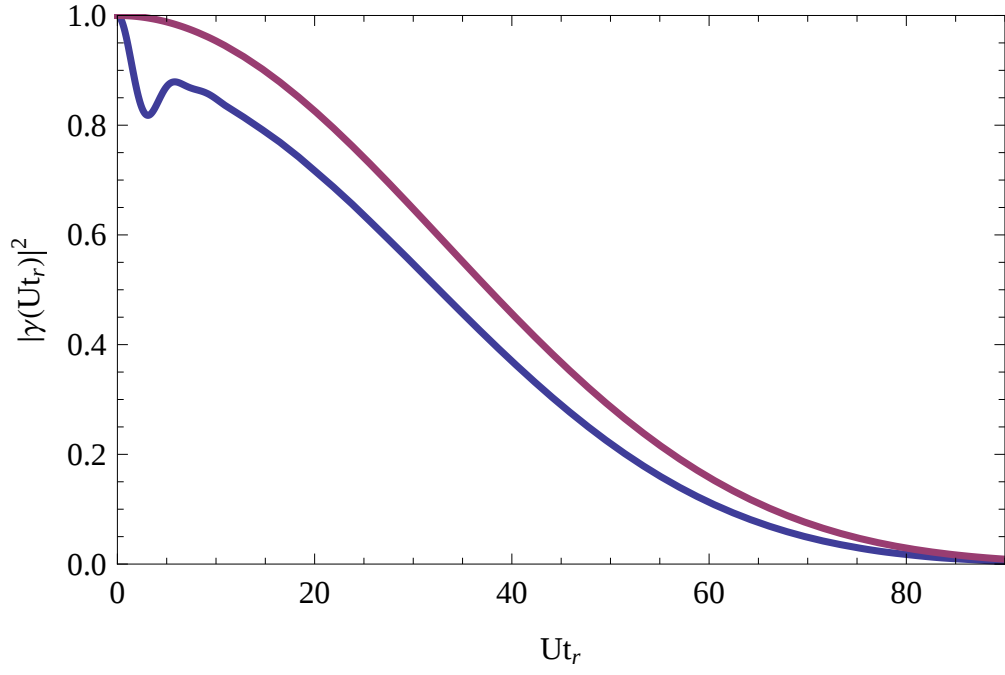


Figure 4.12: Doublon decay on a cubic lattice with $U = 15$ and $W = 12$. The shape of $|\gamma_U(Ut_r)|^2$ (red curve) initially deviates slightly from the exact numerical result (blue curve) due to the neglect of the γ_L term, which decays much more quickly than the UHB contribution.

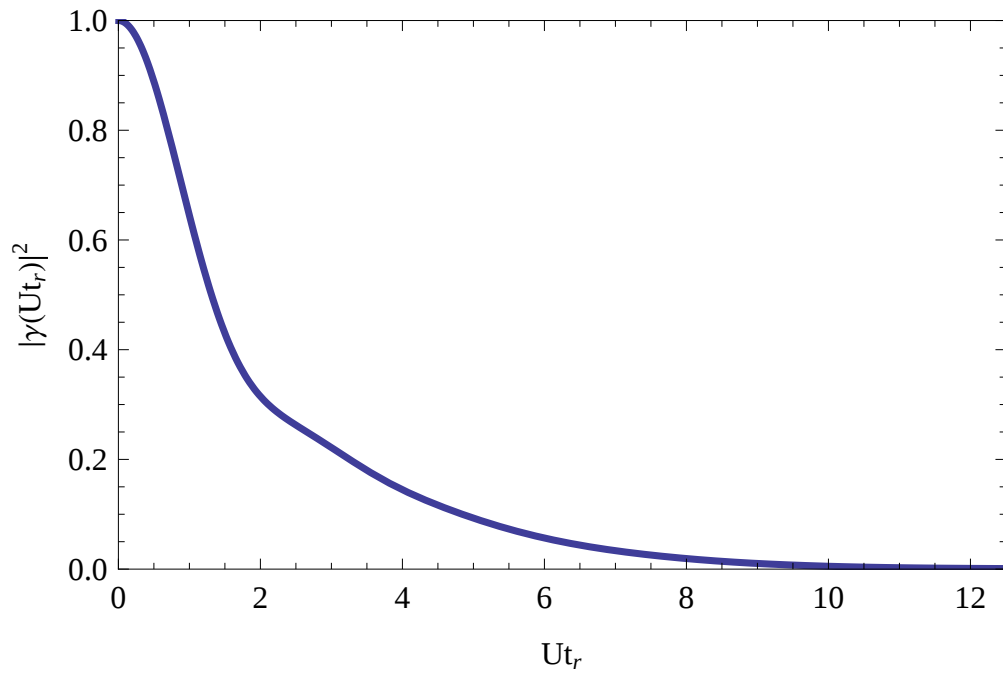


Figure 4.13: Doublon decay on a cubic lattice with $U = 5$ and $W = 12$. In the case $U < W$, it is much more difficult to find an exact analytical form, so only the numerical result is displayed.

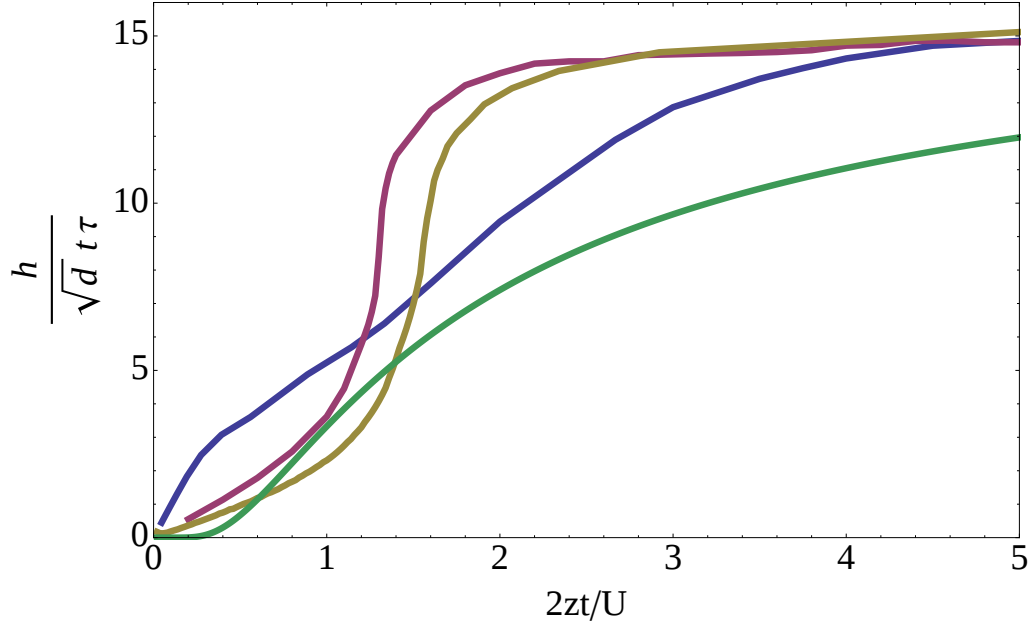


Figure 4.14: Two theoretical calculations, from ladder diagrams of Eq. (4.19) in 2-dimensions (blue) and the exact 2 particle solution from Eq. (4.21) and Eq. (4.33) in 2- and 3- dimensions (red and gold). These are compared to the experiment Eq. (4.22) in 3-dimensions (green), scaled to coincide at weak coupling by a factor 26.4. The theory and experiment are in very different limits of physical parameters, but have a similar shape except at large U/t .

4.4 Conclusions

In conclusion, we have shown that the self consistently computed ladder diagrams provide a detailed picture of the split bands for the Hubbard model. The UHB has a distinct shape that is captured here and related to the shape of the two particle scattering amplitude. We have delineated how the lower Hubbard band occupation is influenced by the passage to large U . Here the background momentum occupancy found in variational studies of the Gutzwiller approximation[25] arise here dynamically. Finally, we have shown that the decay of the doublon in such a system can be calculated by the ladder diagrams as well as by exact methods for very low densities, and the shapes of these curves are fairly close to those found in recent experiments on atomic traps performed under very different physical conditions.

4.A Exact correlation functions for the two particle Hubbard Model

We consider the Hubbard model with two particles, one spin up and the other spin down. Our goal is to calculate the following correlation function.

$$\gamma(t_r) = \langle 0 | c_{i\downarrow} c_{i\uparrow} e^{-iHt_r} c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger | 0 \rangle = \gamma_U(t_r) + \gamma_L(t_r). \quad (4.24)$$

The two parts arise from intermediate states that are in the two split bands. Thus

$$\begin{aligned} \gamma_U(t_r) &= \sum_{\nu \in UHB} | \langle \nu | c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger | 0 \rangle |^2 e^{-iE_\nu t_r} \\ \gamma_L(t_r) &= \sum_{\nu \in LHB} | \langle \nu | c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger | 0 \rangle |^2 e^{-iE_\nu t_r}. \end{aligned} \quad (4.25)$$

We now calculate the eigenvalues and eigenstates for the 2 particle Hubbard model. As our basis we take momentum eigenstates.

$$|Q, k\rangle \equiv c_{Q-k\uparrow}^\dagger c_{k\downarrow}^\dagger |0\rangle \quad (4.26)$$

Q is the total momentum of the state, and both Q and k can be any vector in the first Brillouin zone. The Hamiltonian acts on the basis in the following way.

$$H |Q, k\rangle = E_k |Q, k\rangle + \frac{U}{N_s} \sum_p |Q, p\rangle, \quad (4.27)$$

where $E_k = (\epsilon_{Q-k} + \epsilon_k)$. The Hamiltonian conserves total momentum. Thus, we can diagonalize each total momentum sector independently. Each sector will have N_s eigenstates, where N_s is the size of the lattice. We now fix Q and work in a particular total momentum sector. The basis states now depend on a single index k . The E_k 's will in general be degenerate, and we take an E with degeneracy n , i.e. $\deg(E) = n$, corresponding to states $|Q, k_1\rangle \dots |Q, k_n\rangle$. From these we can make an $n-1$ dimensional degenerate eigenspace of the Hamiltonian with energy E which we shall call $|\psi\rangle_{deg}$.

$$|\psi\rangle_{deg} = \sum_{i=1}^n \alpha_i |Q, k_i\rangle \quad \sum_i \alpha_i = 0 \quad (4.28)$$

One can see that these are eigenstates with energy E since potential energy term goes to zero due to the condition $\sum_i \alpha_i = 0$ and the kinetic energy term gives E times the state. Suppose there are p unique values of E in this total momentum sector.

$$\deg(E_1) + \dots + \deg(E_p) = N_s \quad (4.29)$$

By forming states in the way described above, we can obtain $N_s - p$ eigenstates $|\psi\rangle_{deg}$ that are independent of U . We obtain the remaining non trivial (i.e. U dependent) p eigenstates by plugging the following state into the Hamiltonian.

$$|\psi_Q\rangle = \sum_k \Phi_Q(k) |Q, k\rangle \quad \text{and} \quad H |\psi_Q\rangle = \Lambda_Q |\psi_Q\rangle. \quad (4.30)$$

Here we consider states with a fixed total momentum Q since this object is conserved.

This yields the following results

$$\Phi_Q(k) = \frac{1}{c_Q \sqrt{N_s}} \frac{1}{\Lambda_Q - E_k}, \quad c_Q = \left(\frac{1}{N_s} \sum_k \frac{1}{(\Lambda_Q - E_k)^2} \right)^{\frac{1}{2}}, \quad \frac{U}{N_s} \sum_k \frac{1}{\Lambda_Q - E_k} = 1. \quad (4.31)$$

We can see explicitly from Eq. (4.31) that $\langle \psi_Q | \psi \rangle_{deg} = 0$ since basis states with equal E have equal coefficients, and therefore the condition $\sum_i \alpha_i = 0$ makes this state orthogonal to the degenerate manifold of states in Eq. (4.28). There are $p - 1$ solutions of Eq. (4.31) which lie in between the p distinct E 's. The corresponding states are in the lower Hubbard band. The $|\psi\rangle_{deg}$ found earlier also lie in the lower Hubbard band since these states are independent of U . There is one solution of Eq. (4.31) for which $\Lambda_Q > E_{max}$ and is of order U if $U > W$. The corresponding state lies in the upper Hubbard band. Thus for each fixed Q sector, there is one state in the upper Hubbard band. We now consider the doublon state.

$$|\psi\rangle_d = c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger |0\rangle = \frac{1}{N_s} \sum_{Q,k} e^{-iQ \cdot R_i} |Q, k\rangle \quad (4.32)$$

We can rewrite

$$\gamma(t_r) = \sum_Q |\langle \psi_Q | \psi \rangle_d|^2 e^{-i\Lambda_Q t_r} \quad (4.33)$$

where the Q in the above sum stands for the p states described by Eq. (4.31) in the total momentum sector Q . Since $\langle \psi_d | \psi \rangle_{deg} = 0$ we didn't have to take the degenerate states into account when calculating the correlation function. Furthermore, we see that

$$| \langle \psi_Q | \psi \rangle_d |^2 = \frac{1}{N_s c_Q^2 U^2} \quad (4.34)$$

where c_Q is from Eq. (4.31).

$$\gamma_U(t_r) = \sum_{Q \in UHB} \frac{1}{N_s c_Q^2 U^2} e^{-i\Lambda_Q t_r} \quad (4.35)$$

In the above sum, each Q now represents only one state, since there is only one UHB state in each total momentum sector. We first evaluate this in one dimension, and then generalize to multiple dimensions. The sum can be turned into an integral.

$$\gamma_U(t_r) = \frac{1}{\pi} \int_0^\pi \frac{1}{c_Q^2 U^2} e^{-i\Lambda_Q t_r} dQ \quad (4.36)$$

Converting Eq. (4.31) into integrals, we find that

$$\Lambda_Q = (U^2 + 16t^2 \cos^2 \frac{Q}{2})^{\frac{1}{2}} \quad (4.37)$$

$$c_Q^2 = \frac{1}{U^3} (U^2 + 16t^2 \cos^2 \frac{Q}{2})^{\frac{1}{2}} \quad (4.38)$$

For $U > W$, we keep corrections of $O(\frac{t^2}{U^2})$ in Λ_Q and drop all corrections in c_Q^2 , yielding

$$\gamma_U(t_r) \sim \frac{1}{\pi} \int_0^\pi e^{-iU(1+8\frac{t^2}{U^2} \cos^2 \frac{Q}{2})t_r} dQ \quad (4.39)$$

$$\gamma_U(t_r) \sim e^{-i(U+4\frac{t^2}{U})t_r} J_0(\frac{4t^2}{U}t_r) \quad (4.40)$$

In two dimensions, Eq. (4.31) becomes an elliptic integral so there is no closed form answer for the upper band eigenvalues in terms of elementary functions. However for

$U > W$, keeping corrections to the same order as we did in deriving Eq. (4.39), we can easily generalize to higher dimensions.

$$\Lambda_Q = U(1 + 8 \frac{t^2}{U^2} \sum_{i=1}^d \cos^2 \frac{Q_i}{2}) \quad (4.41)$$

$$c_Q^2 = \frac{1}{U^2} \quad (4.42)$$

$$\gamma_U(t_r) \sim e^{-i(U+4d\frac{t^2}{U})t_r} J_0^d(\frac{4t^2}{U}t_r) \quad (4.43)$$

The other contribution to $\gamma(t_r)$ is $\gamma_L(t_r)$. However, from degenerate perturbation theory, we know that provided $U > W$ $|\langle \nu | \psi \rangle_d|^2$ is $O(\frac{t^2}{U^2})$ smaller for $\nu \in LHB$ than it is for the upper Hubbard band. Hence, $\gamma_L(t_r)$ is a small correction to $\gamma_U(t_r)$.

$$\gamma(t_r) \approx \gamma_U(t_r) \quad (4.44)$$

$$|\gamma(t_r)|^2 \approx J_0^{2d}(\frac{4t^2}{U}t_r) \quad (4.45)$$

In conclusion, the doublon decay in the 2 particle Hubbard model in the regime $U > W$ is dominated by γ_U with the much faster decaying γ_L giving a small correction. To a good approximation, the shape of the decay of $|\gamma(t_r)|^2$ is $J_0^{2d}(\frac{4t^2}{U}t_r)$.

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[26] In [24] Eq. (D4), it is argued that the real part of the self energy, in the range of frequencies $W \ll \omega \ll U$ must have the behavior $\text{Re}\Sigma(\vec{k}, \omega) = -\frac{n}{2-n}\omega + \text{const.}$ Hence at a density $n = .0414$ we expect $\text{Re}\Sigma(\vec{k}, \omega) = -.0212\omega + \text{const.}$, as found numerically.

[27] This is easy to see from the definition of the scattering amplitude and the its result in the ladder scheme:

$$\begin{aligned}
G^{II}(Q, p_1, p_2) &= G(Q/2 + p_1)G(Q/2 - p_1) \\
&\quad - G(Q/2 + p_1)G(Q/2 - p_1)\Gamma(Q)G(Q/2 + p_2)G(Q/2 - p_2) \\
\gamma(Q) &= \sum_{p_1, p_2} G^{II}(Q, p_1, p_2) = \frac{\Pi(Q)}{1 + U\Pi(Q)},
\end{aligned}$$

where we used Eq. (4.1). The spectral density of γ is now easy to find

$$\rho_\gamma = \frac{-\rho_\Pi}{(1 + U\text{Re}\Pi)^2 + (\pi U\rho_\Pi)^2},$$

leading to the quoted result.

Chapter 5

Spectral Functions of the t - J model by ECFL Formalism

5.1 Motivation

While the t - J has received considerable attention over the last two decades, it nonetheless holds many mysteries. The hard core constraint which projects all doubly occupied states from the Hilbert space has been termed by Shastry as Extreme Correlation. It is fundamentally different from strong correlations where high and low energy scales may mix. Standard computational techniques suffer for various reasons. Exact diagonalization and Monte Carlo techniques can provide exact results for very small systems. Standard many-body perturbative methods fail due to the absence of a Wick's theorem. The Dynamical Mean Field Theory offers a way to obtain spectral functions in the limit of infinite U but the spatial resolution is limited by the same constraints which

apply to Monte Carlo and Exact Diagonalization techniques. At present the Density Matrix Renormalization group offers perhaps the best computational results but it does not provide an explicit functional form for the spectral function.

An alternative approach has been initiated by Shastry utilizing the Field theory of Schwinger. Schwinger's formulation of Quantum Field Theory does not rely upon the existence of Wick's theorem. Rather, a hierarchy of Green's functions and vertices may be generated by taking functional derivatives of the Equation of Motion w.r.t some appropriate "source." This technique is powerful in its generality though quite cumbersome as compared to the use of diagrammatic Field Theory. In several papers Ref. ([5]) Ref. ([6]) Ref. ([7]) Ref. ([4]), Shastry has presented a method by which the single particle Green's function of the t - J model may be calculated with the hard core constraint being treated exactly. This chapter presents the results of a rigorous calculation of the t - J model on a 2D square lattice.

The chapter proceeds as follows. In section 2 I present an abbreviated account of Shastry's calculation. In section 3 I put these equations into a form which is appropriate for an explicit calculation. Some tricky aspects of the calculation are discussed. In section 4, I will present a scheme by which the spectral functions can be computed efficiently by FFT. Section 5 presents key results of the calculation in relation to key experimental results of the high T_c Cuprate compounds.

5.2 The Model

The t - J model is given by

$$H = - \sum_{i,j} t_{i,j} \hat{c}_{\vec{r}_j,\sigma}^\dagger \hat{c}_{\vec{r}_i,\sigma} + \frac{1}{2} \sum_{i,j} J_{i,j} \{ \vec{S}_{\vec{r}_i} \cdot \vec{S}_{\vec{r}_j} - \frac{1}{4} n_{\vec{r}_i} n_{\vec{r}_j} + n_{\vec{r}_i} \} - \mu \sum_i n_{\vec{r}_i}, \quad (5.1)$$

where $\hat{c}_{\vec{r}_i,\sigma}^\dagger$ creates a electron at the site i which is *Gutzwiller projected* to the subspace of single occupancy, and the other symbols have their usual meaning. Let us define the Hubbard operators acting upon each site as projected Fermi operators

$$X_i^{\sigma_1\sigma_2} = |\sigma_1\rangle\langle\sigma_2|, \quad X_i^{0\sigma_1} = |0\rangle\langle\sigma_1|, \quad X_i^{\sigma_1 0} = |\sigma_1\rangle\langle 0|, \quad (5.2)$$

in terms of the three possible states at any site, which are $|0\rangle, |\uparrow\rangle, |\downarrow\rangle$ for a two component Fermion. The doubly occupied site is forbidden, and these operators do not connect forbidden states with the allowed ones. Thus an important statement of completeness at any site is the relation

$$X_i^{00} = \mathbf{1} - \sum_{\sigma} X_i^{\sigma\sigma}. \quad (5.3)$$

The first member $X_i^{\sigma_1\sigma_2}$ is Bosonic while the other two are Fermionic with respect to their commutation relations at different sites. The Hamiltonian is expressed in terms of the X operators by

$$H = - \sum_{i,j,\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} - \mu \sum_{i,\sigma} X_i^{\sigma\sigma} + \frac{1}{2} \sum_{i,j} J_{ij} \{ \vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \} + \frac{1}{2} \sum_{i,j,\sigma} J_{ij} X_i^{\sigma\sigma}. \quad (5.4)$$

The last (trivial) term is a shift of the chemical potential, and is added to make the equations more compact.

In what follows we use the abbreviations,

$$\begin{aligned}\delta[i, j] &= \delta_{i,j} \delta(\tau_i - \tau_j), & t[i, j] &= t_{ij} \delta(\tau_i - \tau_j), \\ J[i, j] &= J_{ij} \delta(\tau_i - \tau_j), & \mathcal{V}_r^{\sigma_a \sigma_b} &= \mathcal{V}_r^{\sigma_a \sigma_b}[\tau_r].\end{aligned}\tag{5.5}$$

where $\mathcal{V}$ is the source term. Let $\mathbf{1}$ be the identity matrix in the 2×2 dimensional spin space.

We employ a useful relation with an arbitrary operator $\mathcal{Q}$:

$$\begin{aligned}\langle\langle (\delta_{\sigma_a \sigma_b} - \sigma_a \sigma_b X_a^{\bar{\sigma}_a \bar{\sigma}_b}) \mathcal{Q} \rangle\rangle &= (\Delta_{\sigma_a \sigma_b}[a] + D_{\sigma_a \sigma_b}[a^+]) \langle\langle \mathcal{Q} \rangle\rangle, \\ D_{\sigma_i \sigma_j}[i] &= \sigma_i \sigma_j \frac{\delta}{\delta \mathcal{V}_i^{\bar{\sigma}_i \bar{\sigma}_j}}\end{aligned}\tag{5.6}$$

with

$$\begin{aligned}\Delta_{\sigma_i \sigma_j}[i] &= \delta_{\sigma_i \sigma_j} - \sigma_i \sigma_j \mathcal{G}_{\bar{\sigma}_j \bar{\sigma}_i}[i^-, i] \\ \gamma_{\sigma_i \sigma_j}[i] &= \sigma_i \sigma_j \mathcal{G}_{\bar{\sigma}_j \bar{\sigma}_i}[i^-, i]\end{aligned}\tag{5.7}$$

to write the equation of motion in component form as

$$\begin{aligned}(\partial_{\tau_i} - \boldsymbol{\mu})\mathcal{G}[i, f] &= -\delta[i, f](1 - \gamma[i]) - \mathcal{V}_i \cdot \mathcal{G}[i, f] - X[i, \mathbf{j}] \cdot \mathcal{G}[\mathbf{j}, f] \\ &\quad - Y[i, \mathbf{j}] \cdot \mathcal{G}[\mathbf{j}, f],\end{aligned}\tag{5.8}$$

where the bold $\boldsymbol{\mu}$ is the chemical potential and the other bold symbolized indicate an implied summation. Furthermore we have used the definitions

$$\begin{aligned}X[i, j] &= -t[i, j] (D[i^+] + D[j^+]) + \frac{1}{2} J[i, \mathbf{k}] (D[i^+] + D[\mathbf{k}^+]) \delta[i, j] \\ Y[i, j] &= -t[i, j] (\mathbf{1} - \gamma[i] - \gamma[j]) + \frac{1}{2} J[i, \mathbf{k}] (\mathbf{1} - \gamma[i] - \gamma[\mathbf{k}]) \delta[i, j]\end{aligned}\tag{5.9}$$

to make Eq. (5.8) more compact.

At this point it is useful to define an auxiliary Green's function $\mathbf{g}$ which is related to the physical Green's function by

$$\mathcal{G}[a, b] = \mathbf{g}[a, \mathbf{b}] \cdot \mu[\mathbf{b}, b] \quad (5.10)$$

Here $\mu[p, \mathbf{p}]$ and $\mathbf{g}$ are yet to be determined. Nonetheless we impose this convolution structure where again there is an implied sum over the repeated bold argument on the RHS. Later we will write this in the momentum space and $\mathcal{G}$ will be a simple product of μ and $\mathbf{g}$. Note that the function μ is not bold so that it may be distinguished from the chemical potential $\boldsymbol{\mu}$.

Writing Eq. (5.9) as

$$\begin{aligned} Y[i, j] &= Y_0[i, j] + Y_1[i, j] \\ Y_0[i, j] &= -t[i, j] \mathbf{1} + \delta[i, j] \frac{1}{2} J[i, \mathbf{k}] \mathbf{1} \\ Y_1[i, j] &= t[i, j] (\gamma[i] + \gamma[j]) - \delta[i, j] \frac{1}{2} J[i, \mathbf{k}] (\gamma[i] + \gamma[\mathbf{k}]) \end{aligned} \quad (5.11)$$

and defining

$$\mathbf{g}_0^{-1}[i, f] = \{-(\partial_{\tau_i} - \boldsymbol{\mu})\mathbf{1} - \mathcal{V}_i\} \delta[i, f] - Y_0[i, f], \quad (5.12)$$

the exact EOM Eq. (5.8) becomes

$$\{\mathbf{g}_0^{-1}[i, \mathbf{j}] - Y_1[i, \mathbf{j}] - \Phi[i, \mathbf{j}]\} \cdot \mathbf{g}[\mathbf{j}, \mathbf{f}] \cdot \mu[\mathbf{f}, f] = \delta[i, f] (\mathbf{1} - \gamma[i]) + \Psi[i, f]. \quad (5.13)$$

In order to establish an adiabatic connection to the Fermi gas, we now introduce a convenient parameter λ inserted as follows.

$$\{\mathbf{g}_0^{-1}[i, \mathbf{j}] - \lambda Y_1[i, \mathbf{j}] - \lambda \Phi[i, \mathbf{j}]\} \cdot \mathbf{g}[\mathbf{j}, \mathbf{f}] \cdot \mu[\mathbf{f}, f] = \delta[i, f] (\mathbf{1} - \lambda \gamma[i]) + \lambda \Psi[i, f] \quad (5.14)$$

At $\lambda = 1$ this becomes the exact equation for the EC phase. It has the virtue that as $\lambda = 0$ it gives a canonical equation for $\mathbf{g}$, with $\mu[i, j] = \mathbf{1}\delta[i, j]$. Thus we establish adiabatic continuity with the Fermi gas in the equations of motion. We set $\lambda = 1$ at the end of the calculation. We may now split Eq. (5.14) into two equations:

$$\{\mathbf{g}_0^{-1}[i, \mathbf{j}] - \lambda Y_1[i, \mathbf{j}] - \lambda \Phi[i, \mathbf{j}]\} \cdot \mathbf{g}[\mathbf{j}, f] = \delta[i, f], \quad (5.15)$$

and

$$\mu[i, f] = \delta[i, f] (\mathbf{1} - \lambda \gamma[i]) + \lambda \Psi[i, f]. \quad (5.16)$$

Hence the Eqn. for $\mathbf{g}^{-1}$ reads

$$\mathbf{g}^{-1}[i, m] = \{\mathbf{g}_0^{-1}[i, m] - \lambda Y_1[i, m] - \lambda \Phi[i, m]\} \quad (5.17)$$

Taking functional derivatives w.r.t. $\mathcal{V}$, we generate the standard self energy - vertex hierarchy of Fermionic theory.

5.3 Explicit equations and the Zero source limit in Fourier space

When we turn off the sources, the various matrix function $\mathcal{G}, \mathbf{g}, \mu$ become spin diagonal. We first note the number of particles is given by

$$\sum_p \mu[p] \mathbf{g}[p] = \frac{n}{2} \quad (5.18)$$

and

$$\begin{aligned} \mathcal{G}[k] &= \mathbf{g}[k] \mu[k] \\ \mu[k] &= 1 - \lambda\gamma + \lambda\Psi[k] \\ \mathbf{g}^{-1}[k] &= i\omega_k + \boldsymbol{\mu} - (1 - 2\lambda\gamma) \varepsilon_k - \lambda \Phi[k] \end{aligned} \quad (5.19)$$

with the use of

$$\begin{aligned} \mathbf{g}_0^{-1} &= i\omega_k + \boldsymbol{\mu} - \varepsilon_k \\ Y_0[k] &= \varepsilon_k + \frac{1}{2} \hat{J}[0] \rightarrow \varepsilon_k \\ Y_1[k] &= -2\gamma \varepsilon_k \end{aligned} \quad (5.20)$$

(the constant term $\frac{1}{2} \hat{J}[0]$ can be absorbed into $\boldsymbol{\mu}$ so it is ignored after this point). Finally we set

$$\gamma_{\sigma_i \sigma_j} [i] \rightarrow \gamma = \sum_k \mathbf{g}(k) [1 - \lambda\gamma + \lambda\Psi(k)] \quad (5.21)$$

with a constant γ because we are considering a liquid like state with no broken symmetries. The magnitude of γ is discussed in detail later (see Eqs. (5.37,5.40)).

We proceed with two parallel calculations from Eq. (5.16) and Eq. (5.17) and find equations for Φ and Ψ . We write these together as

$$\begin{aligned}\Phi[k] &= \sum_p E(k, p) \mathbf{g}[p] \Lambda^{(a)}(p, k) e^{i\omega_p 0^+} \\ \Psi[k] &= \sum_p E(k, p) \mathbf{g}[p] \mathcal{U}^{(a)}(p, k) e^{i\omega_p 0^+}\end{aligned}\tag{5.22}$$

where we have defined

$$E(p_1, p_2) = E(p_2, p_1) = \left(\varepsilon_{p_1} + \varepsilon_{p_2} + \frac{1}{2} \left\{ \hat{J}_0 + \hat{J}_{p_1-p_2} \right\} \right) \tag{5.23}$$

with $\hat{J}_p$ defined as the Fourier transform of $J[i, k]$ in the spatial coordinates just as ε_p is the Fourier transform of $t[i, j]$ given by

$$\begin{aligned}J[i, j] &= \sum_p J_p e^{ip(r_i - r_j)} \\ t[i, j] &= \sum_p \varepsilon_p e^{ip(r_i - r_j)}.\end{aligned}\tag{5.24}$$

and the vertex functions $\Lambda^{(a)} = \Lambda^{(2)} - \Lambda^{(3)} = \frac{1}{2}\Lambda^{(s)} - \frac{3}{2}\Lambda^{(t)}$ and $\mathcal{U}^{(a)} = \mathcal{U}^{(2)} - \mathcal{U}^{(3)} = \frac{1}{2}\mathcal{U}^{(s)} - \frac{3}{2}\mathcal{U}^{(t)}$. The notation of the superscripts is given in detail in Ref. ([5]). In brief (s) and (t) refer to the singlet and triplet p-h channels while (a) refers to the antisymmetric channel. The convergence factor $e^{i\omega_p 0^+}$ arises from the time ordering.

5.3.1 Exact equations: reduced vertex function

We will take out the bare vertex to get greater symmetry: write

$$\begin{aligned}\Lambda^{(\alpha)}[p_1, p_2] &= (\delta_{\alpha,1} + \delta_{\alpha,3}) + \bar{\Lambda}^{(\alpha)}[p_1, p_2] \\ \bar{\Lambda}^{(\alpha)}[p_1, p_2] &= -\lambda E(p_1, p_2) \xi^{(\alpha)}[p_1 - p_2] + \lambda A^{(\alpha)}[p_1, p_2] \\ \mathcal{U}^{(\alpha)}[p_1, p_2] &= -\lambda \xi^{(\alpha)}[p_1 - p_2] + \lambda B^{(\alpha)}[p_1, p_2]\end{aligned}\tag{5.25}$$

so that

$$\begin{aligned}\Phi(k) &= -\sum_p E(k,p) \mathbf{g}(p) + \bar{\Phi}(k) \\ &= -\frac{n}{2} \varepsilon_k - \frac{1}{2} \sum_p J_{k-p} \mathbf{g}(p) + \bar{\Phi}(k) + (\text{constant absorbed in } \boldsymbol{\mu}).\end{aligned}\quad (5.26)$$

The first term $\frac{n}{2} \varepsilon_k$ comes from $\varepsilon_k \sum_p \mathbf{g}(p)$ according to the condition Eq. (5.33) which will be discussed later. Hence we may write

$$\begin{aligned}\mathbf{g}^{-1}[k] &= i\omega_k + \boldsymbol{\mu} - (1 - 2\lambda\gamma) \varepsilon_k - \lambda \Phi[k] \\ &= z - x_0 \varepsilon_k + \frac{1}{2} \lambda \sum_q \hat{J}_{k-q} \mathbf{g}(q) - \lambda \bar{\Phi}[k].\end{aligned}\quad (5.27)$$

with

$$x_0 = (1 - 2\lambda\gamma - \lambda \frac{1}{2}n). \quad (5.28)$$

In 2-dimensions on a square lattice

$$\frac{1}{2} \sum_p J_{k-p} \mathbf{g}(p) = c_0 (\cos(k_x) + \cos(k_y)). \quad (5.29)$$

where

$$c_0 = J \sum_p \cos p_x \mathbf{g}[p] > 0 \quad (5.30)$$

and $J_k = 2 J (\cos(k_x) + \cos(k_y))$ where J is the magnitude of the superexchange.

5.3.2 To $O(\lambda^2)$ Theory

This is the first non trivial theory. We want $\mathbf{g}^{-1}$ and μ correctly to $O(\lambda^2)$. For this, it is enough to get Ψ and $\bar{\Phi}$ to $O(\lambda)$ since these are multiplied by λ . Thus we find

$$\begin{aligned}
\bar{\Lambda}^{(a)}(p_1, p_2) &= -2\lambda \times E(p_1, p_2) \chi_0[p_1 - p_2] \\
&\quad - 2\lambda \sum_q E(p_1 - q, p_1) \mathbf{g}(p_1 - q) \mathbf{g}(p_2 - q) \\
\mathcal{U}^{(a)}[p_1, p_2] &= -2\lambda \times \chi_0[p_1 - p_2]
\end{aligned} \tag{5.31}$$

Hence the complete solution to $O(\lambda^2)$ is given by

$$\begin{aligned}
\frac{n}{2} &= \sum_p \mu[p] \mathbf{g}[p] \\
\mathcal{G}[k] &= \mathbf{g}[k] \mu[k] \\
\mu[k] &= 1 - \lambda\gamma + \lambda\Psi[k] \\
\mathbf{g}^{-1}[k] &= i\omega_k + \boldsymbol{\mu} - x_0 \varepsilon_k + \lambda c_0(\cos(k_x) + \cos(k_y)) - \lambda \bar{\Phi}[k] \\
\bar{\Phi}[k] &= -2\lambda \sum_{pq} E(k, p) \left(E(p, k) + E(p + q - k, p) \right) \mathbf{g}[p] \mathbf{g}[q] \mathbf{g}[q + p - k] \\
\Psi[k] &= -2\lambda \sum_{pq} E(k, p) \mathbf{g}[p] \mathbf{g}[q] \mathbf{g}[q + p - k]
\end{aligned} \tag{5.32}$$

From its definition we find that the Luttinger volume of $\mathcal{G}$ is strongly controlled by that of $\mathbf{g}$. Therefore if we want our physical Green's function to obey the volume theorem at any λ both Green's functions must have the same “particle” density. Thus it is essential that we impose a lower level sum rule

$$\sum_k \mathbf{g}[k] = \frac{n}{2}. \tag{5.33}$$

Since this constraint is applied to the auxiliary $\mathbf{g}$ we can use it to simplify the appearance of the physical sumrule

$$\frac{n}{2} = \sum_k \mathcal{G}[k] \tag{5.34}$$

by rewriting it as

$$\frac{n}{2} = \sum_k \mathbf{g}[k] (1 - \lambda\gamma + \lambda\Psi[k]), \quad (5.35)$$

which simplifies to

$$0 = \sum_k (\lambda\Psi[k] - \lambda\gamma) \mathbf{g}[k]. \quad (5.36)$$

This form illustrates the fact that the static renormalization of spectral weight by the term $\gamma \mathbf{g}$ must be balanced by the dynamical redistribution of weight by $\Psi \mathbf{g}$. This equation can usefully be solved for γ ,

$$\gamma = \frac{\sum_k \Psi[k] \mathbf{g}[k]}{n/2}. \quad (5.37)$$

Note now that from Eq. (5.21) we can expand γ itself as a series in λ ,

$$\gamma = \frac{n}{2} - \lambda \frac{n^2}{4} + O(\lambda^2) \quad (5.38)$$

with the $O(\lambda^2)$ terms involving $\Psi(k)$

In making approximations to the exact equations the existence of two sumrules must be handled carefully. In the t -J model we expect the exact equations would yield $\gamma = n/2$, yet in the 2^{nd} order theory we show numerically (below in Fig. (5.1) and Fig. (5.2)) that $\gamma = n/2$ does not allow for a simultaneous solution of both sumrules at all values of n . This is better understood if we recall that γ has an expansion in powers of λ . Alternatively we can implement a scheme which uses γ as an adjustable parameter, i.e. a second chemical potential which may be tuned to satisfy the second

sumrule Eq. (5.37). These are named schemes A and B respectively.

$$\text{Scheme A: } \gamma \rightarrow \gamma_A = \frac{n}{2} - \lambda \frac{n^2}{4} \quad (5.39)$$

$$\text{Scheme B: } \gamma_B = \frac{\sum_k \Psi[k; \gamma_B] \mathbf{g}[k; \gamma_B]}{n/2} \quad (5.40)$$

Scheme A does a significantly better job of satisfying both sumrules than the naive use of $\gamma = n/2$. Fig. (5.1) illustrates this agreement in the region $0 \leq n \leq .5$. On the other hand, Scheme B disturbs the known high frequency behavior of the exact t -J Green's function by an amount that is argued to be small in a certain domain of densities (see inset of Fig. (5.2)).

It is partially a matter of taste to preserve the particle density at the expense of the high frequency behavior. However, it is certainly in line with the philosophy which underlies the t -J model, namely that the low energy properties are more interesting and essential to the problem. Therefore we relax the constraint on the high frequency limit but acquire the correct Luttinger volume by ensuring that $\sum_k \mathbf{g}[k] = \sum_k \mathcal{G}[k]$. Furthermore, in the ECFL equations γ often represents the existence of a correlation hole and in $\mu(k)$ it represents the transfer of spectral weight to the Upper Hubbard band. In these respects it is a measure of the extreme correlations present in this theory. Since we are dealing with a low order treatment of the ECFL it is not wholly unexpected that we will not be able to perfectly capture the EC phase and, recognizing γ 's central importance, it is reasonable to adjust γ to account for the shortcomings of the method.

5.4 Computation of Spectral Functions

Computationally it is expedient to employ a spectral function notation as described for example by Mahan in [10] where, for instance,

$$\rho_{\mathcal{G}}(\nu) = -\frac{1}{\pi} \text{Im}(\mathcal{G}(i\omega \rightarrow \nu + i\eta)) \quad (5.41)$$

and the real part of the analytically continued function can be obtained by Hilbert transform

$$\text{Re}\mathcal{G}(\nu) = \mathcal{H}(\rho_{\mathcal{G}})(\nu) = \text{P.V.} \int_{-\infty}^{\infty} \frac{\rho_{\mathcal{G}}(\omega)}{\nu - \omega} d\omega. \quad (5.42)$$

Analogous definitions exist for $\mathbf{g}$, $\bar{\Phi}$, Ψ , etc. The full set of equations above can be rewritten in terms of this spectral notation. First we have the two sumrules

$$\begin{aligned} \frac{n}{2} &= \sum_k \int d\omega \rho_{\mathbf{g}}(k, \omega) f(\omega) \\ \gamma &= \frac{2}{n} \sum_k \int d\omega \left(\rho_{\mathbf{g}}(k, \omega) \text{Re}\Psi(k, \omega) + \text{Reg}(k, \omega) \rho_{\Psi}(k, \omega) \right) f(\omega) \end{aligned} \quad (5.43)$$

where $f(\omega) = (1 + \exp(\beta\omega))^{-1}$ and $\bar{f}(\omega) = 1 - f(\omega)$. There are also the auxiliary and physical spectral functions

$$\rho_{\mathbf{g}}(k, \omega) = \frac{\rho_{\bar{\Phi}}(k, \omega)}{\left\{ \omega + \boldsymbol{\mu} - x_0 \varepsilon_k + \lambda c_0 (\cos(k_x) + \cos(k_y)) - \lambda \text{Re}\bar{\Phi}(k, \omega) \right\}^2 + (\pi \rho_{\bar{\Phi}})^2} \quad (5.44)$$

and

$$\rho_{\mathcal{G}} = \rho_{\mathbf{g}} (1 - \lambda\gamma + \lambda \text{Re}\Psi) + \text{Reg} \rho_{\Psi}. \quad (5.45)$$

The spectral functions for Ψ and $\bar{\Phi}$ have the form

$$\begin{aligned}
\rho_{\bar{\Phi}}(k, \omega) &= \frac{1}{N_s^2} \sum_{pq} \int d\nu_1 d\nu_2 \rho_{\mathbf{g}}(p, \nu_1) \rho_{\mathbf{g}}(q, \nu_2) \rho_{\mathbf{g}}(p+q-k, \nu_1+\nu_2-\omega) \times \\
&\quad \{f(\nu_1)f(\nu_2)\bar{f}(\nu_1+\nu_2-\omega) + \bar{f}(\nu_1)\bar{f}(\nu_2)f(\nu_1+\nu_2-\omega)\} \times \\
&\quad E(p, k) \left(E(k, p) + E(p+q-k, p) \right) \\
\rho_{\Psi}(k, \omega) &= \frac{1}{N_s^2} \sum_{pq} \int d\nu_1 d\nu_2 \rho_{\mathbf{g}}(p, \nu_1) \rho_{\mathbf{g}}(q, \nu_2) \rho_{\mathbf{g}}(p+q-k, \nu_1+\nu_2-\omega) \times \\
&\quad \{f(\nu_1)f(\nu_2)\bar{f}(\nu_1+\nu_2-\omega) + \bar{f}(\nu_1)\bar{f}(\nu_2)f(\nu_1+\nu_2-\omega)\} \times \\
&\quad E(p, k)
\end{aligned} \tag{5.46}$$

which again differ only through the presence of momentum dependent factors, $E(p_1, p_2)$.

With these equations we can establish an iterative process which leads to a fully self-consistent spectral function, $\rho_{\mathbf{g}}$. The Scheme B loop proceeds as follows.

1. initialize all quantities to those of the Fermi gas: $\boldsymbol{\mu} = \boldsymbol{\mu}_0$, $\gamma = n/2$, $\rho_{\Psi} = \rho_{\bar{\Phi}} = 0$.
2. Build $\rho_{\mathbf{g}}$ from latest instance of $\boldsymbol{\mu}$, $\bar{\Phi}$ and γ .
3. Calculate $\rho_{\bar{\Phi}}$ from latest instance of $\rho_{\mathbf{g}}$ and obtain the real part, via Hilbert transform.
4. Calculate new $\boldsymbol{\mu}$ using a numerical.
5. Repeat steps 2-4 until $\boldsymbol{\mu}$ and $\rho_{\bar{\Phi}}$ have converged to some specified tolerance.
6. Calculate ρ_{Ψ} from latest $\rho_{\mathbf{g}}$ and obtain real part through Hilbert transform according to Eq. (5.42).
7. Calculate γ from Eq. (5.43).

8. Return to Step 2 and repeat loop. Continue to the next step only when γ has converged to specified tolerance.
9. Calculate $\rho_{\mathcal{G}}$.

Scheme A follows a similar loop but is simpler because it lacks the outermost selfconsistency loop for γ . Rather, the code is initialized with a predetermined γ and runs normally skipping over steps 7 and 8 above. Thus the main difference between schemes A and B is that one calculation proceeds from a predetermined value of γ while the other determines γ selfconsistently as described above.

The big step in this loop is the double integration which gives $\rho_{\overline{\Phi}}$. If computed by a direct summation the computational time required will scale as $N_s^2 N_\omega^2$. Furthermore, this slow step is on the innermost loop so it is repeated many times. This leads to unacceptably slow convergence for any reasonable system size. Noting that the summation has the form of a convolution we can make use of FFT routines to calculate $\rho_{\overline{\Phi}}$ with linear scaling in $N_s N_\omega$. This allows us to reach significantly larger systems and lower temperatures than would be possible by a direct approach. The next bottleneck in this flowchart is the calculation of the Hilbert transforms. These can also be made fast through a judicious use of FFT routines.

5.4.1 GGG-type Convolutions

The equations for $\rho_{\overline{\Phi}}$ and ρ_{Ψ} have a form which is very similar to the particle-hole bubble diagrams familiar from a 2^{nd} order perturbation treatment of the Hubbard

model.

$$\Sigma(k)_{2nd} \sim \sum_{pq} G(p)G(q)G(p+q-k) \quad (5.47)$$

In this self energy we have a perfect convolution structure in the frequency and momentum coordinates. The ECFL “self energies” have the same frequency convolution structure which appears only through the frequency arguments of $\mathbf{g}$. However, the $\rho_{\bar{\Phi}}$ and ρ_{Ψ} convolutions suffer from the presence of a momentum-dependent decoration to the convolution. The decorations are such that $\rho_{\bar{\Phi}}$ and ρ_{Ψ} are not actually convolutions in the momentum coordinate as written. Nonetheless we can use FFT routines to solve these summations. The basic strategy is to break up the integral into elementary pieces that do have the form of a convolution. We then avoid the need to do one large integral with quadratic complexity by doing about many small integrals of linear complexity.

To accomplish this we define three p-h like correlation functions

$$\chi_0(Q) = \sum_q \mathbf{g}(q)\mathbf{g}(q+Q) \quad (5.48)$$

$$\chi_1(Q) = \sum_q \varepsilon_q \mathbf{g}(q)\mathbf{g}(q+Q) \quad (5.49)$$

$$\chi_2(Q) = \sum_q \varepsilon_{q+Q} \mathbf{g}(q)\mathbf{g}(q+Q) \quad (5.50)$$

$$(5.51)$$

each of which has a spectral function which can be calculated by FFT. Recall also the each of the summations represent a sum of a vector momentum and matsubara frequency. To be explicit we could write

$$\chi_1(\vec{Q}, i\Omega) = \frac{\beta}{N_s} \sum_{\vec{q}, \omega_n} \varepsilon_{\vec{q}} \mathbf{g}(\vec{q}, i\omega_n) \mathbf{g}(\vec{q} + \vec{Q}, i\omega_n + i\Omega). \quad (5.52)$$

There is a useful symmetry by which we can obtain χ_2 from χ_1 via the relationship

$$\rho_{\chi_1}(Q, \omega) = -\rho_{\chi_2}(Q, -\omega). \quad (5.53)$$

This can be verified algebraically but it is easily understood by noting that χ_1 and χ_2 are related by a time reversal operation (the dressing, ε_q , moves from the particle line to the hole line or vice versa). Time reversal effectively takes $\omega \rightarrow -\omega$ which corresponds to complex conjugation in the Matsubara representation which flips the sign of the imaginary part. Note that χ_0 is time reversal invariant so it satisfies

$$\rho_{\chi_0}(Q, \omega) = -\rho_{\chi_0}(Q, -\omega). \quad (5.54)$$

With these correlation functions many terms of the GGG form can be written as

$$A_{\mathbf{g}\mathbf{g}\mathbf{g}}(k) = F_1(k) \sum_p F_2(p) \mathbf{g}(p) \chi_n(p-k) F_3(p-k). \quad (5.55)$$

where F_1, F_2 , and F_3 are each functions of momentum only and their arguments are carefully matched with the arguments of $A_{\mathbf{g}\mathbf{g}\mathbf{g}}$, $\mathbf{g}$, and χ_n as they appear in the integral such that all factors fit the form of a convolution. In this way we can massage every term of $\rho_{\overline{\Phi}}$ into a convolution of one $\mathbf{g}$ and a χ_n rather than three $\mathbf{g}$'s as originally written. There is one term in this problem which cannot be treated in this way because the argument matching cannot be achieved in such a simple way. This term looks like

$$\overline{\Phi}_{JJ}(k) = \sum_{pq} J_{q-k} J_{p-k} \mathbf{g}(p) \mathbf{g}(q) \mathbf{g}(p+q-k)$$

This issue can be solved by using angle addition identities to decompose one of the J's.

In 2 spatial dimensions this looks like

$$\begin{aligned}
J_{q-k} &= 2J(\cos(q_x - k_x) + \cos(q_y - k_y)) \\
&= 2J(\cos(q_x)\cos(k_x) + \cos(q_y)\cos(k_y) + \sin(q_x)\sin(k_x) + \sin(q_y)\sin(k_y))
\end{aligned} \tag{5.56}$$

To proceed we must define

$$\chi_{cos}(Q) = \sum_q \cos(q_x) \mathbf{g}(q) \mathbf{g}(q + Q) \tag{5.57}$$

$$\chi_{sin}(Q) = \sum_q \sin(q_x) \mathbf{g}(q) \mathbf{g}(q + Q). \tag{5.58}$$

These new functions do not have the full lattice symmetry like each of the χ 's listed above but they are well formed convolutions of a type that can be computed quickly by FFT. We can write convolutions of a type that can be computed quickly by FFT. We can write

$$\begin{aligned}
\bar{\Phi}_{JJ}(k) &= 2J \left(\cos(k_x) \sum_{pq} \mathbf{g}(p) \chi_{cos}(p - k) J_{p-k} + \sin(k_x) \sum_{pq} \mathbf{g}(p) \chi_{sin}(p - k) J_{p-k} \right) \\
&\quad + (k \rightarrow \bar{k})
\end{aligned} \tag{5.59}$$

where $(k \rightarrow \bar{k})$ indicates a momentum reflection across the line $k_x = k_y$ which is needed to restore the lattice symmetry of this term.

The convolutions performed here by FFT come from finite discrete data. This presents no problems for the momentum coordinates which are periodic by definition and therefore amenable to the FFT. However, the frequency dependence is not periodic. The finite list of discrete frequency points is a truncation of an infinite continuum.

Consequently the frequency convolution cannot be naively performed by FFT. Doing so will add spurious terms to the convolution. This is most easily seen by imagining a convolution of some model spectral function made of delta functions $\rho_i(\omega) = \delta(\omega - a_i)$ such that

$$\begin{aligned}\rho_f(\nu) &= \int_{-\infty}^{\infty} g(\omega)\rho_1(\omega)\rho_2(\omega - \nu)d\omega \\ &= g(a_1)\delta(a_1 - \nu - a_2)\end{aligned}\tag{5.60}$$

where $g(\omega)$ is an arbitrary function with compact support. If however we treat these functions as periodic with a range $-\omega_c/2 \leq \omega \leq \omega_c/2$ we obtain

$$\begin{aligned}\rho_f(\nu) &= \int_{-\omega_c/2}^{\omega_c/2} g(\omega)\rho_1(\omega)\rho_2(mod(\omega - \nu))d\omega \\ &= g(a_1)\delta(mod(a_1 - \nu - a_2))\end{aligned}\tag{5.61}$$

where the mod function is defined such that $mod(\omega) = mod(\omega + \omega_c)$ on the range mentioned above. We see that the two methods differ when $mod(a_1 - \nu - a_2) \neq a_1 - \nu - a_2$. For example we may encounter some values a_1 and a_2 for which the difference $a_1 - a_2$ is close to ω_c . If this is the case, the periodic convolution will have a pole at low ν rather than at some high frequency as in the non-periodic convolution. All high frequency spectral weight will be folded back onto the low frequency range. This is akin to an umklapp process but in frequency rather than momentum. These umklapp contributions must be eliminated from the frequency sum so that the result as calculated by FFT will match the exact result. To this end, the frequency data is padded with a string of zeros of length N_ω . In the example above it corresponds to making the $g(\omega)$ finite for the desired terms and zero for the unwanted umklapp terms. The nature of the padding

depends upon the exact structure of the convolution. We have verified numerically that convolutions performed in this way match the direct summations to double precision.

5.4.2 FFT Hilbert Transform

The Hilbert transform defined in Eq. (5.42) is formally a convolution which can in principle be solved with the advantages of the FFT routines. Once again, however, we face the problem that this convolution is a non-periodic frequency integral. Furthermore, the Hilbert kernel $\frac{1}{\omega}$ falls off very slowly at large frequencies so the padding trick from the GGG-convolution will not work well in this case. Consider that imposing periodicity on the Hilbert kernel creates a discontinuity or distortion at some point where the curve must cross zero. This adversely effects the accuracy of the transform and it is found that the use of FFT's to calculate a Hilbert transform will always introduce some error. Fortunately, this error can be controlled and diminished by increasing the length of padding used. There is an explicit Fourier transform for the Hilbert kernel as $-i \operatorname{sgn}(t)$ where t is the time variable conjugate to ω . The function $\operatorname{sgn}(t)$ equals zero when $t = 0, t_c/2$ and the periodic sign function is defined over the range $-t_c/2 < t \leq t_c/2$.

5.5 Results

The program includes several parameters which can be varied. These include bandstructure (through hopping parameters t, t' etc.), the spin coupling J , density, and temperature. The code can furthermore be implemented on a variety on lattices of different size and spatial dimension. For a given choice of these parameters an appropriate

choice must be made for computational grid. This includes the lattice size as well as the discretized frequency grid. We have looked at converged spectral functions for a wide variety of these parameters. As noted in the previous section, the object γ can be handled in a variety of ways. To begin we use the explicit value to $O(\lambda^2)$ expansion. Note that we set $\lambda = 1$ after collecting all terms to the given order. Before proceeding further we first examine Scheme A and quantify the extent to which it is already selfconsistent. For this purpose we use γ_A from Eq. (5.40) and calculate an object Q which measures the validity of the λ expansion to a given order.

$$\begin{aligned}
Q &= \sum_k \mathcal{G}(k) - \frac{n}{2} \\
&= \sum_k \mathbf{g}(k)(1 - \gamma_A + \Psi(k)) - \frac{n}{2} \\
&= \sum_k \Psi(k)\mathbf{g}(k) - \frac{n^2}{4} + \frac{n^3}{8}
\end{aligned} \tag{5.62}$$

The particle sumrule is satisfied when $Q = 0$. Within scheme A we find that Q is a function of the particle density. In fact the curve, Fig. (5.1), (in this case on a 2D square lattice) shows that Q is not zero in general but the error is small (i.e. its ratio with the target density is $|Q|/(n/2) < 1/15$) up to a density of about $n = 3/5$ beyond which point $|Q|/(n/2)$ steadily rises to $\sim 1/4$.

In scheme B we use γ as an adjustable parameter to fix Eq. (5.37). Fig. (5.2) shows the fit of γ for typical parameter choices on 1D, 2D, and 3D lattices at low temperature. The curves overlap in each case and at high density show a marked deviation from the correct formulae Eq. (5.40) for the $O(\lambda^2)$ equations. The inset depicts the ratio of $(1 - \gamma)$ and the exact coefficient, $(1 - \frac{n}{2})$. The term $(1 - \gamma)$ is the

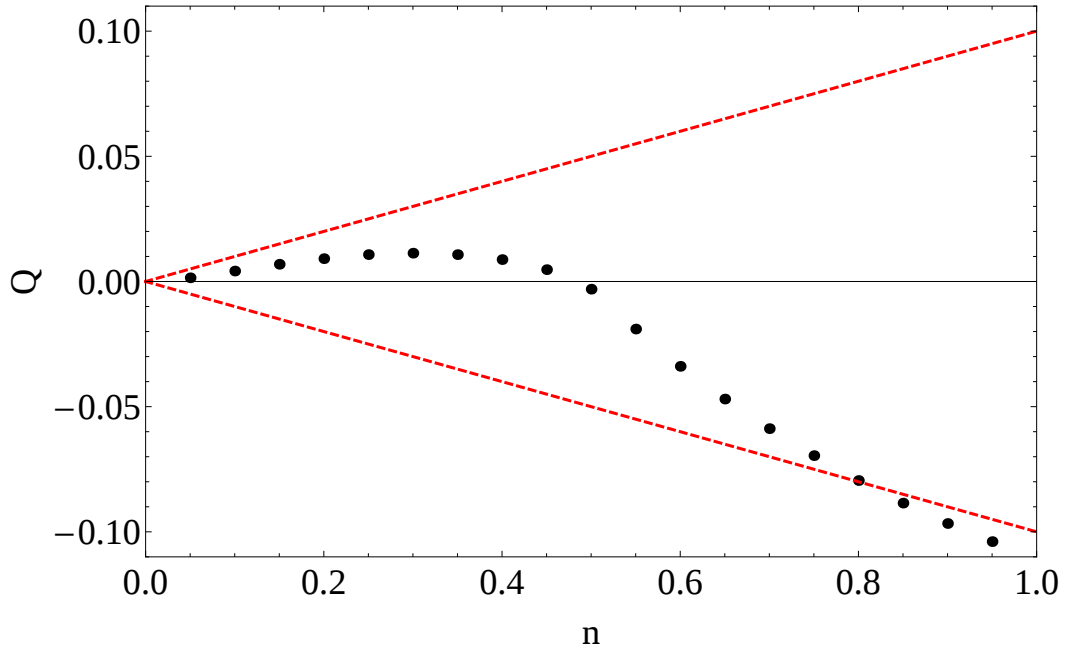


Figure 5.1: In scheme A, we find that the ECFL equations are already nearly selfconsistent over a wide range of densities. At low densities $|Q|/(n/2) < 1/15$ indicating that the error in the particle sumrule is on the order of 5%. Beyond $n \approx .6$ the ratio $|Q|/(n/2)$ grows steadily so that we can identify $n = .6$ as the upper limit for the validity of the $O(\lambda^2)$ ECFL equations.

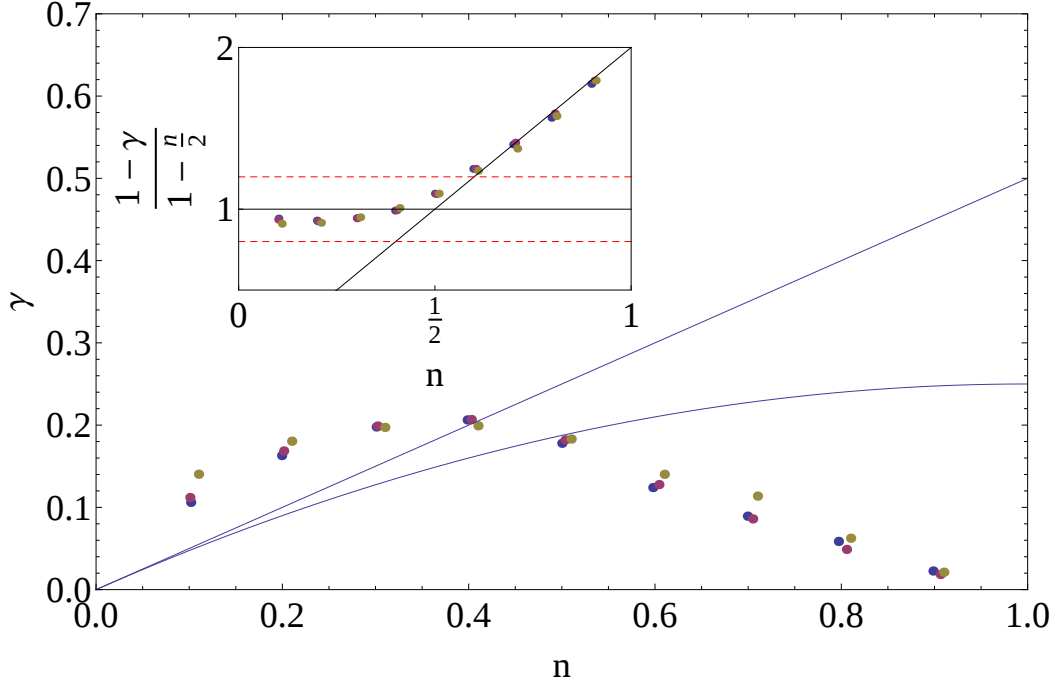


Figure 5.2: In scheme B, γ is used as a free parameter to fix the second level particle sumrule, Eq. (5.37). The figure shows γ for the case $J = 0, t' = -.4$ at low temperature on 1D, 2D, and 3D square lattices. In all three cases γ rises linearly from zero before falling back toward zero at $n = 1$. For comparison note that the exact γ is $n/2$ (straight line) while to $O(\lambda)$ $\gamma = n/2 - \lambda(n/2)^2$ (curve). The inset shows the ratio of lower Hubbard band spectral weight to the exact value. It is found that at low densities the spectral function has nearly the correct weight. At densities greater than $n=.65$ the violation becomes greater than 20% and thus places a limit on the range of validity of scheme B.

coefficient of the high frequency $1/\omega$ tail off of the Green's function and the integral of the total spectral weight and thus for $n > .6$ we have excess spectral weight. The red curves again delimit a region of low fractional error ($< 1/5$) in the total spectral weight. The curve exceeds this limit at $n = 3/5$ as we saw in the previous case. Of further interest is the observation that there is very little difference between these curves which were generated on three very different lattices.

5.5.1 ARPES: Dispersion and Lineshapes

ARPES provides the most direct and meaningful probe of the single particle Green's function. We will first present representative dispersion curves and lineshapes obtained through our calculation. Fig. (5.3) and Fig. (5.4) depict the curves $x_0\varepsilon_k$ and E_k along the high symmetry lines of the 2D square lattice for $n=.3$ and $n=.6$, respectively. At this density x_0 is substantially different from 1 so the bare bandwidth has been renormalized significantly. The original bandwidth was $8t$ but that is has already dropped to $\sim 3.2t$. The renormalization of E_k is given by the solutions of the equation,

$$E_k = x_0 \varepsilon_k - \mu - \lambda c_0(\cos(k_x) + \cos(k_y)) + \lambda \text{Re}\bar{\Phi}(k, E_k). \quad (5.63)$$

It locates the vanishing of the real part of the Green's function and therefore controls the Luttinger volume and any possible changes in the geometry of the Fermi surface. It is clear from the figure that E_k acquires a dynamically generated bandwidth which is narrower than $x_0 \varepsilon_k$. After the two stages of the renormalization, the QP band is about a tenth of its original width. Of particular interest is the shape of E_k near the X-point. The (π, π) QP's which were once at the top of the band have suffered a more significant renormalization than QP's in other regions of the Brillouin Zone thereby resulting in a change in the shape of the dispersion. Effects of this kind should be expected of any strongly k-dependent self energy but the details and location of the minimum near the X-point are specific to our use of $\bar{\Phi}$ from Eq. (5.32). In low order perturbative calculations (like Hubbard) the real part of the self energy tends to

have a very small k -dependence across the QP band and therefore the k -dependence of E_k directly follows the bare dispersion, merely being shifted by μ and k -independent Hartree type terms. In this ECFL calculation the k dependence of $\text{Re}\bar{\Phi}$ at low frequency is comparable to the width of $x_0 \varepsilon_k$ so that the shape change is particularly pronounced. This dispersion (or something like it) may potentially be detected through inverse photo emission experiments. At higher densities for scheme A, say $n=.8$, where our accuracy is admittedly worse than at lower n , we actually see the development of a second Fermi pocket near $k = (\pi, \pi)$ with an area which increases with density.

A further comment should be made regarding of usefulness of tight binding fits of ARPES data. Certainly there is a large literature of ARPES data for which tight binding fits result in hopping parameter which are reasonably accurate. However, the ECFL calculation provides a concrete example of how this methodology needs severe corrections especially in regard to the bandwidth.

Beyond looking at simple dispersions we can break down several curves which help us understand QP lifetimes effects around the BZ. In Figs. (5.5) and (5.6) we plot four distinct curves from $\mathcal{G}$ with and without a finite J respectively. First is E_k (just discussed) which tracks the vanishing of the real part of the spectral function. Second is the position of the QP peak which is defined simply as the frequency at which $\rho_{\mathcal{G}}$ reaches its peak. Finally we can look at the half-max points which give a sense (when viewed on the same plot) of the absolute linewidths and asymmetries involved. Near the Fermi surface all four curves draw very close together and the peak position coincides with the vanishing of the real part. This shows that we are looking at a legitimate

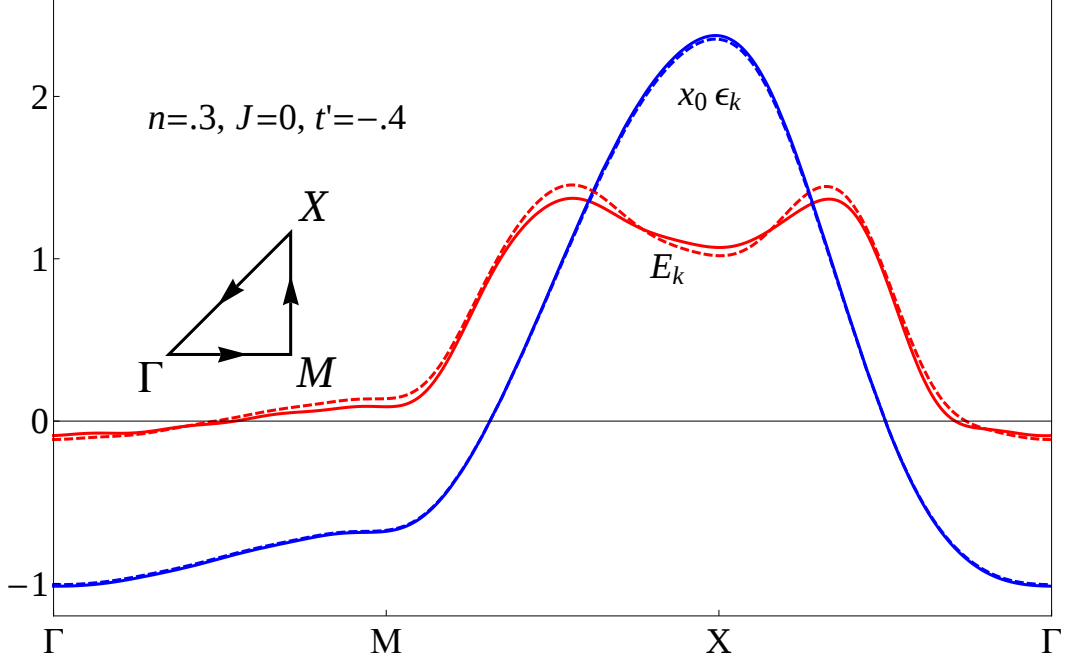


Figure 5.3: The dispersion $x_0 \varepsilon_k$ at $n = .3$ is very narrow compared to the bare bandwidth, $8t$. $x_0 = .43$ and $.44$ for the low ($T=104\text{K}$) and high ($T=288\text{K}$) temperature, respectively. The solid curves depict $T=104\text{K}$ and the dashed depict 288K . However, the QP peaks actually lie on a much smaller bandwidth due to the action of $\bar{\Phi}$ which dynamically renormalizes the dispersion $x_0 \varepsilon_k$. The location of the peaks, E_k , has its own temperature dependence which arises from the temperature dependence of $\text{Re}\bar{\Phi}$. While x_0 is a k -independent rescaling of the bandwidth, the reduction due to $\text{Re}\bar{\Phi}$ is not. This causes the bandwidth to shrink and change shape. A minimum appears near (π, π) . The bandwidth of E_k is approximately $1/5$ of the bare bandwidth, $8t$.

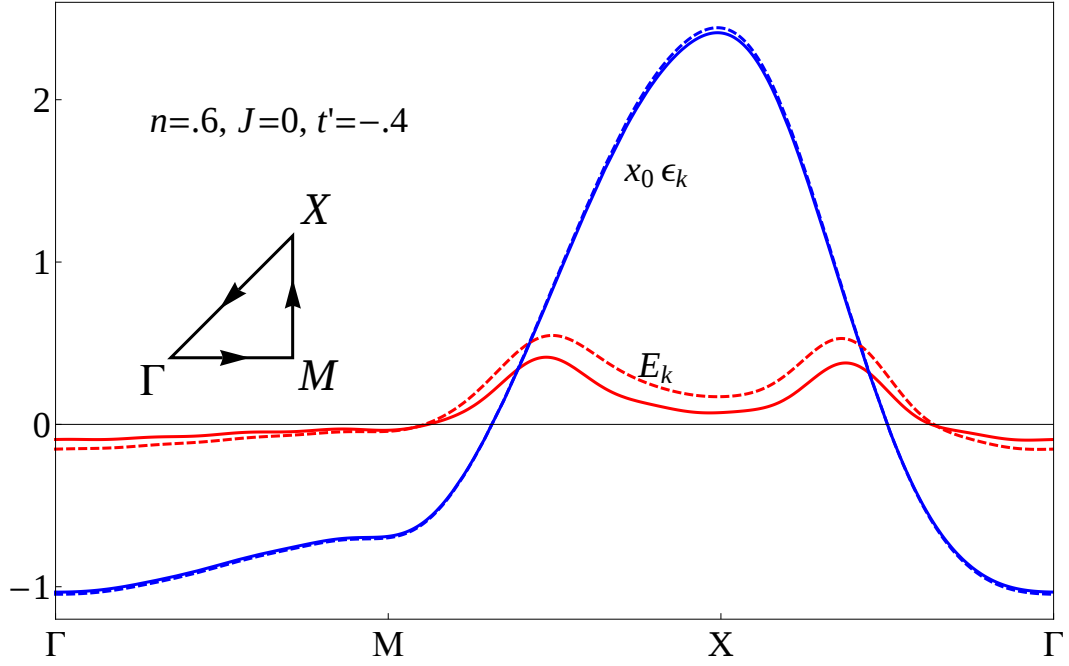


Figure 5.4: As in Eq. (5.3) we plot the dispersion $x_0 \epsilon_k$ and E_k in this case for a density of $n=.6$. While x_0 is similar to $n = .3$, E_k is significantly more narrow at this higher density due to differences in the $\text{Re}\bar{\Phi}$ between the two densities. Furthermore the nascent pocket near $k = (\pi, \pi)$ is more prominent with respect at this density as compared to the total bandwidth of E_k .

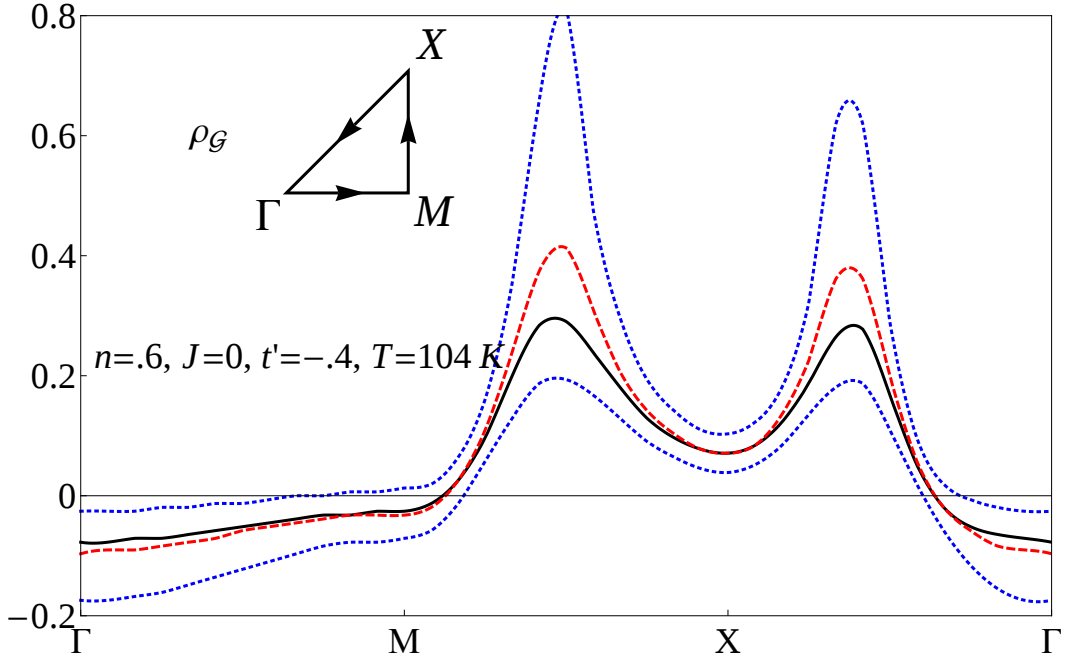


Figure 5.5: We plot the location of the peak of the physical spectral function, ρ_G (Black) and the location of the two half maxima (Blue Dotted), as well as the energy E_k from Eq. (5.63) (Red Dashed). The skew in the lineshapes translates to the nonsymmetric location of the black line relative to the blue dotted lines. This is more clear in Fig. (5.9) where we plot the computed lineshapes.

Fermi liquid with long lived low energy excitations. Away from k_f the QP's develop an asymmetry in the linewidths and the peak position moves to higher frequency than E_k . This is a simple consequence of the steady rise in $\rho_{\overline{k}}$ for increasing $|\omega|$ which causes the development of long high frequency tails as discussed in Gweon et al in Ref. ([4]).

Notice that the difference between figs. (5.5) and (5.6) is small. The inclusion of a finite J apparently has very little effect on the dispersion at these densities. Fig. (5.7) shows a comparison of a single lineshape from a $J=0$ calculation overlayed with it's equivalent from a calculation with $J=.3$. The finite J lineshape has a larger fraction of its weight shifted to higher frequencies in the broad incoherent part of the function.

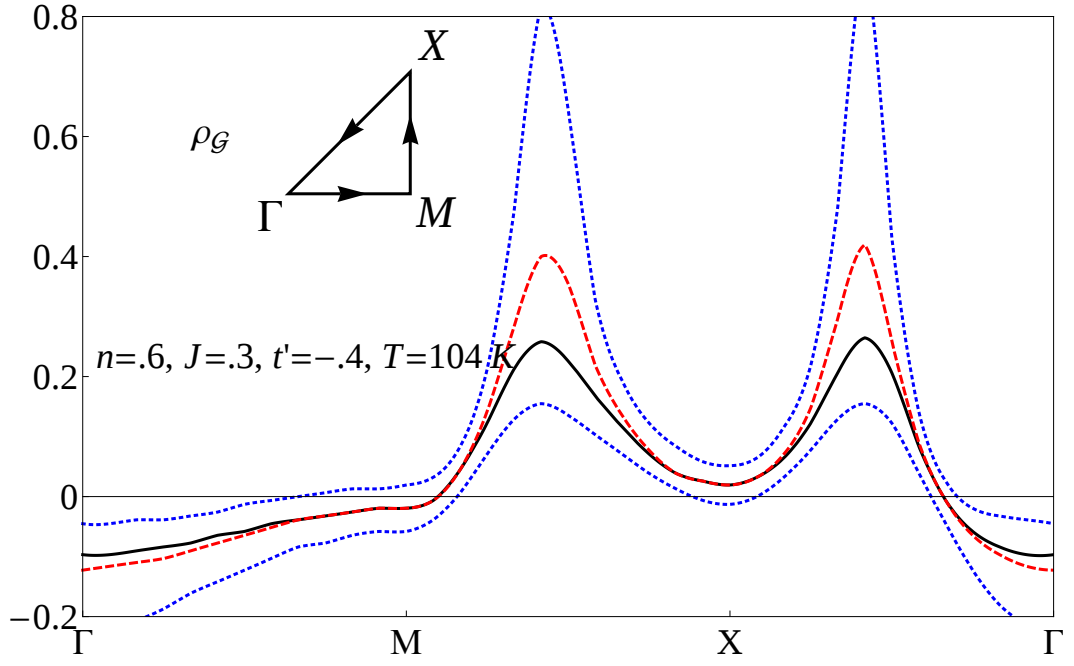


Figure 5.6: The linewidths of the QP peaks change very little in the presence of a finite J . The Fermi surface does not move and the linewidths are nearly the same as in the case where $J = 0$. This plot has all of the same parameters as Fig. (5.8) except for J .

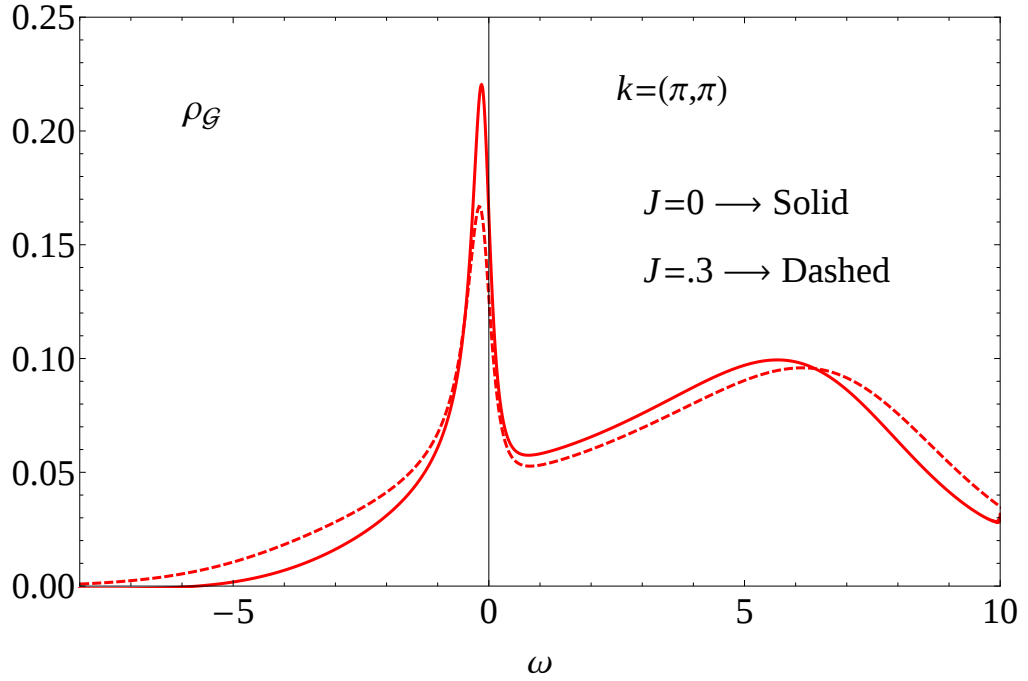


Figure 5.7: This plot compares the $J = 0$ and $J = .3$ cases for a single wavevector outside of the Fermi surface at $T=480K$ and $n=.6$ with a next neighbor hopping $t'=-.4t$. The QP is not shifted or significantly broadened. However, a fraction of the background spectral weight has been shifted to higher frequencies. This result is typical for wavevectors outside the Fermi surface. Close to the Fermi surface, the effect of J is less.

However, the peak has not moved and the lineshape has the same shape qualitatively speaking.

Interestingly the general features observed are present for both $\mathbf{g}$ and $\mathcal{G}$. The effect of $\mu(k)$ has little effect on these plots besides accentuating the skew in the half-max curves. This is not unexpected since we are describing the overdoped region, $n=.6$. Fig. (5.8) shows the linewidths of the auxiliary Fermi liquid which underlies the calculation of Fig. (5.5). Naturally, the E_k curves are the same in each figure but we see that the character and magnitude of the lineshapes is also roughly the same. In

fact, the caparison factor $\mu(k)$ does little to these spectral function besides multiplying by the static factor $1 - \gamma$. The reason for this is that Ψ as calculated from the $O(\lambda^2)$ theory is very small when calculated with full momentum dependence. In a recent paper Gweon et al (Ref. ([4])) used a k-independent approximation to the ECFL equations and was able to obtain ARPES fits of unprecedented quality. A key parameter in these fits was the object Δ_0 which was related to a characteristic inelastic energy scale and was responsible for the development of the extremely skewed lineshapes observed in that paper. In that case δ_0 is fixed by a sumrule in a slightly different way than in our k-dependent calculation. We more usefully define $\Delta = \frac{-\rho_{\bar{\Phi}}}{\rho_{\Psi}}$. To better demonstrate the role of Δ in creating such an asymmetry the equation for the spectral function can be rewritten as

$$\rho_{\mathcal{G}} = \frac{\rho_{\bar{\Phi}}}{|\zeta - \bar{\Phi}|^2} \left(1 - \gamma - \frac{x}{\Delta} + \eta(k, \omega) \right) \quad (5.64)$$

where $\zeta = \omega + \boldsymbol{\mu} - x_0 \varepsilon_k + \lambda c_0(\cos(k_x) + \cos(k_y))$, and $\eta = \text{Re}\Psi + \frac{\text{Re}\bar{\Phi}}{\Delta}$ which canceled to zero exactly in the k-independent model of Gweon et al. In our calculations, $\eta(k)$ is finite but cancels to a subdominant scale at low frequency. The primary difference in this calculation is that our Δ has a much smaller impact in this calculation than the δ_0 used in Ref. ([4]), at least for the low densities considered.

While the action of the caparison factor is considerably less than seen in previous works there is yet an observable skew in the lineshapes. This arises primarily from the action of $\bar{\Phi}$. Fig. (5.9) shows the lineshapes of $\mathbf{g}$ and $\mathcal{G}$ at $k = k_f$ and $k = (\pi, \pi)$ respectively. At the Fermi momentum the skew of the lineshape due to the caparison factor is slight but it does move spectral weight toward negative frequencies. At

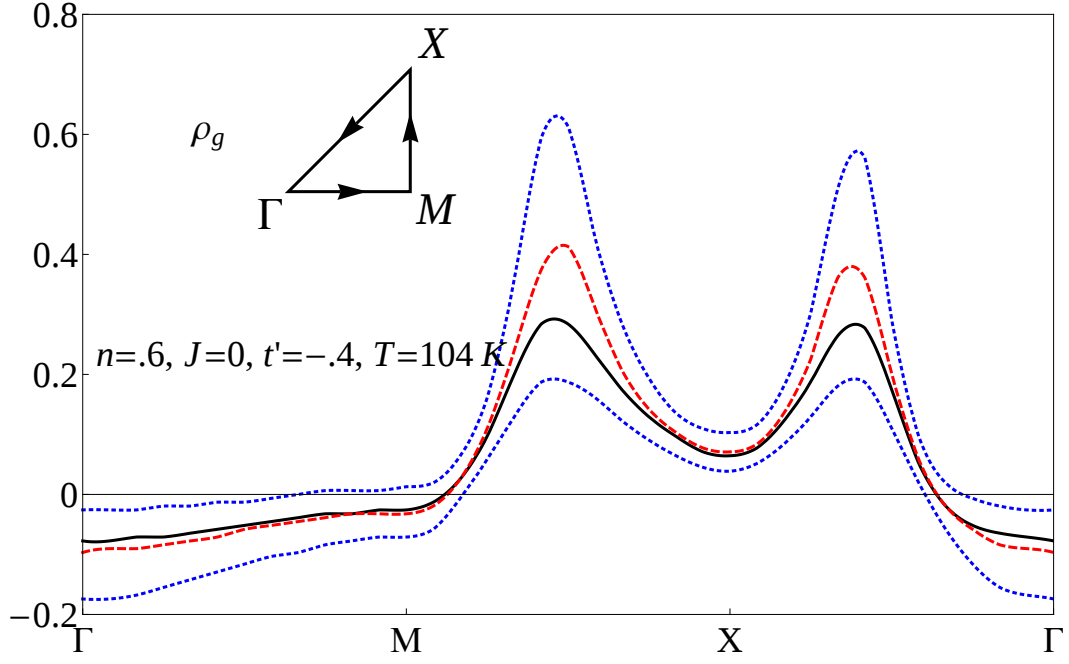


Figure 5.8: We plot the location of the peak of the auxiliary spectral function, ρ_g (Black) and the location of the two half maxima (Blue Dotted), as well as the energy E_k from Eq. (5.63) (Red Dashed). The skew in the lineshapes translates to the nonsymmetric location of the black line relative to the blue dotted lines. This is more clear in Fig. (5.9) where we plot the computed lineshapes.

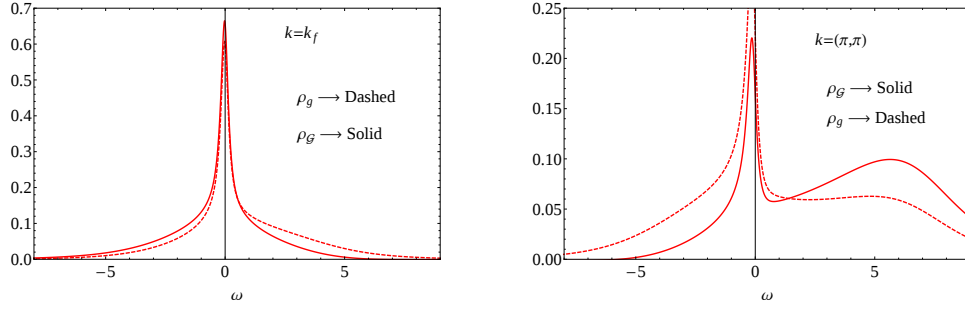


Figure 5.9: The lineshapes of the auxiliary and physical spectral functions are shown together for $k = k_f$ and $k = (\pi, \pi)$. For the smaller magnitude of k the comparison factor shifts the background spectral weight toward negative frequency. Near $k = (\pi, \pi)$ the background spectral is transferred toward positive frequencies.

$k = (\pi, \pi)$ the comparison factor pushes spectral weight in the opposite direction.

5.5.2 Electron pocket and a possible source of quantum oscillations

The dispersion curves shown in the preceding section were calculated in scheme B with a self consistently determined value of γ . The dispersion that comes about from selfconsistency loop is very sensitive to that value of γ . We have already commented that the dispersion develops an interesting minimum near the X-point. It turns out that in our scheme A, that minimum actually drops below the chemical potential, thereby creating an electron pocket centered around (π, π) . For scheme A this pocket forms at a density of $n=.45$. However, we can produce phenomenological variants of scheme A which move that crossing around in density. For instance, we might suggest a scheme A' wherein the value of γ has a larger coefficient on the $O(n^2)$ term. This would put Scheme A' somewhere between schemes A and B making it slightly better than scheme A in terms of satisfying Eq. (5.37) and slightly better than scheme B in that it has a

more appropriate high frequency limit. We find that if we increase the $O(n^2)$ term by a factor of 1.8 we can shift the critical density where the electron pocket forms to $n = .85$.

$$\gamma_A = n/2 - \lambda (n/2)^2 \quad \text{crossing at } n \approx .5 \quad (5.65)$$

$$\gamma_{A'} = n/2 - 1.8\lambda (n/2)^2 \quad \text{crossing at } n = .85 \quad (5.66)$$

$$\gamma_B = \frac{\sum_k \Psi[k] \mathbf{g}[k]}{n/2} \quad \text{no pocket} \quad (5.67)$$

We note of course, that $n = .85$ is beyond the most reliable density range of our calculation. Nonetheless this electron pocket is a striking feature which we suggest may be related to quantum oscillations observed in the Cuprates in recent years (Ref. ([1]) Ref. ([2])). The details of the pocket we observe are likely to be specific to our low order calculation but the feature of the dispersion, E_k , dropping near $k = (\pi, \pi)$ and eventually forming a pocket is robust, appearing on the 1D, 2D, and 3D square lattices. For each dimension $D = 1, 2, 3$ scheme A develops a pocket near Quarter filling, $n = .5$ (highly overdoped regime). This crossing can be tuned to any density by adjusting the value of γ in the same direction that is needed to patch up the particle sumrule. It is interesting to explore the possible dispersions which can arise from taking liberties with the value of γ . In Fig. (5.12) we present the area of the pocket as a function of the density. In scheme A the pocket is a full order of magnitude greater than the pocket measured by QO. However, this pocket becomes smaller in scheme A'. Fig. (5.13) depicts the evolution of the Fermi surface as a function of the density.

The formation of a pocket is seen here through the renormalization of the

dispersion. A related effect can be seen through the QP occupation

$$m_k = \sum_{\omega_n} \mathcal{G}(k, i\omega_n) \exp^{i\omega_n 0^+}. \quad (5.68)$$

Fig. (5.14) and Fig. (5.15) plot the occupation along the high symmetry lines. An increase in m_k in the vicinity of $k = (\pi, \pi)$ has been observed previously through numerical techniques such as Variational Monte Carlo (Ref. ([3])) but no comment has been made regarding the root cause of this phenomenon. This ECFL calculation therefore suggests an explanation of both the measured QO data and the numerically observed n_k curves through a single cause, the reshaping of E_k by a k-dependent self energy.

5.5.3 Optics

The optical conductivity, $\sigma(\Omega)$, is computed within the bubble (throwing out vertex corrections).

$$\text{Re}\sigma(\Omega) = \frac{1}{1-\gamma} \frac{1}{\Omega} \sum_k v_k^2 \int \rho_{\mathcal{G}}(k, \omega) \rho_{\mathcal{G}}(k, \Omega + \omega) (f(\omega) - f(\Omega + \omega)) d\omega \quad (5.69)$$

The imaginary part of the conductivity can be obtained by a Hilbert transform of the real part. Van der marel et al have discussed the universality of certain exponent seen in $\sigma(\Omega)$ near critical points. In this purely t-J calculation we must be careful how we combine the real and imaginary parts because the imaginary part will include contributions from the Upper Hubbard band and from charge transfer processes which can be appreciable at low to intermediate frequencies. For our current purposes we will simply discuss QP lifetime effects of three kinds. First we have $1/\tau_\sigma$ which describes a

characteristic lifetime which can be extracted from the low frequency curve of $\sigma(\Omega)$. To do so we assume a roughly Lorentzian form and define $1/\tau_\sigma$ by

$$\tau_\sigma \int_0^{1/\tau_\sigma} \sigma(\omega)/\sigma(0) d\omega = \pi/4. \quad (5.70)$$

Alternatively we can look at the momentum resolved scattering lifetimes along the nodal and antinodal directions. We call these τ and they are displayed in Fig. (5.17).

Contrary to the standard quadratic picture of a degenerate Fermi Liquid the k-resolved $1/\tau$ curves rise roughly linearly. This indicates that a very low energy scale has emerged, in comparison to which, our lowest temperatures are high. This appears to be the case for the ECFL along both primary directions. As this is not well explained it would be nice to see exactly how the transition from quadratic to linear comes about, ideally, in both the Hubbard and ECFL cases. For this reason we present the an analogous curve at lower density where correlations are proportionally weaker. Consequently, the dispersion still has much of its bare width and shape. Since there is a sharp Fermi surface at this density and relatively weak background spectral weight we should expect to see something much closer to quadratic behavior.

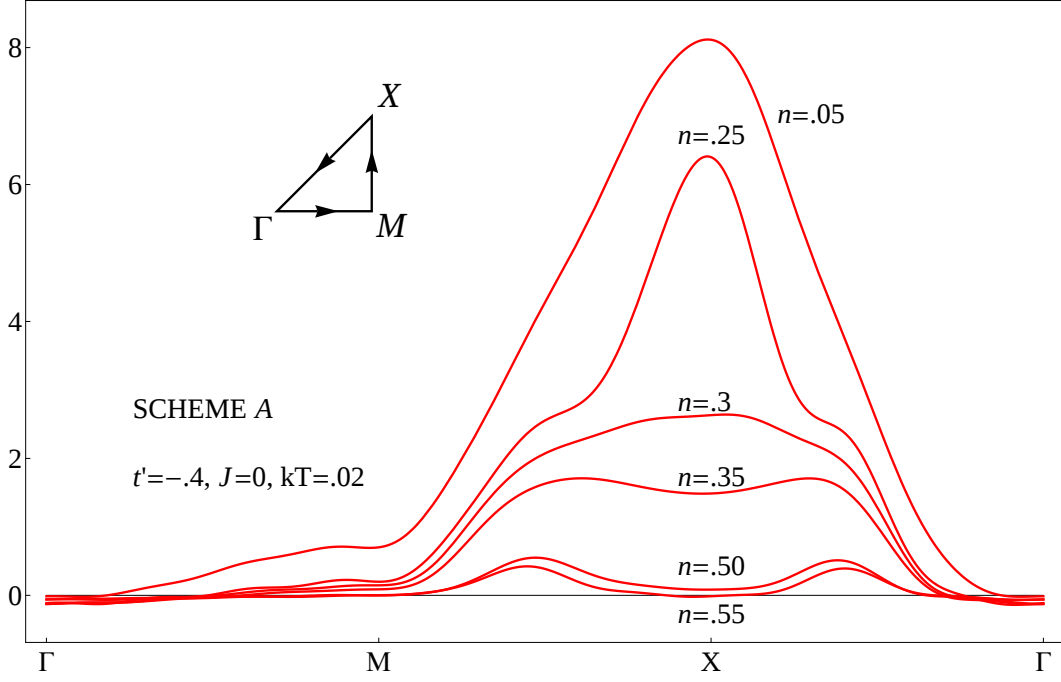


Figure 5.10: The renormalized dispersion E_k which denotes the vanishing of the real part of the $\mathcal{G}$ is shown to evolve as a function of density. With increased density the bandwidth becomes quite narrow and an electron pocket forms near the (π, π) point at a density near $n=1/2$. This crossing is accompanied by a rise in the occupation n_k near (π, π) . Similar pockets form in 1D at $k = \pi$ and in 3D at $k = (\pi, \pi, \pi)$. Variants of scheme A have been explored for which this crossing is moved toward higher density by decreasing γ . At a low enough value of γ the pocket will cross back over the chemical potential and be unoccupied.

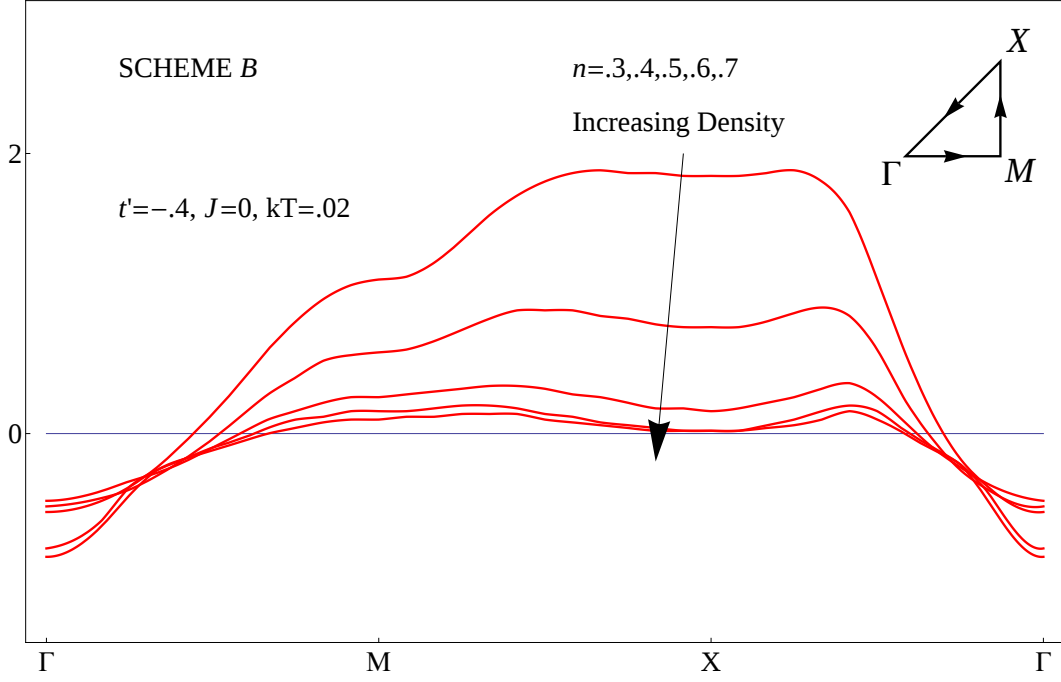


Figure 5.11: In scheme B γ is used as a selfconsistency parameter to fix the sumrule Eq. (5.37). Consequently, the dispersion renormalization factor (x_0) and the static part of $\mu(k)$ are both different than in scheme A. Here we plot the dispersion E_k for scheme B. As in scheme A, the dispersion near the X-point bends downward. However, in this case it does not cross the chemical potential even at the highest densities. Nonetheless at finite temperature, there will be a heightened occupation n_k near $k = (\pi, \pi)$ which would be absent if not for this reshaping of the dispersion.

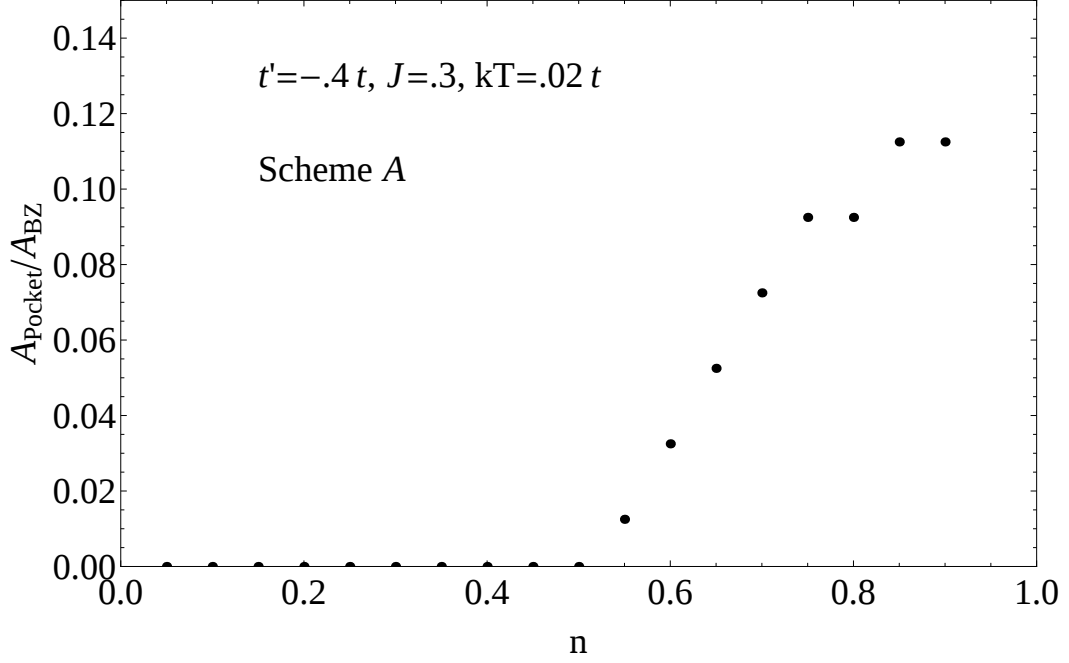


Figure 5.12: In scheme A the point $k = (\pi, \pi)$ drops downward from the top of the band. Near the point $n=.5$ it crosses the chemical potential forming a electron pocket which then grows as a function of density. The figure depicts the fractional of the BZ which is filled by the pocket. A quantum oscillation frequency can be computed for this area through the equation $f = \frac{h}{ea^2} \frac{A}{(2\pi)^2}$ where h is Planck's constant, e is the electron charge and a is the lattice parameter for the Cuprates. This predicts a frequency in the range of $2 * 10^4$ Tesla at the highest densities. The oscillations seen in Cuprates are much smaller and suggest a pocket which occupies only about 2.5% of the Brillouin zone at densities around $n=.9$. The pocket seen in scheme A is an order of magnitude larger. The scheme we call A' adjusts the gamma expansion by some $O(1)$ change and places the critical density of pocket formation at $n=.85$. This results in a much smaller pocket which more accurately predicts the QO frequency near 660T.

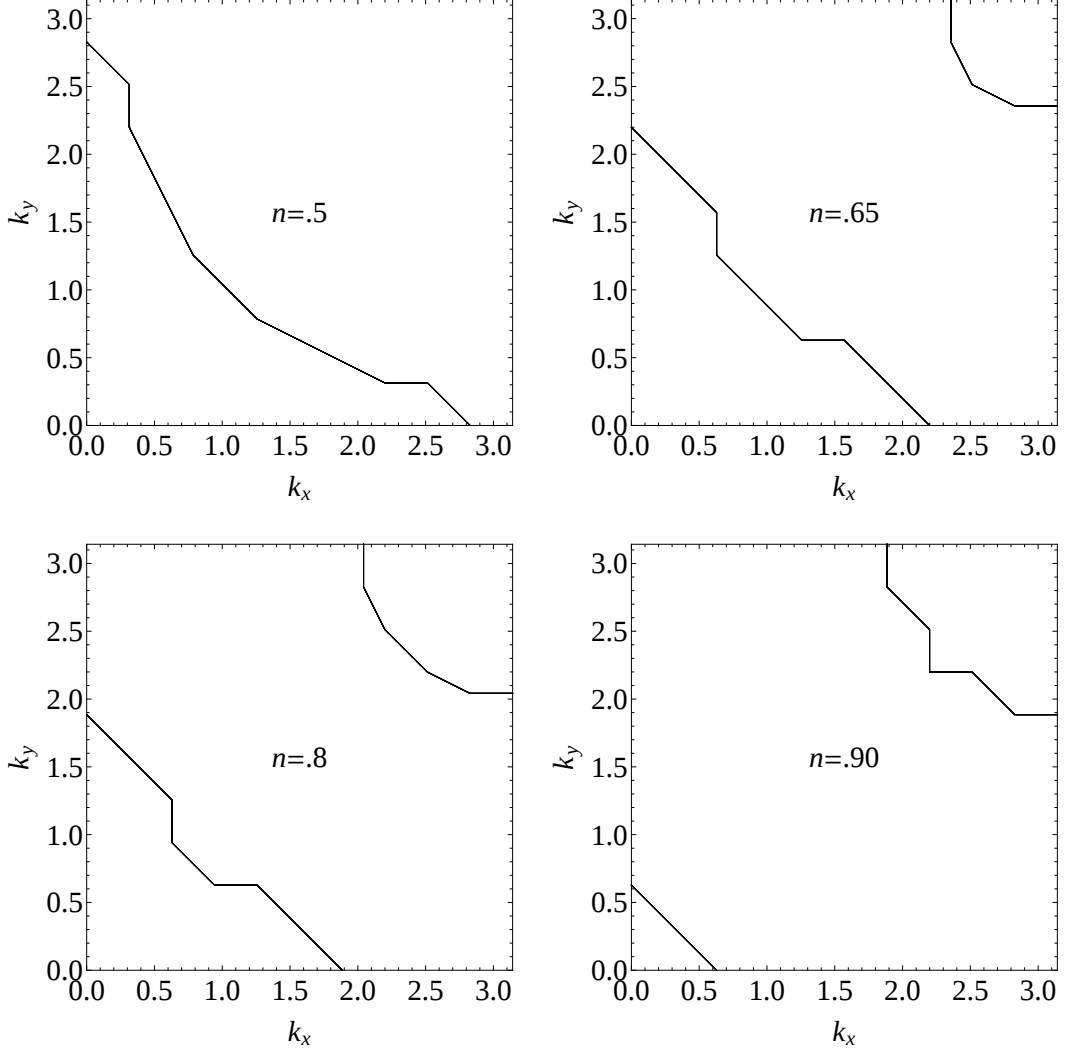


Figure 5.13: In scheme A the dispersion becomes deformed by $\bar{\Phi}$ and a pocket forms near (π, π) . The panel shows the Fermi surface for a series of densities at low temperature (60K) and with a next neighbor hopping $t' = -.4t$ and $J = 0$. The pocket forms at $n=.55$ and grows monotonically with increased density. Note that at $n=.9$ the Fermi volume is quite low. This occurs because at this density the bandwidth has decreased to the extent that this is effectively high temperature. Thus the volume theorem is not strictly satisfied. By altering the density dependence of γ this pocket can be enhanced or diminished. For instance, it is completely absent in scheme B. As noted elsewhere, the highest densities (i.e. $n = .9$) are not as accurate as densities $n < .6$. They are included in this panel to tell a complete story of the evolution of the pocket within scheme A.

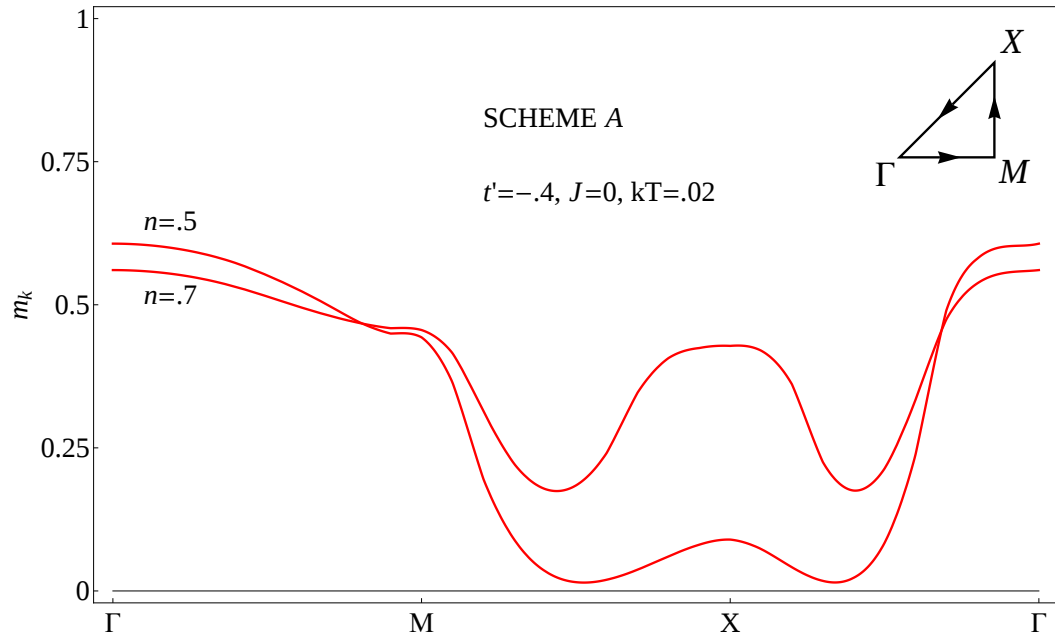


Figure 5.14: In scheme A the point $k = (\pi, \pi)$ drops downward from the top of the band. As a result, the QP occupation has a maximum in this region of the BZ. A feature much like this was found in Ref. ([3]).

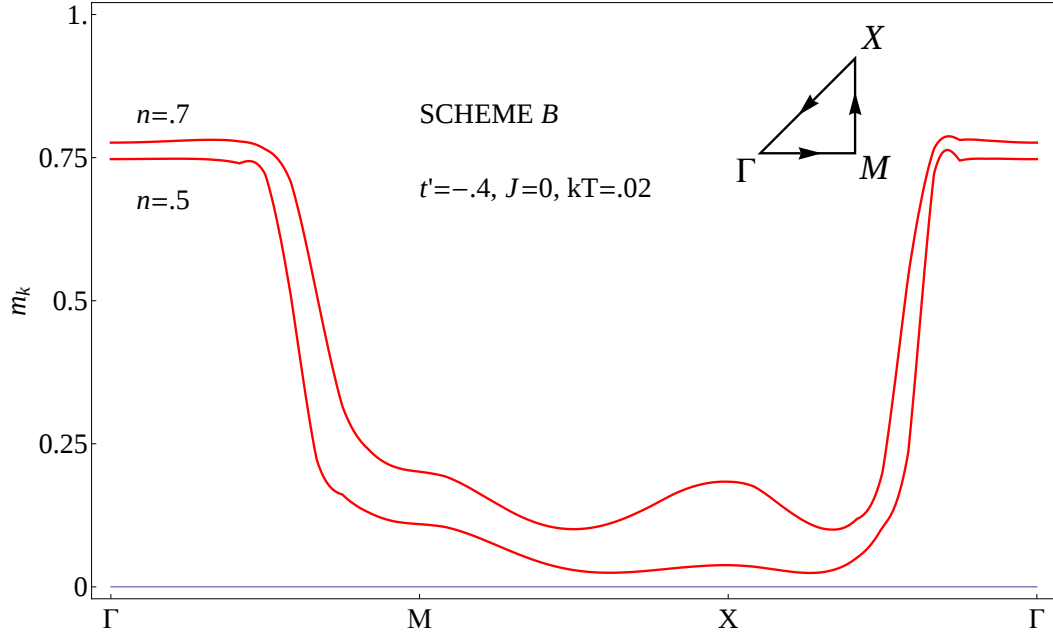


Figure 5.15: In scheme B the dispersion E_k near does dip below the chemical potential to form a Fermi pocket. Nonetheless it has a minimum near (π, π) . Consequently, the QP occupation has a peak in that region because increased portion of the tail of the spectral function will sit at negative frequencies.

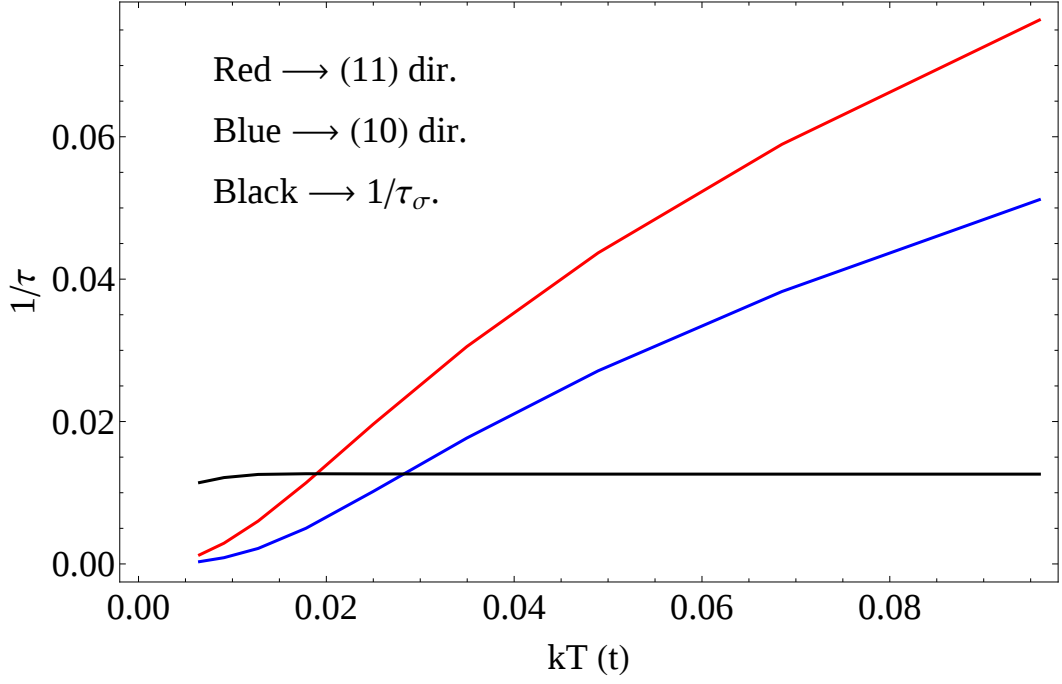


Figure 5.16: The inverse lifetimes for k_f QP's in plotted as a function of temperature for the ECFL along with the momentum averaged inverse lifetime obtained from the optical conductivity. The ECFL has higher k_f scattering rates along the (11) direction than the (10). The temperature dependence is essentially linear until very low temperatures where a quadratic dependence typical of a Fermi liquid takes over. The crossover temperature is at approximately $.02t$ which corresponds to 60K if we take $t=3000K$. In this plot the density is $n = .3$ At higher densities the crossover temperature decreases below our temperature range.

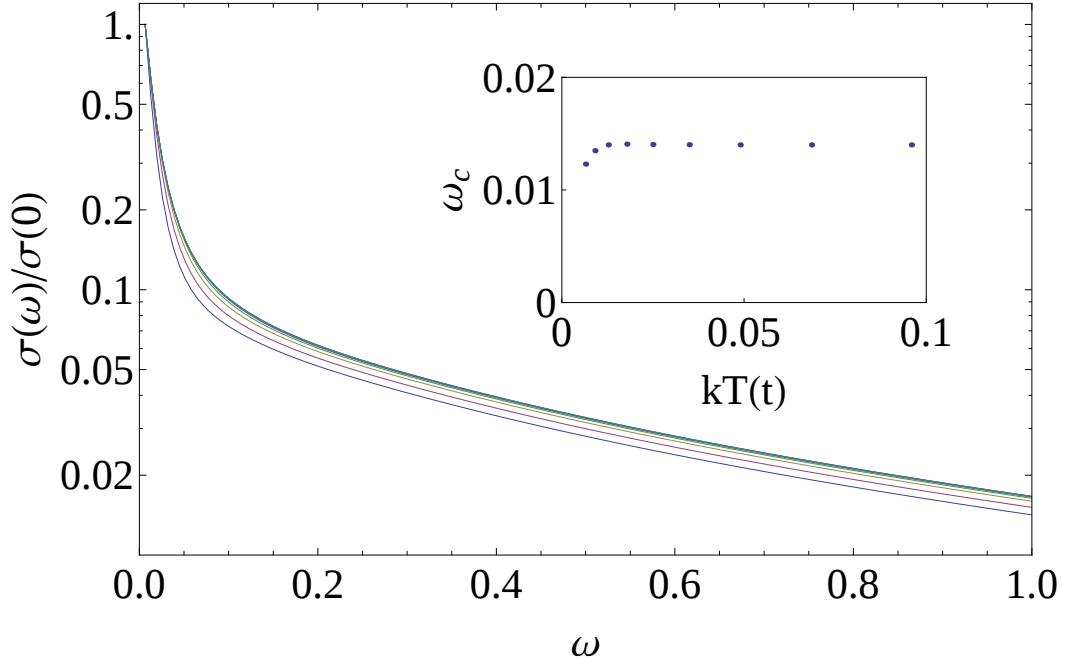


Figure 5.17: The low frequency dependence of the optical conductivity is Lorentzian-like. From the normalized curve we can extract an effective scattering rate from the width of the Lorentzian. In this case there is negligible temperature dependence over nearly the entire temperature range studied. The slight curvature at low kT is caused by the finite η which is intrinsic to the calculation.

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