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The Compressibility in Strongly Correlated Superconductors and Superfluids: From BCS to BEC

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We present a theoretical study of the compressibility, κ , in a Fermi gas with attractive contact interactions, providing predictions for the strongly-attractive regime and the superfluid phase. Our work emphasizes the compressibility sum rule and gauge invariance as constraints on κ and we show how within a particular t -matrix approach, these can be satisfied in the normal phase when no approximations are made. For tractability, approximations must be introduced, and it is believed that thermodynamical approaches to κ are more reliable, than correlation function based schemes. Contrasting with other studies in the literature, we present thermodynamic calculations of κ ; these yield semi-quantitative agreement with experiment and provide physical insight into similar results obtained via quantum Monte Carlo simulations.

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There is extensive recent literature on response functions in strongly correlated superconductors and the counterpart atomic Fermi gas superfluids. Here the correlations are presumed sufficiently strong so that the classic BCS theory, which has been remarkably successful for many decades, is no longer adequate. Among the experiments of interest are thermodynamic response functions [1, 2] as well as dynamical response studies [3] in the Fermi gases which undergo BCS-Bose-Einstein condensation (BEC) crossover. Possibly related are novel probes of the density correlations in the copper oxide superconductors [4].

A particularly important quantity derivable from the response function is the compressibility, κ , because it provides direct signatures of the transition temperature, T_c , which are otherwise difficult to identify in neutral superfluids. Here we discuss the behavior of κ , making contact with recent Fermi gas experiments [1]. Other groups [5, 6] have computed κ , for T strictly above T_c . To calibrate past and future work, we discuss the pitfalls [7] associated with calculating κ in general many-body theories. A consistent theory of the response functions must obey the appropriate “Ward identity”, which imposes gauge invariance on the quantum correlation functions. In this way different theoretical approaches can be assessed according to whether they satisfy the so-called longitudinal and transverse f-sum rules. Moreover, implementation of this gauge invariance is particularly complicated for $T < T_c$ where collective mode effects enter into the density response [8].

Added to this complication is the fact that there are two distinct ways of arriving at a static response such as the compressibility: either through the zero frequency, zero momentum limit of the correlation function or via

direct application of thermodynamics. Consistency is equivalent to imposing a sum rule known as the compressibility sum rule. This latter constraint is known to be problematic in almost every approximate many body theory from quantum hall liquids [9] to the random-phase approximation (RPA) of electron gases [10].

Here we discuss a “ Q -limit Ward identity” [11], which is equivalent to the compressibility sum rule and show how it is necessarily obeyed in our microscopic theory of fermionic superfluids in BCS-BEC crossover. However, for concrete calculations some approximations are required. With these approximations we are able to demonstrate consistency with gauge invariance through analytically satisfying the longitudinal and transverse f-sum rules, but are unable to satisfy the compressibility sum rule. Once approximations are made, as they have been in all BCS-BEC crossover calculations in the literature [5, 6], this consistency requirement is forfeited.

The compressibility $\kappa \equiv n^{-2}(\partial n / \partial \mu)$ must be consistent with the compressibility sum rule [12]

$$\frac{\partial n}{\partial \mu} = -K^{00}(\omega = 0, \mathbf{q} \rightarrow \mathbf{0}), \quad (1)$$

where K^{00} is the density-density component of response function tensor $K^{\mu\nu}(Q)$. defined by $J^\mu(Q) = K^{\mu\nu}(Q)A_\nu(Q)$, where the four-vector potential $A^\mu = (\phi, \mathbf{A})$ incorporates the scalar and vector potential. While our theory is applied to neutral superfluids, we contemplate a weak fictitious electromagnetic (EM) field.

When the compressibility constraint (or the equivalent sum rule) cannot be satisfied, as in the RPA of electron gases, it has been suggested [10] that the more meaningful answer is obtained via a thermodynamic route, where gauge invariance, etc. plays a lesser role. Here we

present our results for κ on either side of unitarity obtained directly from thermodynamics, where we can address the physics both above and below T_c . We find that the compressibility increases as T approaches T_c from above, more dramatically than in a Fermi liquid and that it never diverges, but rather undergoes an upturned step discontinuity at the transition. This upturn reflects the increasing bosonic character, as pairs are formed. Below T_c , the behavior is not so different from that in the BCS regime where it reflects the growth of a fermionic gap which tends to depress κ . These results appear in semi-quantitative agreement with experiment [1] in both the normal and superfluid phases.

The gauge invariant EM response kernel can be expressed as

$$K^{\mu\nu}(Q) = 2 \sum_P \Gamma^\mu(P+Q, P) G(P+Q) \times \gamma^\nu(P, P+Q) G(P) + \frac{n}{m} h^{\mu\nu}, \quad (2)$$

where $h^{\mu\nu} \equiv -g^{\mu\nu}(1 - g^{\nu 0})$ and the diagonal metric tensor $g^{\mu\nu}$ is $(1, -1, -1, -1)$. Throughout we define $Q \equiv q^\mu = (i\Omega_l, \mathbf{q})$ with Ω_l being the boson Matsubara frequency. Similarly, $P \equiv p^\mu = (i\omega_n, \mathbf{p})$ is the 4-momentum of the fermion with ω_n being the fermion Matsubara frequency. The goal of linear response theory is to find the full EM vertex Γ^μ associated with the EM response kernel $K^{\mu\nu}(Q)$. This full EM vertex must obey the Ward identity $q_\mu \Gamma^\mu(P+Q, P) = G^{-1}(P+Q) - G^{-1}(P)$, which implies that $q_\mu K^{\mu\nu}(Q) = 0$ [8]. Here we have introduced the bare EM vertex $\gamma^\mu(P+Q, P) = (1, \frac{\mathbf{p}+\mathbf{q}}{m})$. The noninteracting Green's function is given by $G_0(P) = (i\omega_n - \xi_{\mathbf{p}})^{-1}$ with $\xi_{\mathbf{p}} = \frac{p^2}{2m} - \mu$. $G(P)$ is the single-particle Green's function determined by $G^{-1}(P) = G_0^{-1}(P) - \Sigma(P)$, where $\Sigma(P)$ is the fermion self-energy. Different theories of BCS-BEC crossover will assume different forms for $\Sigma(P)$.

Gauge invariance guarantees that the longitudinal and transverse sum rules are satisfied. A necessary and sufficient condition for the validity of the compressibility sum rule (1) is the Q -limit Ward identity, which can be proven as follows. We have

$$\frac{\partial n}{\partial \mu} = 2 \sum_P \frac{\partial G(P)}{\partial \mu} = -2 \sum_P G^2(P) \left(1 - \frac{\partial \Sigma(P)}{\partial \mu}\right). \quad (3)$$

We show below that this leads to

$$\Gamma^0(P, P)|_{\Omega=0, \mathbf{q} \rightarrow \mathbf{0}} = 1 - \frac{\partial \Sigma(P)}{\partial \mu}, \quad (4)$$

which we refer to as the Q -limit Ward identity. Here Ω is the analytic continuation of $i\Omega_l$. Indeed, comparing with the expression for $K^{00}(\omega = 0, \mathbf{q} \rightarrow \mathbf{0})$ given by Eq.(2), we find $\frac{\partial n}{\partial \mu} = -2 \sum_P \Gamma^0(P, P) G(P) \gamma^0(P, P) G(P)$. When Eq. (4) is satisfied, the compressibility obtained via thermodynamic arguments is related to a two-particle correlation function (K^{00} in this case). The Q -limit Ward

identity serves as an independent constraint on linear response theories [8, 13], separate from the Ward identity reflecting gauge invariance. Because both make a connection between the self energy and the vertex functions, they pose severe challenges to a proper formulation of linear response theory.

We next demonstrate how these consistency conditions are satisfied in BCS-BEC crossover in the pseudogap (pg) phase above T_c . As in all analytic such schemes, we begin with a t -matrix approach [14], where the propagator for the non-condensed pairs is generically given by

$$t_{\text{pg}}^{-1}(Q) = g^{-1} + \chi(Q), \quad (5)$$

Here g is the attractive coupling constant in the Hamiltonian and χ is the pair susceptibility. To capture the physics of Gor'kov theory [14] we take $\chi(Q) = \sum_K G_0(Q-K)G(K)$, with

$$\Sigma(K) \equiv \Sigma_{\text{pg}}(K) = \sum_Q t_{\text{pg}}(Q) G_0(Q-K). \quad (6)$$

The diagrams which are consistent with particle number conservation [14] consist of three types in addition to the bare vertex. They are the so-called Maki Thompson (MT) contribution and two versions of the Aslamazov-Larkin (AL) diagram. These have been presented in the literature [15] and given by

$$\text{MT}_{\text{pg}}^\mu(P+Q, P) = \sum_K t_{\text{pg}}(K) G_0(K-P-Q) \times G_0(K-P) \gamma^\mu(K-P, K-P-Q); \quad (7)$$

$$\text{AL}_1^\mu(P+Q, P) = - \sum_{K,L} t_{\text{pg}}(K) t_{\text{pg}}(K+Q) G_0(K-P) \times G(L) G_0(K-L+Q) G_0(K-L) \times \gamma^\mu(K-L+Q, K-L); \quad (8)$$

$$\text{AL}_2^\mu(P+Q, P) = - \sum_{K,L} t_{\text{pg}}(K) t_{\text{pg}}(K+Q) G_0(K-P) \times G_0(K-L) G(L) G_0(L+Q) \Gamma^\mu(L+Q, L). \quad (9)$$

These diagrams are obtained by inserting the EM vertex in the self-energy diagram in all possible ways and can be shown to be fully consistent with the self energy so that

$$q_\mu [\text{MT}_{\text{pg}}^\mu(P+Q, P) + \text{AL}_1^\mu(P+Q, P) + \text{AL}_2^\mu(P+Q, P)] = \Sigma(P) - \Sigma(P+Q). \quad (10)$$

We write

$$- \frac{\partial \Sigma_{\text{pg}}}{\partial \mu} = \text{MT}_{\text{pg}}^0(P, P) + \text{AL}_1^0(P, P) + \text{AL}_2^0(P, P). \quad (11)$$

Now if we combine the above results with the bare vertex γ^μ , we find that the Ward identity guaranteeing gauge invariance and the Q -limit Ward Identity (4) guaranteeing the compressibility sum rule are both satisfied, providing no approximations [16] are made.

While we have proved the compressibility sum rule on general grounds, it is not in a particularly useful form for numerical application. To make things more transparent and tractable we approximate the normal state contribution to the self energy for temperatures above but near T_c , where $t_{\text{pg}}(Q)$ is peaked near $Q = 0$. We write

$$\Sigma_{\text{pg}}(K) = \sum_Q t_{\text{pg}}(Q)G_0(Q-K) \approx G_0(-K) \sum_Q t_{\text{pg}}(Q). \quad (12)$$

so that

$$\Sigma_{\text{pg}}(K) \approx -G_0(-K)\Delta_{\text{pg}}^2, \quad (13)$$

When extended to include the effects of the condensate, the superconducting order parameter Δ_{sc} is added to Eq.(12), with the usual self energy $\Sigma_{\text{sc}} = \frac{\Delta_{\text{sc}}^2}{\omega + \xi_{\mathbf{k}}}$. In this lowest order approximation we see that the contributions to the self energy from the condensed and non-condensed pairs are not distinguished. The effective gap for fermionic excitations is $\Delta = \sqrt{\Delta_{\text{sc}}^2 + \Delta_{\text{pg}}^2}$. Above T_c , this self energy approximation will lead to an expression for the density-density response function discussed in detail elsewhere [17]. Importantly this result is analytically consistent with the longitudinal and transverse f-sum rules. As in general theories [7, 9, 10], not surprisingly, this approximate density-density response function violates the compressibility sum rule. This means that we will find two different answers for the compressibility via thermodynamics and the response function.

It has been argued [10] that the thermodynamical approach is more reliable. This is due in part to the complexity of satisfying diagrammatic consistency requirements. We, thus, turn to this thermodynamic-based approach [18], later incorporating a parameter choice from radio-frequency spectroscopy [19]. As one departs from the BCS regime, there are additional ‘‘bosonic’’ contributions due to strong pairing fluctuations, besides those associated with the fermionic excitations. The resulting thermodynamical potential $\Omega = \Omega_f + \Omega_b$ including the fermions (f) and composite-bosons (b) can be written as

$$\begin{aligned} \Omega_f &= -\frac{\Delta^2}{g} + \sum_{\mathbf{k}} [(\xi_{\mathbf{k}} - E_{\mathbf{k}}) - \frac{2}{\beta} \ln(1 + e^{-\beta E_{\mathbf{k}}})], \quad (14) \\ \Omega_b &= -a_0 \Delta^2 \mu_p + \sum_{\mathbf{q}} \frac{1}{\beta} \ln(1 - e^{-\beta \omega_{\mathbf{q}}}). \quad (15) \end{aligned}$$

Here μ_p is the pair chemical potential which is non-zero above and zero below T_c and $\omega_{\mathbf{q}}$ is the pair dispersion, which (along with the residue a_0) arises from a small Q expansion of the t-matrix, t_{pg} . $\beta = (k_B T)^{-1}$ and we set $k_B \equiv 1$. The coupling constant g is related to the s-wave scattering length a [14, 19]. Note that Ω_f has a similar structure as that found in BCS theory, but implicitly involves composite-boson contributions.

This thermodynamic potential then yields self consistent conditions on the gap, pseudo-gap and chemical potential via variational conditions: $\frac{\delta \Omega}{\delta \Delta} = 0$, $\frac{\delta \Omega}{\delta \mu_p} = 0$, and

$n = -\frac{\delta \Omega}{\delta \mu}$. For example, these self consistent equations lead to the gap equation

$$g^{-1} + \sum_k \frac{1 - 2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}} = a_0 \mu_p, \quad (16)$$

which is of the familiar BCS form for $T < T_c$, and extends naturally to include a pairing gap in the normal phase as well. One important feature of this thermodynamic approach is that the superfluid transition is second order [19, 20], in contrast to the artificial first order transition found in other work [21]. The compressibility is

$$\frac{\partial n}{\partial \mu} = \left(\frac{\partial n}{\partial \mu} \right)_{\Delta} + \left(\frac{\partial n}{\partial \Delta} \right)_{\mu} \frac{\partial \Delta}{\partial \mu} + \left(\frac{\partial n}{\partial \mu_p} \right)_{\mu} \frac{\partial \mu_p}{\partial \mu}, \quad (17)$$

where this last term vanishes below T_c . From the number equation $n = -\frac{\delta \Omega}{\delta \mu}$, we obtain the following expression for the compressibility above T_c , $\left(\frac{\partial n}{\partial \mu} \right)_{T > T_c}$, given by

$$I_1 + \frac{\Delta^2 \left[\sum_{\mathbf{p}} \frac{\xi_{\mathbf{p}}}{E_{\mathbf{p}}^2} \left(\frac{1 - 2f(E_{\mathbf{p}})}{E_{\mathbf{p}}} + 2 \frac{\partial f(E_{\mathbf{p}})}{\partial E_{\mathbf{p}}} \right) \right]^2}{\sum_{\mathbf{p}} \frac{\Delta^2}{E_{\mathbf{p}}^2} \left(\frac{1 - 2f(E_{\mathbf{p}})}{E_{\mathbf{p}}} + 2 \frac{\partial f(E_{\mathbf{p}})}{\partial E_{\mathbf{p}}} \right) - \frac{4a_0^2 \Delta^2}{\sum_{\mathbf{q}} b'(\omega_{\mathbf{q}})}}. \quad (18)$$

Here $b'(x)$ is the derivative of the usual Bose-Einstein function with respect to its argument. We define

$$I_1 \equiv \sum_{\mathbf{p}} \left[\frac{\Delta^2}{E_{\mathbf{p}}^3} (1 - 2f(E_{\mathbf{p}})) - 2 \frac{\xi_{\mathbf{p}}^2}{E_{\mathbf{p}}^2} \frac{\partial f(E_{\mathbf{p}})}{\partial E_{\mathbf{p}}} \right]. \quad (19)$$

If we extend this calculation below T_c we have for $\left(\frac{\partial n}{\partial \mu} \right)_{T < T_c}$ the following expression

$$I_1 + \frac{\left[\sum_{\mathbf{p}} \frac{\xi_{\mathbf{p}}}{E_{\mathbf{p}}^2} \left(\frac{1 - 2f(E_{\mathbf{p}})}{E_{\mathbf{p}}} + 2 \frac{\partial f(E_{\mathbf{p}})}{\partial E_{\mathbf{p}}} \right) \right]^2}{\sum_{\mathbf{p}} \frac{1}{E_{\mathbf{p}}^2} \left(\frac{1 - 2f(E_{\mathbf{p}})}{E_{\mathbf{p}}} + 2 \frac{\partial f(E_{\mathbf{p}})}{\partial E_{\mathbf{p}}} \right)}. \quad (20)$$

Note that below T_c this has a similar structure as that in BCS theory.

The resulting curves are plotted as black lines in Figure 1, showing the behavior of the compressibility both above and below T_c for three different values of the scattering length. This figure indicates the changes as one varies from the BCS to the BEC side of unitarity. In this lowest order approximation which is based on the net effective gap Δ there is no discontinuity in κ which should be present at a phase transition. Such a signature only arises [22] when one introduces a clearer distinction between the condensed and non-condensed pairs.

A more physical result can be obtained using a variant on this theory in which the non-condensed pairs have a finite lifetime γ so that

$$\Sigma_{\text{pg}} = \frac{\Delta_{\text{pg}}^2}{\omega + \epsilon_{\mathbf{k}} + i\gamma}. \quad (21)$$

Such a broadened BCS-like self energy (with $\gamma \neq 0$) has been applied extensively in cold gas studies, particularly in analyzing experiments involving radio-frequency

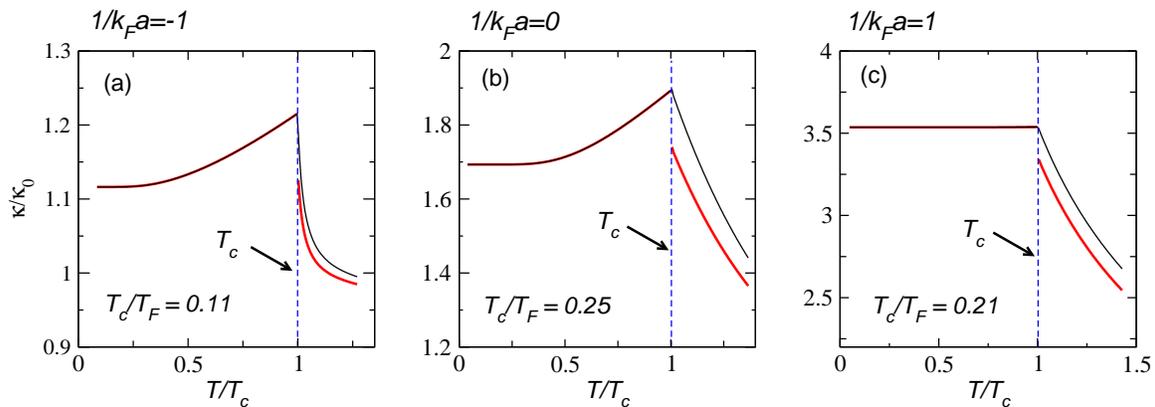


Figure 1: Our BCS-BEC crossover (thermodynamic approach) to compressibility with finite γ (red) and $\gamma = 0$ (black) on (a) BCS side, (b) unitarity, and (c) BEC side. The upturn in the normal state as T decreases is due to the bosonic contribution.

spectroscopy [19, 23]. With this self energy and the addition of the condensate self energy the spectral function $A(\omega, \mathbf{k})$ can be readily calculated [19]. We use $n = \sum_{\mathbf{k}} \int \frac{d\omega}{\pi} A(\omega, \mathbf{k}) f(\omega)$ to directly evaluate [24] the two contributions to the normal state compressibility via $\left(\frac{\partial n}{\partial \mu}\right)_{\Delta}$ and $\left(\frac{\partial n}{\partial \Delta}\right)_{\mu}$. As in RF experiments [19], in the numerics, we take $\gamma/E_F = \alpha T/T_c$ with the constant α of order unity, (although the behavior is extremely insensitive to this parameter). Importantly, the presence of γ then leads to a thermodynamic feature at T_c in the spectral function. This same thermodynamical feature is then mirrored in the compressibility.

The results of this simple modification of the black lines in Figure 1 is plotted as red curves in the figure, which show a discontinuity in the compressibility at T_c . In the normal phase there are two competing terms which one can see directly from comparing the first and second terms in Eq. (18). The first term leads to a contribution to the compressibility which *decreases* with decreasing temperature above T_c . The second term leads to a component which *increases* with decreasing temperature above T_c . We may interpret the first (and second) of these as associated with the fermionic (and bosonic) degrees of freedom. The growth of a fermionic gap tends to depress κ . At the same time the onset of bosonic degrees of freedom leads to a large (but in contrast to Ref. [25],) non-divergent compressibility.

Below T_c , on the other hand, except for a pairing gap which is no longer the same as the order parameter, the behavior of the compressibility is rather similar to that of BCS theory; the decrease with decreasing T reflects the fermionic gap [26]. As one approaches the BEC limit the behavior becomes progressively more temperature independent, essentially because the fermionic parameters, such as Δ and μ , reflected in $\partial n/\partial \mu$, are insensitive to T due to the strong binding energy. In this way, our theory provides predictions for the behavior of κ in BCS-BEC crossover.

We emphasize that while we could, we have not ad-

justed the parameter γ , taken from RF studies, to fit experiment [1] or Monte Carlo simulations [27]. Nevertheless, we point out that the step discontinuity and general behavior for the compressibility found here is within roughly a factor of two as observed experimentally (Figure 2A of Ref. [1]).

Conclusions Past work in the literature has addressed the compressibility [5, 6] using a response function approach. Potentially more reliable [7, 10] are thermodynamical approaches to κ . Because the compressibility is a central means of identifying the transition, it is of particular interest as we do here, to find and apply a thermodynamic methodology which does not predict an unphysical first order transition [21]. An additional advantage is that a thermodynamic approach avoids the complexity of gauge invariance and collective modes which must be included in the superfluid state response functions, thereby allowing κ to be addressed on both sides of T_c .

Our thermodynamic scheme has been applied on both sides of resonance, and thus provides predictions for the BEC regime, showing a step discontinuity which decreases from BCS to BEC, as found earlier [22] for the specific heat. We find no divergences in κ , which are avoided [5, 25] by resumming classes of diagrams in a response function approach. As we have emphasized here and elsewhere [28, 29] such resummations have to be implemented so as not to violate either or both the gauge invariant and Q -limit Ward identities. With improved approximations, it may be possible to recover consistency with these three important (sum rule) constraints, with which our full t -matrix approach to BCS-BEC crossover is manifestly compatible.

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