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ABSTRACT

It is shown that the presence of a singularity in Brueckner's t matrix for an infinite system of Fermions is a sufficient (but not necessary) condition for the existence of a gap in the energy spectrum of the system. On the other hand there are singularities in Galitskii's t-matrix if and only if the system has an energy gap.

Furthermore there are both singularities and an energy gap if the solution of a Schrödinger equation with modified kinetic energy has a positive phase shift δ at the Fermi momentum.

The results are illustrated by deriving approximate expressions for the energy gap and the distances of the singularities from the Fermi surface in terms of the phase shift δ.

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1 INTRODUCTION

In a previous paper[1)] (hereafter called I), it was shown that, for a wide class of potentials, the Brueckner t-matrix for an infinite system of fermions possesses singularities. At that time, it had been speculated that these singularities were associated with the existence of a gap in the energy spectrum of the system and that the low-lying states had a highly collective character - although the relationship between the various phenomena had not been clarified.

Recently, however, Cooper, Mills and Sessler[2)] and Bogoliubov[3)], using a generalization of the superconductivity theory of Bardeen, Cooper and Schrieffer[4)], derived a criterion for the existence of an energy gap which appears to be quite different from the condition for the existence of a singularity of the Brueckner t-matrix, discussed in I. It is therefore of great interest to compare the two criteria in order to see if they are indeed related and to determine the range of validity of the Brueckner method.

In this paper, it will be shown that, if the Brueckner t-matrix possesses singularities, then the Fermi system is in a highly correlated state, but that, in general, the converse is not true.

On the other hand, it will be seen that the t-matrix introduced by Galitskii[5)] is singular if and only if there is an energy gap. This result is physically reasonable since, in contrast to the convential Brueckner method, both Galitskii's theory and the Bardeen, Cooper, Schrieffer theory treat holes and particles symmetrically (see also Iwamoto[6)]).

It is therefore to be expected that Galitskii's approach provides a more accurate description of the normal state in that, in the absence of an energy gap, it may well be a good approximation to a more general theory which is applicable to both correlated and uncorrelated states. This conclusion is of interest since the collective effects are not expected to be of importance far away from the Fermi surface or when two particles have a total momentum very different from zero, so that calculations with the Galitskii t-matrix could give some useful results even when there is an energy gap.

In Section 2, the criterion for the existence of a phase transition of a Fermi system to a highly correlated state is introduced and it is expressed in a form suitable for the comparison with the t-matrix equations which is effected in Sections 3 and 4. In Section 5 the magnitude of the energy gap and distances of the singularities from the Fermi surface are expressed in terms of the Schrödinger equation phase shift to illustrate the results of the previous sections. Section 6 contains a discussion of the results.

2 THE EXISTENCE OF AN ENERGY GAP

In order to avoid the use of the non-linear equation whose solution determines the existence of an energy gap[2], we use the criterion[7] that an infinite Fermi system will undergo a phase transition to a highly correlated state at a temperature $T_c = 1/k\beta_c$. If this criterion is satisfied, the energy spectrum possesses a gap.

A Fermi system has a phase transition if

$$|\chi_K\rangle = - \frac{\tanh 1/4\beta H_0}{H_0} v|\chi_K\rangle \tag{1}$$

has a non-trivial solution for some value β_c of β.

Here, v is the two-particle potential and, in momentum representation,

$$\langle k|H_0|k'\rangle = |\mathcal{E}_0(k)|\ \delta(k - k'), \tag{2}$$

with

$$\mathcal{E}_0(k) = e(k) - e(k_F), \tag{3}$$

where

$$e(k) = k^2 + 2V(k) \tag{4}$$

is the "normal state" energy of a pair of particles with relative momentum $\underset{\sim}{k}$ and total momentum zero. $V(\underset{\sim}{k})$ is the single-particle potential, k_F the Fermi momentum, $\hbar = 1$ and the particle mass is unity.

In eq. (2), $|k\rangle$ is the radial part of the solution with angular momentum ℓ and momentum k of the free-particle Schrodinger equation, i.e.

$$\langle r|k\rangle = kr\, j_\ell(kr) \tag{5}$$

for some ℓ. Here, r is the separation of the particles and $j_\ell(kr)$ is the spherical Bessel function of order . (In the following, the angular momentum label, ℓ, will be suppressed and it is to be understood that all states refer to a fixed but arbitrary angular momentum ℓ.)

Eq. (1) may be rewritten as an eigenvalue equation,

$$|\mathcal{X}_{Ki}\rangle = -\mu_{Ki}(\beta)\,\frac{\tanh 1/4\,\beta H_0}{H_0}\, v\,|\mathcal{X}_{Ki}\rangle, \tag{6}$$

and the condition for a phase transition is that there be a value β_c of β for which

$$\mu_{Ki}(\beta_c) = 1 \tag{7}$$

for some value of i.

Throughout the discussion it will be assumed that the matrix elements $\langle k|v|k'\rangle$ of v are finite although they may be arbitrarily large so that there is no essential physical restriction on v.

Then, by using the methods of I, it may be shown that, for each value of ℓ, there is a set of eigenvalues $\mu_{Ki}(\beta)$ (having the following properties:

I. The eigenvalues are real and discrete and $\mu_{Ki}(\beta) \neq 0$ for finite β.

II. $\frac{\partial}{\partial\beta}\left|\mu_{Ki}(\beta)\right| < 0$ for all β and i.

III. (a) When $\langle k_F | v | k_F \rangle \neq 0$, $\mu_{Ki}(\beta) \longrightarrow 0$ as $\beta \longrightarrow \infty$ for one and only one value, n, of i. If $\langle k_F | v | k_F \rangle < 0$, $\mu_{Kn}(\beta) \longrightarrow 0$ through positive values, otherwise through negative values.

(b) When $\langle k_F | v | k_F \rangle = 0$, $\mu_{Ki}(\beta) \longrightarrow 0$ as $\beta \longrightarrow \infty$ for at least two values of i. In general, there are exactly two such values and one tends to zero from above and the other from below.

IV. $\left|\mu_{Ki}(\beta)\right| \longrightarrow \infty$ as $\beta \longrightarrow 0$

It follows at once that when $\langle k_F | v | k_F \rangle \leqq 0$, eq. (7) can be satisfied for at least one value, n, of i, so that there is a phase transition.

When $\langle k_F | v | k_F \rangle > 0$, every positive eigenvalue $\mu_{Ki}(\beta)$ remains non-zero as $\beta \longrightarrow \infty$, so that it is necessary to show that, for some value of ℓ, at least one eigenvalue is less than unity at $\beta = 0$. This possibility is most conveniently discussed by transforming eq. (6).

Define

$$\langle k | \Delta | k' \rangle = \sqrt{|\mathcal{E}_0(k)|} \quad \delta(k - k') \tag{8}$$

and

$$\langle k | \bar{\mathcal{X}}_{Ki} \rangle = \begin{cases} \lim\limits_{\beta \to \infty} \langle k | \frac{1}{\Delta} v | \mathcal{X}_{Ki} \rangle & \text{for } k \neq k_F \\ 0 & \text{for } k = k_F \end{cases} \tag{9}$$

for all $i \neq n$ ($\lim_{\beta\to\infty} \mu_{Kn}(\beta) = 0$). By using the methods of I, it can be shown that $\langle k_F | v | \mathcal{X}_{Ki} \rangle \to 0$ as $\beta \to \infty$, for $i \neq n$ (so that $\langle k | \bar{\mathcal{X}}_{Ki} \rangle$ is a continuous function of k) and that in the limit as $\beta \to \infty$, all eigenfunctions and eigenvalues of eq.(6), except those with $i = n$, are given by solutions of

$$\left| \bar{\mathcal{X}}_{Ki} \right\rangle = \mu_{Ki} \; G \left| \bar{\mathcal{X}}_{Ki} \right\rangle, \tag{10}$$

where

$$G = -\frac{1}{\Delta} \left\{ v - \frac{v | k_F \rangle \langle k_F | v}{\langle k_F | v | k_F \rangle} \right\} \frac{1}{\Delta} \tag{11}$$

and $\mu_{Ki} = \lim_{\beta\to\infty} \mu_{Ki}(\beta)$. We have now to determine the conditions under which the lowest positive eigenvalue μ_{Kp} is less than unity.

3 THE t-MATRIX AND FREE-SPACE EQUATIONS

In this section, we introduce the t-matrix and free-space equations which are to be compared with eqs. (10) and (11).

In I, it was shown that the criterion for the existence of a singularity in the Brueckner t-matrix for total momentum zero and relative momentum $m < k_F$ is that the equation

$$\left| \mathcal{X}_{Bi} \right\rangle = -\mu_{Bi(m)} \frac{Q}{H_1(m)} v \left| \mathcal{X}_{Bi} \right\rangle \tag{12}$$

have a non-trivial solution with

$$\mu_{Bi} = 1 \tag{13}$$

for some values of m and i.

Here

$$\langle k | H_1 (m) | k' \rangle = \delta(k - k') \, \mathcal{E}_1 (k,m), \tag{14}$$

$$\mathcal{E}_1(k,m) = e(k) - e(m) \tag{15}$$

and

$$\langle k | Q | k' \rangle = \begin{cases} \delta(k - k') & \text{for } k > k_F . \\ 0 & \text{for } k,k' < k_F . \end{cases} \tag{16}$$

Eq. (12) refers to a state of any fixed angular momentum ℓ (although it was derived for $\ell = 0$ in I).

Galitskii's t-matrix (which includes "hole-hole" scattering as well as "particle-particle" scattering (see also Iwamoto[6]) has a singularity for total momentum zero and relative momentum m, if the equation

$$| \mathcal{X}_{Gi} \rangle = - \mu_{Gi} (m) \frac{P}{H_1(m) - i\epsilon} v | \mathcal{X}_{Gi} \rangle \tag{17}$$

has a non-trivial solution with

$$\mu_{Gi}(m) = 1 \tag{18}$$

for some values of $m < k_F$ and i.

Here

$$\langle k | P | k \rangle = \begin{cases} \delta(k - k') & \text{for } k > k_F . \\ - \delta(k - k') & \text{for } k < k_F . \end{cases} \qquad (19)$$

Using the methods of I, it may be shown that both eqs. (13) and (18) can be satisfied if $\langle k_F | v | k_F \rangle \lesseqgtr 0$ and that when $\langle k_F | v | k_F \rangle > 0$, it is necessary to show that $\mu_{Bi} = \mu_{Bi}(k_F)$ and $\mu_{Gi} = \mu_{Gi}(k_F)$ are less than unity* for some value of i.

Now define

$$\langle k | \bar{\chi}_{Bi} \rangle = \begin{cases} \lim_{m \to k_F} \langle k | \frac{Q}{\Delta} v | \chi_{Ki} \rangle & \text{for } k \neq k_F . \\ 0 & \text{for } k = k_F . \end{cases} \qquad (20)$$

and

$$\langle k | \bar{\chi}_{Gi} \rangle = \begin{cases} \lim_{m \to k_F} \langle k | \frac{1}{\Delta} v | \chi_{Gi} \rangle & \text{for } k \neq k_F , \\ 0 & \text{for } k = k_F , \end{cases} \qquad (21)$$

for all $i \neq n$ ($\mu_{Bn} = 0 = \mu_{an}$). Then, as in section 2, $\langle k | \bar{\chi}_{Bi} \rangle$ and $\langle k | \bar{\chi}_{Gi} \rangle$ are continuous functions of k and in the limit as $m \to k_F$, all eigenfunctions and eigenvalues of eqs. (12) and (17) are given by

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* It is also necessary that both $\mu_{Bp}(0)$ and $\mu_{Gp}(0)$ be greater than unity. A sufficient condition for this would be that v have no bound state or at most a weakly bound state. This property is a feature of systems of physical interest so it will be assumed here.

$$|\bar{\mathcal{I}}_{Bi}\rangle = \mu_{Bi}\ QGQ|\bar{\mathcal{I}}_{Bi}\rangle \tag{22}$$

and

$$|\bar{\mathcal{I}}_{Gi}\rangle = \mu_{Gi}\ \ G|\bar{\mathcal{I}}_{Gi}\rangle \tag{23}$$

respectively. Finally, for purposes of comparison with a Schrodinger equation phase shift, δ, we introduce the factor λ_0 by which v has to be multiplied in order that the Schrodinger equation

$$|\Psi\rangle = |k_F\rangle - \mathbb{P}/H_0\, \lambda_0\, v|\Psi\rangle \tag{24}$$

with kinetic energy $e(k)$ should have zero phase shift for momentum k_F, i.e. that

$$\langle k_F|v|\Psi\rangle = 0\ . \tag{25}$$

Using eqs. (8) and (26) and defining

$$|\bar{\Psi}\rangle = \begin{cases} \langle k\ \frac{1}{\Delta}\,v|\Psi\rangle & \text{for}\quad k \neq k_F\ , \\ 0 & \text{for}\quad k = k_F, \end{cases} \tag{26}$$

eq. (24) may be rewritten

$$|\bar{\Psi}\rangle = \lambda_0\ \ GP|\bar{\Psi}\rangle. \tag{27}$$

It is not hard to see that if $\delta(k_F) > 0$ and $\langle k_F|v|k_F\rangle \geq 0$ then $\lambda_0 < 1$; for consider the arbitrary coupling constant λ. When $\lambda << 1$,

$$\tan \delta(k_F) \approx -\lambda\langle k_F | v | k_F \rangle, \tag{28}$$

which is small and negative so that $\delta(k_F) < 0$. However, when $\lambda = 1$, $\delta(k_F) \gg 0$ by assumption, so that there is a value of λ_0 of λ in $0 < \lambda_0 < 1$ for which $\delta(k_F)$ is zero for the potential λ_0 v.

Eqs. (22), (23), and (27) are to be used in the next section.

4 CONDITIONS FOR AN ENERGY GAP

In this section, it will be assumed that $\mu_{Gi}(0) \gg 1$ and $\mu_{Bi}(0) \gg 1$ for all i. This condition is satisfied very well for systems of physical interest and is sufficient to ensure that the t-matrices are singular when $\mu_{Gi} < 1$ and $\mu_{Bi} < 1$.

By using the results of Section 3, the following theorems may be proved (for all relative angular momentum states).

A. The conditions for a singularity in the Galitskii t-matrix and for an energy gap are identical.

B. The presence of a singularity in Brueckner's t-matrix is a sufficient (but not necessary) condition for the existence of and energy gap.

C. A sufficient condition for the existence of a singularity in Brueckner's t-matrix and hence for an energy gap is that the phase shift at momentum k_F in the solution of Schrodinger equation with kinetic energy $\mathcal{E}(k)$ be positive.

The remainder of this section is devoted to proving the theorems.

Eqs. (10) and (23) are identical, which is just the content of theorem A.

Let μ_{Bp} and μ_{Gp} be the smallest positive values of μ_{Bi} and μ_{Gi} respectively. It is not hard to show that

$$\frac{1}{\mu_{Kp}} \geqq \frac{\langle \mathcal{X} | G | \mathcal{X} \rangle}{\langle \mathcal{X} | \mathcal{X} \rangle} \tag{29}$$

and

$$\frac{1}{\mu_{Bp}} \geqq \frac{\langle \mathcal{X} | QGQ | \mathcal{X} \rangle}{\langle \mathcal{X} | \mathcal{X} \rangle} \tag{30}$$

for any trial function $|\mathcal{X}\rangle$. Then, replacing $|\mathcal{X}\rangle$ in the inequality (29) by $|\bar{\mathcal{X}}_{Bp}\rangle$ from eq. (22), we find that

$$\frac{1}{\mu_{Kp}} \geqq \frac{1}{\mu_{Bp}} > 0, \tag{31}$$

so that

$$\mu'_{Bp} \geqq \mu_{Kp} \tag{32}$$

and theorem B follows at once.

Finally, consider the eigenvalue equation

$$|\Psi_1\rangle = \lambda_1 (GP + PG) |\Psi_1\rangle . \tag{33}$$

Then, using the trial wave function $Q|\Psi_1\rangle$ in the inequality (30), we find

$$\frac{1}{\mu_{Bp}} \geqq \frac{1}{2\lambda_1} \tag{34}$$

(since $2Q = 1 + P$).

Then, using $|\bar{\Psi}\rangle$ of eq. (27) as trial wave function,

$$\frac{1}{\lambda_1} \geqslant \frac{\langle\bar{\Psi}|GP + PG|\bar{\Psi}\rangle}{\langle\bar{\Psi}|\bar{\Psi}\rangle} = \frac{2}{\lambda_0} > 0 , \tag{35}$$

so that

$$\lambda_0 \geqq \mu_{Bp} ,$$

which is tantamount to theorem C, since $\lambda_0 < 1$.

5 EXPRESSION FOR THE ENERGY GAP

The rather formal results of Section 4 may be made plausible by deriving an expression for the magnitude of the energy gap and also for the distance of the singularities from the Fermi surface.

First an expression for the transition temperature is obtained. We introduce the function $|\phi\rangle$ as the solution of

$$|\phi\rangle = |k_F\rangle + Fv|\phi\rangle , \tag{36}$$

where

$$F = - \frac{\tanh 1/4\beta H_0}{H_0} + L(\beta)|k_F\rangle\langle k_F| \tag{37}$$

and

$$L(\beta) = \int_0^\infty dk \frac{\tanh 1/4\beta\mathcal{E}_0(k)}{\mathcal{E}_0(k)} . \tag{38}$$

Then, from eqs. (1) and (36),

$$\langle\phi|v|\mathcal{X}_K\rangle = -\langle\phi|v\frac{\tanh 1/4\beta H_0}{H_0} v|\mathcal{X}_K\rangle$$

$$= \langle k_F | v | \mathcal{X}_K \rangle + \langle \phi | v \; K \; v | \mathcal{X}_K \rangle .$$

Thus

$$\langle k_F | v | \mathcal{X}_K \rangle = - L(\beta) \langle \phi | v | k_F \rangle \langle k_F | v | \mathcal{X}_K \rangle \tag{39}$$

and either

$$\langle k_F | v | \mathcal{X}_K \rangle = 0 \tag{40}$$

or

$$L(\beta) = \frac{-1}{\langle \phi | v | k_F \rangle} \quad . \tag{41}$$

For finite β, eq. (40) is not satisfied in general unless $|\mathcal{X}_K\rangle$ is identically zero i.e. there is no phase transition. When there is a phase transition, the transition temperature is given by the value β_c of β for which eq. (41) is satisfied.

Since $L(\beta)$ is positive, $\langle \phi | v | k_F \rangle$ must be negative. This requirement could be satisfied by a repulsive potential, but then $|\mathcal{X}_K\rangle$ would be zero and eq. (41) would not follow. For a very strongly attractive potential, $\langle \phi | v | k_F \rangle$ could be positive for large values of β but it would then be singular for some value β_0 of β and negative for some $\beta < \beta_0$.

$L(\beta)$ has been evaluated elsewhere[7]) and it is found to be sensitive to the form of $e(k)$ only through the effective mass M^* at the Fermi surface. It is found that

$$kT_c = 2.28 \frac{k_F^2}{M^*} \exp\left\{ \pi/2 \; \frac{k_F}{M^*} \; \frac{1}{\langle \phi | v | k_F \rangle} \right\} . \tag{42}$$

In situations of physical interest, v is weakly attractive in that $|\chi_K\rangle$ is not zero and $\langle \phi | v | k_F \rangle$ is negative and the calculated value of β_c is very large. For large β, F is only weakly dependent on and, to a good approximation, we may let $\beta \to \infty$ in eq. (37). Let

$$F_0 = \lim_{\beta \to \infty} F = -\int_0^\infty dk \; \frac{|k\rangle\langle k| - |k_F\rangle\langle k_F|}{|\epsilon_0(k)|} \tag{43}$$

and let $|\phi_0\rangle$ be the solution of the equation obtained by replacing K by K_0 in eq. (36).

If

$$F_1 = -\int_0^\infty dk \; \frac{|k\rangle\langle k| - |k_F\rangle\langle k_F|}{\epsilon_0(k)} , \tag{44}$$

then the equation for the wave matrix Ω for the Schrodinger equation with kinetic energy $\epsilon(k)$ is

$$\Omega = 1 + F_1 v \Omega , \tag{45}$$

from which

$$v|\phi_0\rangle = v\Omega |k_F\rangle + \Omega^+ v \; (F_1 - F_0) \; v | \phi_0 \rangle . \tag{46}$$

This integral equation may be expressed as a convergent iteration series in $v\Omega$ of which the first term gives a good a approximation, so that

$$\langle \emptyset | v | k_F \rangle \approx \langle \emptyset_0 | v | k_F \rangle \approx \langle k_F | v\Omega | k_F \rangle = - k_F \tan \delta(k_F). \tag{47}$$

Using the result of Bardeen, Cooper, and Schrieffer[4)] for the relationship between the magnitude ΔE of the energy gap and the transition temperature, (which is obtained by linearizing the equation[2)] for the energy gap) and, combining eqs. (42) and (47), we find

$$\Delta E = 3.5\ kT_c \approx \frac{8 k_F^2}{M^*} \exp\left\{ - \pi/2 \ \frac{\cot \delta(k_F)}{M^*} \right\} . \tag{48}$$

In a similar manner, it may be shown that if the singularities in Brueckner's t matrix and the real part of Galitskii's t-matrix occur for momenta m_1 and m_2 respectively, then

$$|\varepsilon_0(m_1)| \approx \frac{k_F^2 - m_1^2}{M^*} \approx \frac{4k_F^2}{M^*} \exp\left\{ - \pi \frac{\cot \delta(k_F)}{M^*} \right\} \tag{49}$$

and

$$|\varepsilon_0\ (m_2)| \approx \frac{k_F^2 - m_2^2}{M^*} \approx \frac{4k_F^2}{M^*} \exp\left\{ - \pi/2 \ \frac{\cot \delta(k_F)}{M^*} \right\} \tag{50}$$

in the effective mass approximation and for m_1 and m_2 near to k_F .

Within the range of validity of the approximations (48), (49) and (50), it is clear that $\delta(k_F)$ has to be positive for there to be both an energy gap and t-matrix singularities. $|\varepsilon_0(m_2)|$ is equal to 1/2 ΔE but $|\varepsilon_0\ (m_1)|$ is smaller than $1/2\ \Delta E$ (as a result of the absence of the factor 1/2 in the exponent of eq. (49) compared to eqs. (48) and (50). This fact suggests that, in a more correct expression, a weaker interaction would be required to give an energy gap than to give a singularity in Brueckner's t-matrix. These results are an approximate expression of the content of the theorems proved in section 4.

Eqs. (48), (49), and (50) cannot be used directly to obtain approximate expressions for ΔE, $|\mathcal{E}_0(m_1)|$, and $|\mathcal{E}_0(m_2)|$ from known phase shifts since $\delta(k_F)$ is to be calculated with kinetic energy $e(k)$. The further approximation of replacing $e(k)$ by k^2 is too drastic in general (since it introduces an error into the exponent) although it may be useful for discussing the qualitative features of actual physical systems. (For applications to liquid He^3 and to Nuclear Matter see Emery and Sessler[7,8].)

Finally it should be noted that, in the low-density limit, we can put M^* equal to unity and replace $\tan \delta(k_F)$ by $(-k_F a)$ (a being the scattering length) in eq. (49) to obtain the result of Van Hove[9].

6 DISCUSSION

The results of sections 3, 4, and 5 show that Brueckner's theory of an infinite Fermi system and Galitskii's extension of the theory meet with difficulties when the low-lying energy states of the system have a significantly collective character.

At the same time, if the energy gap is small, Brueckner's approach probably gives an adequate description of states far away from the Fermi surface or of pair states with total momentum appreciably different from zero and so it should be able to reproduce many properties of the system.

For this purpose, it seems to be more accurate to use Galitskii's t-matrix instead of Brueckner's t-matrix and, indeed, the former has summed more terms of the complete perturbation series (although it is not obvious without further discussion that this would result in an improved value of the energy). Consequently it is important to see if the two t-matrices predict significantly different properties of many-Fermion systems, since it may be necessary to amend the extensive calculations already carried out[10,11].

In this connection it should be noted that exclusion principle in intermediate states is doubled in the Galitskii equation with the result that total potential energy would be decreased in magnitude and the rearrangement energy[12] increased. These two effects compensate to some extent and, without further calculation, it is not possible to give a quantitative estimate of the changes.

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