Correlation Energy of a High-Density Gas: Plasma Coordinates

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The model Hamiltonian of Sawada which describes electron correlation at high density is examined. It is shown that the set of scattering modes for momentum transfers below a certain $q_{\max}$ is not complete. It is completed by the plasma mode. $(q_{\max})^{-1}$ is the natural Debye length of the theory.

I. INTRODUCTION

IT is the purpose of this article to supplement the mathematical methods of the preceding paper[1] by a somewhat more detailed analysis. The problem is treated here in the language of continuous spectra. It is then shown that for $q < q_{\max}$, where $q_{\max}$ is given by Eq. (9) of reference 1, the set of scattering states does not form a complete set. The set is completed by the plasma mode. For $q > q_{\max}$, the set of scattering states is complete. This is true only in the infinite limit, for only then will the plasma mode for $q > q_{\max}$ completely dissipate itself into the scattering modes. A similar situation arises in the theory of particle decay as carried out on a simplified model by Glaser and Kallën.[2]

This paper represents work carried out by the author after his remark on the existence of plasma modes in the Sawada theory.[3] The previous paper is, in the main, the work of Sawada, Brueckner, and Fukuda. Though the two independent investigations led to identical results, it was thought to be instructive to the reader to present the two lines of argument concurrently.

2. FORMULATION OF THE THEORY

We shall adopt Sawada's Hamiltonian[3] with some modifications in notation.

We define the creation operator of a pair (excited particle $\mathbf{p}+\mathbf{q}$, hole $\mathbf{p}$) as $d_{\mathbf{q}}^*(\mathbf{p})$, i.e.,

$$d_{\mathbf{q}}^*(\mathbf{p}) = a_{\mathbf{p}+\mathbf{q}}^* b_{\mathbf{p}}^*, \tag{2.1}$$

in Sawada's notation. Then defining the operator (p_F = Fermi momentum)

$$\sigma_{\mathbf{q}}^* = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\substack{|\mathbf{p}|<p_F \\ |\mathbf{p}+\mathbf{q}|>p_F}} d\mathbf{p} [d_{\mathbf{q}}^*(\mathbf{p}) + d_{-\mathbf{q}}(-\mathbf{p})]. \tag{2.2}$$

The Hamiltonian taken by Sawada is ($\hbar=1$, sums on p include spins)

$$H = H_0 + H_c,$$

$$H_0 = \frac{1}{(2\pi)^3}\int_{p>p_F} d\mathbf{p}\,\epsilon_{\mathbf{p}} a_{\mathbf{p}}^* a_{\mathbf{p}} - \frac{1}{(2\pi)^3}\int_{p<p_F} d\mathbf{p}\,\epsilon_{\mathbf{p}} b_{\mathbf{p}}^* b_{\mathbf{p}} + \frac{1}{(2\pi)^3}\int_{p<p_F} d\mathbf{p}\,\epsilon_{\mathbf{p}}, \tag{2.3}$$

$$H_c = \frac{1}{(2\pi)^3}\int d\mathbf{q} \frac{2\pi e^2}{q^2}\left[\sigma_{\mathbf{q}}^*\sigma_{\mathbf{q}} - \frac{1}{(2\pi)^3}\int_{\substack{p<p_F \\ |p+q|>p_F}} d\mathbf{p}\right].$$

(Note that H_c is the usual Coulomb Hamiltonian but with scatterings of excited states to excited states and holes to holes omitted.) The usual operator,

$$\rho_{\mathbf{q}} = \frac{1}{(2\pi)^{\frac{3}{2}}}\int_{p<p_F} a_{\mathbf{p}+\mathbf{q}}^* a_{\mathbf{p}},$$

is now replaced by $\sigma_{\mathbf{q}}$.

In evaluating the commutator of $d_{\mathbf{q}}(\mathbf{p})$ with the Hamiltonian, one makes the further approximation of neglecting the commutator of $d_q(p)$ with all $d_{\mathbf{q}'}^*(\mathbf{p}')$ but for $\mathbf{q}=\mathbf{q}'$. This eliminates the exchange scattering diagrams in the Gell-Mann and Brueckner scheme[4] and is the direct analog of the random phase approximation in the Bohm and Pines theory.[5] With this approximation, the excitations decouple for different $\mathbf{q}$ and behave like bosons, i.e., one may take

$$[d_{\mathbf{q}}^*(\mathbf{p}), d_{\mathbf{q}'}(\mathbf{p})] = (2\pi)^3\delta(\mathbf{q}-\mathbf{q}')\delta(\mathbf{p}-\mathbf{p}'). \tag{2.4}$$

Equations (2.3) and (2.4) define the problem.

The solution runs as follows. One finds the commutators

$$\begin{aligned}
[H, d_{-\mathbf{q}}(-\mathbf{p})] &= \omega_{\mathbf{q}}(\mathbf{p}) d_{-\mathbf{q}}(-\mathbf{p}) + \frac{1}{(2\pi)^{\frac{3}{2}}}\left(\frac{4\pi e^2}{q^2}\right)\sigma_{\mathbf{q}}, \\
[H, d_{\mathbf{q}}^*(\mathbf{p})] &= -\omega_{\mathbf{q}}(\mathbf{p}) d_{\mathbf{q}}^*(\mathbf{p}) - \frac{1}{(2\pi)^{\frac{3}{2}}}\left(\frac{4\pi e^2}{q^2}\right)\sigma_{\mathbf{q}}.
\end{aligned} \tag{2.4'}$$

Equations (2.4′) have the property that although H_0 is not a function of the pair operators, the commutator $[H_0, d_{\mathbf{q}}(\mathbf{p})]$ is nevertheless a function of $d_{\mathbf{q}}(\mathbf{p})$. This

[1] Sawada, Brueckner, Fukuda, and Brout [Phys. Rev. **108**, 507 (1957)], preceding paper.
[2] W. Glaser and G. Kallën, Nuclear Phys. **2**, 706 (1957).
[3] K. Sawada, Phys. Rev. **106**, 372 (1957).
[4] M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).
[5] D. Bohm and D. Pines, Phys. Rev. **92**, 609 (1953).

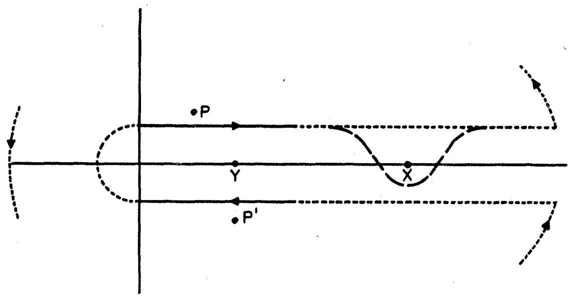

FIG. 1. Contour for the integration of Eq. (2.14).

makes commutators (2.4′) linear functions of $d_{\mathbf{q}}(\mathbf{p})$. One may then introduce the concept of normal modes (i.e., linear combinations of $d_{\mathbf{q}}(\mathbf{p})$, say η, which have the property that $[H,\eta]=\Omega\eta$. We shall work always in the continuous limit though the problem may be equally formulated for the discrete case. In that case consider the set of operators which create the real scattering states corresponding to the excitation $d_q^*(p)$. These are

$$\eta_{\mathbf{q}}^*(\mathbf{p})=d_{\mathbf{q}}^*(\mathbf{p})+\frac{4\pi e^2}{q^2}\left(\frac{1}{(2\pi)^3}\right)\int_{\substack{p'<p_F\\ |\mathbf{p}'+\mathbf{q}|>p_F}} d\mathbf{p}' \times\left[\frac{1}{\varphi_+(\omega_{\mathbf{q}}(\mathbf{p}))}\frac{d_{\mathbf{q}}^*(\mathbf{p}')}{[\omega_{\mathbf{q}}(\mathbf{p})-\omega_{\mathbf{q}}(\mathbf{p}')+i\epsilon]} +\frac{1}{\varphi_+(\omega_q(p))}\frac{d_{-\mathbf{q}}(-\mathbf{p}')}{[\omega_{\mathbf{q}}(\mathbf{p})+\omega_{\mathbf{q}}(\mathbf{p}')]}\right], \quad (2.5)$$

and its complex conjugate. Here

$$\varphi_\pm=1-\frac{4\pi e^2}{q^2}\left(\frac{1}{(2\pi)^3}\right)\int_{\substack{p'<p_F\\ |\mathbf{p}'+\mathbf{q}|>p_F}} d\mathbf{p}' \times\left[\frac{1}{\omega_{\mathbf{q}}(\mathbf{p})-\omega_{\mathbf{q}}(\mathbf{p}')+i\epsilon}-\frac{1}{\omega_{\mathbf{q}}(\mathbf{p})+\omega_{\mathbf{q}}(\mathbf{p}')}\right]. \quad (2.6)$$

With (2.6), it follows from (2.4′) that

$$[H,\eta_{\mathbf{q}}^*(\mathbf{p})]=-\omega_{\mathbf{q}}(\mathbf{p})\eta_{\mathbf{q}}^*(\mathbf{p}). \quad (2.7)$$

Equation (2.7) says that the real pairs have zero self-energy.

The next task is to investigate whether the states (2.5) constitute a complete orthonormal set. That the $\eta_q(p)$ are orthonormal follows immediately from the evaluation of the commutator $[\eta_q^*(p),\eta_q(p')]$. Using Eqs. (2.4) and (2.5), one finds that

$$[\eta_q^*(p),\eta_q(p')]=\delta(p-p')(2\pi)^3. \quad (2.8)$$

The only remaining question, completeness, would be established if the transformation (2.5) is unitary. Let us symbolize (2.5) by

$$\eta=Ud, \quad (2.9)$$

where an annihilation operator in the transformation carries a negative energy in its coefficient in accord with (2.5). The establishment of (2.8) is equivalent to $UU^+=1$. The completeness part of the theorem concerns U^+U and it is here that the plasma mode will appear. For this reason we shall enter into some detail upon the calculation (see also Klein and McCormick[6]).

The off-diagonal element of U^+U is, by direct evaluation,

$$\frac{1}{\varphi_+(\omega_{\mathbf{q}}(\mathbf{p}))}\frac{1}{[\omega_{\mathbf{q}}(\mathbf{p})-\omega_{\mathbf{q}}(\mathbf{p}')+i\epsilon]}+\frac{1}{[\omega_{\mathbf{q}}(\mathbf{p}')-\omega_{\mathbf{q}}(\mathbf{p})-i\epsilon]}\frac{1}{\varphi_-(\omega_{\mathbf{q}}(\mathbf{p}'))}$$
$$+\frac{1}{(2\pi)^3}\left(\frac{4\pi e^2}{q^2}\right)\int_{\substack{p''<p_F\\ |\mathbf{p}''+\mathbf{q}|>p_F}} d\mathbf{p}''\left\{\frac{1}{[\omega_{\mathbf{q}}(\mathbf{p}'')-\omega_{\mathbf{q}}(\mathbf{p})-i\epsilon]}\frac{1}{\varphi_-(\omega_{\mathbf{q}}(\mathbf{p}''))\varphi_+(\omega_{\mathbf{q}}(\mathbf{p}''))}\frac{1}{[\omega_{\mathbf{q}}(\mathbf{p}'')-\omega_{\mathbf{q}}(\mathbf{p}')+i\epsilon]}\right.$$
$$\left.-\frac{1}{[\omega_q(p'')+\omega_q(p)]}\frac{1}{\varphi_-(\omega_q(p''))\varphi_+(\omega_q(p''))}\frac{1}{[\omega_q(p'')+\omega_q(p')]}\right\}. \quad (2.10)$$

The integral in the second half of (2.10) is transformed by using the algebraic relations

$$\frac{1}{[\omega_{\mathbf{q}}(\mathbf{p}'')-\omega_{\mathbf{q}}(\mathbf{p})-i\epsilon]}\frac{1}{[\omega_{\mathbf{q}}(\mathbf{p}'')-\omega_{\mathbf{q}}(\mathbf{p}')+i\epsilon]}=\left\{\frac{1}{\omega_{\mathbf{q}}(\mathbf{p}'')-\omega_{\mathbf{q}}(\mathbf{p})+i\epsilon}-\frac{1}{\omega_{\mathbf{q}}(\mathbf{p}'')-\omega_{\mathbf{q}}(\mathbf{p}')+i\epsilon}\right\}\frac{1}{[\omega_{\mathbf{q}}(\mathbf{p})-\omega_{\mathbf{q}}(\mathbf{p}')+i\epsilon]}, \quad (2.11)$$

$$\frac{1}{\varphi_+\varphi_-}=\left(\frac{1}{\varphi_+}-\frac{1}{\varphi_-}\right)\left(\frac{1}{\varphi_--\varphi_+}\right),$$

$$\varphi_-(\omega_{\mathbf{q}}(\mathbf{p}''))-\varphi_+(\omega_{\mathbf{q}}(\mathbf{p}''))=-\frac{2\pi i}{(2\pi)^3}\left(\frac{4\pi e^2}{q^2}\right)\int\delta(\omega_{\mathbf{q}}(\mathbf{p}''))-\omega_{\mathbf{q}}(\mathbf{p}'''))d\mathbf{p}'''$$
$$\equiv-2\pi i\left(\frac{4\pi e^2}{q^2}\right)E(\omega_{\mathbf{q}}(\mathbf{p}'')). \quad (2.12)$$

[6] A. Klein and B. McCormick, Phys. Rev. 98, 1428 (1955).

Writing

$$\frac{1}{(2\pi)^3}\int d\mathbf{p}''=\int E(\omega_\mathbf{q}(\mathbf{p}''))d\omega_\mathbf{q}(\mathbf{p}''),$$

where the $\omega_\mathbf{q}(\mathbf{p}'')$ are arranged in monotonic sequence, we have for the integral in (2.10) upon using (2.11) and (2.12),

$$-\frac{1}{2\pi i}\left(\frac{1}{\omega_q(p)-\omega_q(p')+i\epsilon}\right)\int d\omega_q(p'')\left[\frac{1}{\varphi_+(\omega_q(p''))}-\frac{1}{\varphi_-(\omega_q(p''))}\right]\left\{\frac{1}{\omega_q(p'')-\omega_q(p)-i\epsilon}+\frac{1}{\omega_q(p'')+\omega_q(p)}-\frac{1}{\omega_q(p'')-\omega_q(p')+i\epsilon}-\frac{1}{\omega_q(p'')+\omega_q(p')}\right\}. \quad (2.13)$$

Changing variable to $\zeta=\omega_q^2(p'')$, (2.13) becomes

$$-\frac{1}{\omega_\mathbf{q}(\mathbf{p})-\omega_\mathbf{q}(\mathbf{p}')+i\epsilon}\left(\frac{1}{2\pi i}\right)\int_C\frac{d\zeta}{\varphi(\sqrt{\zeta})}\left[\frac{1}{\zeta-\omega_\mathbf{q}^2(\mathbf{p})-i\epsilon}-\frac{1}{\zeta-\omega_\mathbf{q}^2(\mathbf{p}')+i\epsilon}\right]. \quad (2.14)$$

The specified contour is shown by the solid lines in Fig. 1.

We must now consider the singularities of φ. Define $\bar{\varphi}$ as the value of φ obtained from taking the principal-value parts of $\varphi_\pm$, i.e., $\bar{\varphi}=\mathrm{Re}\varphi_\pm$, and let $\bar{\omega}_\mathbf{q}$ be the root defined by

$$\bar{\varphi}(\bar{\omega}_\mathbf{q})=0. \quad (2.15)$$

Equation (2.15) is the dispersion relation of Bohm and Pines for the plasma frequency.[7] For $q\to 0$, the solution of (2.15) is $\bar{\omega}_\mathbf{q}=\omega_{\mathrm{pl}}=(4\pi ne^2/m)^{\frac{1}{2}}$.

Now two cases arise:

(a) $\bar{\omega}_\mathbf{q}$ is in the continuum, i.e., $\bar{\omega}_q<(1/2m)(2p_Fq+q^2)$,
(b) $\bar{\omega}_\mathbf{q}$ is out of the continuum, i.e., $\bar{\omega}_q>(1/2m)(2p_Fq+q^2)$.

If one has case (a), then $\lim_{\epsilon\to 0}\varphi(\bar{\omega}_\mathbf{q}\pm i\epsilon)\neq 0$ and the point $\zeta=\bar{\omega}_\mathbf{q}$ will not have pole-like behavior (the point Y in Fig. 1). The deformation indicated by the dotted lines in Fig. 1 is then permitted and one picks up the two poles P and P' as indicated. The result is that (2.14) exactly cancels the first part of (2.10).

If one has case (b), then $\lim_{\epsilon\to 0}\bar{\varphi}(\bar{\omega}_q\pm i\epsilon)=0$ and the point $\zeta=\bar{\omega}_q$ is a pole. In this case a convenient deformation is given by the dashed lines in Fig. 1 around pole X. The remaining poles cancel the first part of (2.10), leaving a residue from X. The final result is that

Case (a):

$$UU^+=U^+U=1,\quad \bar{\omega}_q<\frac{1}{2m}(2p_Fq+q^2).$$

Case (b):

$$UU^+=1,$$

$$(U^+U)_{\mathbf{pp}'}=\frac{4\pi e^2}{q^2}\left(\frac{2\bar{\omega}_\mathbf{q}}{\varphi'(\bar{\omega}_\mathbf{q})}\right)\left[\frac{1}{\bar{\omega}_\mathbf{q}^2-\omega_\mathbf{q}^2(\mathbf{p})}-\frac{1}{\bar{\omega}_\mathbf{q}^2-\omega_\mathbf{q}^2(\mathbf{p}')}\right]+\delta(p-p'),\quad \bar{\omega}_q>\frac{1}{2m}(2p_Fq+q^2). \quad (2.16)$$

The only remaining question is to find the coordinate which, when added to the set $\eta_q(p)$, will complete it. This is the plasma mode for $q<q_{\max}$, where $q_{\max}$ is defined by

$$\bar{\omega}_{q_{\max}}=\frac{1}{2m}[2p_Fq_{\max}+q_{\max}^2]. \quad (2.17)$$

These modes are given by

$$v_\mathbf{q}=\left[\frac{4\pi e^2/q^2}{\varphi'(\bar{\omega}_\mathbf{q})}\right]^{\frac{1}{2}}\left(\frac{1}{(2\pi)^{\frac{3}{2}}}\right)\int_{\substack{p<p_F\\ |\mathbf{p}+\mathbf{q}|>p_F}}d\mathbf{p}\left[\frac{d_\mathbf{q}^*(\mathbf{p})}{\bar{\omega}_\mathbf{q}-\omega_\mathbf{q}(\mathbf{p})}+\frac{d_{-\mathbf{q}}(-\mathbf{p})}{\bar{\omega}_\mathbf{q}+\omega_\mathbf{q}(\mathbf{p})}\right]. \quad (2.18)$$

(Notice that as $q\to 0$, $v_\mathbf{q}\sim\sigma_\mathbf{q}$.) With the addition of $v_\mathbf{q}$, it is readily verified that the $\eta_q(\mathbf{p})$ set is completed. This completes the proof. The calculation of the energy is given in reference 1.

[7] The fact that the inequality $|\mathbf{p}+\mathbf{q}|>p_F$ that arises in (2.15) [see (2.6)] drops by symmetry was pointed out by P. Nozières. This insures that (2.15) is the dispersion relation of Bohm and Pines.