Role of Subsidiary Conditions in the Collective Description of Electron Interactions

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The role of the subsidiary conditions in the Bohm-Pines collective description of electron interactions is discussed in detail. The subsidiary conditions are shown to be compatible with the approximations made in obtaining the Hamiltonian and energy of the many-electron system. Their effect on the ground-state energy and the specific heat is found to be small.

1. INTRODUCTION

IN the development of a quantum collective description of electron interactions,[1] we find it desirable to introduce a set of supplementary field coordinates, N' in number, which describe the collective motion of the electron gas as a whole, the plasma oscillations. We deal then with an extended system of electrons and plasma waves, which possesses a total of $3N+N'$ degrees of freedom. We guarantee that the extended system of electrons and plasma waves has the same physical properties as the original system of interacting electrons by imposing a set of N' subsidiary conditions on the eigenfunctions of the extended system. Such a guarantee is not required for the ground state of the extended system, provided that state is nondegenerate. For, subject to this requirement, it can be shown that the subsidiary conditions are automatically satisfied by the ground-state wave function, so that the ground state of the extended system is identical with the ground state of the original system.

It is then feasible to solve the equations of motion of the extended system *without regard to the subsidiary conditions*, in order to obtain the properties of the ground state of electrons in metals. Indeed, such a solution may be regarded as essentially variational in nature, and its success may be measured by the value of the ground-state energy one obtains. For a suitable choice of the extended-system Hamiltonian, the solution turns out to be relatively straightforward, amounting to a power series expansion in the weak-coupling constant for the electron-plasma interaction.

Adams,[2] in a brief note, has raised the question of whether the approximations which are made in this solution are compatible with the satisfaction of the subsidiary conditions. He purports to prove that if one employs wave functions which satisfy the subsidiary conditions, then the perturbation-theoretic solutions are meaningless. We shall show that this is not true.

We shall discuss the logical development of the collective description in some detail, because we believe that the general method of the collective description may be applied to many other problems in physics.[3] In a many-body system which exhibits collective motion, one introduces new normal modes and associated coordinates because the collective motion is difficult to describe in terms of individual particle coordinates. But how can we do this without actually increasing the number of degrees of freedom of the system? The fact that N' independent collective modes exist must have important consequences for the motion of the individual particles. One of these consequences must be that, for the N-particle system, the number of independent particle degrees of freedom is reduced to $3N-N'$. How can we take such particle correlations into account? The approach adopted in the collective description offers a practical way to do it.

We begin the present discussion by introducing the supplementary field variables in a representation in which the role played by the subsidiary conditions is most evident, and indeed, trivial. We then investigate some properties of this extended system which are invariant under canonical transformations, but which are most easily proved in this representation. Next, we discuss the nature and validity of the approximate solutions we employ for the extended-system Hamiltonian, showing in what sense they are compatible with the subsidiary conditions. We indicate briefly the series of canonical transformations which lead to the final representation utilized for the solutions in BP, and then discuss the role of the subsidiary conditions in the final representation. The essential point here is that to a well-defined order of approximation *the subsidiary conditions in the final representation do not involve the plasma variables*, so that the complete spectrum (ground plus excited states) of the plasma oscillations is correctly given. The subsidiary conditions do affect the electronic motion. Their effect on the ground-state energy and the specific heat at low temperatures will,

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[1] D. Bohm and D. Pines, Phys. Rev. 92, 609 (1953), hereafter referred to as BP.

[2] E. N. Adams, Phys. Rev. 98, 1130 (1955).

[3] T. Miyazima and T. Tamura, Progr. Theoret. Phys. Japan 15, 255 (1956), for example, have treated the collective surface oscillation of a nucleus along similar lines.

however, be small and the physical reason for that will be discussed.

2. FORMULATION OF THE PROBLEM

The basic Hamiltonian for a system of electrons in a uniform background of positive charge may be written as[4]

$$H=\sum_i \frac{p_i^2}{2m}+\frac{1}{2}\sum_{k\neq 0}(\rho_k^*\rho_k-n)v_k, \tag{1}$$

where ρ_k represents the kth density fluctuation of the electron gas and $n=N/V$, where V is the volume of the system, taken to be unity. In this system of units, then, $n=N$, ρ_k is given by

$$\rho_k=\int d\mathbf{r}\rho(\mathbf{r})e^{+i\mathbf{k}\cdot\mathbf{r}}=\sum_i e^{-i\mathbf{k}\cdot\mathbf{r}_i}, \tag{2}$$

and

$$v_k=\int (e^2/r)e^{-i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r}=4\pi e^2/k^2. \tag{3}$$

We know that for long wavelengths the ρ_k very nearly describe independent collective modes for the system—the plasmons.[5] We now introduce explicit plasmon variables (π_k,q_k) (which will later be related to the ρ_k) by adding certain terms to our basic Hamiltonian.[6] The terms we choose to add are given by

$$H_{\text{add}}(k_c)=\tfrac{1}{2}{\sum_{k<k_c}}'(\pi_k^*\pi_k-2\pi_k^*\rho_k\sqrt{v_k}), \tag{4}$$

where the prime on the summation leaves out the term $k=0$, and where k_c is arbitrary. We are, therefore, actually considering a whole family of extended Hamiltonians, each with different degrees of freedom, depending on k_c. The quantities π_k commute with all particle variables, and are defined only by the following requirements:

(1) There must exist canonical conjugates q_k, also commuting with all particle variables, such that

$$[\pi_k,q_{k'}]=-i\delta_{kk'}. \tag{5}$$

(2) The extended Hamiltonian must share all the invariance properties of H under spatial translations, rotation, etc. As a consequence, the transformation properties of π_k, q_k are defined. For example, requiring the extended Hamiltonian to be Hermitian yields the relation

$$\pi_k^*=\pi_{-k},\quad q_k^*=q_{-k}, \tag{6}$$

and from invariance under translation we have

$$U^{-1}\pi_k U=\pi_k e^{i\mathbf{k}\cdot\Delta\mathbf{x}},\quad U^{-1}q_k U=q_k e^{-i\mathbf{k}\cdot\Delta\mathbf{x}}, \tag{7}$$

where $U=U(\Delta\mathbf{x})$ is hereby defined as the translation operator in the extended system. Its effect on ρ_k is already known to be

$$U^{-1}\rho_k U=\rho_k e^{-i\mathbf{k}\cdot\Delta\mathbf{x}}. \tag{8}$$

We need hardly mention that the choice of the form of H_{add} is not unique. In choosing the particular form (4), we are guided only by the desire to end up with an extended Hamiltonian which has a lower bound, and which is simple.[7] It is clear that H_{add} fulfills those requirements because it leads to an H_{ext} which is positive-definite, and it is particularly simple because it merely completes the square of a portion of H. Our family of extended Hamiltonians, labeled by k_c, now can be written

$$\begin{aligned}H_{\text{ext}}(k_c)&=H+H_{\text{add}}(k_c)\\&=T+H_{\text{s.r.}}(k_c)+\tfrac{1}{2}{\sum_{k<k_c}}'[(\pi_k^*-v_k^{\frac{1}{2}}\rho_k^*)\\&\qquad\times(\pi_k-v_k^{\frac{1}{2}}\rho_k)-nv_k],\end{aligned} \tag{9}$$

where

$$T=\sum_{i=1}^{N}\frac{p_i^2}{2m},\quad H_{\text{s.r.}}=\sum_{k>k_c}(\rho_k^*\rho_k-n)v_k. \tag{10}$$

$H_{\text{s.r.}}$ is an interaction which is of shorter range than the original interaction. Each extended Hamiltonian contains $3N+N'$ degrees of freedom, where

$$N'/V=k_c^3/(6\pi^2). \tag{11}$$

The eigenvalue problem

$$H_{\text{ext}}(k_c)\psi_n=E_n\psi_n, \tag{12}$$

subject to the N' subsidiary conditions

$$\pi_k\psi_n=0,\quad (k<k_c) \tag{13}$$

is trivially equivalent to the original eigenvalue problem for all values of k_c.[8] The subsidiary conditions ensure

[4] We follow the notation of BP throughout this paper with the exception that we shall employ Hermitian auxiliary variables π_k, q_k instead of the anti-Hermitian P_k, Q_k of BP. Furthermore, we set $\hbar=1$.

[5] A plasmon is the basic quantum associated with plasma oscillations. The term has recently been introduced because plasma oscillations are found to be a well-defined elementary excitation in nearly all solids. [See D. Pines, Revs. Modern Phys. 28, 184 (1956).]

[6] The procedure followed here is essentially that of BP. See also D. Pines, *Solid State Physics* (Academic Press, Inc., 1955), Vol. 1, p. 373; hereafter referred to as SSP.

[7] In other words if one chooses an extended Hamiltonian which does not have a lower bound, our central theorem regarding the identity of the ground state of the extended system with that of the original system cannot apply. It is then obvious that one has to satisfy the subsidiary conditions exactly at every stage of the calculation in order to obtain correct results. The difficulty with non-positive-definite Hamiltonians has been independently noted by C. G. Kuper [Proc. Phys. Soc. (London) **A69**, 492 (1956)]. Kuper's conclusion, that such difficulties imply that something is not satisfactory in our treatment of the subsidiary conditions, is not correct since we do not propose treating the class of non-positive-definite Hamiltonians with the aid of our central theorem.

[8] It is to be noted that since according to (13) ψ_n is an eigenfunction of π_k, ψ_n is actually non-normalizable because the operator conjugate to π_k, namely q_k, has a continuous spectrum of eigenvalues from $-\infty$ to $+\infty$, as is implied by (5). Any difficulties that may arise from this fact, however, are purely formal. One can normalize ψ_n by artificial devices (for example by limiting the range of q_k from $-L$ to $+L$, and then let L approach ∞ later), and physical quantities calculated will in no way be affected.

that the number of degrees of freedom we deal with is always $3N$, and (12) and (13) are compatible because π_k commutes with H_{ext}.

Formally, nothing has been done so far; but we have prepared the way for the introduction of N' collective variables as independent dynamical ones. In (9), N' of the particle variables ρ_k $(k<k_c)$ have been singled out, indeed, earmarked for liquidation. We plan that in their place N' new independent variables will appear after suitable canonical transformations. The whole formalism would be superfluous if we could solve the eigenvalue problem (12) and (13) exactly for all k_c. Then all extended Hamiltonians $H_{\text{ext}}(k_c)$ would be on the same footing and we might just as well consider $k_c=0$, i.e., the original problem. Of course, we cannot solve the eigenvalue problem (12) and (13) exactly. What we can do is to find a value of k_c for which we can solve the eigenvalue problem approximately. That we can do this is not surprising, because physically there exists a "natural" set of N' collective modes of excitation of the system which is rather well separated from the independent-particle motion. When these modes are properly introduced (via the set of canonical transformations we describe later), we see that the physical and the mathematical description of the electron system is considerably simplified.

We find that we can work with a subfamily of extended Hamiltonians, $H_{\text{ext}}(k_c)$, which are simple in the sense that (1) $H_{\text{ext}}(k_c)$ is of the form of a "particle" Hamiltonian plus a "field" Hamiltonian with only weak coupling between them, and that (2) the corresponding subsidiary conditions restrict only the "particles," but place no constraint on the "field," to a certain well-defined approximation. We shall discuss the exact choice of k_c later.

3. SOME PROPERTIES OF THE EXTENDED SYSTEMS

Before we go on with the formal development, we shall investigate some properties of the extended systems that remain invariant under canonical transformations, but are easier to prove in the representation of (9).

We wish first to emphasize the fact that if the subsidiary conditions are written $\Omega_k\psi=0$, then the Ω_k commute with their corresponding extended Hamiltonian in all representations. Therefore, eigenstates of the Hamiltonian can also be simultaneous eigenstates of Ω_k. To take the subsidiary conditions into account, we may first find all eigenstates of H_{ext}, and only after this is done need we consider the subsidiary conditions. If an eigenstate ψ_n of H_{ext} is nondegenerate, it must also be an eigenstate of Ω_k, while if the states $\psi_n, \psi_m, \cdots$ are degenerate we must take proper linear combinations to form eigenstates of Ω_k. Let us assume that this is done. Then the only effect of the subsidiary conditions is to leave out those eigenstates of H_{ext} which do not satisfy $\Omega_k\psi=0$. To fix this in our minds, we shall represent the situation by the schematic diagram in Fig. 1, where the eigenstates of H_{ext} are represented by the different levels. A cross indicates we must exclude that state because it fails to satisfy $\Omega_k\psi=0$.

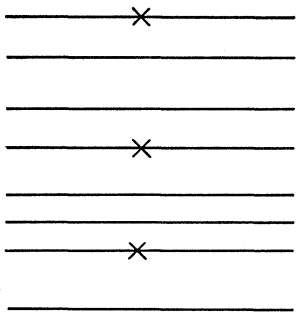

FIG. 1. Schematic diagram of energy levels of H_{ext}.

We can prove that in Fig. 1, the set of crossed-out levels contain only states degenerate with respect to H_{ext}. This is the equivalence theorem proved in BP, which states that *if an eigenvalue of H_{ext} is nondegenerate, then its corresponding eigenfunction automatically satisfies the subsidiary conditions*. We restate the proof as follows:

Let E be a nondegenerate eigenvalue of H_{ext}, and Φ its corresponding eigenstate. Φ is unique. Since π_k and $U(\Delta\mathbf{x})$, the translation operator,[9] both commute with H_{ext}, Φ is also a simultaneous eigenstate of these operators, so that

$$\begin{aligned} H_{\text{ext}}\Phi&=E\Phi,\\ \pi_k\Phi&=\beta_k\Phi,\\ U(\Delta x)\Phi&=\alpha\Phi. \end{aligned} \tag{14}$$

We can conclude, from (14), that

$$U(\Delta\mathbf{x})\pi_k\Phi=\alpha\beta_k\Phi.$$

On the other hand, we also conclude, from (7), that

$$U(\Delta\mathbf{x})\pi_k\Phi=U\pi_kU^{-1}U\Phi=\alpha\beta_ke^{i\mathbf{k}\cdot\Delta\mathbf{x}}\Phi.$$

Therefore

$$\beta_k=\beta_ke^{i\mathbf{k}\cdot\Delta\mathbf{x}}.$$

Since this is true for arbitrary $\Delta\mathbf{x}$,

$$\beta_k\equiv 0,$$

which proves the theorem.

Now, if we know that the lowest state of H_{ext} is nondegenerate, then the equivalence theorem tells us that it coincides with the lowest state of H, since the subsidiary conditions are automatically satisfied. We may rephrase this to say that *if the lowest state of H_{ext} is nondegenerate, then any state of H_{ext} which violates the subsidiary conditions must lie higher in energy than the ground state of H*. This fact has obvious importance for practical calculations, because if we can ascertain the

[9] It is of course not necessary that we use the translation operator. In its place, we may substitute any other operator that commutes with H_{ext} but not with π_k, and which does not have the eigenvalue zero.

ground state of H_{ext} to be nondegenerate, then we can calculate its energy (which is the ground-state energy of H) by a variational method, employing variational wave functions that do not have to take explicit heed of the subsidiary conditions. As long as the wave functions are allowed sufficient freedom of variation, the lowest energy obtained will lie above the true energy by arbitrarily small amounts. This will be a great aid to actual calculations, because the subsidiary conditions are hard to deal with explicitly.

The significance of the equivalence theorem then hinges upon our ability to prove that the ground state of H_{ext} is nondegenerate. We shall not attempt a formal proof here. We first remark that it is generally true that the ground state of a physical system is nondegenerate, or if degenerate, the degeneracy is of a trivial kind that can be easily removed (e.g., spin degeneracies). For all practical purposes, then, we may assume the ground state of H nondegenerate. To see whether the ground state of H_{ext} is then also nondegenerate requires that we understand the effect of H_{add} on H, ignoring the subsidiary conditions. The detailed investigation of this system is carried out in BP and is summarized in the following sections. It is shown that H_{ext} is "well behaved" in the sense that it describes a reasonable physical situation, for which we can obtain an excellent perturbation-theoretic solution. This solution shows that the ground state of H_{ext} is not degenerate.

A physical argument for the general validity of the assumption that the ground state of H_{ext} is nondegenerate may be constructed along the following lines. Let us work in a representation in which all π_k are diagonal with eigenvalues β_k. Then we may consider H_{ext} to be the Hamiltonian for the particles in the presence of external fields β_k:

$$H_{\text{ext}}=H+\tfrac{1}{2}\sum_{k<k_c}{}'\,(\beta_k{}^*\beta_k-2v_k{}^{\frac{1}{2}}\beta_k{}^*\rho_k), \tag{15}$$

where the particles are coupled to the external fields through $\beta_k{}^*\rho_k$. The ground state H_{ext} would be degenerate only if this interaction pushes some excited states of H down to the ground state, and this appears to be highly implausible except possibly for pathological systems. There seems to be a general theorem in physics, so far unproved, which states that *when an external field is applied to a physical system, the reaction of the system will never completely cancel it.* This theorem has been found to be true in practice in all fields of physics.[10] The relevance of this theorem to our problem may be seen by the following argument.

Suppose we phrase our basic problem with the following questions: "If we look upon the β_k in (15) as fixed external parameters and express the lowest eigenstate of (15) in terms of them, then (a) does $\beta_k=0$ give a minimum in the energy, and (b) is it the only minimum?" We can try to answer these questions by calculating the derivative of the energy. Let E, Φ be the lowest eigenvalue and eigenfunction of H_{ext}:

$$H_{\text{ext}}\Phi=E\Phi, \tag{16}$$

where both E and Φ depend on β_k, viewed as external parameters. It is convenient to decompose β_k into their real and imaginary parts:

$$\beta_k=R_k+iI_k,$$

where, from (6), we must require

$$R_k=R_{-k},\quad I_k=-I_{-k}.$$

We can then write

$$H_{\text{ext}}=H+\tfrac{1}{2}\sum_{0<k<k_c}{}'\,[R_k{}^2-2v_k{}^{\frac{1}{2}}R_k\sum_{j=1}^{N}\cos(\mathbf{k}\cdot\mathbf{r}_j),$$
$$+I_k{}^2-2v_k{}^{\frac{1}{2}}I_k\sum_{j=1}^{N}\sin(\mathbf{k}\cdot\mathbf{r}_j)]. \tag{17}$$

Differentiating (17) with respect to R_k, I_k, and then taking expectation values, we have

$$\begin{aligned}\frac{\partial E}{\partial R_k}&=R_k-v_k{}^{\frac{1}{2}}\langle\sum_{j=1}^{N}\cos(\mathbf{k}\cdot\mathbf{r}_j)\rangle,\\ \frac{\partial E}{\partial I_k}&=I_k-v_k{}^{\frac{1}{2}}\langle\sum_{j=1}^{N}\sin(\mathbf{k}\cdot\mathbf{r}_j)\rangle,\end{aligned} \tag{18}$$

where $\langle\ \rangle$ denotes expectation value with respect to Φ. When $R_k=I_k=0$, Φ becomes the ground state of H, which we assume to be nondegenerate, so that in this limit the expectation values $\langle\ \rangle$ vanish, as can be easily shown by the same invariance arguments as are employed in the proof of the eigenvalence theorem. Therefore, $R_k=I_k=0$ is an extremum of E. To show that it is a minimum, and furthermore that it is the only minimum, we have to show that

$$\begin{aligned}|R_k|&>v_k{}^{\frac{1}{2}}|\langle\sum_{j=1}^{N}\cos(\mathbf{k}\cdot\mathbf{r}_j)\rangle|,\\ |I_k|&>v_k{}^{\frac{1}{2}}|\langle\sum_{j=1}^{N}\sin(\mathbf{k}\cdot\mathbf{r}_j)\rangle|.\end{aligned} \tag{19}$$

These inequalities have not been proved; but they represent a mathematical statement of the general theorem whose truth we conjectured earlier. In the appendix we give a simple example to illustrate this point.

[10] As an example, one may cite the fact that when an external magnetic field is applied to an atomic system, the induced field (diamagnetism) is always opposite in direction to the applied field, with a magnitude less than the applied field. Even for a superconductor, the net field inside the system is not zero, although infinitesimal.

4. INTERMEDIATE CANONICAL TRANSFORMATION

In this section we consider the transformation which takes us from (9) to the Hamiltonian used as a starting point in BP. This transformation relates the π_k to the long-wavelength density fluctuations, ρ_k. For this reason, in the new representation, the plasma oscillations which explicitly emerge interact only weakly with the electrons. The transformation carries H_{ext} to

$$H_{\text{ext}}'=e^{-iS}H_{\text{ext}}e^{iS}, \tag{20}$$

where

$$S=i\sum_{k<k_c}{}' v_k^{\frac{1}{2}}q_k\rho_k. \tag{21}$$

The transformed Hamiltonian is

$$H_{\text{ext}}'=H_0+H_1+H_2, \tag{22}$$

where

$$H_0=T+H_{\text{s.r.}}+\tfrac{1}{2}\sum_{k<k_c}{}'\left[(\pi_k^*\pi_k+\omega_p^2q_k^*q_k)-nv_k,\right. \tag{22a}$$

$$H_1=\frac{i}{m}\sum_{k<k_c}{}' v_k^{\frac{1}{2}}q_k\sum_{j=1}^{N}\mathbf{k}\cdot(\mathbf{p}_j-\tfrac{1}{2}\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}_j}, \tag{22b}$$

$$H_2=\frac{1}{2m}\sum_{\substack{k<k_c\\k\neq l}}{}'\sum_{l<k_c}{}'(v_kv_l)^{\frac{1}{2}}(\mathbf{k}\cdot\mathbf{l})q_kq_l^*\rho_{k-l}, \tag{22c}$$

with the "plasma frequency" ω_p defined by

$$\omega_p^2=(nk^2/m)v_k=4\pi ne^2/m. \tag{23}$$

The subsidiary conditions for the wave functions in the new representation are

$$(\pi_k+v_k^{\frac{1}{2}}\rho_k)\psi=0, \quad (k<k_c). \tag{24}$$

The Hamiltonian (22) describes a collection of electrons and plasmons of frequency ω_p. The reason for the particular choice of the additional terms (4) and the generating function (21) is that in this representation the long-range Coulomb interaction between the electrons has been eliminated. There remains only the relatively weak short-range electron-electron interaction, $H_{\text{s.r.}}$, and the last two terms of (22), H_1 and H_2, which describe electron-plasmon interaction.

The theory is useful only if at this point we can say that there is a particular choice of k_c, or a range of k_c, for which $H_{\text{ext}}(k_c)$ really exhibits collective oscillatory motion by virtue of the fact the coupling terms are small. To investigate this question, we may look at the eigenvalues of H_{ext}, ignoring the subsidiary conditions. As we have emphasized before, the only effect of the subsidiary conditions is to throw away some eigenstates of H_{ext} *after* we have diagonalized it.

We may assert that a k_c has been chosen such that the contributions of H_1 and H_2 to the eigenvalues of H_{ext} are small, and then proceed to verify this by perturbation calculations. Whether or not we can do this depends very much on the specific problem, in particular, on the behavior of $H_{\text{s.r.}}(k_c)$. It suffices to summarize here the results in BP.

The interaction term H_1 is linear in the plasma field coordinate q_k. It is shown in BP that for the calculation of low-lying eigenvalues an effective coupling constant for this interaction is

$$g^2=\langle(\mathbf{k}\cdot\mathbf{p}/m\omega_p)^2\rangle, \tag{25}$$

where $\langle\ \rangle$ denotes the expectation value with respect to a low-lying eigenstate of H_0, averaged over k $(k<k_c)$, and p is a particle momentum (any particle). One first assumes that g^2 is small and proceeds to calculate the approximate ground-state energy of H_{ext}, and then chooses that value of k_c which makes the energy a minimum. Substituting this value of k_c back into (25), one verifies that (25) is small. It is shown in SSP that a reasonable choice is

$$k_c/k_f=0.35r_s^{\frac{1}{2}}, \tag{26}$$

where k_f is the wave vector at the Fermi level, and r_s is the average interelectronic distance in units of the Bohr radius.[11] With this choice, one finds that $g^2\approx\frac{1}{16}$ for all metals, so that a perturbation expansion for the low-lying eigenvalues of H_{ext} in powers of g^2 is clearly appropriate. The minimizing procedure thus singles out a particular value k_c, i.e., that given by (26), as physically meaningful in that $H_{\text{ext}}'(k_c)$ describes almost decoupled individual-particle and collective motions.

The nonlinear coupling term H_2 is shown by BP to be even smaller than H_1. An effective coupling constant for H_2 is

$$\tfrac{1}{16}(N'/3N), \tag{27}$$

where N' is the number of plasma degrees of freedom defined in (11). For most metals, this coupling constant is found[4] to be only 2–10% of the magnitude of g^2. We may therefore neglect H_2 entirely. This approximation is known in BP as the "random phase approximation," for it clearly depends upon the fact that the system under consideration contains a very large number, N, of particles, whose correlated collective degrees of freedom are few in number compared with the degrees of individual-particle random motion.

[11] As will be discussed in more detail elsewhere by one of us, there are two kinds of criteria for k_c. One, based on plasmon dynamics, is that k_c be the maximum wave vector for which the plasmon represents an independent elementary excitation weakly coupled to the motion of the individual particles. Such a choice might be defined by $g_0^2=1$, where g_0^2 is the coupling of the k_cth plasmon to the electrons at the top of the Fermi distribution which are moving in the direction of the plasmon. From (25), we have $g_0^2=(k_c^2p_0^2/m^2\omega_p^2)=1$, or $k_c=0.47r_s^{\frac{1}{2}}$. This choice is equivalent to the criterion adopted by R. A. Ferrell (to be published), that it be energetically possible for the plasmon to give up its energy to a single electron. The other choice is related to the system energetics. It is the one used in BP III and SSP, that it be energetically favorable to introduce the k_cth plasmon. A slight improvement of the calculation in SSP which led to (26) yields the result $k_c=0.40r_s^{\frac{1}{2}}$. The close agreement between the two criteria is encouraging, and in all likelihood a choice of k_c between the above values offers a happy compromise.

So far we have been concerned only with the calculation of the eigenvalues of H_{ext}'. Since we believe, as discussed previously, that the ground state of H_{ext}' is nondegenerate, the calculation so far outlined will immediately give us the ground-state energy of the *actual* system. In order to find the excited states of the actual physical system, we have to know which eigenvalues of H_{ext} are spurious on account of the fact that the corresponding wave functions fail to satisfy the subsidiary conditions (24). It is clear that we cannot substitute the wave functions calculated by perturbation theory directly into (24) and test their admissibility, because, being approximate wave functions, *none* of them will satisfy (24) exactly. In order to be consistent with the perturbation procedure, we have to relax the subsidiary conditions (24), and require that they be satisfied only approximately. It is then our task to define a consistent criterion for the approximation satisfaction of the subsidiary conditions.

The detailed developments concerning the consistent changes necessary to relax the subsidiary conditions will be discussed in the next section; but a brief account here is in order. The procedure adopted consists of replacing the simple perturbation treatment of H_{ext}' by a canonical transformation which eliminates the interaction term H_1 to a given order of g^2. Simultaneously, the subsidiary conditions (24) will be transformed into the new representation and assume the form

$$(\Omega_0+\Omega_1+\cdots)\psi=0, \tag{28}$$

where Ω_0 is of zero order in g^2, Ω_1 of first order in g^2, etc. If we wish to calculate the eigenvalues of H_{ext}' correct to first order in g^2, we need the wave function ψ only to zero order in g^2, and then (28) reduces to

$$\Omega_0\psi=0. \tag{29}$$

In this new representation, Ω will still commute with H_{ext} *to the order of approximation desired*, and we can be sure that the subsidiary conditions can always be satisfied. The explicit form of Ω_0, Ω_1 will be given in the next section.

We shall now consider the point raised by Adams[2] concerning the legitimacy of treating H_1 and H_2 as small perturbations. Adams pointed out that the most general wave function which satisfies the subsidiary conditions (24) is

$$\exp(-iv_k^{\frac{1}{2}}\rho_k q_k)\chi(r_1\cdots r_N), \tag{30}$$

where χ is an arbitrary function of the particle coordinates. He pointed out that the expectation values of H_0, H_1, with respect to (30) separately diverge. [Note, however, that H_2 does not diverge. In fact, with respect to (30) $\langle H_2\rangle=0$.] Since H_{ext}' as a whole must have finite eigenvalues [as it clearly does in the original representation (9)], this means that there is a cancellation of infinities among the terms of H_{ext}', if we take its expectation value with respect to an exact eigenfunction which satisfies the subsidiary conditions. Adams, therefore, concludes that the split of H_{ext}' into H_0, H_1, and H_2 in (22) is artificial and meaningless.

This conclusion is incorrect. The fact which Adams pointed out amounts only to the statement that none of the perturbation wave functions can satisfy the subsidiary conditions (24). This is evidently true, because the subsidiary conditions (24) do not commute with H_0; but this is not relevant to the present development, because we do not require (24) to be rigorously satisfied. The logic of the present development consists of first justifying the use of perturbation methods in the calculation of the eigenvalues of $H_{\text{ext}'}$ (and we may ignore the subsidiary conditions while doing so), and then pointing out that in a consistent perturbation treatment it is *necessary* to relax the subsidiary conditions. If we do not relax the subsidiary conditions, the procedure would be inconsistent and meaningless.

To emphasize the logical steps in our development, we shall recapitulate the procedure as follows:

(1) Our primary concern is to calculate the eigenvalues of the physical Hamiltonian H. To do this, we shall first diagonalize H_{ext}'. After this is done, we omit the states of H_{ext}' which do not satisfy the subsidiary conditions (24).

(2) The different operators H_0, H_1, and H_2 in (22) clearly separately have finite eigenvalues. It has been shown, further, that for the low-lying eigenvalues of H_{ext}', the contributions of H_1 and H_2 are small compared to that of H_0. Therefore, we are justified in treating H_1 and H_2 as small perturbations, *insofar as the calculation of eigenvalues are concerned.*

(3) The ground-state energy of H is immediately obtained, because it coincides with the ground-state energy of H_{ext}', as we have argued in the last section.

(4) To obtain the excited energy levels of H, we need to know which states of H_{ext}' satisfy the subsidiary conditions. Since the eigenfunctions of H_{ext}' are calculated only approximately, we only require that they satisfy the subsidiary conditions approximately. It is incorrect to require that they satisfy the subsidiary conditions exactly. The exact subsidiary conditions are incompatible with the approximate Hamiltonian, because they do not commute with the latter.

(5) A consistent procedure can be given in which the subsidiary conditions are satisfied only to a given order in the language of the perturbation theory employed. That this is formally possible and, in fact, physically meaningful renders the whole theory consistent, as the next section shows.

The main emphasis of the present development is on the calculation of the energy levels of H. The approximate wave functions calculated with the present procedure may not be good approximations at all to the actual wave functions. It is well known that for a many-body system, perturbation theory always yields better energies than wave functions. In the formal

structure of this theory, the only purpose the wave functions serve is to provide a correct way to identify which (approximate) eigenvalues of H_{ext} are to be retained (and are approximations to the eigenvalues of H), by virtue of the fact that the corresponding (approximate) wave functions satisfy the (approximate) subsidiary conditions. The essential point is that all the words "approximate" have the same well-defined meaning.

5. FINAL CANONICAL TRANSFORMATION

Once we have ascertained, as in the plasmon problem, that the residual "particles" and the oscillators can be decoupled approximately for some choice of k_c, our object at the outset has largely been won. However, as we have discussed in the last section, the simple perturbation calculation described in the last section is unsatisfactory, because if we diagonalize H_{ext}' approximately in this way, we will find that *none* of our approximate eigenstates satisfy the subsidiary conditions; but some will satisfy them approximately. A systematic approximation procedure must therefore make concomitant approximations in the subsidiary conditions. One way to do this, as mentioned previously, is to make a further canonical transformation to decouple the particles and the oscillators to a given order. The consistent changes required in the subsidiary conditions will then be made automatically.

Again, we shall summarize briefly the results of BP. We drop the nonlinear coupling term in (22), and diagonalize the linear coupling term to order g^2 by a standard perturbation-theoretic canonical transformation. To this order, the collective plasma oscillations and the individual particles become completely decoupled. The particles acquire thereby an effective mass m^*, and the plasma oscillations a new frequency ω_k, slightly different from ω_p. The Hamiltonian in this new representation, neglecting terms of order higher than g^2, is given by

$$H_{\text{ext}}''=\sum_{i=1}^{N}\frac{p_i^2}{2m^*}+\tfrac{1}{2}\sum_{k<k_c}'\left[(\pi_k^*\pi_k+\omega_k^2 q_k q_k)-nv_k\right]+H_{\text{s.r.}}+H_{\text{r.p.}}, \quad (31)$$

where $H_{\text{r.p.}}$ is a weak electron-electron interaction arising from the exchange of virtual plasmons. The effective mass is given by

$$m^*/m=3N/(3N-N'), \quad (32)$$

while ω_k is defined by the dispersion relation

$$1=\sum_{i=1}^{N}\frac{\omega_p^2}{[\omega_k-(\mathbf{k}\cdot\mathbf{p}_i/m)]^2-(k/2m)^2}, \quad (k<k_c). \quad (33)$$

Although ω_k as defined by (33) is strictly speaking an operator involving particle variables, it has been shown in BP that its nondiagonal matrix elements are all of higher order than g^2. It may therefore be considered a c number to order g^2. In fact, for the value of k_c given by (26), we have[5]

$$\frac{\omega_k}{\omega_p}\cong 1+\frac{3}{10}\frac{k_f^2k^2}{m\omega_p^2}+\frac{k^4}{8m^2\omega_p^2}, \quad (34)$$

where k_f is the wave vector of the Fermi level.

The subsidiary conditions now read

$$[\Omega_0(\mathbf{k})+\Omega_1(\mathbf{k})+\cdots]\psi=0, \quad (k<k_c) \quad (35)$$

where

$$\Omega_0(\mathbf{k})=\sum_{j=1}^{N}e^{i\mathbf{k}\cdot\mathbf{r}_j},$$
$$\Omega_1(k)=\sum_{j=1}^{N}(\mathbf{k}\cdot\mathbf{p}_j/m\omega_p)^2e^{i\mathbf{k}\cdot\mathbf{r}_j}. \quad (36)$$

It is clear that Ω_0 is of zero order in g^2, and Ω_1 is of first order in g^2, etc. Since we are solving for the energies of the system to first order in g^2, we need the wave functions only accurate to zero order in g^2. Therefore the subsidiary conditions are

$$\textstyle\sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j}\psi=0, \quad (k<k_c). \quad (37)$$

These conditions are compatible with the Hamiltonian (31), because they commute with the latter, to zero order in g^2. We note that (35) and (37) are independent of the plasma variables. The eigenfunctions of H_{ext}'' are products of particle wave functions and oscillator wave functions. The subsidiary conditions impose restrictions only on the particle wave functions.

To this order of approximation, then, the N' plasma variables become truly independent variables, while the particle degrees of freedom are reduced from $3N$ to $3N-N'$ by the subsidiary conditions (37). The meaning of (37) is clear. It states that the wave functions ψ must vanish for configurations in which $\sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j}\neq 0$, but are otherwise arbitrary. The N' conditions,

$$\sum_{j=1}^{N}e^{i\mathbf{k}\cdot\mathbf{r}_j}=0, \quad (k<k_c)$$

define a $3N-N'$ dimensional subspace in the $3N$-dimensional configuration space. The subsidiary condition specifies that ψ must vanish outside of this subspace.

No problem arises insofar as the plasma variables are concerned. Since the plasma wave functions are not restricted by subsidiary conditions, H_{ext}'' correctly gives the complete spectrum of the plasma oscillations. The lowest energy state of the system thus corresponds to one in which no collective oscillations are excited. The burden of satisfying the subsidiary conditions fall entirely on the "particles," which are actually "bare" electrons surrounded by a cloud of plasmons.

The final variational calculation of the ground state of $H_{\text{ext}}''(k_c)$, which determines k_c by choosing that which

yields the lowest energy, is one for which the error incurred cannot be *a priori* determined—a feature of all variational calculations. It is only when we compare the resulting energy to experimental values that we know how good it is; but once this is done, we have determined N' in terms of physical variables, as given by (26) and (11). It now has definite physical significance. The extended Hamiltonian H_{ext}'' corresponding to N' is then completely fixed, and acquires physical significance, in contradistinction to all others in the family of extended Hamiltonians. The variational method adopted is hence not quite the usual one, because what we do here is to compare the results from *different* Hamiltonians with a fixed type of perturbation wave function, and then pick out the best Hamiltonian. In principle, the low-lying excited states can then be calculated with this Hamiltonian plus subsidiary conditions, with the same value of k_c.

With the above, we have completed the logical development of the collective description of the electron gas.

The Hamiltonian in the representation (31) is the one actually adopted by BP for the calculation of the ground-state energy and the low-temperature specific heat of electrons in metals.[2,12] The results obtained are in good agreement with experiments. However, the subsidiary conditions (37) have not been taken into account in the calculations mentioned. The particle wave functions used consist of a Slater determinant of plane waves, modified slightly by the short-range correlations introduced by $H_{\text{s.r.}}$ and $H_{\text{r.p.}}$, and do not satisfy the subsidiary conditions (37). In view of the agreement with experiments, one must ask why it is that, first, the ground-state energy is so closely approximated; and that, second, the specific heat does not contain spurious contributions from the extra N' degrees of freedom that are in fact quenched by the subsidiary conditions. We shall try to answer these questions on physical grounds.

Let us consider how the particle wave function need be modified in order that it might satisfy the subsidiary conditions and what the effect of such modifications might be on the energy. The desired modification involves the introduction of rather slight and subtle correlations in the electron positions, of just such a kind as to bring about the reduction in the long-range density fluctuations implied by (37). Such modifications will not, however, influence the energy appreciably. First of all, the potential energy (coming from $H_{\text{s.r.}}$) will be relatively unaffected, because $H_{\text{s.r.}}$ involves only short-wavelength density fluctuations ($k>k_c$) while the subsidiary conditions influence only the long-wavelength ones ($k<k_c$). Hence we might expect that terms arising from $H_{\text{s.r.}}$ will be influenced by the subsidiary conditions only to the extent that the long-wavelength density fluctuations are coupled to the short-wavelength ones. This coupling proceeds via H_2, and is, as we have seen, extremely small for any realistic choice of k_c. Secondly, the kinetic energy is also relatively unaffected, because the long-range correlation implied by (37) involves only slowly varying fluctuations in the particle density and hence "costs" little in kinetic energy.

As to the specific heat at low temperatures, one might at first think that since the number of electronic degrees of freedom is reduced from $3N$ to $3N-N'$ by the subsidiary conditions, the specific heat should also be correspondingly reduced if one had taken the subsidiary conditions into account; but this is not true. The effect of the subsidiary conditions becomes important only when we consider an excited level of the system in which an electron has sufficient energy to excite a plasmon (i.e., $\hbar\omega_p\sim 8$ ev), because it is only then that we have to be careful about the degrees of freedom allowed the electrons. Near the ground state, and indeed for levels near the ground state up to an energy large compared to kT, where T is room temperature, no electron can have that much energy. Consequently, calculating the specific heat with or without the subsidiary conditions makes little difference. To put the argument a different way, we may say that the subsidiary conditions "freeze out" certain electron excited states in which an electron has sufficient energy to excite a plasmon; but actually near the ground level there are no such states. Such states, if there were any, have already been "frozen out" by the Pauli principle, which effectively allows not all N, but only a fraction kT/E_F (E_F=Fermi energy) of the electrons to be free. For most metals, $E_F\sim 5$ ev, so that even at room temperature,

$$kT/E_F\sim 1/200.$$

This is to be compared with the fraction of degrees of freedom excluded by the subsidiary condition, namely,

$$N'/3N\sim 1/50 \text{ to } 1/10,$$

for all metals. We see that for temperatures up to room temperature, the inhibition by the Pauli principle is much stronger than that by the subsidiary conditions.

In this connection, it is interesting to note that Kanazawa[13] has recently carried out a calculation of the diamagnetic susceptibility by using the methods of the collective description. In his calculation he explicitly takes the subsidiary conditions into account. The results he obtains differ only slightly from those found by one of us[6] ignoring the influence of the subsidiary conditions.

6. CONCLUSION

We have seen that the subsidiary conditions do not cause any essential complications in the development of our description of electron interaction. Thus we have shown that the physical properties of the electron

[12] D. Pines, Phys. Rev. **92**, 626 (1953).

[13] H. Kanazawa, Progr. Theoret. Phys. Japan **15**, 273 (1956).

system which we calculate ignoring the subsidiary conditions are in fact rather accurate, and we have understood the underlying reasons for the validity of the "no subsidiary condition" approximation. We might summarize these reasons in the following fashion:

(1) The ground state of the extended Hamiltonian, if nondegenerate as it almost certainly is, agrees with the ground state of our original Hamiltonian. This encourages one to attempt an accurate solution for the extended Hamiltonian ground state.

(2) We find that for a suitable choice of k_c, such an accurate solution may be obtained. It is equivalent to a perturbation theory expansion in powers of g^2, where g^2, the plasmon-electron coupling constant, is approximately $\frac{1}{16}$.

(3) To terms of order g^2, the subsidiary conditions can be transformed to a representation in which they do not involve the plasmon variables. Hence the plasmons will be completely unaffected by the subsidiary conditions (up to order g^2). In this representation the subsidiary conditions do act on the electron variables. However, we can neglect their effect on the ground-state properties, to the extent that we have a good solution for our extended Hamiltonian. Furthermore, we have seen, on physical grounds, why the subsidiary conditions will not markedly influence the ground-state energy.

(4) Finally, we find that the subsidiary conditions do not appreciably affect the specific heat, because the degrees of freedom which might be "frozen out" by the subsidiary conditions have long since been frozen out by the Pauli principle.

We should like to remind the reader that the simple determinantal wave function, which has frequently been employed to calculate metallic properties on the above model, certainly does not satisfy the subsidiary conditions. (It does, of course, satisfy $\langle \rho_k \rangle_{\text{Av}} = 0$.) We strongly suspect that the true wave function, which does satisfy the subsidiary conditions, differs drastically from simple determinantal form, though we emphasize our belief that all physical properties calculated with the true wave function will closely resemble those already calculated with the simple determinantal wave function (modified to take into account the short-range electron correlation). How might one, however, try to get an improved wave function? Clearly one way to do this is to get a better solution for the Hamiltonian, H_{ext}'', Eq. (31). As remarked in BP, the improvements must come from taking into account the influence of $H_{\text{r.p.}}$ on the system wave function, since $H_{\text{r.p.}}$ is the only term in (31) capable of modifying the wave function in such a fashion as to enable it to satisfy (35).

Unfortunately, but not surprisingly, one cannot do this simply, i.e., by perturbation theory. If one treats $H_{\text{r.p.}}$ by perturbation theory, one finds that the second-order perturbation-theoretic contribution is of the same size as the zero-order one. Both contributions are extremely small compared to the kinetic energy. (They represent corrections of less than 5%.) Thus we are in no convergence difficulties as far as calculation of the energy is concerned, but it is necessary that we go beyond second-order perturbation theory in treating this term. This we have not yet accomplished.

In conclusion we remark that there now exist two systems for which our assertions concerning the role played by the subsidiary conditions may be rigorously checked. One is the free-electron gas at very high densities ($r_s < 1$). The energy of this system has recently been calculated by Gell-Mann and Brueckner[14] by a quite different method which is valid in the high-density limit. The comparison should be between the two different methods of calculating the long-wavelength part of the Coulomb interaction ($k < k_c$). (The calculation of the energy arising from $H_{\text{s.r.}}$ by second-order perturbation theory is certain to be improved by the adoption of the Gell-Mann-Brueckner techniques.) At this writing a detailed comparison is not possible because Brueckner and Gell-Mann omitted certain terms (analogous to the plasmon modes) which contribute to the correlation energy,[15] but a comparison in the near future should be feasible.

The second system is the dilute hard-sphere boson gas, which has recently been treated by using methods identical to those discussed in the foregoing.[16] Again the energy so obtained agrees with that obtained by a quite different method by several investigators.[17]

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APPENDIX

In this appendix we study a simple example of a particle coupled to an external field via a coupling of the type similar to that encountered in (15). The example chosen is simple enough so that we can calculate the lowest eigenvalue exactly, and see that by increasing the external field in any manner the eigenvalue always increases.

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[14] M. Gell-Mann and K. Brueckner, Phys. Rev. **106**, 364 (1957). We should like to thank Dr. Gell-Mann and Dr. Brueckner for making their manuscript available to us in advance of publication.

[15] K. Brueckner (private communication).

[16] D. Pines and P. Nozieres (to be published).

[17] T. D. Lee and C. N. Yang, Phys. Rev. **105**, 1128 (1957); Lee, Huang, and Yang, Phys. Rev. **106**, 1135 (1957); Proceedings of the Stevens Institute Conference on Many-Body Problems (to be published); K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957); K. Brueckner and K. Sawada, Phys. Rev. **106**, 1117, 1128 (1957).

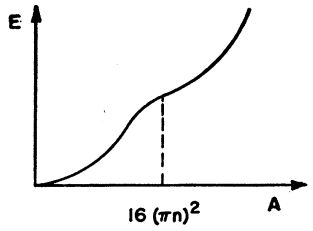

FIG. 2. E as a function of A, showing that in this one-dimensional model, turning on an external field ($A>0$) always increases the energy.

The Hamiltonian in the absence of external field is a very trivial one of a one-dimensional particle in a box of unit length, with periodic boundary conditions:

$$H=-d^2/dx^2. \tag{A1}$$

The lowest eigenvalue is obviously zero. We can rewrite, as an identity,

$$H=-\frac{d^2}{dx^2}+\tfrac{1}{2}(\rho_n{}^*\rho_n-1), \tag{A2}$$

where

$$\rho_n\equiv e^{2\pi inx}, \tag{A3}$$

n being a positive integer not zero. Assume now that an external field C can be turned on by merely letting

$$\rho_n\rightarrow\rho_n+C, \tag{A4}$$

where C is an arbitrary complex number. The Hamiltonian with this field turned on is then

$$H(C)=-\frac{d^2}{dx^2}+\tfrac{1}{2}(C^*C+C^*e^{i2\pi nx}+Ce^{-i2\pi nx}). \tag{A5}$$

In terms of the argument and modulus of C, i.e., writing

$$C=Ae^{i\varphi}, \tag{A6}$$

we have

$$H(A,\varphi)=-\frac{d^2}{dx^2}+\tfrac{1}{2}A^2+A\cos(2\pi nx-\varphi). \tag{A7}$$

We seek the lowest eigenvalue E of $H(A,\varphi)$. Letting

$$z=\pi nx-\tfrac{1}{2}\varphi, \tag{A8}$$

we find that the eigenfunctions ψ satisfy Mathieu's equation,

$$\frac{d^2\psi}{dz^2}+\frac{1}{(\pi n)^2}[(E-\tfrac{1}{2}A^2)-A\cos(2z)]\psi=0, \tag{A9}$$

with the periodic boundary conditions that $\psi(z)$ be periodic in z with period π. The state that has the lowest value, for any value of A, is[18]

$$\psi(z)=Ce_0(z,A), \tag{A10}$$

where $Ce_0(z,A)$ is the Mathieu function which reduces to unity when $A=0$. The corresponding eigenvalue is well known. We shall just quote the results:

$$E=\tfrac{1}{2}\left(1-\frac{1}{4}\frac{1}{(\pi n)^2}\right)A^2+\frac{7}{2048}\left(\frac{A^4}{(\pi n)^6}\right)+O(A^6)$$

$$\text{for } A/[16(\pi n)^2]\ll 1, \tag{A11}$$

and

$$E=\tfrac{1}{2}A^2-(1-\tfrac{1}{4}\sqrt{2})A-(\tfrac{1}{2}\pi n)^2+O(1/A)$$

$$\text{for } A/[16(\pi n)^2]\gg 1. \tag{A12}$$

As a function of A, E shows the qualitative behavior shown in the sketch of Fig. 2. It is clear that $A=0$ is a minimum of E, yielding $E=0$, and that it is the only minimum.

[18] E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, Cambridge, 1948), Chap. XIX.