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ON THE STABILITY OF THE PLANE-WAVE HARTREE-FOCK STATE

by

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ON THE STABILITY OF THE PLANE-WAVE HARTREE-FOCK STATE

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SUMMARY - Considering small deviations from the paramagnetic plane-wave Hartree-Fock state, the condition for the stability of that state is derived using Landau's theory of the Fermi liquid. It is shown that this condition is identical with that derived by other many-body techniques. Comparison is made with Overhauser's theory of giant static spin-density waves.

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Recently some interest has been shown in the problem as to whether the plane-wave Hartree-Fock state is really the ground state of an interacting fermion system. Thouless[1] and Iwamoto and Sawada[2] studied the stability of the plane-wave state by considering an arbitrary, but small deviation from that state. They found that at least in the high-density region the plane-wave state is stable, whereas for lower densities a not explicitly specified state should develop. Iwamoto and Sawada pursued this calculation furthest by taking a screened Coulomb interaction between the particles. Wolff[3] treated the same problem from the standpoint of the spin susceptibility, using the generalized random-phase approximation, however only in the case of short-range interaction. The mentioned authors use apparently distinct methods, which involve rather complicated mathematics. It is the purpose of the present note to treat this problem using Landau's phenomenological theory of the Fermi liquid[4], and show that one gets the same results as the previous authors. This is not surprising, since it is well known that the great variety of existing many-body techniques are in fact equivalent with Landau's theory. The great virtue of Landau's theory is its simplicity and clearness, and it permits one to calculate rather easily many properties of an interacting fermion system. It has not previously been applied in full extent to the stability problem. For an introduction to the theory we refer to Landau's original articles[4] and to the book by Nozières[5], where a complete justification is given.

In Landau's theory of the Fermi liquid the role of particles are played by quasi-particles, i.e. particles moving in the self-consistent field of all the others. These quasi-particles obey Fermi-Dirac statistics. A small variation of the total free energy δF of the system at absolute temperature zero due to a small variation of the distribution function δn is written as

$$\delta F = \mathrm{Sp}\left\{(\varepsilon - \mu)\ \delta n\right\} , \qquad (1)$$

which defines ε as the quasi-particle Hamiltonian. The thermodynamic potential is denoted by μ. The spur in eq. (1) is evaluated in the plane-wave representation, which is appropriate for an extended system. Thus

$$\delta F = \mathrm{Sp}_{\sigma} \sum_{k,q} [\varepsilon(k,q,\sigma) - \mu]\delta n^*(k,q,\sigma) , \qquad (2)$$

where $\varepsilon(k,q,\sigma)$ and $n(k,q,\sigma)$ are the matrix elements of the corresponding operators between plane-wave states k and $k+q$. These quantities also depend on the spin operators. The second fundamental equation relates the change in the quasi-particle Hamiltonian to the change in the distribution function as

$$\delta\varepsilon(k,q,\sigma) = \mathrm{Sp}_{\sigma'} \sum_{k} f(k,\sigma;\ k',\sigma')\ \delta n(k',q,\sigma') . \qquad (3)$$

Here $f(k,\sigma;\ k',\sigma')$ is related to the forward scattering amplitude of two particles, as has been shown by Landau.

Combining eqs. (2) and (3) one can write the variation in the free energy in the form

$$\delta F = \mathrm{Sp}_{\sigma} \sum_{k,q} \left[\varepsilon^{o}(k,q,\sigma) - \mu\right]\ \delta n^*(k,q,\sigma) +$$

$$+ \frac{1}{2}\ \mathrm{Sp}_{\sigma}\ \mathrm{Sp}_{\sigma'} \sum_{k,k',q} f(k,\sigma;\ k',\sigma')\ \delta n(k',q,\sigma')\ \delta n^*(k,q,\sigma),$$

where ε^{o} is the unperturbed quasi-particle Hamiltonian.

If $\delta F > 0$, the state characterized by the distribution function n^{o} will be stable, whereas for $\delta F < 0$ that state will be unstable. Thus by looking at $\delta F = 0$ we can find the critical condition for a transition from one state to another. What remains to be done is to evaluate eq. (4).

Since $\delta\varepsilon$ is small compared to ε^{o}, we can use Schafroth's[6] expansion for the matrix elements of δn in terms of the matrix elements of $\delta\varepsilon$. The result is up to second order

$$\langle k_1|\delta n|k_2\rangle = \frac{n^{o}(k_1) - n^{o}(k_2)}{\varepsilon^{o}(k_1) - \varepsilon^{o}(k_2)} \langle k_1|\delta\varepsilon|k_2\rangle +$$

$$+ \sum_{k_2} \langle k_1|\delta\varepsilon|k_3\rangle \langle k_3|\delta\varepsilon|k_2\rangle \sum_{i=1}^{3} \frac{n^{o}(k_i)}{\prod_{j\neq i} \left[\varepsilon^{o}(k_i) - \varepsilon^{o}(k_j)\right]} , \quad (5)$$

where $n^{o}(k)$ and $\varepsilon^{o}(k)$ are the diagonal matrix elements, which do not depend on the spin.

Using this expansion up to first order, eq. (3) can now be written as

$$\delta\varepsilon(k,q,\sigma) = Sp_{\sigma'} \sum_{k'} f(k,\sigma;\, k',\, \sigma') \frac{n^{o}(k'+q) - n^{o}(k')}{\varepsilon^{o}(k'+q) - \varepsilon^{o}(k')} \delta\varepsilon(k',q,\sigma') \quad (6)$$

which is an integral equation for $\delta\varepsilon(k,q,\sigma)$. In order to find a solution of eq. (6) we use the ansatz

$$\delta\varepsilon(k,q,\sigma) = \alpha(k,q) - \gamma(k,q)\, \sigma\cdot e(q) , \quad (7a)$$

$$\delta n(k,q,\sigma) = \beta(k,q) + \zeta(k,q)\sigma\cdot e(q). \tag{7b}$$

Here $e(q)$ is an arbitrary unit vector and σ the vector spin operator. Further in the isotropic case $f(k,\sigma;k',\sigma')$ can be written as

$$f(k,\sigma;k',\sigma') = \xi(k,k') + \psi(k,k')\,\sigma\cdot\sigma', \tag{8}$$

where $\xi(k,k')$ represents the direct interaction and $\psi(k,k')$ the exchange interaction between particles.

The terms α and ξ lead to changes in the local charge density, whereas the terms γ and ψ result in changes of the local spin density. Changes in the local charge density require large positive energies and therefore tend to desencourage the transition. We therefore do not need to consider the α and ξ terms and may only look for changes in the local spin density.

Hence, with eqs. (7a) and (8) we can finally write eq. (6) in the form

$$\left[\varepsilon^{o}(k+q) - \varepsilon^{o}(k)\right]\varphi(k,q) - \frac{1}{2}\sum_{k'}\left[n^{o}(k'+q) - n^{o}(k')\right]\psi(k,k')\varphi(k',q) = 0 \tag{9}$$

where we have used the definition

$$\gamma(k,q) = \left[\varepsilon^{o}(k+q) - \varepsilon^{o}(k)\right]\varphi(k,q). \tag{10}$$

Gottfried and Goldstone[7] have established the connection with Landau's Boltzmann equation by writing eq. (9) in the co-ordinate representation. However, we prefer to use the momentum representation because the equations are easier to handle. Further the stability condition eq. (4) can now be written as

$$\sum_{k,q}\left[n^{o}(k+q) - n^{o}(k)\right]\varphi(k,q)\left\{\left[\varepsilon^{o}(k+q) - \varepsilon^{o}(k)\right]\varphi(k,q) + \right.$$
$$\left. + \frac{1}{2}\sum_{k'}\left[n^{o}(k'+q) - n^{o}(k')\right]\psi(k,k')\varphi(k',q)\right\} \geqslant 0. \tag{11}$$

We can now establish the connection with the work of Iwamoto and Sawada[2]. Choosing in a plane-wave Hartree-Fock approximation

$$\varepsilon^{o}(k) = \frac{\hbar^2 k^2}{2m} \sum_{k' \text{ occupied}} v(k-k') \qquad (12a)$$

and

$$\psi(k, k') = -2v(k-k') \qquad (12b)$$

with $v(k-k')$ the Fourier transform of the interparticle potential, from eq. (11) it follows

$$N(q) - D_1(q) + D_2(q) \geqslant 0 \ , \qquad (13)$$

where

$$N(q) = \int k \cdot q |\varphi(k,q)|^2 \frac{d^3k}{(2\pi)^3} \ , \qquad (14a)$$

$$D_1(q) = \iint \varphi^*(k,q)[v(k-k') + v(k+k')]\varphi(k',q) \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} \ , \qquad (14b)$$

$$D_2(q) = \iint |\varphi(k,q)|^2 [v(k-k') - v(k+k')] \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} \ . \qquad (14c)$$

The integrations are to be performed for $|k - \frac{1}{2} q| \leqslant k_F \leqslant |k + \frac{1}{2} q|$. Equation (9) goes over in

$$\left[\varepsilon^{o}(k+q) - \varepsilon^{o}(k)\right]\varphi(k,q) + \sum_{k'} \left[n^{o}(k'+q) - n^{o}(k')\right] v(k-k')\varphi(k',q) = 0. \qquad (15)$$

Equations (13), (14a, b, c) and (15) represent actually Iwamoto and Sawada's conditions for the stability of an extended system of electrons in the plane-wave Hartree-Fock state. These authors solve the integral equation and calculate the integrals (14a, b, c) for small q values. They also give a variational expression for the integrals (14a, b, c) for large values of q. It should be noted that eq. (15) is also the same as the integral equation found by Wolff[3], who uses the generalized random-phase approximation. He actually has an additional term which comes from an applied magnetic field. Putting this field zero his equation goes over into eq. (15).

Iwamoto and Sawada have shown that if an electron gas in a plane-wave Hartree-Fock state is unstable, this instability occurs for a value of q different from zero and only in the lower density region. Since from eq. (7b) we have

$$\delta n(k,q,\sigma) = \zeta(k,q)\sigma\cdot e(q) \;,$$

this means that a state with a spin-density wave of small amplitude becomes more stable. Such a state will have an energy spectrum with a gap, which is just given as the solution of the integral equation (15). This is so, because the integral equation is the condition for the stability of the new state.

Overhauser[8], on the other hand, proved that a state characterized by a giant spin-density wave is more stable than the plane-wave Hartree-Fock state for all densities. His condition for the stability of such a state, i.e. his gap equation, has a different form, but in the limit of a small gap, it goes over into eq. (15). Thus considering only small deviations from the plane-wave Hartree-Fock state shows at least that other states (in our case small-amplitude spin-density waves) may be more stable. However, Overhauser's work shows clearly that the conditions for the instability of the plane-wave Hartree-Fock state can never be obtained in this way. Also, one can not predict which state eventually becomes more stable, although the method indicates possible states for which one has to look.

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