On a Quasi-One-Particle Approximation in the Coulomb Many-Particle Problem

1965

SovietRxiv

Abstract

Full Text

Physics

G. L. Krasko

On a Quasi-One-Particle Approximation in the Coulomb Many-Particle Problem

(Presented by Academician G. V. Kurdyumov, 11 II 1965)

It is known (see, for example, ([1])) that in spatially homogeneous compressed systems of interacting electrons the principal contribution to the mass operator M is given by diagrams with the largest number of closed loops*:

$$M = [\text{diagram}] + [\text{diagram}] + [\text{diagram}] + \cdots = [\text{diagram}] \tag{1}$$

The small parameter in the present case is the quantity r_s, the mean distance between particles in units of the Bohr radius.

In (1), as usual, the thin solid line denotes the "unperturbed" Green function G_0, the thin dashed line the Coulomb potential v ($v(p) = 4\pi e^2/p^2$); the bold dashed line in the right-hand side of (1) is the so-called modified potential V:

$$V(p, \omega) = v(p)/\varepsilon(p, \omega), \tag{2}$$

where $\varepsilon(p, \omega) = 1 + v(p)\Pi(p, \omega)$; $\varepsilon(p, \omega)$ is the dielectric permittivity; $\Pi(p, \omega)$ is the polarization operator (p is momentum, ω is frequency).

In analytic form, relation (1) has the form

$$M(p, \omega) = i \int V(p - q, \omega - \tau) G_0(q, \tau)\, dq\, d\tau. \tag{3}$$

Let us replace in this expression the unperturbed Green function $G_0(p, \omega)$ by the full $G(p, \omega)$. Such a procedure, corresponding to the replacement in (1) of the solid thin line by a bold one, obviously introduces an error of higher order than the contribution of the diagrams discarded in (1). Therefore the relation

$$M(p, \omega) = i \int V(p - q, \omega - \tau) G(q, \tau)\, dq\, d\tau \tag{4}$$

has the same accuracy as (3). From the last expression it is seen that the equation for the function $G(q, \tau)$ will now be nonlinear; however, as we shall see, the problem can be made quasi-one-particle.

The modified potential $V(q,t)$ depends on the frequency, and therefore the interaction determined by it is, generally speaking, retarded: the dependence of $V(q,t)$ on the time t does not reduce to $\delta(t)$. Let us average $V(q,t)$ over time:

$$\int_{-\infty}^{+\infty} V(q,t)\,dt = V_{\text{eff}}(q)\int_{-\infty}^{+\infty}\delta(t)\,dt.$$

* We do not write out diagrams that compensate the homogeneous background of positive charge.

The last relation is the definition of the effective static potential $V_{\text{eff}}(q)$ ([1]). It is easy to see that

$$V_{\text{eff}}(q) = v(q)/\varepsilon(q,0). \tag{5}$$

In approximation (1), as is known ([2]),

$$\varepsilon(q,0) = 1 + \frac{\varkappa^2}{q^2}\left[\frac{1}{2} + \frac{p_F}{2q}\left(1 - \frac{q^2}{4p_F^2}\right)\ln\left|\frac{q+2p_F}{q-2p_F}\right|\right], \tag{6}$$

where $\varkappa^2 = 4me^2p_F/\pi$; p_F is the Fermi momentum; $q = |\mathbf{q}|$ ($\hbar = 1$).

In particular, at small transferred momenta q, $V_{\text{eff}}(q)$ is the screened Coulomb potential:

$$V_{\text{eff}}(q) = 4\pi e^2/(q^2 + \varkappa^2).$$

Substituting $V_{\text{eff}}(q)$ into (4) instead of $V(q,\tau)$ and integrating with respect to τ, we obtain

$$M(p,\omega) \equiv M(p) = -\int V_{\text{eff}}(p-q)n(q)\,dq, \tag{7}$$

where $n(q)$ is the "perturbed" density of particles with momentum q.

The equation for the Green function (of a paramagnetic system) thus takes the form

$$\left(G_0^{-1}(p,\omega) + \frac{1}{4}\int V_{\text{eff}}(p-q)n(q)\,dq\right)G(p,\omega) = 1. \tag{8}$$

From (8) it is easy to obtain an equation for the particle density:

$$\frac{1}{2}n(p) = \theta\left\{p^2/2m - \mu - \frac{1}{2}\int V_{\text{eff}}(p-q)n(q)\,dq\right\} \tag{9}$$

($\theta(x)$ is the Heaviside function, μ is the chemical potential).

In the case of nonzero temperature, the preceding arguments can be repeated correspondingly for the temperature Green function. Equation (9) then naturally becomes

$$\frac{1}{2}n(p) = \left[\exp\beta\left\{p^2/2m - \mu - \frac{1}{2}\int V_{\text{eff}}(p-q)n(q)\,dq\right\} + 1\right]^{-1} \tag{10}$$

(β is the inverse temperature).

If the system is not paramagnetic, then, as is easy to show, instead of (10) we shall have the system of equations:

$$\frac{1}{2}(n(p)\pm s(p)) = \left[\exp\beta\left\{p^2/2m - \mu - \frac{1}{2}\int V_{\text{eff}}(p-q)(n(q)\pm s(q))\,dq\right\} + 1\right]^{-1}, \tag{11}$$

where $s(q)$ is the mean spin density.

Equations (9)–(10) are quasi-one-particle; however, the corresponding approximation is by no means the Hartree–Fock approximation. Indeed, as is seen from (1), the approximation made takes into account correlations between particles leading to charge screening. Information about the plasma oscillations themselves (frequency, damping) in the approximation considered, naturally, cannot be obtained, since the potential has previously been averaged over time.

It should be noted that approximation (1), equivalent to the so-called random-phase approximation, gives good results at small transferred momenta also in the interval $1.8 \leq r_s \leq 5.5$ ([2]), i.e., at electron densities actually existing in metals. However, already for $r_s > 1$ interactions with large transferred momentum become substantial, which leads to an increase in the contribution of exchange polarization diagrams not taken into account in (1) (at very large momenta such diagrams compensate by one half the contribution from the direct interaction).

In this connection, in ([3,4]) interpolation procedures (in momentum) were proposed, which make it possible to apply the random-phase approximation with good accuracy to the description of real systems with an intermediate particle density. Hubbard' s interpolation ([3]) consists in replacing the polarization operator $\Pi(p,\omega)$ by the quantity

$$\Pi'(p,\omega) = \Pi(p,\omega)/[1 + f(p)v(p)\Pi(p,\omega)], \tag{12}$$

where $f(p) = \frac{1}{2}p^2/(p^2 + p_F^2)$.

In this case $V(p,\omega)$ and $V_{\text{eff}}(p)$ are correspondingly changed. Obviously, replacing $G_0(p,\omega)$ by $G(p,\omega)$ in (3) should also lead to an improvement of the random-phase approximation, owing to the inclusion of additional diagrams. Moreover,

as is known, many-particle correlations for $r_s > 1$ manifest themselves chiefly in charge screening, whereas plasma oscillations are hardly excited. Therefore, for $r_s > 1$, replacing the retarded potential $V(p, \omega)$ by the static $V_{\text{eff}}(p)$ is the most natural and leads to the smallest error.

The circumstances indicated apparently make it possible to extend the range of applicability of the quasione-particle approximation described above to the density interval $1.8 \leq r_s \leq 5.5$.

It is interesting that equations of the form (11) were obtained and investigated earlier in ([5]). However, in those equations, instead of $V_{\text{eff}}(q)$, there appeared the "bare" potential v from the Hamiltonian; the equations themselves were obtained by the so-called simplest decoupling of the two-particle Green' s function, which does not take correlations into account.

From what has been said one may conclude that the "dressing" of the potential in the simplest decoupling of the two-particle Green' s function, on the one hand, substantially improves this approximation and, on the other, makes it possible to draw a conclusion about the range of its applicability.

Institute of Metallurgy and Physics of Metals
of the Central Scientific-Research
Institute of Ferrous Metallurgy
named after I. P. Bardin

Received
8 II 1965

REFERENCES

1. D. A. Kirzhnits, *Field Methods of the Theory of Many Particles*, 1963.

2. D. Pines, *The Many-body Problem*, 1961; D. Pines, *The Many-Body Problem*, IL, 1963.

3. J. Hubbard, Proc. Roy. Soc., *A243*, 336 (1958); translated in the collection *Problems of the Quantum Theory of Many Bodies*, IL, 1959.

4. P. Nozières, D. Pines, Phys. Rev., *111*, 442 (1958).

5. R. A. Suris, *Fiz. tverd. tela*, 3, No. 6, 1795 (1961).

Note: Figure translations are in progress. See original paper for figures.