

SINGLE-PARTICLE EXCITATIONS IN A NON-DEGENERATE GAS

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We evaluate the single-particle Green's function of a nondegenerate electron gas in the Born approximation. We show that when we take the Coulomb interaction into account the single-particle excitations (plane waves) are distorted because of damping and because of a time modulation of the unperturbed wave.

THE expression $\langle a_p(t') a_p^+(t) \rangle$; $t' > t$ (the averaging is over a canonical ensemble and the operators are in the Heisenberg representation) describes the time-dependence of a particle with momentum p which at time t is in a system of N such particles. When there is no interaction

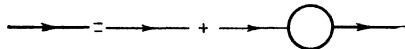
$$\langle a_p(t') a_p^+(t) \rangle \sim \exp(-i\epsilon_p t/\hbar),$$

i.e., the particle is described by a plane wave. When there are interactions the time dependence of $\langle a_p(t') a_p^+(t) \rangle$ will differ from this simple law. One can, however, expect a simple periodic law in the case where the interaction is weak, at least for not too long times, and that the deviations from it will be small. The deviations indicate the order of magnitude of the times during which the particle can be described by a plane wave. In the present paper we consider the time behavior of such a single-particle correlation function (more exactly, a Green's function) for a nondegenerate electron gas in the Born approximation.

1. THE DYSON EQUATION

The Dyson equation for the single-particle thermodynamic Green's function is of the form

$$\begin{aligned} G_p(\tau' - \tau) &= G_p^{(0)}(\tau' - \tau) \\ &+ \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 G_p^{(0)}(\tau_1 - \tau) \Sigma_p(\tau_2 - \tau_1) G_p(\tau' - \tau_2) \end{aligned} \quad (1)$$



(the diagrammatic form is under the equation). The thin, directed full-drawn line corresponds to the zeroth order thermodynamic Green's function:

$$\begin{aligned} G_p^{(0)}(\tau' - \tau) &= -\text{Sp} \{ e^{\beta(\Omega + \mu N - H_0)} T(a_p(\tau') a_p^+(\tau)) \} \\ &= -\langle T a_p(\tau') a_p^+(\tau) \rangle_0; \end{aligned}$$

where

$$\hat{A}(\tau) = e^{\tau(H_0 - \mu N)} \hat{A} e^{-\tau(H_0 - \mu N)}.$$

The thick, directed full-drawn line corresponds to the single-particle thermodynamic Green's function

$$\begin{aligned} G_p(\tau' - \tau) &= -\text{Sp} \{ e^{\beta(\Omega + \mu N - H_0)} T(a_p(\tau') a_p^+(\tau) S(\beta)) \} \\ &= -\langle T(a_p(\tau') a_p^+(\tau) S(\beta)) \rangle_0, \end{aligned}$$

where

$$S(\beta) = T \exp \left(- \int_0^\beta H_i(\tau) d\tau \right),$$

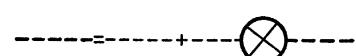
$H_i(\tau)$ is the interaction operator in the interaction representation, and $\Sigma_p(\tau_2 - \tau_1)$ is the mass operator, which is the sum of all possible compact diagrams. In the case of the Coulomb interaction, which we consider henceforth,

$$\begin{aligned} H_0 &= \sum_p \frac{\hbar^2 p^2}{2m} a_p^+ a_p, \\ H_i &= \frac{1}{2V} \sum_{p_1 p_2} \sum_{q \neq 0} V_q a_{p_1}^+ a_{p_2}^+ a_{p_2-q} a_{p_1+q}, \quad V_q = 4\pi e^2/q^2, \end{aligned}$$

 V is the volume of the system.

One can write down a similar equation for the modified interaction potential:

$$W_q(\tau' - \tau) = V_q \delta(\tau' - \tau) + V_q \int_0^\beta \Pi_q(\tau_1 - \tau) W_q(\tau' - \tau_1) d\tau_1. \quad (2)$$



The thick dotted line corresponds to the modified potential $W_q(\tau' - \tau)$; the thin dotted line corresponds to the Coulomb potential; Π_q is the sum of all compact diagrams.

In the following we shall solve Eqs. (1) and (2) in the Born approximation, using for Σ_p an expression which is of second order in the interaction constant; this corresponds to taking the dia-

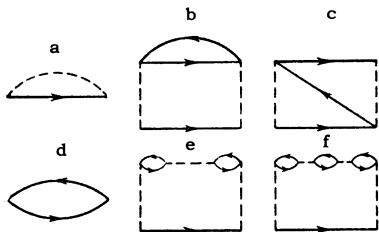


FIG. 1

grams a, b, and c of Fig. 1 into account; for Π_q we retain the lowest order term depicted in Fig. 1d. We must note that the contribution from diagram 1b diverges for small momenta and we need the subsequent diagrams in terms of the Born parameter, such as 1e and 1f, to get rid of this divergence. The diagram 1c takes the second-order exchange effects into account and can be dropped in our case of a nondegenerate gas. In practice one can reduce the evaluation of the contribution of the diagrams 1a and 1b with the corrections 1e, 1f, and so on to evaluating the contribution from diagram 1a where the interaction is replaced by the modified interaction.

One can use the Feynman rules^[1] to write down explicitly the expressions corresponding to the different diagrams: each full-drawn line directed from τ to τ' corresponds to $G_p^0(\tau' - \tau)$, and each dotted line to $V_q \delta(\tau' - \tau)$; in each vertex the momentum conservation law is satisfied; each n-th order diagram has a factor

$$(-1)^{n+L}g/2^n n! V^n,$$

where L is the number of closed electron loops, g a factor which is equal to the number of non-equivalent diagrams which can be obtained from the given one by a permutation of the endpoints of the dotted lines and of pairs of dotted lines. The summation is over all internal momenta and the integration from 0 to β over all internal times. The unperturbed Green's functions are of the form

$$\begin{aligned}\mathfrak{G}_p^{(0)}(\tau' - \tau) &= \begin{cases} (n_p - 1)e^{(\tau' - \tau)(\mu - \varepsilon_p)} & \tau' > \tau \\ n_p e^{(\tau' - \tau)(\mu - \varepsilon_p)} & \tau' < \tau, \end{cases} \\ \mathfrak{G}_p^{(0)}(0) &= -n_p.\end{aligned}$$

In the following we use Boltzmann statistics everywhere: we assume the Born parameter $e^2/\hbar v_T$ to be small ($v_T = \sqrt{2/m\beta}$).

To solve the Dyson equation we use an expansion of the thermodynamic Green's functions in a Fourier series in the variable τ :^[4,6]

$$\mathfrak{G}_p(i\omega_n) = \frac{1}{2} \int_{-\beta}^{+\beta} \mathfrak{G}_p(\tau) e^{i\omega_n \tau} d\tau,$$

$$\mathfrak{G}_p(\tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} \mathfrak{G}_p(i\omega_n), \quad \omega_n = n\pi/\beta. \quad (3)$$

The Dyson equation becomes then

$$\begin{aligned}\mathfrak{G}_p(i\omega_n) &= \mathfrak{G}_p^{(0)}(i\omega_n) + \mathfrak{G}_p^{(0)}(i\omega_n) \Sigma_p(i\omega_n) \mathfrak{G}_p(i\omega_n), \\ \mathfrak{G}_p^{(0)}(i\omega_n) &= (i\omega_n + \mu - \varepsilon_p)^{-1}, \quad \omega_n = (2k+1)\pi/\beta, \\ (k &= 0, \pm 1, \dots).\end{aligned}\tag{4}$$

$$\mathfrak{G}_p^{-1}(i\omega_n) = \mathfrak{G}_p^{(0)-1}(i\omega_n) - \Sigma_p(i\omega_n). \quad (5)$$

2. THE MODIFIED POTENTIAL $W_q(\tau)$

It is not possible to go in Eq. (2) directly over to the Fourier representation, since the function $W_q(\tau)$ does not satisfy the condition $W_q(\tau + \beta) = W_q(\tau)$.^[4] One can, however, write $W_q(\tau)$ in the form

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where the function K_q is the solution of the equation [3]

$$K_q(\tau_2 - \tau_1) = \Pi_q(\tau_2 - \tau_1) + V_q \int_0^{\beta} \Pi_q(\tau - \tau_1) K_q(\tau_2 - \tau) d\tau. \quad (7)$$

$$\square = \text{Diagram A} + \text{Diagram B} - \square$$

We can now go over to the Fourier representation in Eq. (7).

We have

$$K_q(i\omega_n) = \Pi_q(i\omega_n)/[1 - V_q\Pi_q(i\omega_n)], \quad \omega_n = 2n\pi/\beta. \quad (8)$$

We have then

$$W_q(\tau) = V_q \delta(\tau) + \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} \frac{V_q^2 \Pi_q(i\omega_n)}{1 - V_q \Pi_q(i\omega_n)}$$

$$\equiv V_q \delta(\tau) + \tilde{W}_q(\tau). \quad (9)$$

We evaluate $\Pi_Q(\tau)$ in the above-mentioned approximation. Using the Feynman rules we get

$$\Pi_q(\tau) = \frac{1}{V} \sum_{\sigma} \mathfrak{G}_{p-q/2}^{(0)}(\tau) \mathfrak{G}_{p+q/2}^{(0)}(-\tau), \quad (10)$$

from which it is clear that $\Pi_q(-\tau) = \Pi_q(\tau)$ while $\Pi_q(i\omega_n)$ is of the form

$$\Pi_q(i\omega_n) = \frac{1}{2} \int_{-\beta}^{+\beta} e^{i\omega_n \tau} \Pi_q(\tau) d\tau$$

$$= -\frac{1}{(2\pi)^3} \int d^3 p \frac{n_{p+q/2} - n_{p-q/2}}{i\omega_n + \epsilon_{p-q/2} - \epsilon_{p+q/2}} . \quad (11)$$

Calculations give for $\Pi_Q(\tau)$

$$\Pi_q(\tau) = -n_0 \exp\{\beta \varepsilon_{q/2} (2\tau/\beta - 1)^2 - \beta \varepsilon_{q/2}\}, \quad (12)$$

where n_0 is the particle density, $n_0 = N/V$.

For $\Pi_q(i\omega_n) \equiv \Pi_q(n)$ we get

$$\begin{aligned} \Pi_q(2k) &= -\beta n_0 \varphi_k(\sqrt{\beta \epsilon_{q/2}}), \quad \Pi_q(2k+1) = 0, \\ \varphi_k(x) &= (-1)^k e^{-x^2} \int_0^1 \cos k\pi z e^{xz^2} dz. \end{aligned} \quad (13)$$

The function $\varphi_k(x)$ has the following properties

$$\varphi_0(0) = 1, \quad \varphi_k(0) = 0, \quad k \neq 0, \quad \varphi_k(x) \geq 0;$$

for small x

$$\varphi_0(x) = 1 - 2x^2/3, \quad \varphi_k(x) = 2x^2/\pi^2 k^2, \quad k \neq 0.$$

The function $\tilde{W}_q(i\omega_n)$ is of the form

$$\begin{aligned} \tilde{W}_q(i2k\pi/\beta) &= -\frac{4\pi e^2 \kappa^2 \varphi_k(\sqrt{\beta \epsilon_{q/2}})}{q^2(q^2 + \kappa^2 \varphi_k(\sqrt{\beta \epsilon_{q/2}}))} \\ &= 4\pi e^2 \left(\frac{1}{q^2 + \kappa^2 \varphi_k} - \frac{1}{q^2} \right); \\ \tilde{W}_q(i(2k+1)\pi/\beta) &= 0; \end{aligned} \quad (14)$$

where $\kappa^2 \equiv r_D^{-2} \equiv 4\pi e^2 \beta n_0$ is the inverse square of the Debye radius.

3. THE MASS OPERATOR

The mass operator is of the form

$$\begin{aligned} \Sigma_p(\tau) &= -\frac{1}{(2\pi)^3} \int d^3 q W_q(\tau) \mathfrak{G}_{p-q}^{(0)}(\tau) \\ &= -\frac{1}{(2\pi)^3} \int d^3 q V_q \mathfrak{G}_{p-q}^{(0)}(\tau) \delta(\tau) \\ &\quad - \frac{1}{(2\pi)^3} \int d^3 q \tilde{W}_q(\tau) \mathfrak{G}_{p-q}^{(0)}(\tau). \end{aligned} \quad (15)$$

The first term of (15) gives

$$\Sigma_p^{(1)}(i\omega_n) = -(\hbar^2 \kappa^2 / 2m) \varphi_0(\sqrt{\beta \epsilon_p}). \quad (16)$$

This result was obtained by Bonch-Bruevich.^[5]

We note that this is a quantum term. The second term is of the form (after we have changed to the Fourier representation)

$$\begin{aligned} \Sigma_p^{(2)}(i\omega_n) &= -\frac{1}{(2\pi)^3} \int d^3 q \sum_{n_1} \frac{V_q^2 \Pi_q(i\omega_{n_1})}{1 - V_q \Pi_q(i\omega_{n_1})} \\ &\quad \times \frac{1}{i\omega_n + \mu - \epsilon_{p-q} - i\omega_{n_1}}; \\ \omega_{n_1} &= 2n_1\pi/\beta, \quad \omega_n = (2n+1)\pi/\beta. \end{aligned} \quad (17)$$

We note that only the term with $n_1 = 0$ gives a divergence for small q . We can thus drop $V_q \Pi_q(i\omega_{n_1})$ in the denominator when $n_1 \neq 0$. Moreover, we can replace $\Pi_q(0)$ in the term with $n_1 = 0$ by $\Pi_0(0) = -\beta n_0$ since we can neglect this term for not too small values of q . Finally, it is convenient to write the term with $n_1 = 0$ as follows:

$$\frac{\Pi_q(0)}{1 - V_q \Pi_0(0)} \equiv \frac{\Pi_0(0)}{1 - V_q \Pi_0(0)} + \frac{\Pi_q(0) - \Pi_0(0)}{1 - V_q \Pi_0(0)}$$

and to drop the denominator in the second term, since the corresponding integral does not diverge.

As a result we get the following expression for $\Sigma^{(2)}$

$$\begin{aligned} \Sigma_p^{(2)}(i\omega_n) &= -\frac{1}{(2\pi)^3} \int d^3 q \frac{V_q^2 \Pi_0(0)}{1 - V_q \Pi_0(0)} \frac{1}{i\omega_n + \mu - \epsilon_{p-q}} \\ &\quad - \frac{1}{(2\pi)^3} \int d^3 q V_q^2 \frac{\Pi_q(0) - \Pi_0(0)}{i\omega_n + \mu - \epsilon_{p-q}} \\ &\quad - \frac{1}{(2\pi)^3} \int d^3 q V_q^2 \sum_{n_1 \neq 0} \frac{\Pi_q(i\omega_{n_1})}{i\omega_n + \mu - \epsilon_{p-q} - i\omega_{n_1}}. \end{aligned} \quad (18)$$

After summing over n_1 ^[6] we get an expression for the mass operator which has the following necessary analytical properties*

$$\begin{aligned} \Sigma_p^{(2)}(\omega + i\delta) &= -\frac{4}{\beta(2\pi)^4} \int d^3 q V_q^2 \int_{-\infty}^{+\infty} \frac{\Pi_q''(\omega') \coth \beta\omega'/2}{\omega + \mu - \epsilon_{p-q} - \omega' + i\delta} d\omega' \\ &\quad + \frac{1}{(2\pi)^3} \int d^3 q \frac{V_q^2 \Pi_0(0)}{\omega + \mu - \epsilon_{p-q} + i\delta} \\ &\quad - \frac{1}{(2\pi)^3} \int d^3 q \frac{V_q^2 \Pi_0(0)}{1 - V_q \Pi_0(0)} \frac{1}{\omega + \mu - \epsilon_{p-q} + i\delta}. \end{aligned} \quad (19)$$

Here $\Pi_q(\omega) = \Pi'_q(\omega) + i\Pi''_q(\omega)$ is the analytical continuation of $\Pi_q(i\omega_n)$ in the upper half-plane.^[3]

We first evaluate the first term in (19), $\Sigma_{pI}^{(2)}(\omega)$. After some calculations we get for real ω :†

$$\begin{aligned} \text{Re}\Sigma_{pI}^{(2)}(\omega) &= -\frac{me^2}{\beta\hbar^2 p} \left\{ \text{arc tg} \left(\sqrt{\frac{2m(\omega + \mu)}{\hbar^2 \kappa^2}} + p/\kappa \right)^{-1} \right. \\ &\quad \left. - \text{arc tg} \left(\sqrt{\frac{2m(\omega + \mu)}{\hbar^2 \kappa^2}} - p/\kappa \right)^{-1} \right\}, \\ (\omega + \mu > 0); \end{aligned}$$

$$\begin{aligned} \text{Im}\Sigma_{pI}^{(2)}(\omega) &= \frac{me^2}{2\hbar^2 \beta p} \left\{ \ln \left[1 + \frac{\kappa^2}{(\sqrt{2m\hbar^{-2}(\omega + \mu)} + p)^2} \right] \right. \\ &\quad \left. - \ln \left[1 + \frac{\kappa^2}{(\sqrt{2m\hbar^{-2}(\omega + \mu)} - p)^2} \right] \right\}, \\ (\omega + \mu > 0); \end{aligned}$$

$$\text{Im}\Sigma_{pI}^{(2)}(\omega) = 0, \quad (\omega + \mu < 0). \quad (20)$$

We have then

$$\Sigma_{pI}^{(2)}(\omega) = \frac{me^2}{\beta\hbar^2 p} i \ln \frac{1 + i[\sqrt{2m(\omega + \mu)/\hbar\kappa} + p/\kappa]^{-1}}{1 + i[\sqrt{2m(\omega + \mu)/\hbar\kappa} - p/\kappa]^{-1}}. \quad (21)$$

This expression is valid for all ω . It is clear that all its poles lie in the lower half-plane, as should be the case; we must bear in mind here that we choose the branch of the square root which lies in the upper half-plane. An estimate of the remaining terms of the mass operator shows that they are of the order

$$e^2 \kappa \beta \hbar \omega_L \cdot O([\beta(\omega + \mu) - \beta \epsilon_p]^{-2}).$$

They give a small contribution when the condition

$$e^2 \kappa / \beta (\hbar \omega_L)^2 \gg 1, \quad \omega_L^2 = 4\pi e^2 n_0 / m,$$

*cth = coth.

†arctg = tan⁻¹.

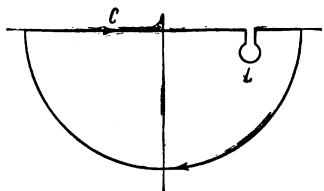


FIG. 2

is satisfied; this is equivalent to $r_D \gg r_B$, where $r_B = \hbar^2/m e^2$ is the Bohr radius. For a sufficiently rarefied plasma this condition is usually satisfied at the same time as the condition for the applicability of perturbation theory.

4. THE GREEN'S FUNCTION

Using the mass operator (21) we find the time dependence of the Green's function. We have

$$G_p(t) = (2\pi\hbar)^{-1} \int_{-\infty}^{\infty} e^{-i\omega t/\hbar} d\omega / [\omega + \mu - \epsilon_p - \Sigma_{fp}^{(2)}(\omega)]. \quad (22)$$

For $t > 0$ [$G_p(t) = 0$ when $t < 0$]. We close the contour of integration in the lower half-plane (see Fig. 2) encircling the branch point of the logarithm,

$$\omega = -\mu + \left(\sqrt{\epsilon_p} - \frac{1}{2} i \sqrt{\beta} \hbar \omega_L \right)^2.$$

The integral along C is equal to the product of $-2\pi i$ by the sum of the residues at the poles of $G_p(\omega)$, which lie all in the lower half-plane. With the above-mentioned accuracy these poles are of the form

$$\omega_p = -\mu + \epsilon_p \pm \sqrt{e^2 \kappa / \beta} - i \hbar^2 p \kappa / 8m$$

(we consider $p \approx p_T = \sqrt{m/\beta}$). The integral over L gives a small contribution and we get finally

$$G_p(t) \sim e^{-i(\epsilon_p - \mu)t/\hbar} e^{-\Gamma_p t} \cos(\sqrt{e^2 \kappa / \beta} t / \hbar), \quad (23)$$

where $\Gamma_p = \hbar p \kappa / 8m$.

The plane wave is thus damped when the interaction is taken into account, and its amplitude is modulated in time with a frequency

$$\sqrt{e^2 \kappa / \beta / \hbar}.$$

Since $\Gamma_p \ll \sqrt{e^2 \kappa / \beta} / \hbar$ the difference from a plane wave will become appreciable after periods of the order

$$t \gtrsim \hbar \sqrt{\beta / e^2 \kappa}.$$

5. THE DISTRIBUTION FUNCTION AND THE CHEMICAL POTENTIAL

Using the well-known relation between the spectral density of the correlation function $\langle a_p^\dagger(t) a_p(0) \rangle$ and the Fourier components of the retarded and

advanced Green's functions^[7] we have the following equation for the chemical potential

$$n = (-2\pi)^{-3} \int d^3 p \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\text{Im} \Sigma_p}{(\omega + \mu - \epsilon_p - \text{Re} \Sigma_p)^2 + (\text{Im} \Sigma_p)^2} \times \frac{d\omega}{1 + e^{\beta\omega}}. \quad (24)$$

If we approximate the spectral density of the correlation function by a δ -function, we get

$$n = (2\pi)^{-3} \int d^3 p \int_{-\infty}^{\infty} \delta(\omega + \mu - \epsilon_p - \text{Re} \Sigma_p) \frac{d\omega}{1 + e^{\beta\omega}}. \quad (25)$$

Substituting here the values of the roots

$$\omega = -\mu + \epsilon_p \pm \sqrt{e^2 \kappa / \beta},$$

we get*

$$n_p = \int_{-\infty}^{\infty} \delta(\omega + \mu - \epsilon_p - \text{Re} \Sigma_p) \frac{d\omega}{1 + e^{\beta\omega}} = e^{\beta(\mu - \epsilon_p)} \text{ch} \sqrt{\beta e^2 \kappa}, \quad (26)$$

which is the momentum distribution function when the interaction is taken into account. We also obtain easily the corrected value of the chemical potential

$$\mu = \mu_0 + \delta\mu, \quad \mu_0 = \mu|_{e^2=0}; \quad \delta\mu = -e^2 \kappa / 2,$$

from which follows the well-known Debye correction to the free energy, $-e^2 N \kappa / 3$.

In conclusion the authors express their sincere gratitude to V. L. Gurevich and Yu. A. Firsov for valuable advice and to A. G. Samoilovich for discussing their results.

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