

The thermodynamics of normal Fermi-systems

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Using Keldysh's diagram technique we show that it is possible to write the Hamiltonian of a normal Fermi system of strongly interacting particles in the statistical limit in the form of a functional of the quasi-particle occupation numbers. Landau's Fermi-liquid theory is generalized to the case of arbitrary temperatures. We show that a low-temperature specific-heat singularity may occur at a certain density.

1. Landau's phenomenological Fermi-liquid theory^{1,2} is based on the existence of quasi-particles for which the damping is small compared to their energy. In the microscopic derivation^{3,4} Landau's quasi-particles are interpreted as the poles of the single-particle Green function lying close to the real axis in the complex frequency plane. The smallness of the quasi-particle damping is caused by the scattering suppression due to the Pauli principle and by the presence of a jump in the Fermi-particle momentum distribution function in the ground state. When the temperature increases the jump in the distribution function vanishes and the quasi-particle damping increases. The Landau theory therefore describes only weakly excited states of the Fermi system and holds at temperatures which are low compared to the Fermi energy ε_F . Landau's Fermi-liquid theory was generalized in Refs. 5 to 9 to finite temperatures under the assumption that the single-particle Green function of the system has a pole in the complex momentum plane rather than in the complex frequency plane.

It was shown in Ref. 10 that not only the energy of weakly excited states but the whole spectrum of a normal Fermi-system with strong interactions can be expressed in the form of a functional of the quasi-particle distribution function, the existence of the quasi-particles not being connected with the presence or absence of poles in the Green functions. In contrast to the Landau theory, the quasi-particle lifetime then turns out to be infinite, and the states of the system with different numbers of quasi-particles are found to be stationary. This fact enables us to generalize Landau's Fermi-liquid theory to the case of arbitrary temperatures. One should note that the possibility to write the free energy (but not the spectrum of the system) in the form of a functional of the quasi-particle distribution function was established before in Refs. 11 to 15.

The possibility to express the energy as a functional of the occupation numbers can be most clearly seen when one attempts to find an operator \hat{S} which changes the system Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$ to a possibly simpler form $\hat{E} = \hat{S}\hat{H}\hat{S}^{-1}$. Formally one can choose the operator \hat{S} such that \hat{E} will commute with the Hamiltonian of non-interacting particles \hat{H}_0 . It has not been possible to overcome the difficulties arising when one tries to perform the calculations based on these considerations. The main obstacle is clearly the degeneracy of the spectrum of \hat{H}_0 . However, the difficulty disappears if we assume the system to be normal. This

assumption means, in particular, that the spectrum of a system of N particles is continuous for any fixed N when the volume is infinite. Thanks to the presence of Møller operators it is possible in that case to number the spectrum of \hat{H} by the spectrum of \hat{H}_0 . This procedure is carried out in the present paper using Keldysh's diagram technique.¹⁶ Its result reduces to the diagonalization of the Hamiltonian \hat{H} and to expressing it as a non-linear functional of the momentum-density operators $\hat{n}_p = \hat{\alpha}_p^+ \hat{\alpha}_p$.

We note that it is far from trivial that it is possible to apply the diagram technique to excited system states which are multiply degenerate. This possibility is produced by the properties of a normal Fermi-system in the thermodynamic limit, and first and foremost by the continuity of its energy spectrum. We emphasize that in the present paper we are dealing with the determination of the true spectrum of the Hamiltonian of a system which lies on the physical sheet of the resolvent and not with the poles of the analytical continuation of the Green functions which are well known to lie on the non-physical sheet. The latter determine quasi-stationary states with energies close to the energies of stationary states, provided that the damping is sufficiently small.

The quasi-particle operators $\hat{\alpha}_p$ turn out to be statistically independent with respect to the Gibbs distribution. Thanks to this the free energy of a normal Fermi system can be obtained as the solution of an equation in functionals of first order derivatives which in this paper is solved "explicitly" using a trivial generalization of the well known Cauchy method for solving analogous equations in the finite-dimensional case. As a result we express the free energy as a functional of the Fermi distribution function $\bar{n}(p)$ of a perfect gas of quasi-particles which has an energy spectrum $\varepsilon(p)$ which is determined by the functional derivative of the mean energy of the system. The entropy is expressed in terms of the quasi-particle distribution function $\bar{n}(p)$ by the same formula as in the case of a perfect gas. Since the total number of particles is equal to the number of quasi-particles in the system, it follows immediately that the Fermi momentum of the quasi-particle distribution is connected at zero temperature with the system density in the same way as for a perfect gas. This approach is attractive because it yields these results without resorting to additional considerations (such as a maximum entropy principle).

The thermodynamic quantities can thus be determined completely once the quasi-particle energy $\varepsilon(p)$ is known.

One should note that, notwithstanding the simplicity in principle of the thermodynamic formulae, the evaluation of the quasi-particle energy spectrum $\varepsilon(p)$ for a system with strong interactions is in the general case a problem which is not less complicated than the evaluation of the Green functions by the usual temperature diagram technique.⁴

In the present paper we study the thermodynamic characteristics of a system at low temperatures and show that if the quasi-particle energy $\varepsilon(p)$ as function of the momenta changes discontinuously, there occurs for a certain particle-number density a singularity of the form $C_V \approx \alpha T(\ln T)^2$ in the specific heat C_V as a function of the temperature T . The reason for this behavior of the specific heat is the instability of the Fermi jump in the quasi-particle distribution which leads to complete restructuring rather than smoothing of the jump when the temperature is increased. We emphasize that this result is obtained for a fermion system with strong interactions; in particular, the coefficient α in the temperature dependence of the specific heat is determined solely by Landau's Fermi-liquid quasi-particle interaction function $f(p, p')$.

It is of interest to compare the quasi-particles considered here with the quasi-particles whose spectrum is determined by the poles of the Green functions. The existence of poles lying close to the real axis in the complex frequency plane means that the state $\hat{a}_p^+ |\psi_0\rangle$, where \hat{a}_p^+ is a particle creation operator and $|\psi_0\rangle$ the exact ground state of the system, is almost stationary. Hence it follows that in Landau's theory when the interaction is switched on not only does the ground state $|\psi_0^{(0)}\rangle$ of the perfect particle gas change to the state $|\psi_0\rangle$, but the state $\hat{a}_p^+ |\psi_0^{(0)}\rangle$ change also to the state $Z_p \hat{a}_p^+ |\psi_0\rangle$ (Z_p is a renormalization constant). In that sense one can state that in the Landau theory a state with a single excited particle is represented with high probability by a state with a single quasi-particle. In contrast, the state $\hat{a}_p^+ |\psi_0\rangle$ with a single quasi-particle considered in the present paper is a superposition of excited many-particle states of the system. Only at temperatures close to zero, when the degeneracy of the energy levels E is small, is the quasi-particle energy the same as the Landau quasi-particle energy determined by the real part of the mass operator.

2. We consider a system of N particles, in a volume V , described by the Hamiltonian

$$\hat{H} = \sum_p \varepsilon_0(p) \hat{a}_p^+ \hat{a}_p + \frac{1}{2} \sum_{p_1, p_2, p_1', p_2'} \langle p_1 p_2 | U | p_1' p_2' \rangle \hat{a}_{p_1}^+ \hat{a}_{p_2}^+ \hat{a}_{p_1'} \hat{a}_{p_2'} = \hat{H}_0 + \hat{H}_1, \quad (1)$$

where \hat{a}_p^+ and \hat{a}_p are the Fermi creation and annihilation operators for a particle in a state $p = (\mathbf{p}, \sigma)$ with momentum \mathbf{p} and spin σ , $\varepsilon_0(p) = \mathbf{p}^2/2m$ is the kinetic energy of a particle, and

$$\langle p_1 p_2 | U | p_1' p_2' \rangle = \frac{1}{V} U(|\mathbf{p}_1 - \mathbf{p}_1'|) \delta_{\mathbf{p}_1 + \mathbf{p}_2, \mathbf{p}_1' + \mathbf{p}_2'} \delta_{\sigma_1 \sigma_1'} \delta_{\sigma_2 \sigma_2'} \quad (2)$$

is the interaction potential energy for a pair of particles.

Let $|\psi\rangle$ be any eigenstate of the Hamiltonian

$$\hat{H} |\psi\rangle = E |\psi\rangle. \quad (3)$$

We define for each stationary state $|\psi\rangle$ the Green function

$$iG(t, t', p) = \langle \psi | T \hat{a}_p(t) \hat{a}_p^+(t') | \psi \rangle, \quad (4)$$

where T is the chronological ordering operator,⁴ while the $\hat{a}_p(t)$ are operators in the Heisenberg representation. Since the Hamiltonian commutes with the total momentum operator $\hat{\mathbf{P}}$ one can choose the base $|\psi\rangle$ to be common to the operators \hat{H} and $\hat{\mathbf{P}}$, and the Green function (4) is diagonal in the momentum representation. Changing to the interaction representation we write

$$iG(t, t', p) = \langle \psi^{(0)} | \hat{S}^{-1}(t_m, t_0) T \hat{a}_p^{(0)}(t) \hat{a}_p^{(0)\dagger}(t') \hat{S}(t_m, t_0) | \psi^{(0)} \rangle = \langle \psi^{(0)} | T_c \hat{a}_p^{(0)}(t) \hat{a}_p^{(0)\dagger}(t') \hat{S}_c | \psi^{(0)} \rangle, \quad (5)$$

where $t_m = \max\{t, t'\}$, $t_0 < 0$ is some initial time,

$$|\psi\rangle = \hat{S}(0, t_0) |\psi^{(0)}\rangle, \quad \hat{S}(t_2, t_1) = T \exp \left[-i \int_{t_1}^{t_2} dt \hat{H}_I(t) \right], \quad (6)$$

T_c is the ordering operator along a contour c going from t_0 to t_m (the branch designated in what follows by a minus sign) and back from t_m to t_0 (the branch designated by a plus sign).^{16,17} The Green function of (6) can be represented by a sum of diagrams^{18,19}

$$iG = \text{---} + \text{---} + \text{---} + \dots \quad (7)$$

containing the free Green function

$$iG^{(0)}(t, t', p) = \{\theta_c(t-t') [1-n_p] - \theta_c(t'-t) n_p\} \exp[-i\varepsilon_0(p)(t-t')] \quad (8)$$

and the correlation functions

$$g^{(k)}(p_1 \dots p_k, p_1' \dots p_k') \times \exp \left\{ i \sum_{j=1}^k [\varepsilon_0(p_j')(t_j' - t_0) - \varepsilon_0(p_j)(t_j - t_0)] \right\}, \quad k=2, 3, \dots, N, \quad (9)$$

depicted by two lines connecting each of two, three, ... Green functions. Here $\theta_c(t-t') = 1$ if the time t' precedes t on the contour c , and $\theta_c(t-t') = 0$ in the opposite case, and $n_p = \langle \psi^{(0)} | \hat{a}_p^+ \hat{a}_p | \psi^{(0)} \rangle$ are the occupation numbers for the state $|\psi^{(0)}\rangle$. The correlation functions $g^{(k)}$ are defined using the single-time k -particle density matrices

$$f^{(k)}(p_1 \dots p_k, p_1' \dots p_k') = \langle \psi^{(0)} | \hat{a}_{p_1}^+ \dots \hat{a}_{p_k}^+ \hat{a}_{p_k} \dots \hat{a}_{p_1} | \psi^{(0)} \rangle, \quad k=1, 2, \dots, N$$

through the relations

$$f^{(k)}(p_1 \dots p_k, p_1' \dots p_k') = \gamma_{1 \dots k} \left\{ \prod_{i=1}^k f^{(1)}(p_i, p_i') + \sum_{1 \leq i < j \leq k} g^{(2)}(p_i, p_j, p_i', p_j') \prod_{\substack{l=1 \\ l \neq i, j}}^k f^{(1)}(p_l, p_l') + \dots + g^{(k)}(p_1 \dots p_k, p_1' \dots p_k') \right\}, \quad k=2, 3, \dots, N, \quad (10)$$

where

$$\gamma_{1\dots n} = (1 - P_{12})(1 - P_{13} - P_{23}) \dots (1 - P_{1n} - \dots - P_{n-1, n}) \quad (11)$$

is the antisymmetrization operator, and P_{ij} the operator which interchanges a pair of particles, acting on the unprimed variables p_i and p_j .

We shall assume that all correlation functions are continuous functions of the momenta in the statistical limit as $N \rightarrow \infty$, $V \rightarrow \infty$, and $N/V = \rho = \text{constant}$. This assumption means that there is no discrete spectrum, and in particular that there are no bound states of two, three, . . . particles. It means also that there is no long-range order and, hence, it excludes from our considerations crystalline, superfluid, and superconducting systems. The continuity of the correlation functions in the momentum representation is destroyed also near second-order phase transition points when the spatial correlation length tends to infinity. The continuity of the correlation functions causes the contribution from (9) to (7) to tend to zero in the statistical limit as $t_0 \rightarrow -\infty$, according to the Riemann-Lebesgue theorem, in view of the oscillating behavior of (9).

As a result the Green function (5) reduces in the statistical limit to an average over the state of a perfect gas with some integrable particle momentum distribution function $n(p)$. One can write this average as the limit of averages over states of a perfect gas with a finite number of particles N in a volume V as $N \rightarrow \infty$, $V \rightarrow \infty$, and $N/V = \rho$. Let

$$|\psi_{N, V}^{(0)}\rangle = \hat{a}_{p_1}^+ \dots \hat{a}_{p_N}^+ |0\rangle \quad (12)$$

be states of a perfect gas determined by the occupation numbers $n_p = 1$ or 0 of the single-particle states; $W = V\Delta p / (2\pi)^3$ is the number of such levels corresponding to a given value of spin and belonging to a volume Δp in momentum space; $N(p, \Delta p)$ is the number of particles in those levels. We consider also a sequence of states (12) for which the ratio $N(p, \Delta p) / W$ tends to a limit $n(p)$. For sufficiently large N , V , $|t_0|$ we then understand the function $\psi^{(0)}$ to mean the corresponding function (12) and put $n_p = 1$ or 0 in (8).

It was shown in Ref. 20 that when one averages over a mixed state there are secular divergences in the expansion of the Green function. The presence of these divergences precludes the use of perturbation theory and the ability to "number" the Green function by the occupation numbers n_p . We show that when one averages over the pure state (12) the divergences do not occur. To do that it is sufficient to consider the "dangerous" diagrams containing irreducible insertions in the Green function²⁰:



$$= \int_{\circ} dt_2 \int_{\circ} dt_3 \{ \theta_c(t_1 - t_2) [1 - n_p] - \theta_c(t_2 - t_1) n_p \} \\ \times \Sigma(t_2 - t_3, p) \{ \theta_c(t_3 - t_4) [1 - n_p] \\ - \theta_c(t_4 - t_3) n_p \} \exp[-i\varepsilon_0(p)(t_1 - t_4)]. \quad (13)$$

Since $n_p(1 - n_p) = 0$ we see that the terms in (13) which diverge as $t_0 \rightarrow -\infty$, and which contain an integration over the interior times t_2, t_3 with infinite limits along the contour

c , vanish. On the other hand, in the remaining non-divergent terms the integration over t_2, t_3 along the contour c takes place over a finite interval limited by the values of the exterior times t_1, t_4 . As a result, perturbation theory turns out to be applicable in the case considered by us and we can express the exact Green function of the pure state as a function of the occupation numbers n_p of a state of a perfect fermion gas. We can thus put in (5) $t_0 = -\infty$, insert a factor $\hat{S}^{-1}(\infty, t_m) \hat{S}(\infty, t_m)$ which is identically equal to unity, and use Keldysh's diagram technique¹⁶ to evaluate the Green function G . We note that owing to the degeneracy of the energy levels $E^{(0)}$ of the excited states of a fermion system without interactions the S -matrix changes the state $\psi^{(0)}$ with energy $E^{(0)}$ into a superposition of states belonging to the same energy level $E^{(0)}$ of the unperturbed Hamiltonian. This fact prevents us from "removing" the operator $\hat{S}^{-1}(\infty, -\infty)$ from under the averaging sign as can be done for the ground state.⁴

The energy spectrum E can be expressed in the usual way in terms of the exact Green function⁴ in the form

$$E = \frac{i}{2} \sum_p \int \frac{d\omega}{2\pi} [\omega + \varepsilon_0(p)] G^{-+}(\omega, p) \quad (14)$$

or in the form, which contains an integral over a parameter:

$$E = E^{(0)} + \int_0^1 \frac{d\lambda}{\lambda} \frac{i}{2} \sum_p \int \frac{d\omega}{2\pi} [\omega - \varepsilon_0(p)] G^{-+}(\omega, p). \quad (15)$$

Here $iG^{-+}(\omega, p)$ is the Fourier transform of the Green function (4) with respect to $t - t'$:

$$iG^{-+}(t, t', p) = -\langle \psi | \hat{a}_p^+(t') \hat{a}_p(t) | \psi \rangle,$$

in which the time t lies on the "minus" branch and the time t' on the "plus" branch of the contour c , while λ is a parameter varying from 0 to 1 and introduced through the substitution $U \rightarrow \lambda U$ in (2). Expressions (14), (15) enable us to construct an expansion of the energy spectrum in a perturbation-theory series in powers of the interaction or the density and to "number" it by the occupation numbers n_p of the states of a perfect Fermi gas. In the limit as $V \rightarrow \infty$ this expansion determines the energy per unit volume in the form of a functional of the continuous distribution density $n(p)$ which satisfies the condition

$$\sum_{\sigma} \int \frac{d\mathbf{p}}{(2\pi)^3} n(p) = \frac{N}{V} = \rho, \quad 0 \leq n(p) \leq 1. \quad (16)$$

We consider, for instance, the expansion of the energy in powers of the density:

$$E = \sum_p \varepsilon_0(p) n_p + \sum_{p_1, p_2} f_{p_1, p_2}^{(V)} n_{p_1} n_{p_2} + \dots \quad (17)$$

The volume dependence of the coefficients of the expansion can be determined, with an accuracy which is sufficient for us, from the following considerations. If we fix N and let V tend to ∞ we must obtain the spectrum of an N -particle scattering problem. As this spectrum is the same as the spectrum of the unperturbed problem, the coefficients $f^{(V)}$ must tend to zero as $V \rightarrow \infty$. On the other hand, as $N \rightarrow \infty$, $V \rightarrow \infty$,

$N/V = \rho$ the energy must be proportional to V . To the main order of magnitude, therefore

$$f_{\mathbf{p}_1 \dots \mathbf{p}_k}^{(V)} \approx f(\mathbf{p}_1 \dots \mathbf{p}_k) / V^{k-1},$$

where $f(\mathbf{p}_1, \dots, \mathbf{p}_k)$ is independent of the volume. When taking the limit $V \rightarrow \infty$, $N/V = \rho$ we assume that it is sufficient to consider the configurations n_p which have a density $n(p)$, i.e., such for which the number of points falling in a small volume Δ with center at the point p is equal to $n(p)\Delta$. Clearly,

$$\sum_p n(p) = N, \quad 0 \leq n(p) \leq 1,$$

whence we obtain Eq. (16). Taking the limit we get the limiting spectrum in the form of a functional of the momentum density $n(p)$:

$$E = E[n(p)] = V \left\{ \sum_{\sigma} \int \frac{d\mathbf{p}}{(2\pi)^3} \varepsilon_{\sigma}(p) n(p) + \sum_{\sigma_1, \sigma_2} \int \frac{d\mathbf{p}_1 d\mathbf{p}_2}{(2\pi)^6} f(\mathbf{p}_1, \mathbf{p}_2) n(p_1) n(p_2) + \dots \right\}. \quad (18)$$

The expansion coefficients $f(\mathbf{p}_1, \dots, \mathbf{p}_k)$ can be determined by a diagram method and can be expressed in terms of the Møller operators of k -particle problems ($k = 2, 3, \dots$).

3. The discussions given here mean that it is possible to reduce the total Hamiltonian to the form

$$\hat{S}^+(0, -\infty) \hat{H} \hat{S}(0, -\infty) = E[\hat{N}_p], \quad \hat{N}_p = \hat{a}_p^+ \hat{a}_p, \quad (19)$$

which is diagonal in the representation of the occupation numbers n_p . The unitarity of $\hat{S}(0, \infty)$ is a consequence of the fact that the Fermi system is normal. Formula (19) is symbolic, i.e., indicates a means of evaluating approximations for the operator $E[\hat{N}_p]$. (The operator \hat{H} is not defined for $N = \infty$ and neither are its eigenfunctions. The usual, somewhat slipshod terminology which we use in what follows presupposes that N is very large but finite.)

Introducing the quasi-particle operators

$$\hat{\alpha}_p = \hat{S}(0, -\infty) \hat{a}_p \hat{S}^+(0, -\infty), \\ \hat{\alpha}_p^+ = \hat{S}(0, -\infty) \hat{a}_p^+ \hat{S}^+(0, -\infty), \quad (20)$$

we find from (19) that

$$\hat{H} = E[\hat{n}_p], \quad \hat{n}_p = \hat{\alpha}_p^+ \hat{\alpha}_p. \quad (21)$$

We evaluate now the partition function:

$$\exp(-\beta\Omega) \equiv \exp(\beta VP) = \text{Sp} \exp(-\beta \hat{H}') \\ = \sum_{\{n_p\}} \exp(-\beta V E_V' [n_p]), \quad (22)$$

$$H' \equiv H - \mu N, \quad E_V' = E_V - \mu \rho, \quad \beta = 1/T,$$

$E_V = E/V$ is the energy per unit volume, μ the chemical potential, P the pressure, Ω the thermodynamic potential. We add to the Hamiltonian a term with an auxiliary external field $\varphi(p)$ which is momentum-dependent and we consider instead of (22) the more general expression:

$$\exp(\beta VP(t, \varphi)) = \text{Sp} \exp \left\{ -t\beta \hat{H}' - \beta \sum_p \varphi(p) \hat{\alpha}_p^+ \hat{\alpha}_p \right\} \\ = \sum_{\{n_p\}} \exp \left\{ -t\beta V E_V' [n_p] - \beta \sum_p \varphi(p) n_p \right\}, \quad (23)$$

which changes into (22) when $t = 1, \varphi = 0$.

We consider the set of n_p configurations having a density as defined in section 2 and determine the average value of the functional $\Phi(n)$, putting

$$\bar{\Phi} = \lim_{V \rightarrow \infty} \exp(-\beta VP) \\ \times \sum_{\{n_p\}} \exp \left\{ -t\beta V E_V' [n_p] - \beta \sum_p \varphi(p) n_p \right\} \Phi(n). \quad (24)$$

Replacing in (23) $\varphi(p)$ by $\varphi(p) + \varepsilon \eta(p)$ and differentiating we get

$$\left. \frac{\partial P}{\partial \varepsilon} \right|_{\varepsilon=0} = - \sum_{\sigma} \int \frac{d\mathbf{p}}{(2\pi)^3} \bar{n}(p) \eta(p) \quad (25)$$

or

$$\delta P / \delta \varphi(p) = -\bar{n}(p) / (2\pi)^3. \quad (26)$$

Replacing now in (23) the function $\varphi(p)$ by $\varphi(p) + \varepsilon \eta(p) + \delta \chi(p)$ and differentiating with respect to ε and δ we get

$$\left(\beta V \frac{\partial^2 P}{\partial \varepsilon \partial \delta} + \beta^2 V^2 \frac{\partial P}{\partial \varepsilon} \frac{\partial P}{\partial \delta} \right)_{\varepsilon=\delta=0} = \exp(-\beta VP) \\ \times \sum_{p,q} \sum_{\{n_p\}} \exp \left\{ -t\beta V E_V' [n_p] - \beta \sum_p \varphi(p) n_p \right\} \\ n_p n_q \eta(p) \chi(q) \Big|_{\varepsilon=\delta=0},$$

which after division by V and taking the limit gives

$$\left. \frac{\partial P}{\partial \varepsilon} \frac{\partial P}{\partial \delta} \right|_{\varepsilon=\delta=0} \\ = \overline{\sum_{\sigma_1} \int \frac{d\mathbf{p}_1}{(2\pi)^3} n(p_1) \eta(p_1) \sum_{\sigma_2} \int \frac{d\mathbf{p}_2}{(2\pi)^3} n(p_2) \chi(p_2)}. \quad (27)$$

It now follows from (27) and (25) that

$$\overline{n(p)n(q)} = \bar{n}(p)\bar{n}(q). \quad (28)$$

Equation (28) holds only almost everywhere (for instance, it is incorrect when $p = q$). It is clear that the discussion given here can be extended and we are led to the conclusion that our quasi-particles (20) are statistically independent in the sense of the definition (24).

The statistical independence of $n(p)$ gives us a basis to consider that class Γ of functionals $\Phi(n)$ for which $\Phi(n) = \Phi(\bar{n})$. For instance, functionals such as

$$\Phi(n) = \sum_{\sigma_1 \dots \sigma_k} \int \frac{d\mathbf{p}_1 \dots d\mathbf{p}_k}{(2\pi)^{3k}} \Phi(p_1 \dots p_k) n(p_1) \dots n(p_k) \quad (29)$$

belong to that class. We assume that $E_V' [n(p)]$ belongs to that class. This assumption enables us, by differentiating (23) with respect to t and using (28), to obtain for P an equation in functional derivatives:

$$-\frac{\partial}{\partial t}P(t, \varphi) = E_{\nu}' \left[-(2\pi)^3 \frac{\delta P}{\delta \varphi(p)} \right] \quad (30)$$

with the initial condition

$$P(0, \varphi) = \frac{1}{\beta} \sum_{\sigma} \int \frac{dp}{(2\pi)^3} \ln [1 + e^{-\beta \varphi(p)}] = P_0[\varphi(p)]. \quad (31)$$

This problem is the continuum analog of the Cauchy problem:

$$\begin{aligned} \frac{\partial}{\partial t}P(t, x) &= D(y), & P(0, x) &= P_0(x), \\ x &= (x_1 \dots x_n), & y &= (y_1 \dots y_n), & y_i &= \frac{\partial P}{\partial x_i}, \end{aligned} \quad (32)$$

and its solution can be written down using characteristics¹⁰

$$P(t, x) = tD(y(\xi)) - t \sum_{i=1}^n y_i(\xi) \frac{\partial D(y(\xi))}{\partial y_i} + P_0(\xi), \quad (33)$$

where $y_i(\xi) = \partial P_0(\xi) / \partial \xi_i$ while the parameters $\xi = (\xi_1 \dots \xi_n)$ can be expressed in terms of the coordinates x from the equation

$$x_i = \xi_i - t \partial D(y(\xi)) / \partial y_i, \quad i=1, \dots, n. \quad (34)$$

Accordingly the solution of Eq. (30) has the form

$$\begin{aligned} P(t, \varphi) &= -t E_{\nu}'[\bar{n}(p)] \\ &+ \sum_{\sigma} \int \frac{dp}{(2\pi)^3} \bar{n}(p) \frac{\delta E_{\nu}'[\bar{n}(p)]}{\delta \bar{n}(p)} + P_0[\varepsilon'(p)], \end{aligned} \quad (35)$$

where

$$\bar{n}(p) = -(2\pi)^3 \frac{\delta P_0[\varepsilon'(p)]}{\delta \varepsilon'(p)} = (\exp[\beta \varepsilon'(p)] + 1)^{-1}, \quad (36)$$

while $\varepsilon'(p)$ is determined from the equation

$$\varphi(p) = \varepsilon'(p) - (2\pi)^3 t \delta E_{\nu}'[\bar{n}(p)] / \delta \bar{n}(p), \quad (37)$$

which is the continuum analog of (34). Putting in $t=1$ and $\varphi(p)=0$ (35) and (37) we get the final expression for the thermodynamic potential and the entropy of the system:

$$\Omega = -PV = E'[\bar{n}(p)] + \beta^{-1}S, \quad (38)$$

$$S = -V \sum_{\sigma} \int \frac{dp}{(2\pi)^3} \{ \bar{n}(p) \ln \bar{n}(p) + [1 - \bar{n}(p)] \ln [1 - \bar{n}(p)] \}, \quad (39)$$

where $\bar{n}(p)$ is the Fermi quasi-particle distribution function (36), and the quasi-particle energy is given by the equation

$$\varepsilon'(p) = (2\pi)^3 \delta E_{\nu}'[\bar{n}(p)] / \delta \bar{n}(p). \quad (40)$$

4. In what follows we shall show that for rather general forms of functionals of the energy $E(n)$ a singularity may occur in the specific heat at a temperature which tends to zero (and a certain fixed density). We start with the problem of finding the quasi-particle distribution function at zero temperature. This problem reduces to finding the minimum of $E(n)$ under the limitations (16).

The corresponding general discrete problem is the following: find $\min F(x)$, $x = (x_1 \dots x_n)$ under the condi-

tions $g(x) = 0$ and $\lambda_1(x) \geq 0, \dots, \lambda_k(x) \geq 0$, where g and λ are given.

If the minimum is reached at the point \bar{x} lying inside the admissible domain, i.e., if $\lambda_i(\bar{x}) > 0, i=1, \dots, k$ the limitations are unimportant and the minimum is looked for, using Lagrangian multipliers, as the minimum of the function $F - \mu g$.

Assume, however, that the minimum is reached at a point \bar{x} lying on the boundary: $\lambda_i(\bar{x}) = 0, i=1, \dots, l, l < k$. In that case we must have at the point \bar{x} $F(\bar{x} + \delta) \geq F(\bar{x})$ for any sufficiently small vector δ satisfying the condition $g(\bar{x} + \delta) = 0, \lambda_i(\bar{x} + \delta) \geq 0, i=1, \dots, l$. This requirement is equivalent to the inequality $(\delta, \nabla F) \geq 0$, if $(\delta, \nabla \lambda_i) > 0, i=1, \dots, l$ which means

$$\nabla F(\bar{x}) = c_1 \nabla \lambda_1 + \dots + c_l \nabla \lambda_l + \mu \nabla g, \quad c_i \geq 0,$$

or

$$\nabla (F - c_1 \lambda_1 - \dots - c_l \lambda_l - \mu g) = 0. \quad (41)$$

A final conclusion: there must exist a μ and non-negative c_1, \dots, c_l such that for them \bar{x} is a stationary (minimum) point of the function

$$\Gamma(x) = F(x) - \mu g(x) - \sum_{i=1}^l c_i \lambda_i(x). \quad (42)$$

Transferring this discrete formulation to the continuum case and taking into account that our limitations are $n(p) \geq 0, 1 - n(p) \geq 0$ we get the following problem: We need a constant μ and also non-negative functions $\lambda_1(p), \lambda_2(p)$ with the limitation $\lambda_1(p)\lambda_2(p) = 0$, such that the functional

$$\begin{aligned} \Gamma(n) &= E(n) - \mu \sum_{\sigma} \int \frac{dp}{(2\pi)^3} n(p) - \sum_{\sigma} \int \frac{dp}{(2\pi)^3} \lambda_1(p) n(p) \\ &- \sum_{\sigma} \int \frac{dp}{(2\pi)^3} \lambda_2(p) [1 - n(p)] \end{aligned} \quad (43)$$

reaches a minimum.

Calculating the variation of Γ leads to the problem of finding functions $0 \leq n(p) \leq 1$ and $\mu, \lambda_1, \lambda_2$ such that

$$\begin{aligned} \varepsilon'(p, n) &= \varepsilon(p, n) - \mu = \lambda_1(p) - \lambda_2(p), \\ \varepsilon(p, n) &= (2\pi)^3 \delta E_{\nu}' / \delta n(p). \end{aligned} \quad (44)$$

We note that in the region ω_+ , where $n(p) = 1$ the functions $\lambda_1(p) = 0, \lambda_2(p) > 0$ and hence the function $\varepsilon'(p) < 0$ in this region.

Introducing similarly a region ω_- :

$$n(p) = 0, \quad \lambda_2(p) = 0, \quad \lambda_1(p) > 0, \quad \varepsilon'(p) > 0$$

and a region ω_0 :

$$\lambda_1(p) = \lambda_2(p) = 0, \quad \varepsilon'(p) = 0,$$

we are led to the following conclusion: the solution of our problem is a function $0 \leq \bar{n}(p) \leq 1$ such that the regions ω_+ ($\bar{n}(p) = 1$) and ω_- ($\bar{n}(p) = 0$) are the same as the regions ω'_+ ($\varepsilon'(p, n) < 0$) and ω'_- ($\varepsilon'(p, n) > 0$). In the region complementary to $\omega_+ + \omega_-$ the function $\varepsilon'(p, n)$ vanishes.

In what follows we only consider the isotropic case. We

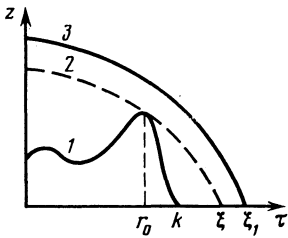


FIG. 1. Momentum dependence of the quasi-particle energy: 1: $z = f(r, \bar{n})$; 2: $z = \bar{\eta} - r^2$; 3: $z = \eta - r^2$.

also assume that $\varepsilon(p, n)$ has the form

$$\varepsilon(p, n) = [r^2 + f(r, n)]/2m, \quad (45)$$

where $r = |p|$ and that 1) $f(r, n) \geq 0$ and continuous; 2) there exists a constant k such that

$$E_1(n) = E(n) - \sum_p \int \frac{dp}{(2\pi)^3} \varepsilon_0(p) n(p) \quad (46)$$

does not change when we vary $n(p)$ solely in the region $r \gg k$; 3) if $\bar{n}(r) = 1$ when $r \leq k$ the function $f(r, \bar{n})$ has the form shown in the figure.

These requirements can be greatly relaxed, as they are a compromise between the consideration of an actual model and an excessively general one. Assumption 2 is a generalization of the condition $f(\mathbf{p}, \mathbf{q}) = 0$, $|\mathbf{p}| > k$, $|\mathbf{q}| > k$, if

$$E_1(n) = \sum_{\alpha_1, \alpha_2} \int \frac{dp_1 dp_2}{(2\pi)^6} f(\mathbf{p}_1, \mathbf{p}_2) n(p_1) n(p_2),$$

and assumption 3 is that there exists a parabola $z = \bar{\eta} - r^2$ touching the curve $z = f(r, \bar{n})$ in a point r_0 and intersecting it only once. To simplify the calculations in what follows we consider the simplest case $k < \xi$ (see the figure).

One shows easily that for any $\eta \geq \bar{\eta}$ the solution of our extremum problem is a Fermi jump $n_\eta(r) = 1$ when $r \leq \xi_1$ and $n_\eta(r) = 0$ when $r > \xi_1$. Indeed, by virtue of assumption 3 the function

$$v_\eta = -2m\varepsilon'(p) = \eta - r^2 - f(r, n_\eta), \quad \eta = 2m\mu \quad (47)$$

is non-negative in the region where $n_\eta(r) = 1$ and negative there where $n_\eta(r) = 0$.

In what follows we consider the limiting situation $\eta = \bar{\eta}$. In that case the corresponding functions $n_{\bar{\eta}}$ and $v_{\bar{\eta}}$ are denoted by \bar{n} and \bar{v} . We denote by

$$\bar{\rho} = \frac{8\pi}{(2\pi)^3} \int_0^\xi r^2 dr$$

the density corresponding to $\bar{\eta}$. To find the distribution function

$$n(p) = \frac{\exp(v(p)/\varepsilon)}{1 + \exp(v(p)/\varepsilon)}, \quad \varepsilon = \frac{2m}{\beta}$$

for a given density $\bar{\rho}$ and a non-zero temperature ε we must solve Eq. (40)

$$v(p) = \bar{\eta} + \sigma - r^2 - f(r, n) \quad (48)$$

under the condition

$$\rho = \frac{1}{\pi^2} \int_0^\infty \frac{\exp(v(r)/\varepsilon)}{1 + \exp(v(r)/\varepsilon)} r^2 dr = \frac{1}{\pi^2} \int_0^\xi r^2 dr = \rho \quad (49)$$

(here the addition σ to the chemical potential $\bar{\eta}$ is determined by specifying ε). We have

$$n(r) = \bar{n}(r) + \frac{\exp(v(r)/\varepsilon)}{1 + \exp(v(r)/\varepsilon)} - \bar{n}(r) = \begin{cases} n(r) - \frac{1}{1 + \exp(v(r)/\varepsilon)}, & r \leq \xi, \\ \frac{\exp(v(r)/\varepsilon)}{1 + \exp(v(r)/\varepsilon)}, & r > \xi. \end{cases} \quad (50)$$

By virtue of assumption 2 we can write

$$v(r) = \sigma + \bar{v}(r) + f(r, \bar{n}) - f\left(r, \bar{n} - \frac{1}{1 + \exp(v(r)/\varepsilon)}\right) \approx \sigma + \bar{v}(r) + \frac{1}{\pi^2} \int_0^k f(r, r_1, \bar{n}) \frac{r_1^2 dr_1}{1 + \exp(v(r_1)/\varepsilon)}. \quad (51)$$

Here $f(r, r_1, \bar{n}) \geq 0$ is the second variation of $E(n)$.

It is clear that only the vicinities of the points r_0 and ξ are important for finding the asymptotic behavior of v as $\varepsilon \rightarrow 0$. However, when $r = r_0 + s$ ($s \ll r_0$) we have

$$v(r_0 + s) \approx \sigma + \frac{1}{2} v''(r_0) s^2 + \frac{1}{\pi^2} \int_0^k f(r_0 + s, r_1, \bar{n}) \frac{r_1^2 dr_1}{1 + \exp(v(r_1)/\varepsilon)}. \quad (52)$$

In what follows we shall show that σ is positive. We may thus assume that $v(r_0 + s) \geq \frac{1}{2} v''(r_0) s^2$, since $f(r_0, n) > 0$.

We take now $0 < \alpha < 1/3$. In that case

$$\exp(v(r)/\varepsilon) \geq \exp(v''(r_0) r_0^2 \alpha / 2\varepsilon)$$

when $|s| \geq \varepsilon^\alpha$ and, hence, Eq. (51), apart from exponential corrections, is

$$v(r) = \sigma + \bar{v}(r) + \frac{1}{\pi^2} \int_{r_0 - \varepsilon^\alpha}^{r_0 + \varepsilon^\alpha} dr_1 \frac{r_1^2 f(r, r_1, \bar{n})}{1 + \exp(v(r_1)/\varepsilon)} \equiv \sigma + \bar{v}(r) + \gamma(r), \quad (53)$$

where

$$\gamma(r) \approx \pi^{-2} f(r, r_0, \bar{n}) r_0^2 \bar{v}, \quad (54)$$

$$\bar{v} = \int_{r_0 - \varepsilon^\alpha}^{r_0 + \varepsilon^\alpha} dr \frac{\exp(-v(r)/\varepsilon)}{1 + \exp(-v(r)/\varepsilon)}. \quad (55)$$

We shall find below the point $r_0 + h$ where $v'(r_0 + h) = 0$ and show that $|h| \sim \varepsilon(-\ln \varepsilon)$. Using that we can rewrite (55) in the form

$$\bar{v} \approx \int_{-\infty}^{\infty} ds \frac{\exp[-v(r_0 + h)/\varepsilon - v''(r_0 + h) s^2 / 2\varepsilon]}{1 + \exp(-v(r_0)/\varepsilon)} = \exp\left(-\frac{v(r_0 + h)}{\varepsilon}\right) \varepsilon^{1/2} D(\varepsilon), \quad (56)$$

where $D(\varepsilon)$ is bounded and non-vanishing as $\varepsilon \rightarrow 0$. Using (53) and (54) we now get

$$\bar{\nu} \approx \varepsilon^{1/2} \exp[-(\sigma + \bar{f}\bar{\nu})/\varepsilon] D, \quad (57)$$

where

$$\bar{f} = \pi^{-2} f(r_0, r_0, \bar{n}) r_0^2.$$

We now must determine $\bar{\nu}$ and σ from (57) and (49). To do this we must first find the points in which $\nu'(r_0 + h) = \nu(\xi + l) = 0$. From (53) we get

$$\sigma \approx -\bar{\nu}'(\xi) l. \quad (58)$$

Moreover, from (53) and (54) we have

$$\nu'(r_0 + h) \approx \bar{\nu}''(r_0) h + \bar{f}\bar{\nu}, \quad h \approx -\bar{f}\bar{\nu}/\bar{\nu}''(r_0). \quad (59)$$

We now rewrite (49) in the form

$$\int_{\xi}^{\xi+l} r^2 dr + \int_{\xi+l}^{\infty} \frac{\exp(\nu(r)/\varepsilon) r^2 dr}{1 + \exp(\nu(r)/\varepsilon)} - \int_0^{\xi+l} \frac{r^2 dr}{1 + \exp(\nu(r)/\varepsilon)} = J_1 + J_2 - J_3 = 0. \quad (60)$$

Evaluating J_2 and J_3 we restrict ourselves to contributions from the vicinities of r_0 and the (one-sided) vicinities of $\xi + l$. From the expression

$$J_3 = \int_{(r_0)} \frac{\exp(-\nu/\varepsilon) r^2 dr}{1 + \exp(-\nu/\varepsilon)} + \int_{(\xi+l)} \frac{\exp(-\nu/\varepsilon) r^2 dr}{1 + \exp(-\nu/\varepsilon)} = g_1 + g_2 \quad (61)$$

we get

$$g_1 = r_0^2 \int_{r_0 - \varepsilon^\alpha}^{r_0 + \varepsilon^\alpha} \frac{\exp(-\nu/\varepsilon) dr}{1 + \exp(-\nu/\varepsilon)} = r_0^2 \bar{\nu}, \quad g_2 = O(\varepsilon). \quad (62)$$

Similarly $J_2 = O(\varepsilon)$. Assuming that $\varepsilon \bar{\nu}^{-1} = O(\varepsilon)$ (as will be checked below) we find now from Eq. (60)

$$l \approx r_0^2 \bar{\nu} / \xi^2, \quad (63)$$

whence, using (58) we get

$$\sigma \approx \bar{\nu}'(\xi) r_0^2 \bar{\nu} / \xi^2 = a \bar{\nu}, \quad a > 0. \quad (64)$$

Assuming $\bar{\nu} = \varepsilon^{1/2} \kappa$ and using (64) we now find from (57) that

$$(a + \bar{f}) \kappa = -1/2 \ln \varepsilon - \ln \kappa + \ln D, \quad (65)$$

where

$$\kappa \sim 1/2 (-\ln \varepsilon) / (a + \bar{f}). \quad (66)$$

We note finally that (see (57), (66))

$$\bar{f}\bar{\nu} + \sigma \sim -1/2 \varepsilon \ln \varepsilon. \quad (67)$$

We now study the calculation of the specific heat C_ν . We must evaluate $dE_\nu/d\varepsilon$ under the condition (49). However,

$$\frac{dE_\nu}{d\varepsilon} = 2 \int \frac{dp}{(2\pi)^3} \frac{\delta E}{\delta n(p)} \frac{\partial n(p)}{\partial \varepsilon} = \frac{1}{\pi^2} \int_0^\infty dr [r^4 + r^2 f(r, n)] \frac{\partial n}{\partial \varepsilon}. \quad (68)$$

From (49) it follows that

$$\int_0^\infty r^2 \frac{\partial n}{\partial \varepsilon} dr = 0.$$

We can therefore rewrite (68) in the form

$$\frac{dE_\nu}{d\varepsilon} = \frac{1}{\pi^2} \int_0^\infty dr \{ [r^4 + r^2 f(r, \bar{n}) - \xi^2 r^2] n + r^2 [f(r, n) - f(r, \bar{n})] \} \frac{\partial n}{\partial \varepsilon}, \quad (69)$$

or

$$\frac{dE_\nu}{d\varepsilon} = \frac{1}{\pi^2} \int_{(r_0+h)} dr u(r) \Phi(r) + \frac{1}{\pi^2} \int_{(\xi+l)} dr u(r) (r^4 - \xi^2 r^2) + \frac{1}{\pi^2} \int_0^h dr u(r) \left[f\left(r, \bar{n} - \frac{1}{1 + \exp(\nu/\varepsilon)}\right) - f(r, \bar{n}) \right] = J_1' + J_2' + J_3', \quad (70)$$

where we have put

$$\Psi(r) = r^4 + r^2 f(r, \bar{n}) - \xi^2 r^2, \quad u(r) = \left(\frac{d\nu}{d\varepsilon} - \frac{\nu}{\varepsilon} \right) \frac{\exp(\nu/\varepsilon)}{[1 + \exp(\nu/\varepsilon)]^2}. \quad (71)$$

However,

$$\Psi(r_0) = \Psi'(r_0) = \Psi(\xi) = 0, \quad (72)$$

as follows easily from the equations

$$\bar{\nu}(r_0) = \bar{\nu}'(r_0) = 0, \quad \xi^2 = \bar{\nu}.$$

Moreover, from the estimate $\nu(r_0) \approx \sigma + \bar{f}\bar{\nu}$ and (67) it follows that

$$\left(\frac{d\nu}{d\varepsilon} - \frac{\nu}{\varepsilon} \right)_{r_0} \approx \frac{d}{d\varepsilon} (\sigma + \bar{f}\bar{\nu}) = -\frac{1}{2}, \quad (73)$$

whence

$$J_1' \approx -\frac{1}{2\pi^2} \int_{-\infty}^\infty ds [\Psi(r_0 + h) + s\Psi'(r_0 + h) + s^2\Psi''(r_0 + h) + \dots] \times \frac{\exp[-\nu(r_0 + h)/\varepsilon - \nu''(r_0 + h)s^2/2\varepsilon]}{[1 + \exp(-\nu/\varepsilon)]^2}, \quad (74)$$

$$\nu(r_0 + h) = \nu(r_0) + 1/2 h^2 \nu''(r_0) \approx \sigma + \bar{f}\bar{\nu} \quad (75)$$

and, hence, (see (67))

$$\exp[-\nu(r_0 + h)/\varepsilon] \sim \varepsilon^{1/2}. \quad (76)$$

Taking now (72) and (59) into account we find that

$$J_1' < \varepsilon^2 \ln \varepsilon, \quad J_2' < \varepsilon^2 \ln \varepsilon. \quad (77)$$

Finally, when $r \approx s + \xi + l$ and $s \ll r_0$ we have

$$\frac{d\nu}{d\varepsilon} = \frac{d\sigma}{d\varepsilon} \approx -a \ln \varepsilon, \quad \frac{\nu}{\varepsilon} \approx \frac{\nu'(\xi + l)s}{\varepsilon}. \quad (78)$$

Therefore

$$\begin{aligned}
J_2' \approx & -\frac{1}{\pi^2} a \ln \varepsilon \int_{-\infty}^{\infty} ds v(s) \{2\xi^3 l + 2(\xi+l) [2(\xi+l)^2 - \xi^2] s \\
& + O(l^2)\} - \frac{1}{\pi^2} \int_{-\infty}^{\infty} ds v(s) \left[\frac{v'(\xi+l)s}{\varepsilon} + \frac{v''(\xi+l)s^2}{2\varepsilon} \right] \\
& \times \{2\xi^3 l + 2(\xi+l) [2(\xi+l)^2 - \xi^2] s + O(l^2)\}, \\
v(s) = & \frac{\exp(v'(\xi+l)s/\varepsilon)}{[1 + \exp(v'(\xi+l)s/\varepsilon)]^2}. \quad (79)
\end{aligned}$$

It is clear that the first term is of order $\alpha(-\ln \varepsilon) \ln \varepsilon = \alpha \varepsilon^2 \ln^2 \varepsilon$, where $\alpha > 0$, while the second term is much smaller than the first since $v(s)$ is an even function. Combined with (77) this finally gives us

$$\left. \frac{dE_V}{d\varepsilon} \right|_0 = C_V \approx \alpha \varepsilon (\ln \varepsilon)^2. \quad (80)$$

As should have been expected the main contribution to the specific heat C_V comes from the edge ξ of the Fermi jump. The specific heat is thus discontinuous and tends to zero as $\varepsilon \rightarrow 0$ in agreement with Nernst's theorem, but its derivative with respect to the temperature becomes infinite at a temperature which tends to zero.

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