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A GENERALIZED HARTREE APPROXIMATION AND INTEGRAL EQUATIONS FOR CORRELATIONS IN QUANTUM FLUIDS

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A Generalized Hartree Approximation and Integral Equations for Correlations in Quantum Fluids

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With the use of Mori's continued-fraction method and by taking the collisionless approximation and assuming the vertex part in Dyson's equation to depend only on the momentum transfer Q, a generalized Hartree equation and the density-density response function $\chi_Q(\omega)$ are obtained in terms of the density-density canonical correlation χ_Q. This generalized Hartree equation contains the self-energy effect through the effective interaction and the streaming term.

On the basis of this equation, the direct correlation function and the Ornstein-Zernike relation in a classical fluid are extended to the case of a quantum fluid. These results give a generalization of the Hohenberg-Kohn-Mermin theory for a nonuniform electron gas applicable to a quantum fluid and also give an extension of the Percus method for deriving equations for the radial distribution function g(r) in such a way as to treat a quantum fluid. By applying this method to a neutral quantum fluid, quantal versions of the Percus-Yevick

and the hypernetted chain equations are derived. For a charged quantum fluid (electron gas), new integral equations are obtained by dividing an interatomic potential into strong short-range and slowly-varying long-range parts, and these equations give the compressibility sum rule taking into account the role of the short-range part of the potential in a similar way as Landau's Fermi-liquid theory.

The generalized Hartree equation combined with these integral equations for neutral and charged quantum fluids yields extensions of the Landau kinetic equation in the Fermi-liquid theory and of the Landau-Silin equation for the electron gas, respectively, to large wavevectors and high frequencies at non-zero temperatures.

In conjuction with these integral equations, a method for determining the dynamic and static structure factors, $S(Q,\omega)$ and $S(Q)$, and the self-energy $\Sigma_p^R(\varepsilon)$ in a self-consistent manner is set up.

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一般化されたハートリー近似と量子流体の相関関数にたいする積分方程式

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森の連分数の方法を用いて，衝突を無視する近似と2体グリーン関数にたいするダイソン方程式の結節部分が移行運動量Qのみの関数であるとする近似をもとに一般化されたハートリー方程式を導いた。この方程式は，普通のハートリー方程式と較べて，生のポテンシャルと流れの項が，密度のカノニカル相関χ_Qで表現される実効ポテンシャルと自己エネルギー$\Sigma_p^R(\epsilon)$の汎関数になっている流れの項でおきかえられている。

この方程式をもとに，古典流体におけるオルンシュタイン＝ゼルニケの関係式・直接相関関数を量子流体の場合に拡張した。この拡張は，第1に，外場中の電子ガスにたいするホーヘンバーグ＝コーン＝マーミンの理論の一般の量子流体への一般化を与え，第2に，古典液体の動径分布関数g(r)にたいする積分方程式を導くバーカスの方法の量子流体に適用できるような拡張を与える。この方法を用いて，バーカス＝イェビックの方程式・ハイパーネッティド＝チェーン方程式を中性量子流体の場合に拡張した。荷電量子流体（電子ガスを含む）にたいしては，相互作用をレンジの短い部分と長く弱い部分に分けることにより，新しい積分方程式を導いた。

中性および荷電量子流体にたいするこれらの方程式と組みあわせることにより，一般化されたハートリー方程式は，それぞれフェルミ流体におけるランダウ方程式・電子ガスにたいするランダウ＝シリン方程式の大波数Q・高周波ωかつ有限温度の場合への拡張を与えていることが示される。

さらに一般化されたハートリー方程式をもとに，中性および荷電量子流体（フェルミオンおよびボソン）における動径分布関数g(r)・時空間相関関数G(r, t)・分布関数n_pの3つの量を自己無撞着な形で，相互作用の強弱によらず，定める体系的な方法を導いた。この方法は巨視的なランダウのフェルミ液体の理論と微視的な乱雑位相近似にもとづく理論との関係を明らかにする。

Contents

§1. Introduction

There have been proposed numerous successful but apparently different approaches to the quantal many-body problem. Among them, the so-called random-phase approximation (RPA), originally developed by Bohm and Pines[1] in treating the electron gas, has been applied to a wide variety of many-body calculations. The RPA is essentially a weak-coupling approximation. When an interaction plays a dominant role, therefore, it is necessary to go beyond the RPA in order to calculate properties of the system. The Landau theory of Fermi liquids and also the Landau-Silin theory of the electron gas[2], though formal, have the advantage of being exact for any normal liquid, irrespective of its density and its strength of interaction, as long as the temperature is sufficiently low. These theories, however, can not treat phenomena involving large wavevectors and high frequencies. It should be also noted that these methods can provide no account of equilibrium properties such as the ground state energy and radial distribution function. Thus, it is necessary to generalize the Landau theory and also the Landau-Silin theory so as to be applicable to microscopic phenomena involving large wavevectors and high frequencies at nonzero temperatures and to bridge the gap between this macroscopic approach and microscopic theories such as the RPA theory.

We consider the case of the electron gas as a typical example of many-body problems. Equilibrium properties of the electron gas have been investigated exhaustively in the RPA. In the high-density limit the behaviour of the electron gas is well described by the RPA because the average potential energy

is small compared to the kinetic energy due to the presence of the Fermi surface. The high-density limit is expressed by the parameter r_s as $r_s \ll 1$ where r_s is defined by $4\pi r_s^3 a_0^3/3 = 1/n_0$ (n_0; the number density, a_0, the Bohr radius), while the region of actual metallic densities is an intermidiate regime ($1.8 \leq r_s \leq 5.6$). In the region of actual metallic densities, the RPA suffers from the drawback that the radial distribution function g(r) becomes negative for small distance r.[3] Hubbard[4] has given the correction to the RPA, but his result also has this drawback[5]. Nozieres and Pines[6] came to the conclusion that it was not especially fruitful to pursue the systematic study of corrections to the RPA because it is intrinsically a high density expansion.

In recent years, Singwi et al.[7] and Hubbard[8] calculated the radial distribution function in the range of actual metallic densities and improved this drawback fairly well by using the following semi-classical approach. They[7] have solved the equation of motion for the classical one-particle distribution f(r,p,t)(i.e. the BBGKY equation) in the presence of an external potential U(r), by assuming the ansatz for the two-particle distribution function

$$f_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}' \mid t) = f(\mathbf{r}, \mathbf{p}, t) f(\mathbf{r}', \mathbf{p}', t) g(|\mathbf{r} - \mathbf{r}'|), \quad (1.1)$$

and obtained a classical dielectric constant in the form

$$\varepsilon(Q, \omega) = 1 + \frac{v(Q) \cdot n_0 \beta \bar{\chi}_Q^0(\omega)}{1 - v(Q) G(Q) \cdot n_0 \beta \bar{\chi}_Q^0(\omega)}, \quad (1.2)$$

with

$$G(Q) = -\frac{1}{n_0}\int \frac{Q q}{q^2}\left[S(|Q-q|)-1\right]\frac{dq}{(2\pi)^3} \quad . \qquad (1.3)$$

Here, $\bar{\chi}_Q^o(\omega)$ is the classical free-electron polarizability and S(Q) is the structure factor and v(Q) is the Fourier transform of the Coulomb interaction. To obtain the quantal dielectric constant they made the assumption that in the classical dielectric constant the classical free-electron polarizability and the classical structure factor can be replaced by their quantal analogs. Thus, they proposed a quantal method of determining of S(Q) in a self-consistent manner since the structure factor is expressed in terms of the dielectric constant owing to the sum rule. In their calculation, the radial distribution function is positive for all values of the density up to $r_s=4$. However, their dielectric constant (1.1) has an unsatisfactory feature that the compressibility obtained from its long wavelength limit becomes negative for $r_s>3$.

In order to obtain a more satisfactory expression for the compressibility, two ways of refinements have been proposed. The first approach is due to Singwi et al.[9] who derived an improved dielectric constant with

$$G(Q) = -\frac{1}{n_0}\int \frac{Q q}{q^2 \varepsilon(q)}\left[S(|Q-q|)-1\right]\frac{dq}{(2\pi)^3}, \qquad (1.4)$$

where

$$\varepsilon(Q) \equiv \varepsilon(Q,0) \quad .$$

The second approach is to determine the radial distribution function with the aid of the virial form of the equation of

state. Thus Schneider[10] obtained

$$G(Q) = -\frac{1}{n_0}\int \frac{\mathbf{Q}\cdot\boldsymbol{\eta}}{\eta^2}\left[S(|\mathbf{Q}-\boldsymbol{\eta}|)-1+n_0\frac{\partial}{\partial n_0}S(|\mathbf{Q}-\boldsymbol{\eta}|)\right]\frac{d\boldsymbol{\eta}}{(2\pi)^3}, \quad (1.5)$$

and Vashishter and Singwi[11] gave

$$G(Q) = (1+an_0\frac{\partial}{\partial n_0})\left[-\frac{1}{n_0}\int \frac{\mathbf{Q}\cdot\boldsymbol{\eta}}{\eta^2}\left\{S(|\mathbf{Q}-\boldsymbol{\eta}|)-1\right\}\frac{d\boldsymbol{\eta}}{(2\pi)^3}\right], \quad (1.6)$$

where a is to be treated as a parameter. Although these two refinements improved values of the compressibility fairly well, the positiveness of the radial distribution function at small r became slightly worse than the earlier Singwi et al. result[7].

Concerning the Singwi et al. approach[7] to the electron gas, the following two remarks should be mentioned. The replacement of the classical structure factor S(Q) by the quantal one in the translation from the classical into quantal dielectric constant is not unique since there are many functions which become the classical structure factor in the classical limit. Secondly, the Singwi et al. treatment is essentially limited to the systems with a slowly varying potential, so that their treatment cannot describe g(r) in small interparticle separation at the low-density region where the strong and steep part of the Coulomb potential plays an important role. Concerning the compressibility, the situation is the same as the positiveness of g(0). Therefore, refinements of their approach should be performed in such a way that the strong and steep part of the Coulomb interaction is treated correctly.

On the other hand, the classical statistical-mechanical method for treating the many-body problem has several points superior to the quantal one. For instance, a wide variety of integral

equations for the radial distribution function g(r) such as the Percus-Yevick (PY) and hypernetted chain (HNC) equations have been proposed and shown to give the results in fair agreement with experiments. However, it is difficult in quantum fluids to derive integral equations for g(r) because phase space cannot be separated into coodinate and momentum spaces. There are three methods for deriving approximate integral equations (for example, the PY equation) for g(r) in classical fluids; (i) the diagrammatic technique[12], (ii) the functional-expansion method[13], (iii) the use of collective coodinates[14]. Among them the functional-expansion method developed by Percus yields the PY, HNC equations and others in a systematic way and has the advantage of indicating how corrections can be made to them. Recently we have obtained integral equations[15] for a fluid with a potential with slowly= varying and strong short-range parts, such as a charged particle system, by using the functional-expansion method. Therefore, if we can make this method applicable to quantal systems, these integral equations for classical neutral and charged fluids can be transformed in the case of quantum fluids in a systematic manner. Previously Percus[16] has tried to extend the PY equation to quantum fluids by the use of collective coodinates, but his attempt is not quite successful .

Recently a generalized Vlasov equation[17)-20] has been proposed and used to describe new collective modes observed by the inelastic neutron scattering experiments in classical liquids. This generalized Vlasov equation involves an effective interaction expressed in terms of the direct correlation function

instead of a bare potential v(r). Consequently, this equation is applicable even to the hard-sphere system in contrast to the usual Vlasov equation. In this sense, the generalized Vlasov equation offers an extension of the RPA for treating a strong-coupling system, and a quantal version of this equation is expected to give an approach to a quantal strong-coupling many-body system.

The purpose of the present study is to extend the above-mentioned advantageous treatment of the classical many-body problem to the quantal one, and thus to obtain the method by which Boson, Fermion, and classical fluids can be treated from a unified point of view.

In §2, the density-density relaxation function is obtained with the use of Mori's continued-fraction method[21] and the dynamic structure factor $S(Q,\omega)$ is represented in terms of the self-energy $\Sigma_p^R(\varepsilon)$ and the density-density canonical correlation χ_Q, which are to be determined in a self-consistent manner. In §3, the self-consistent equation for the self-energy $\Sigma_p^R(\varepsilon)$ is given. In §4, moments of the canonical correlation of the density fluctuation $\gamma_Q(\omega)$ are investigated up to the fourth moment.

In §5, we obtain expressions for quantal versions of the direct correlation function and the Ornstein-Zernike relation. With the use of the results in §5, the Hohenberg-Kohn-Mermin theory in a nonuniform electron gas is generalized to the case of quantum fluids in §6.

In §7, quantal extensions of the PY anf HNC equations are derived and then in §8, the generalized Hartree equation derived

in §2 in conjuction with these equations is shown to give a generalization of the Landau kinetic equation in the Fermi= liquid theory.

In §9, we obtain integral equations for charged quantum fluids and then in §10, the generalized Hartree equation combined with these equations is shown to yield a generalization of the Landau-Silin kinetic equation for the electron gas. In §11, one of our equations derived in §9 is numenically solved in the case of the electron gas and the result is compared with that of Singwi et al. The last section is devoted to summary concluding remarks.

§2. Relaxation function and generalized Hartree equation

Let us consider the following relaxation function $\Gamma_Q^{pp'}[z]$ with momentum variables p and p'

$$\Gamma_Q^{pp'}[z] = \int_{-\infty}^{\infty} e^{-zt} \langle \rho_{pQ}(t) ; \rho_{p'Q}(0) \rangle \, dt \ , \tag{2.1}$$

where

$$\langle A ; B \rangle \equiv \frac{1}{\beta} \int_0^{\beta} \langle e^{\lambda(\hat{H}-\mu\hat{N})} A \, e^{-\lambda(\hat{H}-\mu\hat{N})} B^{\dagger} \rangle \, d\lambda \ , \tag{2.2}$$

$$\rho_{pQ} \equiv a^{\dagger}_{p-Q/2} a_{p+Q/2} \ . \tag{2.3}$$

Here, $a_p^{\dagger}$ and a_p are, respectively, the creation and annihilation operators of the free-particle states with momentum p, μ is the chemical potential, the dagger, $\dagger$, denotes Hermite conjugate, $\beta = 1/k_B T$, and $\hat{H}$ and $\hat{N}$ are the Hamiltonian and the particle number operator, respectively. The angular bracket indicates the average over the grand canonical ensemble.

According to Mori's continued-fraction method[21] this relaxation function $\Gamma_Q^{pp'}[z]$ may be expressed in the form

$$\Gamma_Q^{pp'}[z] = \sum_{p''} (p | \{ z - i\hat{\omega}_0 + \hat{\phi}(z) \}^{-1} | p'') (p'' | \hat{\chi}_Q | p') \ , \tag{2.4}$$

where

$$(p | \hat{\chi}_Q | p') \equiv \langle \rho_{pQ} ; \rho_{p'Q} \rangle \equiv \chi_Q^{pp'} \ , \tag{2.5}$$

$$(p | i\hat{\omega}_0 | p') \equiv \sum_{p''} \langle \dot{\rho}_{pQ} ; \rho_{p'Q} \rangle (p'' | \hat{\chi}_Q^{-1} | p') \ . \tag{2.6}$$

Here $(p|\hat{A}|p')$ and $(p|\hat{A}^{-1}|p')$ denote, respectively, the p-p' element of a matrix $\hat{A}$ and the inverse matrix $\hat{A}^{-1}$ and $\hat{\phi}(z)$ is the damping function.

In the present study we take $\hat{\phi}(z)=0$, which means the collisionless approximation. Then, to calculate the relaxation function $\Gamma_Q^{pp'}[z]$ by means of Eq.(2.4), we must evaluate $\chi_Q^{pp'}$ and $\langle\dot{\rho}_{pQ};\rho_{p'Q}\rangle$. In the first place we are concerned with the calculation of $\chi_Q^{pp'}$. This static correlation can be calculated with the use of the temperature Green's function method as below.

In general the temperature Green's function;

$$K_{pp'}(Q,\omega_m) \equiv \int_0^\beta e^{i\omega_m\tau}\langle e^{(\hat{H}-\mu\hat{N})\tau}\rho_{pQ}\, e^{-(\hat{H}-\mu\hat{N})\tau}\rho^{+}_{p'Q}\rangle d\tau, \quad (2.7)$$

with

$$\omega_m = 2m\pi/\beta, \quad (2.8)$$

obeys the following Dyson's equation:[22]

$$K_{pp'}(Q,\omega_m) = \frac{1}{\beta}\sum_n G_{p+Q/2}(\varepsilon_n+\omega_m)G_{p-Q/2}(\varepsilon_n)\delta_{pp'}$$
$$-\frac{1}{\beta^2}\sum_{nn'} G_{p+Q/2}(\varepsilon_n+\omega_m)G_{p-Q/2}(\varepsilon_n)\Gamma^{Q}_{pp'}(\varepsilon_n,\varepsilon_{n'};\omega_m)\chi$$
$$\times G_{p'+Q/2}(\varepsilon_{n'}+\omega_m)G_{p'-Q/2}(\varepsilon_{n'}), \quad (2.9)$$

where

$$\varepsilon_n \equiv \begin{cases} 2n\pi/\beta & \text{(Boson)} \\ (2n+1)\pi/\beta & \text{(Fermion)} \end{cases}, \qquad \zeta \equiv \begin{cases} 1 & \text{(Boson)} \\ -1 & \text{(Fermion)} \end{cases}, \quad (2.10)$$

and $G_p(\varepsilon_n)$ denotes the one-particle temperature Green's function defined at the set of points ε_n and $\Gamma^Q_{pp'}(\varepsilon_n, \varepsilon_{n'}: \omega_m)$ is the vertex part. From Eq.(2.7) we can see that $\chi_Q^{pp'}$ is obtained by setting $\omega_m=0$ in Eq.(2.9), that is,

$$\beta\langle \rho_{pQ} ; \rho_{p'Q} \rangle = K_{pp'}(Q, \omega_m = 0) = \beta \chi_Q^{pp'}$$

$$= \frac{2}{\beta} \sum_n G_{p+Q/2}(\varepsilon_n) G_{p-Q/2}(\varepsilon_n) \delta_{pp'}$$

$$- \frac{1}{\beta^2} \sum_{n,n'} G_{p+Q/2}(\varepsilon_n) G_{p-Q/2}(\varepsilon_n) \Gamma^Q_{pp'}(\varepsilon_n, \varepsilon_{n'} ; \omega_m = 0)$$

$$\times G_{p+Q/2}(\varepsilon_{n'}) G_{p-Q/2}(\varepsilon_{n'}) \quad . \qquad (2.11)$$

It is difficult to evaluate $\chi_Q^{pp'}$ without the use of approximations, as is seen from Eq.(2.11). When the parameters ε_n and $\varepsilon_{n'}$ are small, $\Gamma^Q_{pp'}(\varepsilon_n, \varepsilon_{n'} : \omega_m = 0)$ is shown to depend on ε_n, $\varepsilon_{n'}$ weakly for Fermions.[23] Moreover, in the classical limit, $\Gamma^Q_{pp'}(\varepsilon_n, \varepsilon_{n'} : \omega_m = 0)$ is the function of only the wave-vector Q, and as will be shown later,

$$\lim_{\hbar \to 0} \Gamma^Q_{pp'} = S(Q) - 1 \quad ,$$

where S(Q) is the structure factor. Considering these features, we make the following approximation

$$\Gamma^Q_{pp'}(\varepsilon_n, \varepsilon_{n'} ; \omega_m = 0) = \Gamma^Q \quad , \qquad (2.12)$$

that is, $\Gamma^Q_{pp'}$ is independent of ε_n, $\varepsilon_{n'}$ and p, p'. This approximation simplifies the calculation of $\chi_Q^{pp'}$ and reduces Eq.(2.11) to

$$\langle \rho_{pQ} ; \rho_{p'Q} \rangle = f_Q(p) \delta_{pp'} - f_Q(p) \beta \Gamma^Q f_Q(p') \quad . \qquad (2.13)$$

where

$$f_Q(p) \equiv \frac{1}{\beta}\frac{\hbar}{\beta}\sum_n G_{p+Q/2}(\varepsilon_n)\,G_{p-Q/2}(\varepsilon_n)$$

$$= \frac{1}{\pi\beta}\int_{-\infty}^{\infty} d\varepsilon\, \frac{1}{e^{\beta\varepsilon}-\eta}\, \mathrm{Im}\left\{G^R_{p+Q/2}(\varepsilon)\,G^R_{p-Q/2}(\varepsilon)\right\}$$

$$= \frac{1}{\beta\pi}\int_{-\infty}^{\infty} d\varepsilon\, \frac{1}{e^{\beta\varepsilon}-\eta}\, \mathrm{Im}\,\frac{G^R_{p+Q/2}(\varepsilon) - G^R_{p-Q/2}(\varepsilon)}{\varepsilon^0_{p+Q/2}+\Sigma^R_{p+Q/2}(\varepsilon)-\varepsilon^0_{p-Q/2}-\Sigma^R_{p-Q/2}(\varepsilon)} \,. \qquad (2.14)$$

Here

$$G^R_p(\varepsilon) \equiv \frac{1}{\varepsilon - \varepsilon^0_p + \mu - \Sigma^R_p(\varepsilon)} \,, \qquad (2.15)$$

is the analytically continued function of $G_p(\varepsilon_n)$ with a discrete set of points ε_n throughout the entire upper half-plane, so that

$$G^R_p(i\varepsilon_n) = G_p(\varepsilon_n) \quad \text{for} \quad \varepsilon_n > 0 \,,$$

and ε^0_p is the kinetic energy of a free particle and $\Sigma^R_p(\varepsilon)$, the self-energy.

As an illustration of the function $f_Q(p)$, we take two simple cases below. First in the absence of interactions ($\Sigma^R_p(\varepsilon)=0$), $f_Q(p)$ is reduced to

$$f_Q(p) = -\frac{1}{\beta}\,\frac{n(\varepsilon^0_{p+Q/2}) - n(\varepsilon^0_{p-Q/2})}{\varepsilon^0_{p+Q/2} - \varepsilon^0_{p-Q/2}} \,, \qquad (2.15)'$$

where

$$n(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} - \eta} \,,$$

and second in the classical limit, $f_Q(p)$ is shown to be proportional to the normalized Maxwell distribution function $\Phi_M(p)$:

$$\lim_{\hbar\to 0} \frac{1}{N} f_Q(p) = \Phi_M(p), \tag{2.16}$$

where N is the average total number of particles.

On the other hand, there is an exact relation concerning $\chi_Q^{pp'}$;

$$\frac{1}{N}\sum_{pp'} \chi_Q^{pp'} = \frac{1}{N}\sum_{pp'} \langle \rho_{pQ} ; \rho_{p'Q} \rangle$$
$$= \frac{1}{N}\langle \rho_Q ; \rho_Q \rangle \equiv \chi_Q, \tag{2.17}$$

where

$$\rho_Q \equiv \sum_p \rho_{pQ} = \sum_p a^+_{p-Q/2}\, a_{p+Q/2} .$$

Owing to Eqs.(2.17) and (2.13), Γ^Q has the form

$$\beta\Gamma^Q = -\left(\frac{\chi_Q}{\chi_Q^\circ} - 1\right)\frac{1}{\chi_Q^\circ}\,\frac{1}{N}, \tag{2.18}$$

where

$$\chi_Q^\circ \equiv \frac{1}{N}\sum_p f_Q(p) . \tag{2.19}$$

With the use of Eqs.(2.18) and (2.13), there results finally

$$\chi_Q^{pp'} = f_Q(p)\,\delta_{pp'} + f_Q(p)\left(\frac{\chi_Q}{\chi_Q^\circ} - 1\right)\frac{1}{\chi_Q^\circ} f_Q(p)\,\frac{1}{N} . \tag{2.20}$$

It should be mentioned that although Eq.(2.20) is an approximation, $\chi_Q^{pp'}$ given by Eq.(2.20) has the exact classical limit, as shown below. Taking account of

$$\lim_{\hbar\to 0} \chi_Q = S(Q), \quad \lim_{\hbar\to 0} \chi_Q^\circ = 1 ,$$

and Eq.(2.16), the classical limit of $\chi_Q^{pp'}$ is written as

$$\lim_{\hbar\to 0}\frac{1}{N}\langle \rho_{pQ};\rho_{p'Q}\rangle = \frac{1}{N}\Big\langle \sum_{i=1}^{N'} e^{-iQr_i}\delta(p-p_i)\cdot\sum_{j=1}^{N'} e^{iQr_j}\delta(p'-p_j)\Big\rangle_c$$
$$= \Phi_M(p)\delta(p-p') + \Phi_M(p)\{S(Q)-1\}\Phi_M(p'), \qquad (2.21)$$

where $\langle A_{N'}\rangle_c$ denotes the classical average over the grand canonical ensemble, that is,

$$\langle A_{N'}\rangle_c \equiv \sum_{N'=0}^{\infty}\exp(-\beta\mu N')\int \exp(-\beta H_{N'})A_{N'}d\Gamma$$
$$\times\left(\sum_{N'=0}^{\infty}\exp(-\beta\mu N')\int\exp(-\beta H_{N'})d\Gamma\right)^{-1}.$$

This result is exact in the classical mechanical case.

Next, we calculate $\langle\dot{\rho}_{pQ};\rho_{p'Q}\rangle$ which is necessary to evaluate Eq.(2.6), and obtain the result

$$\langle\dot{\rho}_{pQ};\rho_{p'Q}\rangle = -\frac{1}{\beta}\frac{i}{\hbar}[n_{p-Q\hbar}-n_{p+Q\hbar}]\delta_{pp'} \equiv g_Q(p)\delta_{pp'}, \qquad (2.22)$$

where

$$n_p \equiv \langle a_p^{+}a_p\rangle .$$

From Eq.(2.20), the inverse matrix to $\chi_Q^{pp'}$ is easily calculated in the form

$$(p|\hat{\chi}_Q^{-1}|p') = \frac{\delta_{pp'}}{f_Q(p)} - \left\{\frac{1}{\chi_Q^0}-\frac{1}{\chi_Q}\right\}\frac{1}{N}. \qquad (2.23)$$

Now, we find from a combination of Eqs.(2.22) and (2.23) that

$$(p|i\hat{\omega}_0|p') = -i\omega_{pQ}\delta_{pp'} - \left(\frac{1}{\chi_Q^0}-\frac{1}{\chi_Q}\right)\frac{1}{N}g_Q(p), \qquad (2.24)$$

where

$$i\omega_{pQ} \equiv -g_Q(p)/f_Q(p)$$
$$= \frac{i}{\hbar}[n_{p-Q/2}-n_{p+Q/2}]\Big/\frac{1}{\pi}\int_{-\infty}^{\infty}d\varepsilon\,\frac{1}{e^{\beta\varepsilon}-\eta}\,\mathrm{Im}\left\{G^R_{p+Q/2}(\varepsilon)G^R_{p-Q/2}(\varepsilon)\right\}. \quad (2.25)$$

This quantity $i\omega_{pQ}$ is a complicated functional of the self-energy In the case of $\Sigma^R_p=0$, $i\omega_{pQ}$ takes a simple form

$$i\omega_{pQ} = \frac{i}{\hbar}[\varepsilon^0_{p+Q/2}-\varepsilon^0_{p-Q/2}] = \frac{i}{\hbar}\frac{pQ}{m}. \quad (2.26)$$

Thus we can obtain the relaxation function using Eqs.(2.20) and (2.24). In Mori's method the continued-fraction representation is obtained by use of a generalized Langevin equation of motion.[21] Before calculating the relaxation function, we investigate here a generalized Langevin equation of motion associated with the continued-fraction representation of the relaxation function in our approximations. Also, from this equation the meaning of the approximations used above and of our continued-fraction representation becomes clear as shown later.

Making use of Eq.(2.24), we obtain the equation for

$$\phi_{pQ}[z] = \int_0^\infty \phi_{pQ}(t)\,e^{-zt}\,dt,$$

where

$$\phi_{pQ}(t) = e^{i\hat{H}t/\hbar}\,\phi_{pQ}\,e^{-i\hat{H}t/\hbar},$$

in the following form

$$(z+i\omega_{pQ})\phi_{pQ}[z] + \frac{1}{n_0\beta}\left\{\frac{1}{\chi^0_Q}-\frac{1}{\chi_Q}\right\}\frac{i}{\hbar}\left\{n_{p+Q/2}-n_{p-Q/2}\right\}\frac{1}{V}\sum_{p'}\phi_{p'Q}[z]=0, \quad (2.27)$$

where n_o is the number density. Here we have put $\rho_{pQ}(t=0)=0$. If we make an approximation for $\Sigma^R_p(\varepsilon)$ to be independent of ε, then

$$\hbar\omega_{pQ} = E_{p+Q/2} - E_{p-Q/2} ,$$

$$\chi^0_Q = -\frac{1}{\beta}\frac{1}{N}\sum_p \frac{n(E_{p+Q/2})-n(E_{p-Q/2})}{E_{p+Q/2}-E_{p-Q/2}} ,$$

where

$$E_p = \varepsilon^0_p + \Sigma^R_p ,$$

so that Eq.(2.27) becomes

$$\left\{z+\frac{i}{\hbar}(E_{p+Q/2}-E_{p-Q/2})\right\}\rho_{pQ}[z] - \frac{1}{n_o\beta}\left\{\frac{1}{\chi^0_Q}-\frac{1}{\chi_Q}\right\}\frac{i}{\hbar}\left\{n(E_{p+Q/2})-n(E_{p-Q/2})\right\}\frac{1}{V}\sum_{p'}\rho_{p'Q}[z] = 0 . \tag{2.28}$$

In comparison with the usual Hartree equation, we can see that Eq.(2.27) is regarded as a generalized Hartree equation in the following two points: (i) The bare potential in the usual Hartree equation is replaced by the effective one:

$$n_o\beta V_{eff}(Q) \equiv -\left\{\frac{1}{\chi^0_Q}-\frac{1}{\chi_Q}\right\} , \tag{2.29}$$

which becomes the direct correlation function C(Q) in the classical limit

$$n_o\beta V_{eff}(Q) = -n_o C(Q) = \frac{1}{S(Q)} - 1 .$$

(ii) The streaming term, $(i/h)[\varepsilon^0_{p+Q/2}-\varepsilon^0_{p-Q/2}]$, in the usual Hartree equation is replaced by $i\omega_{pQ}$, which depends on the self-energy $\Sigma^R_p(\varepsilon)$ in a complicated way.

Though there is no explicit Fock term in the generalized Hartree equation, Eq.(2.27), the exchange effect is taken into account in this equation due to the generalization in (i) and (ii). The average of ρ_{pQ} in Eq.(2.27) gives a quantal generalized Vlasov equation for the Wigner function,

$$F_W(Q,p,z) \equiv \langle \rho_{pQ} \rangle [z] ,$$

and the classical limit of this equation becomes a generalized Vlasov equation.[17)-20)]

Now, we compute the relaxation function with the use of the above results as follows: From Eq.(2.24), we get

$$(p|\{z-i\hat{\omega}_0\}^{-1}|p') = \frac{g_Q(p)}{\Lambda_Q(z,p)}\delta_{pp'} + \frac{\beta g_Q(p)}{\Lambda_Q(z,p)} \frac{V_{eff}(Q)}{\varepsilon(Q,z)} \frac{1}{\Lambda_Q(z,p')} \frac{1}{V} , \quad (2.30)$$

where

$$\Lambda_Q(z,p) \equiv z + i\omega_{pQ} , \quad (2.31)$$

$$\varepsilon(Q,z) \equiv 1 - V_{eff}(Q) \frac{1}{V} \sum_p \frac{\beta g_Q(p)}{\Lambda_Q(z,p)} , \quad (2.32)$$

so that, with the aid of Eq.(2.20), the relaxation function $\Gamma_Q^{pp'}[z]$ is written as

$$\begin{aligned}\Gamma_Q^{pp'}[z] &= \sum_{p''} (p|\{z-i\hat{\omega}_0\}^{-1}|p'')(p''|\hat{\chi}_Q|p') \\ &= \sum_{p''} \left\{ \frac{g_Q(p)}{\Lambda_Q(z,p)}\delta_{pp'} + \frac{\beta g_Q(p)}{\Lambda_Q(z,p)} \frac{V_{eff}(Q)}{\varepsilon(Q,z)} \frac{g_Q(p'')}{\Lambda_Q(z,p'')} \frac{1}{V} \right\} \\ &\quad \times \left\{ f_Q(p'')\delta_{p''p} + f_Q(p'') \left\{ \frac{\chi_Q}{\chi_Q^0} - 1 \right\} \frac{1}{\chi_Q^0} f_Q(p') \frac{1}{N} \right\} . \end{aligned} \quad (2.33)$$

On the other hand, it can be easily shown that

$$\sum_{p''}(p|i\hat{\omega}_0|p'')(p''|\hat{\chi}_Q|p') = -i\omega_{pQ} f_Q(p)\delta_{pp'} = g_Q(p)\delta_{pp'}, \quad (2.34)$$

under the condition that Eq.(2.29) holds. It should be noted that Eq.(2.34) cannot be derived, if the potential contained in $(p|i\hat{\omega}_0|p')$ is the bare one.*)

By use of Eq.(2.34) and the identity

$$(z - i\hat{\omega}_0)^{-1} = \{(z-i\hat{\omega}_0)^{-1} i\hat{\omega}_0 + 1\}/z, \quad (2.35)$$

Eq.(2.33) may be written as

$$\Gamma_Q^{pp'}[z] = \frac{1}{z}\left\{\frac{g_Q(p)}{\Lambda_Q(z,p)}\delta_{pp'} + \frac{\beta g_Q(p)}{\Lambda_Q(z,p)}\frac{V_{eff}(Q)}{\varepsilon(Q,z)}\frac{g_Q(p')}{\Lambda_Q(z,p')}\frac{1}{V} + \chi_Q^{pp'}\right\}. \quad (2.36)$$

In general, the relaxation function $\Gamma_Q^{pp'}[z]$ and the response function $\chi_Q^{pp'}[z]$ defined by

$$\chi_Q^{pp'}[z] \equiv -\frac{1}{\beta}\int_0^\infty e^{-zt}\left\langle\frac{1}{i\hbar}[\rho_{pQ}(t), \rho_{p'Q}^\dagger]\right\rangle dt, \quad (2.37)$$

are related as follows:

$$\Gamma_Q^{pp'}[z] = \frac{1}{z}\left\{-\chi_Q^{pp'}[z] + \chi_Q^{pp'}\right\}, \quad (2.38)$$

which is derived by partial integration of Eq.(2.1). Comparison of Eq.(2.36) with Eq.(2.38) gives the expression of the response

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*) Equation (2.29) is the quantal extension of the condition that the three kinetic methods [(i) initial-value approach, (ii) dielectric approach and (iii) method of fluctuations in distribution function] of calculating the space-time correlation function should be equivalent to one another as is reported elsewhere.[24]

function in the form

$$\chi_Q^{pp'}[z] = -\frac{g_Q(p)}{\Lambda_Q(z,p)}\delta_{pp'} - \frac{\beta g_Q(p)}{\Lambda_Q(z,p)}\frac{V_{eff}(Q)}{\varepsilon(Q,z)}\frac{g_Q(p')}{\Lambda_Q(z,p')}\frac{1}{V} . \quad (2.39)$$

At first glance Eq.(2.39) has a simple structure similar to the expression obtained by use of the usual Hartree approximation,[25] which is obtained by replacing $V_{eff}(Q)$ by $v(Q)$, the Fourier transform of the bare potential, and $i\omega_{pQ}$ by $(i/\hbar)[\varepsilon^0_{p+Q/2}-\varepsilon^0_{p-Q/2}]$ in Eq.(2.39). But the expression of Eq.(2.39) is not so simple in general, since χ_Q^0, χ_Q and $i\omega_{pQ}$ contained in $V_{eff}(Q)$ and $\Lambda_Q(z,p)$ are related to the function, $f_Q(p)$ defined by Eq.(2.14). Also, the density-density response function $\chi_Q(\omega)$ is expressed as

$$\chi_Q(\omega) \equiv \frac{1}{N}\sum_{pp'}\chi_Q^{pp'}[-i(\omega+i0^+)]$$

$$= \chi_Q^0(\omega)\Big/\{1+n_0\beta V_{eff}(Q)\chi_Q^0(\omega)\} , \quad (2.40)$$

where

$$\chi_Q^0(\omega) = \frac{1}{N\beta}\sum_p \frac{n_{p+Q/2}-n_{p-Q/2}}{\hbar\omega-\hbar\omega_{pQ}+i0^+} .$$

With the aid of the general relation between the canonical correlation function and the relaxation function,[26] the dynamic structure factor $S(Q,\omega)$ is given by the formula

$$S(Q,\omega) = \frac{\beta\hbar\omega}{2}\left\{1+\coth\left(\frac{\beta\hbar\omega}{2}\right)\right\}\gamma_Q(\omega) . \quad (2.41)$$

where

$$\gamma_Q(\omega) \equiv \frac{1}{\pi} \mathrm{Re}\left\{\frac{1}{N}\sum_{pp'} \Gamma_Q^{pp'}[i\omega]\right\}$$
$$= \frac{1}{\pi}\frac{1}{\omega}\,\mathrm{Im}\left\{\chi_Q(\omega)\right\}$$
$$= -\frac{1}{\pi}\frac{1}{\omega}\frac{1}{n_0\beta V_{eff}(Q)}\,\mathrm{Im}\left\{\frac{1}{\varepsilon(Q,-i\omega)}\right\}. \quad (2.42)$$

Consequently, structure factor S(Q) is determined by the sum rule

$$S(Q) = \int_{-\infty}^{\infty} S(Q,\omega)\,d\omega = \int_{-\infty}^{\infty} \frac{\beta\hbar\omega}{2}\coth\left(\frac{\beta\hbar\omega}{2}\right)\gamma_Q(\omega)\,d\omega. \quad (2.43)$$

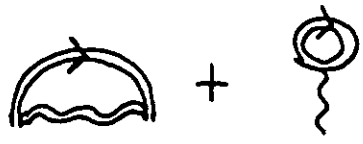
§3. Equation for self-energy $\Sigma_p^R(\varepsilon)$

In the preceding section we obtained the response function in Eq.(2.39), where the vertex part

$$\Gamma(p,z) \equiv V_{eff}(q)/\varepsilon(q,z), \tag{3.1}$$

involves χ_Q^o, χ_Q and the self-energy $\Sigma_p^R(\varepsilon)$ through the definitions of $\varepsilon(p,z)$ and $V_{eff}(p)$. In this section we obtain the expression of $\Sigma_p^R(\varepsilon)$ in terms of the vertex part $\Gamma(p,z)$; that is, the self-consistent equation for $\Sigma_p^R(\varepsilon)$ with the use of the Hartree-Fock approximation as follows:

With the Hartree-Fock approximation, the self-energy $\Sigma_p(\varepsilon_n)$ is determined by the sum of the following two terms

$\Sigma_p(\varepsilon_n) =$  , (3.2)

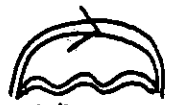
where ⇒ denotes the one-particle Green's function $G_p(\varepsilon_n)$, ~~ denotes the interaction $V_{eff}(p)$ and ≈ means the vertex part

$$\tilde{\Gamma}(p,\varepsilon_n) = V_{eff}(p)/\hat{\varepsilon}(p,\varepsilon_n) . \tag{3.3}$$

Here

$$\hat{\varepsilon}(p,\varepsilon_n) \equiv \varepsilon(p,-i\varepsilon_n) \quad \text{for } \varepsilon_n > 0 .$$

In the first place, we compute the first term in Eq.(3.2) as follows:

$\Sigma_1(p,\varepsilon_{n_0}) \equiv$ 

$$= -\frac{1}{\beta}\sum_{\omega_n}\int\frac{dp_1}{(2\pi)^3}\tilde{\Gamma}(p-p_1,\varepsilon_{n_0}-\omega_n)G_{p_1}(\omega_n)$$

$$= \frac{-\eta}{4\pi i}\int\frac{dp_1}{(2\pi)^3}\oint_C d\omega\,\Gamma^{RA}(p-p_1,\varepsilon_{n_0}-\omega)G^{RA}_{p_1}(\omega)f_\eta(\omega) \tag{3.4}$$

$$-\frac{1}{\beta}\int\frac{dp_1}{(2\pi)^3}\tilde{\Gamma}(p-p_1,0)G_{p_1}(\varepsilon_{n_0}) ,$$

where

$$f_\zeta(\varepsilon) \equiv \begin{cases} \coth\left(\frac{\beta\varepsilon}{2}\right), & (\zeta=1, \text{Boson}) \\ -\tanh\left(\frac{\beta\varepsilon}{2}\right), & (\zeta=-1, \text{Fermion}) \end{cases} \tag{3.5}$$

$$\tilde{\Gamma}(p, \varepsilon_n) \equiv \begin{cases} \Gamma^R(p, i\varepsilon_n) & \text{for } \varepsilon_n > 0, \\ \Gamma^A(p, i\varepsilon_n) & \text{for } \varepsilon_n < 0, \end{cases} \tag{3.6}$$

and

$$G_p(\varepsilon_n) \equiv \begin{cases} G_p^R(i\varepsilon_n) & \text{for } \varepsilon_n > 0, \\ G_p^A(i\varepsilon_n) & \text{for } \varepsilon_n < 0. \end{cases} \tag{3.7}$$

Here, the sum over ω_n is replaced by the contour integral and C, the contour of integration, is shown in Fig. 1. We can now easily perform the analytic continuation with respect to ε_n in Eq.(3.4) into the real axis, thereby obtaining the retarded function $\Sigma_1^R(p,\varepsilon)$. Since the integral over the large arcs is equal to zero, Eq.(3.4) is shown to be

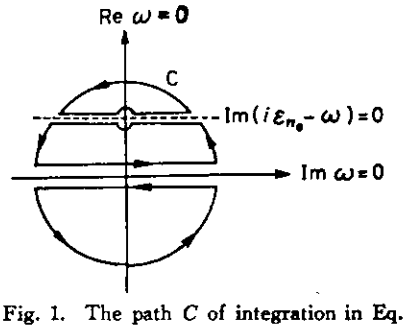


Fig. 1. The path C of integration in Eq. (3·4).

$$\Sigma_1^R(p,\varepsilon) = \frac{\hbar}{2\pi}\int\frac{dp_1}{(2\pi)^3}\int_{-\infty}^{\infty}d\omega\int_{-\infty}^{\infty}d\varepsilon_1 \frac{\mathrm{Im}\,G_{p_1}^R(\varepsilon)\cdot\mathrm{Im}\,\Gamma^R(p-p_1,\omega)}{\omega+\varepsilon_1-\varepsilon+i0^+} \times\left\{f_{-\zeta}(\omega)-f_\zeta(\varepsilon)\right\}. \tag{3.8}$$

Here, the details of the calculation of the above result are omitted, for the derivation is similar to that given by Abrikosov et al.[27]

On the other hand, the second term in Eq.(3.2) is given in

the form

$$\Sigma_2^R(p, \varepsilon_n) \equiv$$  $$= n_0 V_{eff}(0). \qquad (3.9)$$

Combinining Eqs.(3.8) and (3.9), we obtain a self-consistent equation for $\Sigma_p^R(\varepsilon)$.

§4. Sum rules

In this section we compute moments of the function $\gamma_Q(\omega)$ defined by Eq.(2.42), with respect to ω, Since $\gamma_Q(\omega)$ is an even function concerning ω, we have only to calculate even moments

$$\langle\langle \omega^{2n} \rangle\rangle \equiv \int_{-\infty}^{\infty} \omega^{2n} \gamma_\alpha(\omega)\, d\omega \,. \tag{4.1}$$

From Eq.(2.27), we obtain the equation for

$$\rho_{p\alpha}(\omega) \equiv \int_{-\infty}^{\infty} \rho_{p\alpha}(t)\, e^{i\omega t}\, dt \,,$$

in the form

$$\omega \rho_{p\alpha} = \omega_{p\alpha} \rho_{p\alpha} + n_0 \beta V_{\mathrm{eff}}(\alpha) \frac{1}{N} \omega_{p\alpha} f_\alpha(p) \rho_\alpha \,, \tag{4.2}$$

from which, with the use of the relation

$$\sum_p \omega_{p\alpha} f_\alpha(p) = 0 \,, \tag{4.3}$$

the equation of continuity is derived as

$$\omega \rho_\alpha = \sum_p \omega_{p\alpha} \rho_{p\alpha} \equiv Q \cdot j_\alpha(\omega) \,. \tag{4.4}$$

Here, the current $j_Q(\omega)$ is a complicated functional of the self-energy. The equation of continuity (4.4) plays an important role in the calculation of $\langle\langle \omega^{2n} \rangle\rangle$ below.

(i) $\langle\langle 1 \rangle\rangle$

With the aid of the Krammers-Kronig relation, the zeroth moment $\langle\langle 1 \rangle\rangle$ is easily given by,

$$\int_{-\infty}^{\infty} \gamma_\alpha(\omega)\, d\omega = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{1}{\omega} \mathrm{Im} \left\{ \frac{1}{N} \sum_{p,p'} \chi_\alpha^{pp'}[-i\omega] \right\} = \chi_\alpha \,. \tag{4.5}$$

This is the exact zeroth moment relation.

(ii) $\ll\omega^2\gg$

With the help of the equation of continuity (4.4) the second moment $\ll\omega^2\gg$ may be written as

$$\int_{-\infty}^{\infty}\omega^2\gamma_\alpha(\omega)d\omega = \frac{1}{N}\int_{-\infty}^{\infty}\langle\omega\rho_\alpha(\omega);\omega\rho_\alpha(\omega)\rangle d\omega$$

$$= \frac{1}{\pi}\mathrm{Re}\left\{\frac{1}{N}\sum_{pp'}\int_{-\infty}^{\infty}\omega_{p\alpha}\omega_{p'\alpha}\Gamma_\alpha^{pp'}[i\omega]d\omega\right\}. \quad (4.6)$$

Due to the relation between $\Gamma_Q^{pp'}[i\omega]$ and $\chi_Q^{pp'}[i\omega]$, and the Krammers-Kroning relation, the above equation becomes

$$\int_{-\infty}^{\infty}\omega^2\gamma_\alpha(\omega)d\omega = \frac{1}{N}\omega_{p\alpha}\omega_{p'\alpha}\int_{-\infty}^{\infty}\frac{1}{\pi\omega}\mathrm{Im}\chi_\alpha^{pp'}[-i\omega]d\omega$$

$$= \frac{1}{N}\sum_{pp'}\omega_{p\alpha}\omega_{p'\alpha}\chi_\alpha^{pp'}$$

$$= \frac{1}{N}\sum_{p}\omega_{p\alpha}^2 f_\alpha(p) - N\beta\Gamma^\alpha\left\{\frac{1}{N}\sum_{p'}\omega_{p'\alpha}f_\alpha(p')\right\}^2$$

$$= \frac{1}{N}\sum_{p}\omega_{p\alpha}^2 f_\alpha(p). \quad (4.7)$$

Here we have used Eq.(4.3). If we take either the classical limit or put $\Sigma_p^R(\varepsilon)=0$ in the quantal case, we obtain the following result

$$\frac{1}{N}\sum_{p}\omega_{p\alpha}^2 f_\alpha(p) = \frac{Q^2}{m\beta}. \quad (4.8)$$

That is, the right-hand side of Eq.(4.7) becomes identical with the exact second moment. In general, if we want to have the exact second moment, we must regard Eq.(4.8) as a condition to be imposed on $f_Q(p)$.

(iii) $\langle\!\langle\omega^4\rangle\!\rangle$

Due to the equation of continuity, the fourth moment becomes

$$\int_{-\infty}^{\infty}\omega^4\gamma_a(\omega)d\omega = \frac{1}{N}\sum_{pp'}\int_{-\infty}^{\infty}d\omega\,\omega_{pa}\omega_{p'a}\langle\omega\rho_{pa};\omega\rho_{p'a}\rangle .$$

Let us replace $\omega\rho_{pQ}$ in the above equation by

$$\omega_{pa}\rho_{pa}+n_0\beta V_{eff}(a)\frac{1}{N}\omega_{pa}f_a(p)\rho_a ,$$

which is obtained from Eq.(4.2), then the fourth moment $\langle\!\langle\omega^4\rangle\!\rangle$ yields four terms. We repeat the procedures leading to Eq.(4.7) and sum up these four terms, then we obtain

$$\langle\!\langle\omega^4\rangle\!\rangle = \left\{\frac{1}{N}\sum_p\omega_{pa}^4 f_a(p)\right\}+\left\{\frac{1}{N}\sum_p\omega_{pa}^2 f_a(p)\right\}^2 n_0\beta V_{eff}(a) . \quad (4.9)$$

If we make $\Sigma_p^R(\varepsilon)=0$, then the first term of the above equation is written as

$$\frac{1}{N}\sum_p\omega_{pa}^4 f_a(p) = \frac{a^2}{2m}\left\{\frac{\hbar^2a^2}{2m}+4\langle KE\rangle\right\}\frac{a^2}{m\beta} , \quad (4.10)$$

where

$$\langle KE\rangle \equiv \frac{1}{N}\sum_p\frac{p^2}{2m}\langle a_p^+a_p\rangle . \quad (4.11)$$

This term reduces to the exact classical limit since

$$\lim_{\hbar\to 0}\langle KE\rangle = \frac{3}{2}\frac{1}{\beta} .$$

If we assume here that the relation (4.10) as well as (4.8) is generally valid, the fourth moment $\ll\omega^4\gg$ is finally written in the form

$$\ll\omega^4\gg = \frac{Q^2}{2m}\left\{\frac{\hbar^2Q^2}{2m}+4\langle KE\rangle\right\}\frac{Q^2}{m\beta} + \left(\frac{Q^2}{m\beta}\right)^2 n_0\beta V_{eff}(Q), \quad (4.12)$$

while the exact one is

$$\ll\omega^4\gg = \frac{Q^2}{2m}\left\{\frac{\hbar^2Q^2}{2m}+4\langle KE\rangle\right\}\frac{Q^2}{m\beta} + \frac{n_0}{m}\int dr\, g(r)\left[1-\cos(Qz)\right]\frac{\partial^2 U(r)}{\partial z^2}\frac{Q^2}{m\beta}, \quad (4.13)$$

where

$$z = (Qr)/Q.$$

§5. Quantal Ornstein-Zernike relation

In classical fluids the Ornstein-Zernike (OZ) relation plays an important role in treating integral equations for g(r). Thus, in this section we derive a quantal extention of the OZ relation.

For a classical system, the OZ relation is written as

$$g(r)-1 = C(r) + n_0\int C(|r-r'|)\{g(r')-1\}dr' , \tag{5.1}$$

which is obtained from the relation between the functional derivatives[13]

$$\int \left.\frac{\delta[-\beta U(r)]}{\delta n(r'')}\right|_0 \left.\frac{\delta n(r'')}{\delta[-\beta U(r')]}\right|_0 dr'' = \delta(r-r') , \tag{5.2}$$

where

$$\left.\frac{\delta[-\beta U(r)]}{\delta n(r')}\right|_0 \equiv -C(|r-r'|) + \delta(r-r')/n_0 , \tag{5.3}$$

$$\left.\frac{\delta n(r|U)}{\delta[-\beta U(r')]}\right|_0 = n_0\delta(r-r') + n_0^2\{g(|r-r'|)-1\} . \tag{5.4}$$

Here, n(r) or n(r|U) denotes the density in a nonuniform fluid due to an imposed external potential U(r) and $|_0$ means the functional derivative being taken at U(r)=0, that is, n(r)=n_0 (n_0; the average density) and C(r), the direct correlation function. From these equations, we can obtain the Fourier transforms of functional derivatives.

Because of

$$\mathcal{F}_Q\left[\left.\frac{\delta n(r|U)}{\delta[-\beta U(r')]}\right|_0\right] = n_0 S(Q) , \tag{5.5}$$

where

$$S(Q)-1 = n_0 \cdot \mathcal{F}_Q\{g(r)-1\}, \tag{5.6}$$

$$\mathcal{F}_Q[f(r)] \equiv \int f(r) e^{iQr} dr , \tag{5.7}$$

there follows from Eq.(5.2)

$$\mathcal{F}_Q\left[\left.\frac{\delta[-\beta U(r)]}{\delta n(r')}\right|_0\right] = \frac{1}{n_0 S(Q)} . \tag{5.8}$$

From the above consideration in the case of classical fluids, we can derive a quantal OZ relation through the replacement of the functional derivatives, $\left.\frac{\delta n(r|U)}{\delta[-\beta U(r')]}\right|_0$ and $\left.\frac{\delta[-\beta U(r)]}{\delta n(r')}\right|_0$, by quantal ones respectively as follows.

For this purpose, in the first place we must obtain a quantal extension of the direct correlation function, C(r). In a quantal system, according to the linear response theory[28] Eq.(5.5) is replaced by

$$\mathcal{F}_Q\left[\left.\frac{\delta n(r|U)}{\delta[-\beta U(r')]}\right|_0^{QM}\right] = n_0 \chi_Q , \tag{5.9}$$

where χ_Q is defined by Eq.(2.16),so that Eq.(5.2) yields

$$\mathcal{F}_Q\left[\left.\frac{\delta[-\beta U(r)]}{\delta n(r')}\right|_0^{QM}\right] = \frac{1}{n_0 \chi_Q} . \tag{5.10}$$

Since in a classical system the Fourier transform of the direct correlation function satisfies the relation

$$\mathcal{F}_Q[n_0 C(|r-r'|)] = 1 - n_0 \cdot \mathcal{F}_Q\left[\left.\frac{\delta[-\beta U(r)]}{\delta n(r')}\right|_0\right] , \tag{5.11}$$

the Fourier transform of a quantal direct correlation function must be expressed in the form

$$\mathcal{F}_Q\left[n_0\tilde{C}(|r-r'|)\right] = h(Q) - n_0\mathcal{F}_Q\left[\frac{\delta[-\beta U(r)]}{\delta n(r')}\Big|_0^{QM}\right]$$

$$= h(Q) - 1/\chi_Q \,, \qquad (5.12)$$

where h(Q) is a certain function which satisfies

$$\lim_{k\to 0} h(Q) = 1 \,.$$

On the other hand, the average of the equation of motion (2.27) in the classical limit reduces to a generalized Vlasov equation[17)-20)] with an effective interaction

$$n_0\beta V_{eff}(Q) = -\left\{1 - \frac{1}{S(Q)}\right\} = -n_0 C(Q) \,. \qquad (5.13)$$

That is, the term in Eq.(2.27)

$$n_0\beta V_{eff}(Q) = -\left\{\frac{1}{\chi_Q^0} - \frac{1}{\chi_Q}\right\}, \qquad (5.14)$$

becomes the direct correlation function in the classical limit, where χ_Q^0 is defined by Eq.(2.19). Thus, in a quantum fluid, the effective potential (5.14) plays the same role in determining atomic motions as the direct correlation function does in a classical fluid and also the function, $\{1/\chi_Q^0 - 1/\chi_Q\}$, satisfies the condition (5.12) necessary to be a quantal direct correlation function.

Consequently, it is appropriate in our framework to choose

$$\mathcal{F}_Q\left[n_0\tilde{C}(r)\right] = n_0\tilde{C}(Q) \equiv 1/\chi_Q^0 - 1/\chi_Q \,, \qquad (5.15)$$

as a quantal direct correlation function $\tilde{C}(r)$.

In the second place, we extend the relation[13] between the density distribution n(r|U) under an external potential U(r) and the radial distribution function g(r) in a classical system

$$n(r|U=v) = n_0 g(r) , \tag{5.16}$$

where v(r) is the interatomic potential, to a quantal system on the basis of the relation in the classical system,

$$\int \left.\frac{\delta[-\beta U(r)]}{\delta n(r')}\right|_0 \left\{ n(r'|U=v) - n_0 \right\} dr' = C(r) . \tag{5.17}$$

Here, we make the ansatz that the relation (5.17) remains valid in the quantal system if we replace the classical quantities in Eq.(5.17) by their quantal analogs; that is,

$$\int \left.\frac{\delta[-\beta U(r)]}{\delta n(r')}\right|_0^{QM} \left\{ n(r'|U=v) - n_0 \right\}^{QM} dr' = \tilde{C}(r) . \tag{5.18}$$

Usefulness of the ansatz (5.18) can only be judged a posteriori.

By taking Fourier transformation of Eq.(5.18), we obtain an equation for $\mathcal{F}_Q[n(r|U=v)-n_0]$ in the form

$$\mathcal{F}_Q\left[\left.\frac{\delta[-\beta U(r)]}{\delta n(r')}\right|_0^{QM}\right] \cdot \mathcal{F}_Q\left[\left\{ n(r|U=v) - n_0 \right\}^{QM}\right] = \mathcal{F}_Q[\tilde{C}(r)] = \frac{1}{n_0}\left\{\frac{1}{\chi_Q^0} - \frac{1}{\chi_Q}\right\} .$$

From this equation and (5.10), we get finally

$$\mathcal{F}_Q\left[n(r|U=v) - n_0 \right] = \frac{\chi_Q}{\chi_Q^0} - 1 \quad ; \tag{5.19}$$

this reduces to Eq.(5.16) as seen from the fact $\lim_{k\to 0} \chi_Q = S(Q)$ and $\lim_{k\to 0} \chi_Q^0 = 1$.

Between the quantal direct correlation function $\tilde{C}(r)$ and $\{n(r|U=v)-n_0\}$ given by Eq.(5.19), we can set up a relation as follows. The identity $\frac{1}{\chi_Q} \cdot \chi_Q = 1$ given by the Fourier transform of Eq.(5.2) is rewritten as

$$\frac{\chi_Q}{\chi_Q^0} - 1 = \chi_Q^0 \, n_0 \tilde{C}(Q) + \frac{\left[\chi_Q^0 \cdot n_0 \tilde{C}(Q)\right]^2}{1 - \chi_Q^0 \cdot n_0 \tilde{C}(Q)} \quad . \tag{5.20}$$

With the use of Eqs.(5.15) and (5.19), this equation is transformed into

$$\frac{n(r|v)}{n_0} - 1 = \hat{B} \cdot \tilde{C}(r) + n_0 \int \left\{\hat{B} \cdot \tilde{C}(|r-r'|)\right\} \left\{\frac{n(r'|v)}{n_0} - 1\right\} dr' , \tag{5.21}$$

where $\hat{B}$ is an operator defined by

$$\mathcal{F}_Q\left[\hat{B} \cdot f(r)\right] = \chi_Q^0 \cdot \mathcal{F}_Q\left[f(r)\right] , \tag{5.22}$$

and $n(r|v) = n(r|U=v)$.

This equation (5.21) is a quantal extension of the OZ relation (5.1).

It should be noted that $\{n(r|v)-n_0\}$ given by Eq.(5.19) represents a non-linear response to imposition of an external field $U(r)=v(r)$ which is identical with the interatomic potential at the origin, and also the relation (5.19) offers a quantal version of the Percus method as shown later.

§6. Generalization of Hohenberg-Kohn-Mermin Theory

Hohenberg and Kohn[29] and Mermin[30] have shown that the thermodynamic potential Ω in a nonuniform electron gas due to imposion of an external potential U(r) is represented as

$$\Omega = \int U(r')\, n(r'|U)\, dr' + F[n(r|U)] \quad , \tag{6.1}$$

where n(r|U) denotes the density at r and F[n(r|U)] is a functional independent of U(r). On the basis of Eq.(6.1), they have derived the Thomas-Fermi equation and the expression of F[n] as a functional Taylor's expansion with respect to $\{n(r|U)-n_0\}$.

In this section, on making use of Eq.(6.1) and the results in §5 we extend the results of Hohenberg-Kohn-Mermin in more general form suitable not only for an electron gas but also for quantum fluids whose potential need not be able to be Fourier-transformed.

Since $\frac{\delta\Omega}{\delta n(r)}$ at the equilibrium satisfies the relation

$$\left.\frac{\delta\Omega}{\delta n(r)}\right|_{eq} = U(r) + \left.\frac{\delta F[n]}{\delta n(r)}\right|_{eq} = 0 \quad , \tag{6.2}$$

there follows

$$\frac{\delta}{\delta n(r')}\left[\left.\frac{\delta F[n]}{\delta n(r)}\right|_{eq}\right] = -\frac{\delta U(r)}{\delta n(r')} \quad . \tag{6.3}$$

If we put

$$F[n(r|U)] = H[n(r|U)] - \mu\int n(r|U)\, dr \quad , \tag{6.4}$$

we find from Eq.(6.2)

$$\left.\frac{\delta H[n]}{\delta n(r)}\right|_{eq} = \mu - U(r) \equiv \Gamma(r|n) , \tag{6.5}$$

where $\int U(r')n(r'|U)dr' + H[n]$ is the free energy and μ, the chemical potential. A functional Taylor's expansion of $\left.\frac{\delta H[n]}{\delta n(r)}\right|_{eq} \equiv \Gamma(r|n)$ around a constant function $n(r|U)$, where r is a fixed point, is expressed as

$$\Gamma(r|n) = \Gamma(r|c)_{c=n(r|U)} + \int \left.\frac{\delta\Gamma(r|n)}{\delta n(r')}\right|_{c=n(r|U)} \{n(r'|U)-n(r|U)\}dr' . \tag{6.6}$$

Here,

$$\Gamma(r|c)_{c=n(r|U)} = \mu_0(n(r|U)) , \tag{6.7}$$

where $\mu_0(c)$ is the chemical potential in a uniform system at the density c. By making an approximation

$$\left.\frac{\delta\Gamma(r|n)}{\delta n(r')}\right|_{c=n(r|U)} = -\left.\frac{\delta U(r)}{\delta n(r')}\right|_{c=n(r|U)} \tag{6.8}$$

$$\doteqdot -\left.\frac{\delta U(r)}{\delta n(r')}\right|_0 \equiv \frac{-1}{\beta}\left\{\tilde{C}(|r-r'|) - \frac{h(|r-r'|)}{n_0}\right\} ,$$

where

$$\mathcal{F}_Q\left[h(r)/n_0\right] = h(Q)/n_0 = 1/n_0\chi_Q^0 , \tag{6.9}$$

and using Eq.(6.8), Eq.(6.6) is expressed as

$$\beta\mu = \beta\mu_0(n(r|U)) + \beta U(r) - \int \tilde{C}(|r-r'|)\{n(r'|U)-n(r|U)\}dr' + \int \frac{h(|r-r'|)}{n_0}\{n(r'|U)-n(r|U)\}dr' . \tag{6.10}$$

If we make another approximation

$$h(|r-r'|) \doteqdot \delta(r-r') , \tag{6.11}$$

noting the relation $\lim_{k\to 0} h(r)=\delta(r)$, Eq.(6.10) is written in the form

$$\beta\mu = \beta\mu_0(n(r|U)) + \beta U(r) - \int \tilde{C}(|r-r'|)\{n(r'|U)-n_0\}dr' + \left\{\frac{n(r|U)}{n_0}-1\right\}\beta\left(\frac{1}{\chi_T^0}-\frac{1}{\chi_T}\right), \tag{6.12}$$

where κ_T is the isothermal compressibility and $n_0\kappa_T^0=\beta\chi_{Q=0}^0$. This is a quantal extension of the previous result[15]. In the case of $\kappa_T^0/\kappa_T \doteq 1$ we obtain the relation

$$\beta\mu = \beta\mu_0(n(r|U)) + \beta U_H^D(r) , \tag{6.13}$$

where

$$\beta U_H^D(r) = \beta U(r) - \int \tilde{C}(|r-r'|)\{n(r'|U)-n_0\}dr' . \tag{6.14}$$

In the Hohenberg-Kohn-Mermin theory, $-\tilde{C}(r)$ is replaced by $\beta v(r)$. On the other hand, in the case of $|n(r|U)-n_0|/n_0 \ll 1$, Eq.(6.12) is written in the form

$$\frac{\beta}{n_0\chi_T^0}\nabla n(r|U) + n(r|U)\nabla\beta U_H^D(r) = 0 . \tag{6.15}$$

Next, we consider the functional Taylor's expansion of $F[n(r|U)]$ around n_0 for the case of $|n(r|U)-n_0|/n_0 \ll 1$. Since from Eq.(6.3)

$$\frac{\delta^2}{\delta n(r)\delta n(r')}F[n]\Big|_0 = \frac{1}{\beta}\frac{\delta[-\beta U(r)]}{\delta n(r')} \equiv -\frac{1}{\beta}\left\{\tilde{C}(|r-r'|)-\frac{h(|r-r'|)}{n_0}\right\}, \tag{6.16}$$

and $\delta F[n]/\delta n|_0=0$, $F[n]$ is represented as

$$F[n] \doteq F[n_0] + \frac{1}{2}\int\left\{-\tilde{C}(|r-r'|)/\beta\right\}\Delta n(r)\Delta n(r')\,dr dr' + \frac{1}{2}\int\frac{h(|r-r'|)}{n_0\beta}\Delta n(r)\Delta n(r')\,dr dr' , \tag{6.17}$$

where

$$\mathcal{F}_Q[\,h(r)] = 1/\chi_Q^0 ,$$

and $\Delta n(r) \equiv n(r|U)-n_0$. In the case of the electron gas, Eq.(6.17) reduces to the result of Hohenberg-Kohn if we use the RPA, that is, $-\tilde{C}(r)/\beta \doteqdot v(r)$ and $\Sigma_p^R(\varepsilon)\doteqdot 0$. This fact shows that our choice of a quantal direct correlation function (5.15) is appropriate.

Here, we should mention that Eq.(6.17) is equivalent to the result of Hohenberg-Kohn as shown below. Equation (6.17) is rewritten in the form

$$\begin{aligned} F[n] &= F[n_0] + \frac{1}{2}\int \frac{1}{\beta}\frac{\delta[-\beta U(r)]}{\delta n(r')}\Big|_0 \Delta n(r)\Delta n(r')\,dr\,dr' \\ &= F[n_0] + \frac{1}{2}\int U(|r-r'|)\,\Delta n(r)\Delta n(r')\,dr\,dr' \\ &\quad + \frac{1}{2}\int\left\{\frac{1}{\beta}\frac{\delta[-\beta U(r)]}{\delta n(r')}\Big|_0 - U(|r-r'|)\right\}\Delta n(r)\Delta n(r')\,dr\,dr' . \end{aligned} \tag{6.18}$$

With the aid of Eq.(5.10), the Fourier transform of the kernel $K(|r-r'|)$ of the third term in Eq.(6.18) is expressed as

$$\begin{aligned} K(Q) \equiv \mathcal{F}_Q[K(|r-r'|)] &= \mathcal{F}_Q\left[\frac{1}{2\beta}\frac{\delta[-\beta U(r)]}{\delta n(r')}\Big|_0 - \frac{U(|r-r'|)}{2}\right] \\ &= \frac{1}{2\beta}\left\{\frac{1}{n_0\chi_Q} - \beta U(Q)\right\} \\ &= \frac{1}{2}U(Q)\Big/\{\varepsilon(Q)-1\} , \end{aligned} \tag{6.19}$$

where

$$\varepsilon(Q) \equiv 1/\{1-n_0 U(Q)\cdot\beta\chi_Q\} \equiv 1/\{1-\alpha(Q)\} . \tag{6.20}$$

This is nothing but the result of Hohenberg-Kohn. Essentially, Eqs.(6.17) and (6.18) are two different ways of separations of the functional derivative $\delta[-\beta U(r)]/\delta n(r')|_0$ into the two parts; the one separation is into $-\tilde{C}(|r-r'|)$ and $h(|r-r'|)/n_0$, the other, $\beta v(|r-r'|)$ and $\frac{\delta[-\beta U(r)]}{\delta n(r')}\Big|_0 - \beta v(|r-r'|)$.
The definition of a direct correlation function (5.15) gives the separation (6.17) automatically.

In contrast to the expression (6.18), Eq.(6.17) is applicable to a system interacting via a potential which can not be Fourier-transformed.

§7. PY and HNC equations for neutral quantum fluids

In this section we extend the Percus method[13] to treat a quantal system on the basis of the results in §5 and obtain quantal PY and HNC equations.

If the density $n(r|U)$ in a nonuniform system due to imposition of an external potential $U(r)$ is approximately determined by a functional equation $F[n(r|U)] \doteqdot F[n_0]$, the Percus method yields an improved integral equation for $n(r|U)$ in a nonuniform system by making a functional-expansion of $F[n]$, for example, around the average density n_0:

$$F[n] \doteqdot F[n_0] + \int \left.\frac{\delta F[n]}{\delta n(r')}\right|_0 \{n(r'|U) - n_0\}\, dr' , \tag{7.1}$$

truncated at the first order. Then, by using the relation (5.16) between the density in the nonuniform system and $g(r)$ in the uniform system, this improved equation for $n(r|U)$ becomes an integral equation for $g(r)$ in the uniform system, if the external potential $U(r)$ is set equal to the interatomic potential $v(r)$. Owing to the relation (5.19), the same procedure is applicable to a quantal system.

In the first place, we derive a quantal PY equation. In a nonuniform fluid interacting via a short-range potential, the density $n(r|U)$ under an external potential $U(r)$ is approximately described by

$$n(r|U) \approx \int \frac{dp}{(2\pi)^3} \frac{1}{e^{\beta\left(\frac{p^2}{2m} + U - \mu\right)} - \eta} \equiv \mathcal{N}[U] , \tag{7.2}$$

and more generally is determined by

$$n(r|U) \approx n^{\circ}(r|U) , \tag{7.3}$$

where $n^0(r|U)$ is the density of a noninteracting fluid with the streaming term $i\omega_{PQ}$ defined by Eq.(2.25). From this fact it is proper to take

$$G[n] = n(r|U)/n^0(r|U), \tag{7.4}$$

for a generating functional in the Percus method in order to obtain an integral equation for $n(r|U=v)$ in a fluid with a short-range interaction. On account of

$$\mathcal{F}_Q\left[\frac{\delta n^0(r|U)}{\delta[-\beta U(r')]}\bigg|_0\right] = n_0 \chi_Q^0, \tag{7.5}$$

which is derived from Eq.(2.27) setting $V_{eff}(Q)=0$, we obtain the functional derivative of Eq.(7.4) at n_0

$$\frac{\delta G[n]}{\delta n(r')}\bigg|_0 = \frac{\delta(r-r')}{n_0} - \frac{1}{n_0}\int \frac{\delta n^0(r|U)}{\delta[-\beta U(r'')]}\bigg|_0 \frac{\delta[-\beta U(r'')]}{\delta n(r')}\bigg|_0 dr''$$

$$= \frac{\delta(r-r')}{n_0} - \hat{B}\cdot\frac{\delta[-\beta U(r)]}{\delta n(r')}\bigg|_0, \tag{7.6}$$

where $\hat{B}$ is the operator defined by Eq.(5.22). Consequently, the functional-expansion of Eq.(7.4) is represented as

$$\frac{n(r|U)}{n^0(r|U)} = \frac{n(r|U)}{n_0} - \hat{B}\int \frac{\delta[-\beta U(r)]}{\delta n(r')}\bigg|_0 \{n(r'|U) - n_0\} dr'. \tag{7.7}$$

By putting U=v in the above equation and using Eq.(5.19) we obtain a quantal PY equation in the form

$$\hat{B}\,\tilde{C}(r) = -\frac{n(r|U)}{n_0}\left\{\frac{n_0}{n^0(r|U)} - 1\right\}. \tag{7.8}$$

Here we make a further approximation,

$$n^0(r|U) \doteqdot \mathcal{K}[U] \tag{7.9}$$

in order to obtain an explicit expression for $n^{o}(r|v)$ in Eq.(7.8). Since the Fourier transforms of $\tilde{C}(r)$ and $n(r|v)$ are expressed in terms of χ_Q and χ_Q^o as seen from Eqs.(5.15) and (5.19), the Fourier transform of Eq.(7.8) is an equation for χ_Q, so that the combined use of Eqs.(7.8), (2.41), (2.43) and (3.2) determines $S(Q,\omega)$, $g(r)$ and $\Sigma_p^R(\varepsilon)$ in a self-consistent manner.

In the classical limit, Eq.(7.8) reduces to the classical PY equation since

$$\lim_{\hbar\to 0}\hat{B}=1\,,\quad \lim_{\hbar\to 0}\mathcal{R}[v]=n_0 e^{-\beta v}\quad\text{and}\quad \frac{n(r|v)}{n_0}=n_0 g(r)\,.$$

Furthermore, we remark here that in a Fermi system at zero temperature, the function $\mathcal{R}[v]$ is written as

$$\frac{\mathcal{R}[v]}{n_0}=\begin{cases}[1-v(r)/E_F]^{3/2}\,, & (v/E_F<1)\\ 0\,, & (v/E_F\geqq 1)\,,\end{cases}\qquad (7.10)$$

so that the potential in $\mathcal{R}[v]$ plays the same role as the hard-sphere potential when $v(r)/E_F\geqq 1$ (E_F; the Fermi energy).

On making use of the OZ relation (5.21), Eq.(7.8) can be put in an alternative form,

$$n(r|v)=n^{o}(r|v)\{1+\tilde{\gamma}(r)\}\,, \qquad (7.11)$$

where

$$\tilde{\gamma}(r)=n_0\int\{\hat{B}\hat{C}(|r-r'|)\}\left\{\frac{n(r'|v)}{n_0}-1\right\}dr'\,. \qquad (7.12)$$

If we put here

$$\tau(r)\equiv n(r|v)/n^{o}(r|v)=1+\tilde{\gamma}(r)\,, \qquad (7.13)$$

$$e(r) \equiv n^{\circ}(r|v)/n^{\circ} , \tag{7.14}$$

$$f(r) \equiv e(r) - 1 , \tag{7.15}$$

then Eq.(7.11) is rewritten as

$$\tau(r) = 1 - n_0\int \tau(r')f(r')dr' + n_0\int \tau(r')f(r')\tau(|r-r'|)e(|r'-r|)dr' , \tag{7.16}$$

which is the identical form to the classical PY equation[31]. Therefore, in the case of the hard-sphere system with a diameter σ_H, because of

$$e(r) = \begin{cases} 1 , & (r > \sigma_H) \\ 0 , & (r < \sigma_H) , \end{cases} \tag{7.17}$$

the solution of Eq.(7.16) is nothing but the classical one obtained by Wertheim[31] in the closed form, so that for quantum hard-sphere fluids (Fermions or Bosons) the quantal direct correlation function $\tilde{C}(r)$ is expressed in terms of the classical direct correlation function $C_H(r)$, as

$$\chi_Q^{\circ}\,\tilde{C}(Q) = C_H(Q) , \tag{7.18}$$

where

$$n_0 C_H(Q) = \mathcal{F}_Q[n_0 C_H(r)] = -24\eta\int_0^1 d\lambda\,\lambda^2 \frac{\sin(\lambda\cdot\sigma_H Q)}{\lambda\cdot\sigma_H Q}(\alpha+\beta\lambda+\gamma\lambda^3) , \tag{7.19}$$

$$\eta = (\pi/6)\,n_0\sigma_H{}^3 , \tag{7.20}$$

$$\alpha = (1+2\eta)^2/(1-\eta)^4 \;;\; \beta = -6\eta(1+\tfrac{1}{2}\eta)/(1-\eta)^4 ,$$

$$\gamma = \tfrac{1}{2}\eta(1+\eta)^2/(1-\eta)^4 .$$

The canonical density-density correlation function χ_Q is also expressed as

$$\chi_Q = \chi_Q^0 \Big/ \{1 - n_0 C_H(Q)\} . \tag{7.21}$$

In the second place, we are concerned with the derivation of a quantal extension of HNC equation. For this purpose by analogy with the classical case, we take as a generating functional

$$G[n] = \ln \frac{n(r|U)}{n^0(r|U)} , \tag{7.22}$$

whose functional derivative at n_0 is given by

$$\frac{\delta}{\delta n(r')}\left[\ln \frac{n(r|U)}{n^0(r|U)}\right]\Big|_0 = \frac{\delta(r-r')}{n_0} - \hat{B}\,\frac{\delta[-\beta U(r)]}{\delta n(r')}\Big|_0 . \tag{7.23}$$

Thus, the functional Taylor's expansion of Eq.(7.22) truncated at the first order is written as

$$\int\left\{\hat{B}\,\frac{\delta[-\beta U(r)]}{\delta n(r)}\Big|_0\right\}\{n(r'|U)-n_0\}\,dr' = \frac{n(r|U)}{n_0} - \ln\frac{n(r|U)}{n^0(r|U)} . \tag{7.24}$$

By putting U=v in Eq.(7.24), we obtain a quantal HNC equation

$$\hat{B}\,\hat{C}(r) = \frac{n(r|U)}{n_0} - \ln\frac{n(r|U)}{n_0} + \ln\frac{n^0(r|U)}{n_0} , \tag{7.25}$$

which is rewritten by using the OZ relation (5.21) in the form

$$n(r|U) = n^0(r|U)\exp\{\tilde{\gamma}(r)\} , \tag{7.26}$$

where $\tilde{\gamma}(r)$ is defined by Eq.(7.12). Obviously Eq.(7.25) in the classical limit reduces to the usual HNC equation. It should be mentioned here that in addition to Eq.(7.25) there is another quantal extension of the HNC equation as will be shown in §9B.

§8. Generalization of Landau kinetic equation

In this section we show that Eq.(2.27) with an effective interaction $\beta V_{eff}(Q)=-\tilde{C}(Q)$ obtained by the quantal PY or HNC equations derived in §7 gives an extension of the Landau kinetic equation in the Fermi-liquid theory to the case of Fermion and Bosons in the large (Q,ω) region at $T\neq 0$. In Eq.(2.27), however, the momentum dependence of the scattering amplitude function $f_{pp'}$ in the Landau theory is neglected.

Considering the fact the PY equation (7.11) is written as

$$\hat{B}\tilde{C}(r) = n(r|v)/n_0 - 1 - \tilde{\gamma}(r) \qquad (8.1)$$
$$= \{\psi[v]-1\}\{1+\tilde{\gamma}(r)\} ,$$

where

$$\psi[v] \equiv n^{\circ}(r|v)/n_0 \doteqdot \mathcal{E}[v]/n_0 , \qquad (8.2)$$

we can represent the Fourier transform of the direct correlation function in the form

$$\chi_0^{\circ}\cdot n_0\tilde{C}(Q) = n_0F_s^{\circ}(\bar{Q}) + \int_0^{\infty} K(\bar{Q},\bar{q})\, n_0\tilde{\gamma}(\bar{q})\, d\bar{q} \qquad (8.3)$$
$$\equiv -n_0F(\bar{Q}) ,$$

where

$$n_0F_s^{\circ}(\bar{Q}) = n_0\int\{\psi[v]-1\}e^{iQr}dr , \qquad (8.4)$$

$$K(\bar{Q},\bar{P}) = \frac{3\bar{P}}{4\bar{Q}}\int_{|\bar{Q}-\bar{P}|}^{\bar{Q}+\bar{P}} \bar{t}\cdot n_0F_s^{\circ}(\bar{t})\, d\bar{t} , \qquad (8.5)$$

$$\bar{Q} \equiv Q/Q_F \quad ; \quad Q_F \equiv (3\pi^2 n_0)^{1/3} . \qquad (8.6)$$

In the special case of the hard-sphere, it has been shown in §7 that

$$n_0 F(Q) = -n_0 C_H(Q) . \tag{8.7}$$

From the above consideration and Eqs.(2.27) and (8.3), we can write a kinetic equation for $\delta n_p(Q,\omega)=\langle \rho_{pQ} \rangle [z=-i\omega]$ as

$$(\hbar\omega - \hbar\omega_{pQ})\delta n_p(Q,\omega) + \left\{ n_{p+Q/2} - n_{p-Q/2} \right\} \frac{F(Q)}{\beta \chi_Q^0} \frac{1}{V} \sum_{p'} \delta n_{p'}(Q,\omega) = 0 . \tag{8.8}$$

In the case of Fermion this equation reduces to the Landau equation if we take the wave-vector Q small and T=0 as shown below: If we define $\varepsilon_p = \mathrm{Re}(\varepsilon)$ and neglect $\mathrm{Im}(\varepsilon)$, where ε is the solution of

$$\varepsilon - \varepsilon_p^0 - \Sigma_p^R(\varepsilon) = 0 , \tag{8.9}$$

the function $f_Q(p)$ defined by Eq.(2.14) in the small Q limit is expressed as

$$\lim_{Q \to 0} f_Q(p) = -\frac{1}{\beta} \frac{\partial n(\varepsilon_p)}{\partial \varepsilon_p} , \tag{8.10}$$

with the use of the relation

$$\left\{ G_p^R(\varepsilon) \right\}^2 \doteqdot \frac{\partial}{\partial \varepsilon_p} G_p^R(\varepsilon) , \tag{8.11}$$

where $n(\varepsilon)=\exp[\beta(\varepsilon-\mu)-\eta]^{-1}$.

Because of Eq.(8.10) and the relation in the small Q

$$n(\varepsilon_{p+Q/2}) - n(\varepsilon_{p-Q/2}) \doteqdot \frac{\partial n(\varepsilon_p)}{\partial \varepsilon_p} Q \frac{\partial \varepsilon_p}{\partial p} , \tag{8.12}$$

Eq.(2.25) is written as

$$i\omega_{pQ} \equiv -g_Q(p)/f_Q(p) \doteqdot \frac{i}{\hbar} Q \frac{\partial \varepsilon_p}{\partial p} . \tag{8.13}$$

Also, by using Eq.(8.10), Eq.(2.19) in the small Q limit becomes

$$\lim_{Q\to 0}\beta\chi_Q^0 = -\frac{1}{N}\sum_p\left\{\lim_{Q\to 0} f_Q(p)\right\}$$
$$= -\frac{1}{N}\sum_p \frac{\partial n(\varepsilon_p)}{\partial \varepsilon_p} = \frac{1}{N}\sum_p \delta(\varepsilon_p-\mu)$$
$$= 3m^*/p_F^2 \equiv \nu(0)/N\ , \qquad (8.14)$$

where m* is the effective mass and $\nu(0)$ the density of states; P_F, the Fermi momentum. Hence, finally Eq.(8.8) in the small Q region is shown to become

$$(\hbar\omega - Qv_p)\delta n_p(Q,\omega) + Qv_p \frac{\partial n(\varepsilon_p)}{\partial \varepsilon_p} f_{00}\frac{1}{V}\sum_p \delta n_p(Q,\omega) = 0\ , \qquad (8.15)$$

where

$$v_p = \nabla_p \varepsilon_p\ , \qquad (8.16)$$

$$f_{00} = F(0)/\{\nu(0)/N\}\ . \qquad (8.17)$$

This is the Landau equation with an approximate scattering amplitude function $f_{pp'}\doteqdot f_{00}$. Note that, in Eq.(8.15), f_{00} is determined by the quantal PY equation; for example, in the case of the hard-sphere

$$f_{00} = \frac{p_F^2}{3m^*}\frac{(1+2\zeta)^2}{(1-\zeta)^4}\ . \qquad (8.18)$$

From Eq.(8.15) the sound velocity s is represented as

$$s^2 = \frac{p_F^2}{3mm^*}\left\{1 + F(0)\right\}\ , \qquad (8.19)$$

which is identical to the formula given by Landau. Thus we can consider Eq.(8.8) as an extended Landau kinetic equation for the large (Q,ω) region at non-zero temperatures. This situation is not altered if we use the quantal HNC equation (7.26) instead of Eq.(7.11).

§9. Integral equations for charged quantum fluids

Since the Coulomb potential consists of both long-range and strong short-range parts, the PY and HNC equations are not applicable to a charged particle system even in the classical case when the density of a system increases[32]. Remedying these defects, we have previously derived integral equations[15] suitable for a charged particle system even in the high density region. In this section, we extend these integral equations applicable to a quantum system such as an electron gas at zero temperature.

(A) Equations appropriate to a slowly varying potential

As shown in §6, the density $n(r|U)$ in a nonuniform system due to a slowly-varying external potential U, that is, in the case of $|n(r|U)-n_0|/n_0 \ll 1$, is approximately determined by

$$\frac{1}{n_0 \chi_T^0} \nabla n(r|U) + n(r|U) \nabla U_H^D(r) = 0, \tag{9.1}$$

where $U_H^D(r)$ is defined by Eq.(6.14).

This fact suggests that to derive an integral equation suitable for fluids interacting via a slowly varying potential we should take

$$G[n] = \frac{1}{n_0 \chi_T^0} \nabla n(r|U) + n(r|U) \nabla U_H^D(r), \tag{9.2}$$

for a generating functional, whose functional derivative with respect to $n(r')$ is written as

$$\left.\frac{\delta G[n]}{\delta n(r')}\right|_0 = \frac{1}{n_0 \chi_T^0} \nabla \delta(r-r') + n_0 \nabla \left.\frac{\delta U(r)}{\delta n(r')}\right|_0 + n_0 \nabla U^D, \tag{9.3}$$

where

$$\beta v^D(r) \equiv -\tilde{C}(r) . \tag{9.4}$$

Hence, the functional Taylor's expansion of G truncated at the first order is

$$\frac{n_0}{\beta}\nabla\int\left.\frac{\delta[-\beta U(r)]}{\delta n(r')}\right|_0\{n(r'|U)-n_0\}dr' \tag{9.5}$$
$$= -n(r|U)\nabla v_H^D(r) + n_0\nabla\int v^D(|r-r'|)\{n(r'|U)-n_0\}dr' ,$$

from which by setting U(r)=v(r) an integral equation is derived in the form

$$\nabla\tilde{C}(r) = -\frac{n(r|v)}{n_0}\nabla\beta v_H^D(r) + \nabla\beta\{v(r)-v_H^D(r)\} , \tag{9.6}$$

where

$$v_H^D(r) \equiv v(r) + \int v^D(|r-r'|)\{n(r'|U)-n_0\}dr' . \tag{9.7}$$

This equation is rewritten by taking Fourier transform in the form

$$\frac{1}{\beta}\tilde{C}(q) = v(q) + \frac{1}{n_0}\int\frac{Qq}{Q^2}v_H^D(\xi)\left\{\frac{\chi_{|Q-\xi|}}{\chi^0_{|Q-\xi|}}-1\right\}\frac{d\xi}{(2\pi)^3} \tag{9.8}$$
$$\equiv v(q)\{1-G(q)\} ,$$

where

$$v_H^D(q) \equiv v(q) + \frac{1}{n_0\beta}\left(\frac{1}{\chi_q}-\frac{1}{\chi^0_q}\right)\left(\frac{\chi_q}{\chi^0_q}-1\right) \tag{9.9}$$
$$\equiv v(q)/\tilde{\varepsilon}(q) ,$$

$$1/\tilde{\varepsilon}(q) \equiv \chi_q/\chi^0_q - G(q)\{\chi_q/\chi^0_q-1\} , \tag{9.10}$$

$$G(q) = -\frac{1}{n_0}\int\frac{Qq}{Q^2}\frac{v(\xi)}{v(q)}\frac{1}{\tilde{\varepsilon}(\xi)}\left\{\frac{\chi_{|Q-\xi|}}{\chi^0_{|Q-\xi|}}-1\right\}\frac{d\xi}{(2\pi)^3} , \tag{9.11}$$

Remenbering the relation

$$\chi_Q = \chi_Q^0 / [\,1+n_0\beta v(Q)\{1-G(Q)\}\chi_Q^0\,],$$

we obtain from Eq.(6.11) the recurrence formula for G(Q)

$$-G(Q) = \frac{1}{n_0}\int \frac{dq}{q^2}\left\{\frac{\chi_q}{\chi_q^0} - G(q)\left(\frac{\chi_q}{\chi_q^0}-1\right)\right\}\left\{\frac{\chi_{|Q-q|}}{\chi_{|Q-q|}^0}-1\right\}\frac{dq}{(2\pi)^3}, \quad (9.12)$$

in the case of an electron gas.

With the aid of Eqs.(9.5) and (5.10), an integral equation for the density (charge) distribution n(r|U) under the external potential U(r) is expressed as

$$\mathcal{F}_Q[n(r|v)-n_0] \quad (9.13)$$
$$= -\left\{v(Q)+\int \frac{dq}{Q^2} v_H^D(q)\cdot \mathcal{F}_{|Q-q|}[n(r|v)-n_0]\frac{dq}{(2\pi)^3}\right\} n_0\beta\chi_Q,$$

where

$$v_H^D(Q) \equiv v(Q) + \frac{1}{\beta}\left(\frac{1}{\chi_Q}-\frac{1}{\chi_Q^0}\right)\mathcal{F}_Q[n(r|v)-n_0]. \quad (9.14)$$

Since the function χ_Q can be determined from Eq.(9.6), this equation contains only one unknown function n(r|U). If we take only the first term of Eq.(9.13), we obtain the linear response formula

$$\mathcal{F}_Q[n(r|v)-n_0] = -v(Q)\cdot n_0\beta\chi_Q, \quad (9.15)$$

which is written for U(r)=v(r) in the form

$$\mathcal{F}_Q[n(r|v)-n_0] = -v(Q)\cdot n_0\beta\chi_Q \equiv \frac{1}{\varepsilon(Q)}-1, \quad (9.16)$$

where

$$\varepsilon(Q) \equiv 1 + v(Q)\pi(Q), \quad (9.17)$$

$$\pi(Q) \equiv n_0\beta\chi_Q^0 / \{1-v(Q)G(Q)n_0\beta\chi_Q^0\}. \quad (9.18)$$

while the nonlinear response n(r|v) to the external potential U=v is determined by

$$\mathcal{F}_a[n(r|v)-n_0] = \chi_a/\chi_a^\circ - 1 \quad . \tag{9.19}$$

Therefore, Eq.(9.13) determines the nonlinear density response n(r|U) to the external potential U. Due to the condition $|n(r|U)-n_0|/n_0 \ll 1$ under which Eq.(9.13) is derived, Eq.(9.13) does not give n(r|U) so well in the small r region where the Coulomb potential is strong and steep.

We give here the two remarks concerning Eq.(9.8). If we make an approximation, $U_H^D(r) \doteqdot U(r)$ in Eq.(9.2), Eq.(9.11) reduces to

$$G(Q) = -\frac{1}{n_0}\int \frac{Qq}{q^2}\left[\frac{\chi_{|Q-q|}}{\chi^\circ_{|Q-q|}} - 1\right]\frac{dq}{(2\pi)^3} \quad , \tag{9.20}$$

that is, $\varepsilon(Q)=1$, in Eq.(9.11). In comparison of Eq.(9.20) with the result of Singwi et al.[7], their equation is obtained from Eq.(9.20) by replacing $\chi_{|Q-q|}/\chi^\circ_{|Q-q|}$ by $S(|Q-q|)$ which is the classical limit of the former.

Next, if we make an appromimation, $\tilde{C}(r) \doteqdot -\beta v(r)$, that is, if we use in Eq.(9.6)

$$v_H(r) = v(r) + \int v(|r-r'|)\{n(r'|v)-n_0\}\,dr' \quad , \tag{9.21}$$

instead of $v_H^D(r)$, we obtain

$$G(Q) = -\frac{1}{n_0}\int \frac{Qq}{q^2}\,\frac{\chi_q}{\chi^\circ_q}\left\{\frac{\chi_{|Q-q|}}{\chi^\circ_{|Q-q|}} - 1\right\}\frac{dq}{(2\pi)^3} \quad . \tag{9.22}$$

In comparison of Eq.(9.22) with a later work of Singwi et al.[9] there are the following two differences;

(i), the factor $\chi_{|Q-q|}/\chi^\circ_{|Q-q|}$ in Eq.(9.22) is replaced by

$S(|Q-q|)$ and (ii), $\chi_q^o/\chi_q = 1+v(1-G)\chi_q^o \equiv \varepsilon_e(q)$ is replaced by $\varepsilon(q) \equiv 1+v(q)\pi(q)$ where $\pi(q)$ is defined by Eq.(9.18). The difference (ii) means that in the result of Singwi et al. $\mathfrak{F}_Q[n(r|v)-n_o]$ is approximated by the linear response, $1/\varepsilon(Q)-1$, as shown by Eqs.(9.16) and (9.19).

(B) PY equation with a screened potential

In a fluid interacting via a long-range potential the Hartree field (the screening effect) plays an important role. The Thomas-Fermi method taking account of this effect gives the density $n(r|U)$ in a nonuniform electron gas due to imposition of the external potential $U(r)$ in the form

$$n(r|U) = \mathcal{N}[U_H(r)] , \tag{9.23}$$

where

$$U_H(r) = U(r) + \int v(|r-r'|)\{n(r'|U)-n_o\}dr' . \tag{9.24}$$

From this fact we can see that in order to derive an equation in such a way as to take account of the Hartree field we should take

$$G[n] = n(r|U)/n^o(r|U_H) , \tag{9.25}$$

for a generating functional, whose functional derivative is written as

$$\left.\frac{\delta G[n]}{\delta n(r')}\right|_o = \frac{\delta(r-r')}{n_o} - \hat{B}\left\{\left.\frac{\delta[-\beta U(r)]}{\delta n(r')}\right|_o - \beta v(|r-r'|)\right\} . \tag{9.26}$$

Here, $\hat{B}$ is the operator defined by Eq.(5.22). Consequently an equation for $n(r|U)$ in the external potential $U(r)$ is expressed as

$$\hat{B}\int \left.\frac{\delta[-\beta U(r)]}{\delta n(r')}\right|_0 \{n(r'|U)-n_0\}dr' \qquad (9.27)$$
$$= -\frac{n(r|U)}{n_0}\left\{\frac{n_0}{n^0(r|U_H)}-1\right\}+\hat{B}\int U(|r-r'|)\{n(r'|U)-n_0\}dr'.$$

By putting $U(r)=v(r)$ in Eq.(9.27), we obtain an equation for $n(r|v)$

$$\tilde{C}(r) = -\hat{B}^{-1}\frac{n(r|v)}{n_0}\left\{\frac{n_0}{n^0(r|v_H)}-1\right\}$$
$$-n_0\beta\{v(r)-v_H(r)\}, \qquad (9.28)$$

where v_H is defined by Eq.(9.21). This equation (9.28) may be rewritten with the use of the OZ relation (5.21) in a different form

$$n(r|v) = n^0(r|v_H)\{1+\tilde{\gamma}(r)+\hat{B}\cdot n_0\beta(v-v_H)\}. \qquad (9.29)$$

For a moment, we are concerned with the case of an electron gas. As is shown in the classical case[15], if we use $\{n(r|v)-n_0\}$ obtained by the Thomas-Fermi theory in an electron gas at T=0 as an approximation, Eq.(9.28) is written as

$$\tilde{C}(r) = -\hat{B}^{-1}\frac{n(r|v)}{n_0}\left\{n_0/\mathcal{L}\left[\frac{e^2}{r}e^{-Q_{TF}r}\right]-1\right\}$$
$$-n_0\beta\frac{e^2}{r}\{1-e^{-Q_{TF}r}\}, \qquad (9.30)$$

where Q_{TF} is the Thormas-Fermi constant, so that the direct correlation function $\tilde{C}(r)$ and the potential e^2/r are automatically separated into the short-range and long-range parts.

Since Eq.(7.2) for zero temperature reduces to

$$\frac{n^{\circ}(r|U_H)}{n_0} \doteqdot \frac{\gamma\zeta[U_H]}{n_0} = \begin{cases} 0 & , (U_H/E_F \geqq 1) \\ (1-U_H/E_F)^{3/2} & , (U_H/E_F < 1) , \end{cases} \tag{9.31}$$

there follows from Eq.(9.29)

$$n(r|U) = 0 \quad \text{for} \quad U_H(r)/E_F \geqq 1 , \tag{9.32}$$

so that $n(r|v)$ never becomes negative near the origin. If we evaluate $v_H(r)$ by applying the RPA in the calculation of $\{n(r|v)-n_0\}$ in Eq.(9.21), this screened potential in the small distance is expressed as[32]

$$U_H(r)/E_F \doteqdot 2\alpha r_s \frac{1}{x} e^{-ax} \cos ax , \tag{9.33}$$

where $x=p_F r$, $a=2\left\{\frac{\alpha r_S}{3\pi}\right\}^{1/4} \cdot \frac{p_F}{h}$ and $\alpha=(4/9\pi)^{1/3}$, whence we can estimate x_0 which satisfies $n(r|v)=0$ for $rp_F \leqq x_0$; for example, $x_0=0.75$ for $r_s=4$. Note that this analysis (9.33) cannot be applied to an electron gas of high density since Eq.(9.23) does not take account of the exchange effect. From the above consideration we can expect that Eq.(9.28) could determine $g(r)$ in the small distance correctly.

Next, we proceed to the derivation of another type of quantal HNC equation besides Eq.(7.26). In §6, we have shown that the Thomas-Fermi method can be generalized by replacing $U_H(r)$ by $U_H^D(r)$ defined by Eq.(6.14). This fact suggests that $n^{\circ}(r|U_H)$ in the generating functional (9.25) may be replaced by $n^{\circ}(r|U_H^D)$.

Therefore, we choose as a generating functional

$$G[n] = n(r|v)/n^{\circ}(r|v_H^D), \tag{9.34}$$

where U_H^D is defined by Eq.(6.14). In this case, the functional derivative of Eq.(9.34) with respect to n(r) at n_0 is shown to becomes zero:

$$\left.\frac{\delta G[n]}{\delta n(r')}\right|_0 = \frac{\delta(r-r')}{n_0} - \hat{B}\left\{\left.\frac{\delta[-\beta v]}{\delta n(r')}\right|_0 - \beta v^D\right\} \equiv 0, \tag{9.35}$$

since the Fourier transform of the above equation becomes

$$\mathcal{F}_q\left[\left.\frac{\delta G[n]}{\delta n(r')}\right|_0\right] = \frac{1}{n_0} - \chi_q^0\left[\frac{1}{n_0\chi_q} - \frac{1}{n_0}\left(\frac{1}{\chi_q} - \frac{1}{\chi_q^0}\right)\right] \equiv 0, \tag{9.36}$$

so that the functional Taylor's expansion of Eq.(9.34) truncated at the first order reduces to

$$n(r|v) = n^{\circ}(r|v_H^D) \quad . \tag{9.37}$$

By putting U=v in Eq.(9.37), we obtain an integral equation

$$n(r|v) = n^{\circ}(r|v_H^D) \doteq \int \frac{dp}{(2\pi)^3}\left\{\exp\left[\beta\left(\frac{p^2}{2m} + v_H^D(r) - \mu\right)\right] - 1\right\}^{-1}, \tag{9.38}$$

where

$$\beta v_H^D(r) \equiv \beta v(r) - \int \tilde{C}(|r-r'|)\{n(r'|v) - n_0\}\,dr', \tag{9.39}$$

and this equation can be written in an alternative form

$$\tilde{C}(r) = -\hat{B}^{-1}\frac{n(r|v)}{n_0}\left\{\frac{n_0}{n^{\circ}(r|v_H^D)} - 1\right\} - \beta\left(v - v_H^D\right) \quad . \tag{9.40}$$

In the classical limit, Eq.(9.38) reduces to the classical HNC equation. In this sense we can regard Eqs.(9.38) as well as (7.26) as a quantal HNC equation.

(C) Equations involving separated potentials

Though the short-range effect has been taken into account to some extent, Eq.(9.6) is essentilly appropriate to fluids with slow-varying long-range potentials. On the contrary, Eq.(9.28) is suitable for systems with short-range potential, the long-range part being taken into account in a type of the RPA, that is, $\frac{1}{\beta}\tilde{C}^{L}(r)=-v^{L}(r)$. In this section we derive combined equations of Eqs.(9.6) and (9.28) by dividing the potential into the short-range and long-range parts.

As shown in classical fluids[15], we can show that if direct correlation functions $\tilde{C}_i(r|v)$ (i=1.. m) are derived from generating functionals $G_i[n]$, respectively, by the Percus method, new integral equations are given by

$$\tilde{C}(r|v) = \tilde{C}_1(r|\mathcal{P}_1 v) + \cdots + \tilde{C}_m(r|\mathcal{P}_m v), \tag{9.41}$$

$$\tilde{C}(r|v) = \alpha_1 \tilde{C}_1(r|v) + \cdots + \alpha_m \tilde{C}_m(r|v), \tag{9.42}$$

where $\mathcal{P}_i$'s are operators separating the potential v(r) into the i-th component ($\mathcal{P}_1+\mathcal{P}_2+\cdots \mathcal{P}_m=1$), and α_i's arbitrary constants ($\alpha_1+\cdots +\alpha_m=1$).

According to Eq.(9.41) we obtain an integral equation by combining Eqs.(9.6) and (9.28)

$$\nabla\tilde{C}(r) = -\nabla\left[\hat{B}^{-1}\frac{n(r|v)}{n_0}\left\{\frac{n_0}{n^{\circ}(r|v_H^S)}-1\right\}\right] + \nabla\beta v_H^S - \frac{n(r|v)}{n_0}\nabla\beta v_H^L - \nabla\beta\{v-v_H^L\}, \tag{9.43}$$

where

$$U_H^i \equiv U^i + \int U^i(|r-r'|)\{n(r'|U) - n_0\}dr' ; \ (i = S, L), \quad (9.44)$$
$$U^S = \mathcal{P}_S U \quad ; \ U^L = \mathcal{P}_L U \ .$$

With the aid of Eq.(5.21), this equation is rewritten in the form

$$n(r|U) = n^0(r|U_H^S)\left[1 + \tilde{\gamma}(r) + \hat{B}\left\{\beta U_H^S + \tilde{C}_L(r)\right\}\right] \quad (9.45)$$

where

$$\nabla \tilde{C}_L(r) \equiv -\frac{n(r|U)}{n_0}\nabla\beta U_H^L - \beta\nabla(U - U_H^L) \ . \quad (9.46)$$

As is shown in §6, the bare potential v(r) in the Hartree field may be replaced by the direct correlation function $\tilde{C}(r)$, that is, $U_H(r)$ by $U_H^D(r)$. Hence, we can generalized Eq.(9.45) with the replacements of $v_H^i(r)$ by

$$U_H^{Di}(r) \equiv U^i(r) + \int U^{Di}(|r-r'|)\{n(r'|U) - n_0\}dr', \quad (9.47)$$
$$U^{Di} \equiv \mathcal{P}_i U^D \quad ; \ (i = S, L) \ ,$$

and the result is written in the form

$$n(r|U) = n^0(r|U_H^{DS})\left\{1 + \hat{B}\cdot\tilde{C}_L(r|U_H^{DL})\right\} . \quad (9.48)$$

Here,

$$\nabla \tilde{C}_L(r|U_H^{DL}) \equiv -\frac{n(r|U)}{n_0}\nabla U_H^{DL} \ . \quad (9.49)$$

The density (charge) distribution n(r|U) under the external potential U(r), associated with Eq.(9.48), is given by

$$n(r|U) = n^{\circ}(r|U_H^{DS})\left\{1 + \hat{B}\cdot P(r|U_H^{DL})\right\} \tag{9.50}$$

where

$$\nabla P(r|U_H^{DL}) \equiv -\frac{n(r|U)}{n_0}\nabla\beta U_H^{DL} \tag{9.51}$$

$$U_H^{Di}(r) \equiv \beta_i U(r) + \int v^{Di}(|r-r'|)\{n(r'|U)-n_0\}dr' ; \quad (i=S,L). \tag{9.52}$$

When we apply these equations to an electron gas, it is proper to adopt

$$\beta_S = erf(\zeta r) \quad ; \quad \beta_L = 1 - erf(\zeta r), \tag{9.53}$$

as separating operators according to Ewald[34].

§10. Generalization of Landau-Silin kinetic equation

In this section, on the basis of integral equations derived in §9, we prove that Eq.(2.27) in conjunction with Eq.(9.43) or (9.48) becomes the Landau-Silin kinetic equation[2] in the case of an electron gas.

In the first place, the Fourier transform of Eq.(9.43) is written in the form

$$n_0\hat{C}(\bar{a}) = n_0\hat{C}_S(\bar{a}) + n_0\hat{C}_L(\bar{a}) \qquad (10.1)$$
$$\equiv -n_0 F(\bar{a})/\chi^0_{\bar{a}} - n_0\beta U(\bar{a})\{1-G(\bar{a})\},$$

where

$$\chi^0_{\bar{a}}\cdot n_0\hat{C}_S(\bar{a}) \equiv \int_0^\infty K(\bar{a},\bar{q})\left[n_0\hat{\gamma}(\bar{q}) + \chi^0_{\bar{q}}\{\beta U^S_H(\bar{q}) + n_0\hat{C}_L(\bar{q})\}\right] d\bar{q}$$
$$+ n_0 F_S(\bar{a}) + n_0\beta U^S_H(\bar{a})\cdot\chi^0_{\bar{a}} \equiv -n_0 F(\bar{a}), \qquad (10.2)$$

$$-n_0\hat{C}_L(\bar{a}) \equiv n_0\beta U(a) + \frac{3}{8}\frac{1}{\bar{a}^3}\int_0^\infty d\bar{q}\,\bar{q}\,h(\bar{a},\bar{q})\left[\frac{\chi_{\bar{q}}}{\chi^0_{\bar{q}}} - 1\right] d\bar{q}$$
$$\equiv n_0\beta U(\bar{a})\{1 - G(\bar{a})\}, \qquad (10.3)$$

$$h(\bar{a},\bar{q}) \equiv \int_{|\bar{a}-\bar{q}|}^{\bar{a}+\bar{q}} d\bar{\xi}\cdot\bar{\xi}\, n_0\beta U^L_H(\bar{\xi})(\bar{\xi}^2 + \bar{a}^2 - \bar{q}^2), \qquad (10.4)$$

$$U^i_H(\bar{a}) = U^i(\bar{a})\chi_{\bar{a}}/\chi^0_{\bar{a}} \quad ; (i = S, L), \qquad (10.5)$$

from which there follows

$$\chi_Q = \frac{\chi_Q^\circ}{1+[n_0\beta v(Q)\{1-G(Q)\}+n_0F(Q)/\chi_Q^\circ]\chi_Q^\circ} \quad (10.6)$$

Here, the term $n_0\beta v(Q)\{1-G(Q)\}$ comes mainly from the long-range part of the potential and the term $n_0F(Q)$ from the short-range part. As for Eq.(9.48), the above situation is quite similar. From Eqs.(10.1) and (2.29), Eq.(2.27) is written for $\delta n_p(Q,\omega)=\langle\rho_{pQ}\rangle[z=-i\omega]$ in the form

$$(\hbar\omega-\hbar\omega_{pQ})\delta n_p(Q,\omega)+\{n_{p+Q/2}-n_{p-Q/2}\}\left[v(Q)\{1-G(Q)\}+\frac{F(Q)}{\beta\chi_Q^\circ}\right]\frac{1}{V}\sum_{p'}\delta n_{p'}(Q,\omega) = 0. \quad (10.7)$$

Following the same procedure as in §8, Eq.(10.7) in the small Q limit is rewritten as

$$(\hbar\omega-Qv_p)\delta n_p(Q,\omega)+Qv_p\frac{\partial n(\varepsilon_p)}{\partial\varepsilon_p}\left[v(Q)\{1-G(Q)\}+\frac{F(0)}{\{\nu(0)/N\}}\right]\frac{1}{V}\sum_{p'}\delta n_{p'}(Q,\omega) = 0, \quad (10.8)$$

which is to be compared with the Landau-Silin equation

$$(\hbar\omega-Qv_p)\delta n_p(Q,\omega)+Qv_p\frac{\partial n(\varepsilon_p)}{\partial\varepsilon_p}\frac{1}{V}\sum_{p'}\{v(Q)+f_{pp'}\}\delta n_{p'}(Q,\omega)=0. \quad (10.9)$$

From Eq.(10.8) the compressibility sum rule in an electron gas is drived as

$$\begin{aligned}\frac{\kappa_I^\circ}{\kappa_T}-1 &= \lim_{Q\to0}\left\{\frac{n_0\beta\chi_Q^\circ}{\pi(Q)}-1\right\}\\ &= \lim_{Q\to0}\left\{\frac{\chi_Q^\circ}{\chi_Q}-1-v(Q)\,n_0\beta\chi_Q^\circ\right\}\\ &= \lim_{Q\to0}\left\{F(Q)-v(Q)\,G(Q)\,n_0\beta\chi_Q^\circ\right\}\\ &= F(0)-\frac{1}{2}G''(0)(Q_{TF}/Q_F)^2, \end{aligned} \quad (10.10)$$

where Q_F is the Fermi wavevector and $\kappa_T^o = 3m^*/n_o p_F^2$.

In contrast with Eq.(10.10), the Landau-Silin equation yields

$$\frac{\gamma_T^o}{\gamma_T} - 1 = F(0) , \qquad (10.11)$$

since $G(Q) \equiv 0$ in Eq.(10.9), and the treatment of Singwi et al.[7),9)] gives

$$\frac{\gamma_T^o}{\gamma_T} - 1 = -\frac{1}{2} G''(0) (Q_{TF}/Q_F)^2 , \qquad (10.12)$$

which means that the short-range effect is not taken into account appropriately in their treatment. Thus, we can see from Eq.(10.10) that there is a close relation between the violation of the compressibility sum rule and the behaviour of g(r) in the small distance as mentioned in §9B.

§11. Application to the electron gas

In §9, we have derived integral equations appropriate to charged particle systems. An essential difference between one of our equations and the Singwi et al. equation[7] is expressed by Eqs.(9.20) and (1.3), that is, $\chi_{|Q-q|}/\chi^{o}_{|Q-q|}$ is replaced by $S(|Q-q|)$ in their equation. For comparison with the Singwi et al. result, we solved numerically the equation for χ_Q;

$$\tilde{C}(q)/\beta = v(q)\{1-G(q)\}, \tag{11.1}$$

with G(Q) defined by Eq.(9.20) in the approximation, $\Sigma^{R}_{p}(\varepsilon)=0$, and with the aid of Eqs.(2.43) and (5.19) we obtain g(r) and n(r|v).

The results are shown in Fig.2(A)-2(C) for the values of r_s=2, 3 and 5, respectively. In these figures, g(r)'s are expressed in Fig.(a); the full lines denote our results and the dotted lines, the Singwi et al. results. The curves of the density n(r|v) in the presence of the external field U(r)=v(r) are shown in Fig.(b); full lines (i) and (ii) denote our calculation and the results calculated from the linear response formula (9.16), respectively, and the dotted curves are obtained from the nonlinear formula (9.19) with the use of χ_Q of Singwi et al.

It should be noted that in our calculation, g(r) remains positive at r_s=5 where the results of Singwi et al. become negative. Even at r_s=6, g(r) obtained from our formula remains positive, that is, g(0)=0.146 whereas in the Singwi et al. result g(0)=-0.03, and becomes identical with their result in the large distance. However, the density n(r|v) in the small r becomes

negative at $r_s=3$; this breakdown is natural because Eq.(9.20) is drived under the condition that the potential is slowly varying. As r_s increases, the difference between $n(r|v)$ calculated from the nonlinear formula and that obtained in the linear approximation becomes large. The linear response theory gives quite unsatisfactory $n(r|v)$ and yields an overestimated amplitude of oscillations in the charge density around the impurity.

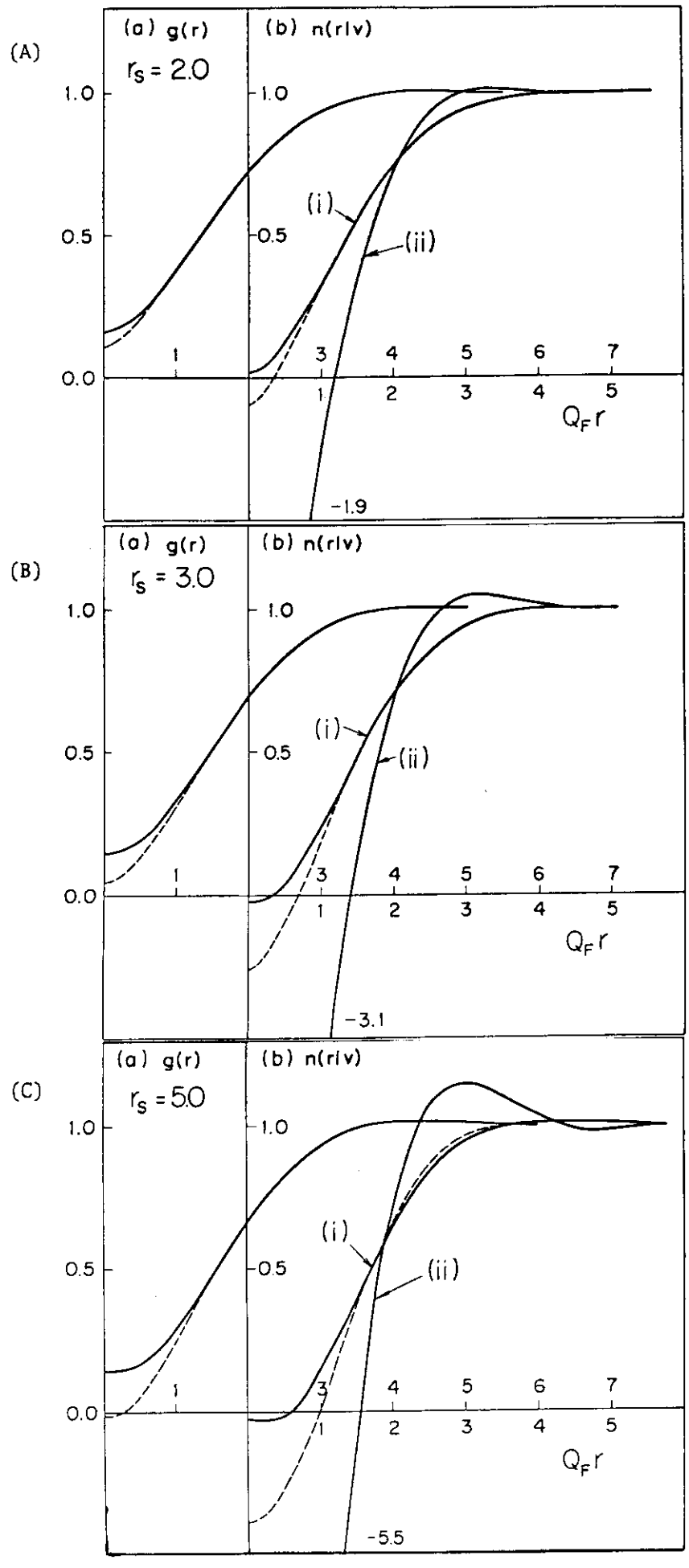


Fig. 2

(a) The radial distribution function g(r) and (b) the density n(r|v)

The present theory, the full curves in (a) and (i) in (b); the Singwi et al. results, the dotted curves; the linear theory, the full curves (ii). the number associated with curves (ii) denotes the value of n(r=0|v).

§12. Summary and concluding remarks

In the present study, we have obtained a set of self-consistent equations for the density-density response function $\chi_Q(\omega)$, the density-density canonical correlation χ_Q and the self-energy $\Sigma^R_p(\varepsilon)$, which are given by Eqs.(2.40), (3.2) and an integral equation such as Eq.(9.8); these equations can be considered to determine, in a self-consistent manner, the dynamic and static structure factors, $S(Q,\omega)$ and $S(Q)$, and the distribution function n_p due to the relations (2.41) and (2.43) and

$$n_p = -\frac{1}{\pi}\int_{-\infty}^{\infty} d\varepsilon \frac{1}{e^{\beta\varepsilon}-\eta} \, \mathrm{Im}\left\{\frac{1}{\varepsilon-\varepsilon^0_p+\mu-\Sigma^R_p(\varepsilon)}\right\} . \tag{12.1}$$

In the first place, we have derived an approximate equation of motion (2.27) for $\rho_{pQ} = a^\dagger_{p-Q/2}a_{p+Q/2}$, that is,

$$i\hbar\dot{\rho}_{pQ} = \hbar\omega_{pQ}\rho_{pQ} + \left\{n_{p-Q/2} - n_{p+Q/2}\right\} V_{\mathrm{eff}}(Q)\frac{1}{V}\sum_{p'}\rho_{p'Q}, \tag{12.2}$$

as a generalized Langevin equation in the Mori theory. In comparison with the usual Hartree equation which is obtained with the use of the RPA:

$$i\hbar\dot{\rho}_{pQ} = \frac{pQ}{m}\rho_{pQ} + \left\{n(\varepsilon^0_{p-Q/2}) - n(\varepsilon^0_{p+Q/2})\right\} v(Q)\frac{1}{V}\sum_{p'}\rho_{p'Q}, \tag{12.3}$$

Eq.(12.2) is different in the following points: the streaming term pQ/m in Eq.(12.3) is replaced by $\hbar\omega_{pQ}$ which is a functional of the self-energy as defined by Eq.(2.25), and also the bare potential $v(Q)$ and the distribution function $n(\varepsilon^0_p)$ for an ideal gas in Eq.(12.3) are replaced, respectively, by the effective potential $V_{\mathrm{eff}}(Q)$, which is represented in terms of χ_Q and χ^0_Q as shown by Eq.(2.29), and the distribution function n_p determined

by Eq.(12.1). In this sense, Eq.(2.27) can be regarded as a generalized Hartree equation. From Eq.(12.2) or (2.27), the density-density response function $\chi_Q(\omega)$ is expressed as Eq.(2.40) which is quite similar to the formula obtained by the use of the usual Hartree approximation.

In the expression for $\chi_Q(\omega)$ and n_p and also in the equation of motion (12.2), the functions, χ_Q and $\Sigma_p^R(\epsilon)$, remain to be determined. In the second place, we have obtained an equation (3.2) for the self-energy with the use of the Hartree-Fock approximation.

In the third place, we have set up integral equations for χ_Q by extending the Percus method to the case of quantum fluids. For this purpose, a quantal direct correlation function $\tilde{C}(r)$ was obtained as Eq.(5.15) on the basis of a generalized Hartree equation (12.2). By making the ansatz (5.18), a quantal Ornstein-Zernike relation (5.21) was derived as a relation between $\tilde{C}(r)$ and the inhomogeneous density $n(r|v)$ in the presence of an external potential $U(r)=v(r)$. Our definition of quantal direct correlation function, (5.15), gave extensions of the results of the Hohenberg-Kohn-Mermin theory for a nonuniform electron gas in the forms of (6.13) and (6.17), and also extended the Percus method to treat quantum fluids. Thus, we have derived a quantal PY equation (7.8) and two quantal HNC equations, (7.25) and (9.38), by applying the Percus method to neutral quantum fluids. For charged quantum fluids such as an electron gas, we have obtained three types of equations for χ_Q. The first type of equation , (9.8), is appropriate to treat a fluid with a slowly varying potential, and includes the Singwi et al. equation,[7] as a special case. The second equation is an improved quantal

PY equation (9.28), in which the long-range potential is taken into account in the form of the Hartree field. The third type of equation is Eq.(9.45) or (9.48), which is composed of two equations; One is the improved PY equation (9.28) involving the short-range part of the potential and the other, the equation (9.8) involving the long-range part.

Also, we have derived formulas (9.13), (9.27) and (9.50) for the nonlinear density response $n(r|U)$ to a static external potential $U(r)$. These equations for $n(r|U)$ contain χ_Q which can be determined by a suitable integral equation for $n(r|v)$. By using these formulas, we can calculate, for example, the electron density around an impurity in the electron gas.

Our generalized Hartree equation (2.27) for the case of neutral and charged quantum fluids has provided us with Eqs.(8.8) and (10.7), which are shown to be microscopic generalizations of the Landau equation and of the Landau-Silin equation for large wavevectors Q and high frequencies ω, respectively.

Important points of our method may be emphasized in the following way. The ordinary equation of motion in the RPA (12.3) offers microscopic description of quantum fluids; this description, however, gives correct results only in the case where the interaction is sufficiently weak and the average potential energy is small compared to the kinetic energy. On the other hand, although the Landau theory of Fermi liquids (or the Landau-Silin theory of the electron gas) has the advantage of being applicable to any normal liquid, irrespective of its density and its strength of interaction, this theory can provide no account of microscopic properties such as the radial distribution function, and its validity is limited to phenomena in the macroscopic regime, small

wavevectors and low frequencies, and in the low-temperature limit. As was shown by Eqs.(8.8) and (10.7), our generalized Hartree equation (12.2) led to extensions of the Landau and the Landau-Silin equations to describe microscopic phenomena involving large values of Q and ω at nonzero temperature not only in Fermion, but also in Boson systems. Moreover, this equation, with the combined use of integral equations for χ_Q and $\Sigma_p^R(\varepsilon)$, gave a systematic method for obtaining explicit results (not in the formal way) for the radial distribution function g(r), the space-time correlation function G(r,t) and the distribution n_p for both neutral and charged quantum fluids (Fermions or Bosons) including classical ones, irrespective of law of interaction, from a unified point of view, and bridged the gap between the macroscopic Landau approach and the RPA theory.

In our treatment, we neglected the damping function $\hat{\phi}(z)$, that is, we adopted the collisionless approximation. In consequence, our results are not applicable to the hydrodynamical region. The fundamental approximation in our method is represented by Eq.(2.12). Relation (2.20) is derived in this approximation and is exact in the classical limit. Neglect of momentum dependence in Eq.(2.12) corresponds to the approximation that, in Landau's Fermi-liquid theory, the scattering amplitude function $f_{pp'}$ is independent of p and p'. The meaning of the approximation involved in the expression of $\chi_Q(\omega)$ or $S(Q,\omega)$ can be understood from our generalized Hartree equation (12.2) since this equation is nothing but a generalized Langevin equation of motion associated with the representation of $\Gamma_Q^{pp}[Z]$ in the Mori

theory.

In order to extend our method to the hydrodynamic regime, we must evaluate the damping function $\hat{\phi}(z)$. This is not an easy work for a quantal system.

It should be noted that quantal integral equations are set up not for the radial distribution function g(r) but for n(r|v). The function n(r|v) is not so strongly coupled with the dynamics of atoms as g(r) in the sense that the function n(r|v) is related to $\chi_Q=\chi_Q(\omega=0)$ whereas the radial distribution function g(r) to $S(Q)=\int_{-\infty}^{\infty}\frac{\hbar\beta}{2\pi}\coth\left(\frac{\beta\hbar\omega}{2}\right)\mathrm{Im}\,\chi_Q(\omega)d\omega$, that is, to the all ω-range of $\chi_Q(\omega)$.

In the present study, we have made the approximation

$$n^0(r|U)\doteqdot\int\frac{dp}{(2\pi)^3}\left[\exp\left\{\beta\left(\frac{p^2}{2m}+U(r)-\mu\right)-\gamma\right]^{-1}, \qquad (12.4)$$

but this approximation is improved if we use the relation

$$n^0(r|U)\doteqdot-\frac{1}{\pi}\int\frac{dp}{(2\pi)^3}\int_{-\infty}^{\infty}d\varepsilon\,\frac{1}{e^{\beta\varepsilon}-\gamma}\,\mathrm{Im}\left\{\frac{1}{\varepsilon-\varepsilon_p^0+\mu_0(r)-\Sigma_p^R(\varepsilon)}\right\}, \qquad (12.5)$$
$$\equiv\mathcal{N}_1[U]$$

where

$$\mu_0(r)\equiv-U(r)+\mu\ .$$

In Eqs.(7.8), (7.26) and (9.28), the exchange effect is not taken into account so that, for example, Eq.(9.28) is not applicable to an electron gas in the high densities. It is not difficult, however, to take account of the exchange effect in Eqs.(7.8) and (9.28), as was done in the Thomas-Fermi theory.

We remark that the functional derivative, with respect to U, of $\mathcal{N}_1[U]$ defined by Eq.(12.5) gives

$$\mathcal{F}_Q\left[\left.\frac{\delta\gamma_1[U]}{\delta[-\beta U(r')]}\right|_0\right] = \frac{1}{\beta}\frac{\partial n_0}{\partial\mu} = \chi^0_{Q=0}\,, \tag{12.6}$$

while

$$\mathcal{F}_Q\left[\left.\frac{\delta n^0(r|U)}{\delta[-\beta U(r')]}\right|_0\right] = \chi^0_Q\,. \tag{12.7}$$

Thus, approximate expressions for $n^0(r|U)$ which satisfy Eq.(12.7) are required in order to improve integral equations such as Eqs.(7.8) and (9.43).

Concerning the ansatz (5.18), that is,

$$\mathcal{F}_Q[n(r|U)-n_0] = \chi_Q/\chi^0_Q - 1\,, \tag{12.8}$$

we give here three remarks. Recently Sjolander and Stott[35] have derived an integral equation for the electron density around a point particle in the electron gas, taking into account nonlinear effects. Their equation for an impurity with an infinite mass and the same charge as an electron is rewritten in our notation

$$\gamma^{+-}(Q) = -\left\{v(Q)+\frac{1}{n_0}\int\frac{Qq}{Q^2}v(q)\gamma^{+-}(|Q-q|)\frac{dq}{(2\pi)^3}\right\}\beta\chi_Q\,, \tag{12.9}$$

where

$$\gamma^{+-}(Q) \equiv \mathcal{F}_Q[n(r|U)/n_0-1]\,. \tag{12.10}$$

In this equation, they have used

$$G(Q) = -\frac{1}{n_0}\int\frac{Qq}{q^2}\{S(|Q-q|)-1\}\frac{dq}{(2\pi)^3}\,, \tag{12.11}$$

in the calculation of $\chi_Q=\chi^0_Q/[1+v(Q)\{1-G(Q)\}\chi^0_Q]$. If we use

$$G(Q) = -\frac{1}{n_0}\int\frac{Qq}{q^2}\left\{\frac{\chi_{|Q-q|}}{\chi^0_{|Q-q|}}-1\right\}\frac{dq}{(2\pi)^3}\,, \tag{12.12}$$

instead of Eq.(12.11), then the solution for Eq.(12.9) is written in the form,

$$\gamma^{+-}(Q) = \frac{1}{n_0}\left\{\chi_Q/\chi_Q^0 - 1\right\}; \qquad (12.13)$$

this is nothing but the ansatz (12.8). Moreover, our evaluation of $n(r|v)$ shows a fairly good agreement with the results of Sjolander and Stott[37].

Also, it is important to note that, in contrast to the result of a later Singwi et al. work[9], the ansatz (12.8) gives the so-called "electron-dielectric constant"[36], $\epsilon_e(Q)=\chi_Q^0/\chi_Q=1+v(1-G)\chi_Q^0$, in Eq.(9.22).

The last remark is that, as is seen from Eq.(9.16), the ansatz (12.8) combined with χ_Q and χ_Q^0 obtained by using RPA gives the density response $n(r|v)$ in the linear approximation. In other words, the RPA result is obtained in our method as follows: with the aid of the ansatz (12.8), the functional expansion of $n(r|U)$ with respect to $U(r)$

$$n(r|U) \doteqdot n_0 + \int \left.\frac{\delta n(r|U)}{\delta[-\beta U(r')]}\right|_0 \{-\beta U(r')\}\, dr', \qquad (12.14)$$

yields the RPA result;

$$\chi_Q = \chi_Q^0 / \{1 + v(Q)\chi_Q^0\},$$

by putting $U(r)=v(r)$ and by taking the Fourier transform. All these facts indicate that the ansatz (12.8) is reasonable in our framework.

An extension of this method to systems of binary mixtures[37] and to systems with spin variables, can be performed without further difficulties. The momentum dependence in the vertex

part $\Gamma^{Q}_{pp'}(\varepsilon_n, \varepsilon_{n'}; \omega_m=0)$ in Eq.(2.12) may be taken into account, as was done in the Landau theory, by expanding in a series of Legendre polynomials. It is important to generalize this method to be applicable to the hydrodynamic regime and also to extend the linearized equation of motion (12.2) so as to treat nonlinear effects such as in critical phenomena.

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References

1) D. Bohm and D. Pines, Phys. Rev. 92 (1953), 609.

2) D. Pines and P. Nozieres, The Theory of Quantum Liquids. (Benjamin, 1966), 157.

3) A. Glick and R. A. Ferrell, Ann. Phys. 11 (1959), 359.
L. Hedin, Phys. Rev. 139 (1965), A796.
F. Brouers, Phys. Stat. Sol. 19 (1967), 867.

4) J. Hubbard, Proc. Roy. Soc. A243 (1957), 336.

5) P. R. Antoniewicz and L. Kleinman, Phys. Rev, B2 (1970), 2808.

6) P. Nozieres and D. Pines, Phys. Rev. 111 (1958), 442.

7) K. S. Singwi, M. P. Tosi and R. H. Land, Phys. Rev. 176 (1968), 589.

8) J. Hubbard, Phys. Letters 25A (1967), 709.

9) K. S. Singwi, A. Sjolander, M. P. Tosi and R. H. Land Phys. Rev. B1 (1970), 1044.

10) T. Schneider, Physica 52 (1971), 481.

11) P. Vashishta and K. S. Singwi, Phys. Rev. B6 (1972), 875.

12) G. Stell, The equilibrium Theory of Classical Fluids, edited by H. L. Frisch and J. L. Lebowitz (Benjamin, 1964), II-171.

13) J. K. Percus, (a); Phys. Rev. Letters 8 (1962), 462.
(b); Ref.12), II-33.

14) J. K. Percus, Phys. Rev. 110 (1958) 1.

15) J. Chihara, JAERI-memo 5101 (1973) (preprint)

16) J. K. Percus, The Many-Body Problem, edited by J. K. Percus (Interscience, 1963), 303.

17) R. Zwanzig, Phys. Rev. 144 (1966), 170.

18) M. Nelkin and S. Ranganathan, Phys. Rev. 164 (1967), 222.

19) J. Chihara, Prog. Theor. Phys. 41 (1969), 285.

20) A. Z. Akcasu and J. J. Duderstadt, Phys. Rev. 188 (1969), 479.

21) H. Mori, Prog. Theor. Phys. 34 (1965), 399.

22) G. M. Eliashberg, Soviet Phys. -JETP 14 (1962), 886.

23) A.A. Abrikosov, L. P. Gor'kov and I. Ye. Dzyaloshinskii, Quantum Field Theoretical Methods in Statistical Physics (Pergamon, Oxford, 1965), P. 356.

24) J. Chihara, K. Sasaki and Y. Obata, J. Phys. Soc, Japan 31 (1971), 1323.

25) S. V. Tyablikov and V. L. Bonch-Bruevich, Adv. in Phys. 11 (1962), 317.

26) R. Kubo, Reports on Progress in Physics. 19 Part. 1 (1966), 248.

27) Reference 10), P. 182.

28) For example. Ref.26), P. 279.

29) P. Hohenberg and W. Kohn, Phys. Rev. 136 (1964), B864.

30) N. D. Mermin, Phys. Rev. 137 (1965), A1441.

31) M. S. Wertheim, J. Math. Phys. 5 (1964), 643.

32) D. D. Carley, Phys. Rev. 131 (1963), 1406.

33) V. L. Bonch-Bruevich and S. V. Tyablikov, The Green Function Method in Statistical Mechnics. (North-Holland, 1962), 144.

34) P. P. Ewald, Ann. Physik 64 (1921), 253 .

35) A. Sjolander and K. J. Stott, Phys. Rev. B5 (1972), 2109.

36) R. W. Shaw, Jr., J. Phys. C3 (1970), 1140.

37) J. Chihara, JAERI-memo-5163 (1973).