PHYSICAL REVIEW B VOLUME 14, NUMBER 3 1 AUGUST 1976

Formalism of distribution-function method in impurity screening*

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(Received 4 April 1974; revised manuscript received 16 December 1975)

Using the Weyl-Wigner formulation of quantum mechanics, a rigorous quantum-mechanical basis of the distribution-function method in potential screening, both with and without an externally applied magnetic field, is given. An expansion of the local particle density, up to order $\hbar^2$, leads to a quantum correction of the Thomas-Fermi self-consistent potential approximation and to the so-called "quasiclassical approximation" for nonzero magnetic field. The important results are nonlinear in the potential characteristic of the distribution-function method. They are compared with the results of Horing, based on linear response and random-phase approximation using Green's function, for the low- and very-high-field regime, thus, clarifying the exact nature of the "quasiclassical approximation" as a leading term (zero order in $\hbar$) in a very-high-magnetic-field approximation. The formalism sheds some light on some of the unfamiliar aspects of the results based on linear response.

I. INTRODUCTION

Several studies[1] have been made on the effect of a uniform external magnetic field on the screening of a charged impurity by a quantum plasma. Recently, Das and de Alba[1] and Das and Hebborn,[2] employing a distribution-function approach to the problem, presented a physically and mathematically simple model, the so-called "quasiclassical approximation," for studying the effect. This model was also investigated by Horing,[3] by the use of dielectric-function formalism, and its potential in tremendously simplifying the problem was then recognized. The distribution-function approach, in fact, has an added merit in that it is nonlinear in the potential, and the calculation for the screening length is straightforward by simply linearizing the Poisson equation in electrostatics.

The basic physical and mathematical simplicity of the distribution-function method in impurity potential screening, both in the presence and absence of the magnetic field, calls for the examination of the rigorous quantum-mechanical basis of this method and for a systematic way of improving this approach. The purpose of this paper is to lay down the quantum-mechanical foundation of the method and to point out a systematic way of improving the existing approximation,[1,2] based on the distribution-function approach. It is shown that quantum effects to order $\hbar^2$ can easily be incorporated in this approach, leading to an improvement of the Thomas-Fermi[4] and Debye-Huckel[5] screening in the absence of the magnetic field and to a remarkable improvement of the quasiclassical approximation, by exhibiting the desired anisotropy in the screening.

It must be emphasized that the theory to be presented here is nonlinear, characteristic of the original Thomas-Fermi statistical approach.[6] Although several theories[1] on impurity screening in the absence and presence of the magnetic field already exist, which include quantum effects to all orders, they are usually mathematically more complicated and are based on linear-response theory from the very beginning. As we shall soon see, the nonlinear distribution-function theory presented here does not contain any other approximations beyond the basic physical assumption that independent particles move in a self-consistent potential. Indeed, exact expression to order $\hbar^2$ for the particle density is readily obtained by simple and straightforward calculations. Application of the Poisson equation in electrostatics then yields a nonlinear equation for the self-consistent potential. In principle, all the results can be given to all orders in $\hbar^2$. It is, therefore, clear that all the results of this paper, which are nonlinear in the self-consistent potential, are expected to complement, not duplicate, the previous results based on linear-response theory. Comparison with previous results to order $\hbar^2$ can of course be easily carried out by linearizing in the potential, and this is always done at the end of all calculations. Perhaps the main contribution of this paper lies in the expression of the particle density; it serves as a finite temperature- and magnetic-field-dependent generalization of previous nonlinear results[7] which are only valid at zero temperature and zero magnetic field.

The outline of the paper is as follows. Section II gives the general formulation of the local particle density $n(q)$ which appears in the Poisson equation. The expression for $\mathrm{Tr}(\mathcal{H}-\mu)^n$ indeed leads to a systematic expansion in powers of $\hbar^2$ for $n(q)$. Section III gives the expression for $n(q)$ in the presence of a uniform magnetic field, the treatment being confined to the low-field regime. Section IV greatly transcends the quasi-classical approximation employed by other workers. Calculation for the screening effects is given for the intermediate field strength and in the quantum limit. These calculations were carried out to exhibit the remarkable simplicity of the method. The significance of the results on recent very-high-field experiments is discussed. Comparison with Horing's work is given in Appendix A; this helps to clarify the nature of the approximation used in Sec. IV and sheds some light on some of the unfamiliar aspects of Horing's result.

II. GENERAL FORMULATION OF THE LOCAL PARTICLE DENSITY $n(q)$

Let N be the total number of electrons and N_0 the positive background in a quantum plasma. Then

$$N_0 = n_0 V \ , \tag{1}$$

$$N = -\frac{\partial}{\partial\mu}\,\mathrm{Tr}F(\mathcal{K}) \tag{2}$$

$$= \int d^3q\, n(q) \ , \tag{3}$$

where

$$F(\mathcal{K}) = -k_B T \ln(1 + e^{-\mathcal{K}/k_B T}) \ .$$

Then the self-consistent potential due to an impurity charge Ze located at the origin must satisfy the Poisson equation in electrostatics,

$$\nabla^2 V(q) = 4\pi e n(q) - 4\pi e n_0 - 4\pi Z e \delta(q) \ . \tag{4}$$

Thus the problem is reduced to the calculation of $\mathrm{Tr}F(\mathcal{K})$ expressed as a volume integral which will then define $n(q)$.[8] In this respect, the problem is identical to the calculation of the magnetic susceptibility. $\mathcal{H}$ can be a general Hamiltonian operator, such as the Dirac Hamiltonian which includes the Pauli anomalous term[9] or the Hamiltonian for Bloch electrons.[10] The result using these Hamiltonians will be reported elsewhere. In this paper we will consider a quantum plasma where the carriers are described by a free-electron dispersion law. Thus, in the presence of a magnetic field and an impurity potential $V(q)$, we have

$$\mathcal{H} = [P + (e/c)A(Q)]^2/2m - eV(Q) + g\mu_B s_z B \ . \tag{5}$$

To avoid ambiguity, we write capital letters for quantum operators and small letters for their eigenvalues. The starting point for calculating $\mathrm{Tr}F(\mathcal{K})$ is Eq. (37) of Ref. 9 (to be referred to as I) which can also be written, using $\mathcal{K} = \mathcal{H} - \mu$ instead of an arbitrary operator A, as

$$\mathrm{Tr}\mathcal{K}^n = \frac{\tilde{\mathrm{Tr}}}{h^3}\int d^3p\, d^3q \cos\left[\frac{\hbar}{2}\sum_{\substack{j>k=1\\ j<k}}^{n-1}\left(\frac{\partial^{(j)}}{\partial p}\cdot\frac{\partial^{(k)}}{\partial q} - \frac{\partial^{(j)}}{\partial q}\cdot\frac{\partial^{(k)}}{\partial p}\right)\right] \times \prod_{l=1}^{n} K^{(l)}(p,q) \ , \tag{6}$$

where $\tilde{\mathrm{Tr}}$ means taking the trace over spin indices. $K(p,q)$ is a classical function of p and q and is referred to in I as the Weyl transform of the operator $\mathcal{H} - \mu$. $K(p,q)$ provides the correct Weyl correspondence between the classical function and quantum-mechanical operator, thus $\mathcal{K} \rightleftharpoons K(p,q)$. Indeed Eq. (6) will give us a systematic expansion of $\mathrm{Tr}\mathcal{K}^n$ and hence of $\mathrm{Tr}F(\mathcal{K})$ and finally of $n(q)$ in powers of $\hbar^2$. The explicit expansion up to second order in $\hbar$ is

$$\begin{aligned}\mathrm{Tr}\mathcal{K}^n = \frac{\tilde{\mathrm{Tr}}}{h^3}\int d^3p\, d^3q \Bigg\{ & [K(p,q)]^n - \frac{1}{2!}\left(\frac{\hbar}{2}\right)^2 [K(p,q)]^{n-2}(n-1)(n-2)\left[\left(\frac{\partial^2 K}{\partial p\partial p}:\frac{\partial^2 K}{\partial q\partial q}\right) - \left(\frac{\partial^2 K}{\partial p\partial q}:\frac{\partial^2 K}{\partial q\partial p}\right)\right] \\ & - \frac{1}{2!}\left(\frac{\hbar}{2}\right)^2 [K(p,q]^{n-3}\frac{(n-1)(n-2)(n-3)}{3}\left[\left(\frac{\partial^2 K}{\partial p\partial p}:\frac{\partial K}{\partial q}\frac{\partial K}{\partial q}\right)\right. \\ & \left. + \left(\frac{\partial^2 K}{\partial q\partial q}:\frac{\partial K}{\partial p}\frac{\partial K}{\partial p}\right) - 2\left(\frac{\partial^2 K}{\partial p\partial q}:\frac{\partial K}{\partial p}\frac{\partial K}{\partial q}\right)\right]\Bigg\} \ ,\end{aligned} \tag{7}$$

where the double dot indicates tensor contraction, i.e.,

$$\frac{\partial^2 K}{\partial p\partial q}:\frac{\partial^2 K}{\partial q\partial p} = \frac{\partial^2 K}{\partial p_i \partial q_j}\,\frac{\partial^2 K}{\partial q_i \partial p_j} \ , \tag{8}$$

repeated indices being summed over. The last term in Eq. (7) can be reduced to the form of the second term, plus terms which are gradient with respect to p and q. We obtain

$$\mathrm{Tr}\mathcal{K}^n = \frac{\mathrm{Tr}}{h^3}\int d^3p\,d^3q\,\Big\{[K(p,q)]^n - \frac{1}{2!}\Big(\frac{\hbar}{2}\Big)^2\frac{n(n-1)}{3}[K(p,q)]^{n-2}\Big[\Big(\frac{\partial^2 K}{\partial p\partial p}:\frac{\partial^2 K}{\partial q\partial q}\Big) - \Big(\frac{\partial^2 K}{\partial p\partial q}:\frac{\partial^2 K}{\partial q\partial p}\Big)\Big]$$
$$- \frac{1}{2!}\Big(\frac{\hbar}{2}\Big)^2\frac{(n-1)(n-3)}{3}\Big[\frac{\partial}{\partial q}\cdot\Big(\frac{\partial^2 K}{\partial p\partial p}\cdot\frac{\partial K}{\partial q}[K(p,q)]^{n-2}\Big) + \frac{\partial}{\partial p}\cdot\Big(\frac{\partial^2 K}{\partial q\partial q}\cdot\frac{\partial K}{\partial p}[K(p,q)]^{n-2}\Big)$$
$$- \frac{\partial}{\partial q}\cdot\Big(\frac{\partial^2 K}{\partial q\partial p}\cdot\frac{\partial K}{\partial p}[K(p,q)]^{n-2}\Big) - \frac{\partial}{\partial p}\cdot\Big(\frac{\partial^2 K}{\partial p\partial q}\cdot\frac{\partial K}{\partial q}[K(p,q)]^{n-2}\Big)\Big]\Big\}. \tag{9}$$

The above expression gives $\mathrm{Tr}\mathcal{K}^n$ for all integer n including $n=0$. For $n=2$, the $\hbar^2$ terms cancel out and for $n=0$, the surviving $\hbar^2$ terms integrate out to zero. Using Eqs. (33) and (34) in I, $(\partial/\partial\mu)\mathrm{Tr}F(\mathcal{K})$ can thus be obtained as a volume integral, and through Eq. (3), we have for $n(q)$

$$n(q) = \frac{\tilde{\mathrm{Tr}}}{h^3}\int d^3p\Big\{f(K(p,q)) - \frac{\hbar^2}{24}f''(K(p,q))\Big[\Big(\frac{\partial^2 K}{\partial p\partial p}:\frac{\partial^2 K}{\partial q\partial q}\Big) - \Big(\frac{\partial^2 K}{\partial p\partial q}:\frac{\partial^2 K}{\partial q\partial p}\Big)\Big]$$
$$- \frac{\hbar^2}{24}\Big[\frac{\partial}{\partial q}\cdot\Big(\frac{\partial^2 K}{\partial p\partial p}\cdot\frac{\partial K}{\partial q}f''(K(p,q))\Big) + \frac{\partial}{\partial p}\cdot\Big(\frac{\partial^2 K}{\partial q\partial q}\cdot\frac{\partial K}{\partial p}f''(K(p,q))\Big)$$
$$- \frac{\partial}{\partial q}\cdot\Big(\frac{\partial^2 K}{\partial q\partial p}\cdot\frac{\partial K}{\partial p}f''(K(p,q))\Big) - \frac{\partial}{\partial p}\cdot\Big(\frac{\partial^2 K}{\partial p\partial q}\cdot\frac{\partial K}{\partial q}f''(K(p,q))\Big)\Big]$$
$$- \frac{\hbar^2}{8}\Big[\frac{\partial}{\partial q}\cdot\Big(\frac{\partial^2 K}{\partial p\partial p}\cdot\frac{\partial}{\partial q}\frac{\partial}{\partial\mu}\Big[\frac{F(K)}{K}\Big]\Big) + \frac{\partial}{\partial p}\cdot\Big(\frac{\partial^2 K}{\partial q\partial q}\cdot\frac{\partial}{\partial p}\frac{\partial}{\partial\mu}\Big[\frac{F(K)}{K}\Big]\Big)$$
$$- \frac{\partial}{\partial q}\cdot\Big(\frac{\partial^2 K}{\partial q\partial p}\cdot\frac{\partial}{\partial p}\frac{\partial}{\partial\mu}\Big[\frac{F(K)}{K}\Big]\Big) - \frac{\partial}{\partial p}\cdot\Big(\frac{\partial^2 K}{\partial p\partial q}\cdot\frac{\partial}{\partial q}\frac{\partial}{\partial\mu}\Big[\frac{F(K)}{K}\Big]\Big)\Big]\Big\}, \tag{10}$$

where $f(x)$ is the Fermi-Dirac distribution function. By virtue of the presence of $f(x)$ and $F(x)$, the gradient terms in p do not contribute after integration with respect to p. In the absence of an impurity potential, the second term in $n(q)$ gives the leading quantum correction owing to the quantization of the (p,q) space. It is the one responsible for the Landau-Peierls diamagnetism which arises primarily from the quantization of the components, transverse to the magnetic field, of the canonical conjugate momentum. At zero temperature, the last $\hbar^2$ term of Eq. (10) drops out; in what follows, we will continue to neglect this $\hbar^2$ term for the degenerate case, $k_BT \ll \mu$. In principle, the formalism used enables one to calculate $(\partial/\partial\mu)\mathrm{Tr}\,F(\mathcal{K})$ to all orders in $\hbar^2$; however, the calculation beyond $\hbar^2$ is already very tedious. In Sec. IV we will show how to partly avoid this procedure by using the Weyl correspondence principle to fully take into account the important quantum effects of the problem. The situation discussed in that section is very closely related to the phenomenon of magnetic breakdown in solid-state theory. The expression for $n(q)$, Eq. (10) as it stands, is expected to be applicable to the screening at low field and this is discussed in Sec. III.

It is easy to verify that $H(p,q)$ for the Hamiltonian operator given in Eq. (5) is indeed[11] $[K(p,q) = H(p,q) - \mu]$

$$K(p,q) = [p + (e/c)A(q)]^2/2m - eV(q) + g\mu_B s_z B - \mu, \tag{11}$$

which coincide with the nonrelativistic Hamiltonian function in classical mechanics if spin is neglected [in the general case, $H(p,q)$ may also contain quantum-mechanical effects with powers of $\hbar$ occurring; an example is the Weyl transform of the Hamiltonian for a Dirac particle and Bloch electrons in a uniform magnetic field].

For the rest of this section, we will consider the screening in the absence of a magnetic field and indicate quantum corrections to the Thomas-Fermi and Debye-Huckel self-consistent-potential approximation. From Eqs. (10) and (11) the Poisson equation which determines the self-consistent potential is

$$\nabla^2 V(q) = 4\pi e\Big\{\frac{2}{h^3}\int d^3p\Big[f(K(p,q)) + \frac{\hbar^2 e}{12m}\nabla^2 V(q) f''(K(p,q)) - \frac{\hbar^2 e^2}{24m}|\nabla V(q)|^2 f'''(K(p,q)) - \frac{\hbar^2}{8m}\nabla^2\frac{\partial}{\partial\mu}\Big(\frac{F(K)}{K}\Big)\Big]\Big\}$$
$$- 4\pi e\,n_0 - 4\pi Ze\,\delta(q), \tag{12}$$

where the factor of 2 in front of the integral accounts for the spin degeneracy. By neglecting the $\hbar^2$ terms in the square brackets, we obtain the Thomas-Fermi self-consistent-potential approximation and, by using the classical Boltzmann distribution instead of the Fermi-Dirac distribution, the Debye-Huckel screening. Our purpose here is to incorporate the $\hbar^2$ terms and calculate the screening for $T=0$. At $T=0$, the last term within the curly bracket of Eq. (12) does not contribute. By writing

$$f''(K(p,q)) = \frac{\partial^2}{\partial\mu^2} f(K(p,q)),$$

we immediately obtain

$$\nabla^2 V(q) = 4\pi e\left(\rho(q) + \frac{\hbar^2 e}{12m}\nabla^2 V(q)\frac{\partial^2}{\partial\mu^2}\rho(q) + \frac{\hbar^2 e^2}{24m}|\nabla V(q)|^2\frac{\partial^3}{\partial\mu^3}\rho(q)\right) - 4\pi e\, n_0 - 4\pi Ze\,\delta(q), \tag{13}$$

where

$$\rho(q) = (1/3\pi^2)(2m/\hbar^2)^{3/2}[\mu + eV(q)]^{3/2}. \tag{14}$$

Therefore the effective Poisson equation is

$$\nabla^2 V(q) = \left[4\pi e\left(\rho(q) + \frac{\hbar^2 e^2}{24m}|\nabla V(q)|^2\frac{\partial^3}{\partial\mu^3}\rho(q)\right) - 4\pi e n_0 - 4\pi Ze\,\delta(q)\right] \times\left(1 - \frac{4\pi e^2\hbar^2}{12m}\frac{\partial^2}{\partial\mu^2}\rho(q)\right)^{-1}. \tag{15}$$

The result, upon expanding the right-hand side up to terms linear in $V(q)$ [valid for $eV(q)/\mu \ll 1$], is

$$\nabla^2 V(q) = \left(\frac{6\pi e^2 n_0}{\mu} + \frac{3}{2}\frac{\pi^2 e^4 n_0^2\hbar^2}{m\mu^3}\right)V(q) - 4\pi Ze\,\delta(q), \tag{16}$$

where the factor multiplying $4\pi Ze\,\delta(q)$ is taken as unity since we expect $V(q)\to\infty$ as $q\to 0$. Finally, we have

$$\nabla^2 V(q) = \lambda_0^2\left[1 + \frac{1}{3\pi}\left(\frac{e^2}{2a_0\mu}\right)^{1/2}\right]V(q) - 4\pi Ze\,\delta(q), \tag{17}$$

where λ_0 is the reciprocal of the Thomas-Fermi screening length and a_0 is the Bohr radius. Thus the net effect of the quantum corrections to the Thomas-Fermi approximation results in a decrease in the screening length from the Thomas-Fermi value. This is not surprising since our treatment here goes beyond the Thomas-Fermi statistical approach; we have in fact included quantum effects due to the presence of the potential. Our calculation shows that indeed quantum effects modify the Thomas-Fermi screening length. More pronounced quantum effects exist in the presence of a uniform magnetic field. The next section starts the discussion on the effect of a uniform magnetic field on the screening of charged impurity by quantum plasma.

A similar $\hbar^2$ correction, as that of Eq. (17), is implicit in the dielectric-function formulation of Lindhard and Horing,[1] the nonlinear result given by Eq. (13) is in complete agreement with the work of DuBois and Kivelson,[7] Golden,[6] and many others (Appendix B). In Appendixes C and D, we further show how the thermodynamic potential obtained from Eq. (9) gives the correct answer for the following two cases:

(a) $A(q)\neq 0$, $V(q)=0$ in Eq. (11) and substituted in Eq. (9) yield the correct expression for the magnetic susceptibility of free electrons.

(b) $A(q)=0$, $V(q)\neq 0$ in Eq. (11) and substituted in Eq. (9), the resulting expression for the thermodynamic potential reduces to the correct nondegenerate zero magnetic field limit given by Landau and Lifshitz.[12]

The important result of this section is given by Eqs. (12) and Eq. (13). These are nonlinear equations for the self-consistent potential. Equations (12) and (13), as they stand are exact to order $\hbar^2$; Eq. (13) has been given in the literature.[7] However, the derivation given in this paper is much simpler and straightforward.

III. EXPRESSION FOR $n(q)$ IN THE PRESENCE OF UNIFORM MAGNETIC FIELD: LOW-FIELD CASE

The effect of a uniform magnetic field on the screening of charged impurity at low fields deserves a separate discussion. It is at low field where one expects to see and understand how the electrons redistribute themselves in response to the application of the magnetic field. The quantum dynamical properties of charged particles, in fact, manifest themselves from the nature of the particles response to low-magnetic-field strength.[9] In this section we will evaluate the screening at low fields for $T=0$.[13]

For the low-field case the expression for $n(q)$ is obtained by substituting Eq. (11) into Eq. (10). After integration with respect to p, the result is

$$n(q) = \rho(q,B) - \frac{\hbar^2}{24}\left[\left(\frac{eB}{mc}\right)^2 - \frac{2e}{m}\nabla^2 V(q)\right]\frac{\partial^2}{\partial\mu^2}\rho(q,B) + \frac{\hbar^2 e^2}{24m}|\nabla V(q)|^2\frac{\partial^3}{\partial\mu^3}\rho(q,B), \quad (18$$

where

$$\rho(q,B) = \frac{\tilde{\mathrm{T}}\mathrm{r}}{\hbar^3}\int d^3p\, f(K(p,q)).$$

We will evaluate $n(q)$ only up to second order in the magnetic field strength B. This is conveniently done by first expanding $\rho(q,B)$ in powers of B up to the second order. The validity of this procedure can, of course, only be expected in the asymptotic sense.[13] We have

$$f(K(p,q))=f(K^0(p,q))+f'(K^0(p,q))\Sigma^{(1)}B+\frac{1}{2!}[f''(K^0(p,q))(\Sigma^{(1)})^2+f'(K^0(p,q))\Sigma^{(2)}]B^2+O(B^3)\,, \quad (19)$$

where

$$\Sigma^{(1)}=\frac{e}{2mc}(q_xp_y-q_yp_x)+g\mu_Bs_z\,,$$

$$\Sigma^{(2)}=\frac{e^2}{4mc^2}(q_x^2+q_y^2)\,.$$

These, substituted into Eq. (18), will give

$$n(q)=\frac{\tilde{\mathrm{T}}\mathrm{r}}{h^3}\int d^3p\Bigg\{f(K^0)+B^2\left(\frac{1}{2!}[f'(K^0)\Sigma^{(2)}+f''(K^0)(\Sigma^{(1)})^2]-\frac{1}{24}\left(\frac{e\hbar}{mc}\right)^2f''(K^0)\right)$$
$$+\frac{\hbar^2e}{12m}\nabla^2V(q)\left(f''(K^0)+\frac{B^2}{2!}[f^{\mathrm{V}}(K^0)(\Sigma^{(1)})^2+f'''(K^0)\Sigma^{(2)}]\right)$$
$$-\frac{\hbar^2e^2}{24m}|\nabla V(q)|^2\left(f'''(K^0)+\frac{B^2}{2!}[f^{\mathrm{V}}(K^0)(\Sigma^{(1)})^2+f^{\mathrm{V}}(K^0)\Sigma^{(2)}]\right)\Bigg\}\,, \quad (20)$$

where we have left out in the integral first-order terms in B since they do not contribute. The angular momentum component in $f''(K^0)(\Sigma^{(1)})^2$ can be written in the form of $f'(K^0)\Sigma^{(2)}$. We have

$$\frac{\tilde{\mathrm{T}}\mathrm{r}}{h^3}\int d^3p f''(K^0)(\Sigma^{(1)})^2=\frac{\partial^2}{\partial\mu^2}\frac{\tilde{\mathrm{T}}\mathrm{r}}{h^3}\int d^3p f(K^0)(\Sigma^{(1)})^2\,. \quad (21)$$

Since

$$(\Sigma_{L_z}^{(1)})^2=\left(\frac{e}{2mc}\right)^2(q_x^2p_y^2-2q_xq_yp_xp_y+q_y^2p_x^2)\,, \quad (22)$$

the angular momentum part of the integral reduces to

$$\frac{\partial^2}{\partial\mu^2}\frac{\tilde{\mathrm{T}}\mathrm{r}}{h^3}\int d^3pf(K^0)(\Sigma_{L_z}^{(1)})^2=\frac{\partial^2}{\partial\mu^2}\frac{\tilde{\mathrm{T}}\mathrm{r}}{h^3}\frac{2}{3}\int d^3pf(K^0)\frac{e^2}{4mc^2}(q_x^2+q_y^2)\frac{p^2}{2m}\,. \quad (23)$$

It is easy to verify that for $T=0$

$$\frac{\partial^2}{\partial\mu^2}\frac{\tilde{\mathrm{T}}\mathrm{r}}{h^3}\int d^3pf(K^0)(\Sigma_{L_z}^{(1)})^2=-\frac{\tilde{\mathrm{T}}\mathrm{r}}{h^3}\int d^3pf'(K^0)\Sigma^{(2)}\,. \quad (24)$$

By a similar procedure, the angular momentum part of $f^n(H^0)(\Sigma^{(1)})^2$ can be written in the form of $f^{n-1}(H^0)\Sigma^{(2)}$ term with an opposite sign.

Thus, to order B^2, we have for $n(q)$,

$$n(q)=S(q,B)-\frac{B^2}{24}\left(\frac{e\hbar}{mc}\right)^2\frac{\partial^2}{\partial\mu^2}\rho(q)+\frac{\hbar^2e}{12m}\nabla^2V(q)\frac{\partial^2}{\partial\mu^2}S(q,B)+\frac{\hbar^2e^2}{24m}|\nabla V(q)|^2\frac{\partial^3}{\partial\mu^3}S(q,B)\,, \quad (25)$$

where

$$S(q,B)=\rho(q)+(\mu_BB)^2\frac{1}{2!}\frac{\partial^2}{\partial\mu^2}\rho(q)\,,$$

$$\rho(q)=\frac{2}{h^3}\int d^3p\, f(K^0(p,q))\,.$$

The positive and negative B^2 terms in $n(q)$, with $V(q)$ set equal to zero, correspond to the Pauli and Landau susceptibility, respectively. The effective Poisson equation is

$$\nabla^2V(q)=\left[4\pi e\left(S(q,B)+\frac{\hbar^2e^2}{24m}|\nabla V(q)|^2\frac{\partial^3}{\partial\mu^3}S(q,B)-\tfrac{1}{6}(\mu_BB)^2\frac{\partial^2}{\partial\mu^2}\rho(q)\right)-4\pi en_0-4\pi Ze\delta(q)\right]\times\left(1-\frac{\pi e^2\hbar^2}{3m}\frac{\partial^2}{\partial\mu^2}S(q,B)\right)^{-1}\,. \quad (26)$$

The linearized Poisson equation is

$$\nabla^2V(q)=\lambda^2V(q)-4\pi Ze\delta(q)\,, \quad (27)$$

where

$$\lambda^2=A(1+C)\,, \quad (28)$$

$$A=\frac{4\pi e^2n_0}{\mu}\left[\frac{3}{2}-\frac{1}{8}\left(\frac{\mu_BB}{\mu}\right)^2\right]\,, \quad (29)$$

$$C=\left[\frac{3}{4}+\frac{9}{32}\left(\frac{\mu_B B}{\mu}\right)^2\right]\frac{4\pi e^2\hbar^2}{12m}\frac{n_0}{\mu^2}\,, \tag{30}$$

$$\rho_0=\frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\mu^{3/2}=n_0\,. \tag{31}$$

And these substituted in the expression for λ^2, we obtain

$$\lambda^2=\lambda_0^2\left\{\left[1-\frac{1}{48}\left(\frac{\hbar\omega_c}{\mu}\right)^2\right]+\frac{1}{3\pi}\left(\frac{e^2}{2a_0\mu}\right)^{1/2}\left[1+\frac{7}{96}\left(\frac{\hbar\omega_c}{\mu}\right)^2\right]\right\}, \tag{32}$$

where λ_0 is the inverse Thomas-Fermi screening length. Equation (32) reduces to the λ^2 of Eq. (17) in the absence of the magnetic field. The first term of Eq. (32) was also obtained by Horing by the use of dielectric-function formalism and contour integration.[3] The spherically symmetric solution to the potential is

$$V(q)=(Ze/|q|)\exp(-\lambda|q|)\,. \tag{33}$$

These results may be interpreted as follows. The application of the magnetic field causes the electrons to redistribute themselves resulting in the net increase in the screening length. The spatial anisotropy in the screening does not show up at low fields, up to the second order in the field strength. In Sec. IV, we will discuss how to take into account, to all orders in the field strength, important quantization caused by the magnetic field while partly including quantum effects due to the presence of the impurity potential.

IV. QUASICLASSICAL APPROXIMATION AND BEYOND

The aim of this section is to derive the so-called quasiclassical approximation,[2] for obtaining the self-consistent potential in the presence of a magnetic field, as a zero-order term in a power-series expansion in $\hbar^2$. The important results are of course nonlinear and this is given by Eqs. (39) and (46). The discussion of the approximation involved in arriving at Eqs. (39) and (46) constitutes the main part of this section; this serves to elucidate the exact quantum-mechanical nature of the so-called quasiclassical approximation, first used by Das and de Alba[1] and later investigated by Horing.[3] Comparison with linear-response theory results for very high magnetic field, where the approximations used in this section are good, is given in Appendix A. In this section, it is assumed that the important quantum effects due to the magnetic field are represented by the Landau orbits, a situation very closely related to the phenomenon of magnetic breakdown in solids.

The quasiclassical approximation (QCA) of impurity shielding by quantum plasma is very fascinating since its justification lies deep in the basic philosophy of quantum theory. The concept, in its embryonic form, dates back to the days of the old quantum theory. This is the Bohr correspondence principle,[14] i.e., correspondence between the classical Hamiltonian function and discrete energy values, which lead to the Bohr-Sommerfield quantization rules so successful in the theory of periodic and multiply periodic systems. Now the inability of the Bohr-Sommerfield quantization rules in describing aperiodic systems clearly shows that the Bohr-Sommerfield quantization rules is an especial consequence of the Bohr correspondence principle. Thus the idea of a correspondence between the classical function and discrete values can be accepted as fundamental, and one may expect generalized quantization rules as a consequence.

In modern quantum theory, however, the correct correspondence between the classical function and a quantum-mechanical operator is given by the Weyl correspondence.[15] A one-to-one correspondence between the classical function and a quantum-mechanical operator is obtained by the use of the Weyl transform. In general the Weyl transform of an arbitrary quantum-mechanical operator also contains quantum-mechanical quantities, i.e., the presence of $\hbar$, Planck's constant. For the $\mathcal{H}$ operator given by Eq. (5), the Weyl transform coincides with the classical Hamiltonian except for the presence of a Zeeman term. To summarize, the Weyl correspondence in modern quantum theory involves (i) finding eigenvalues of a quantum-mechanical operator, (ii) finding the Weyl transform of the quantum-mechanical operator, and (iii) equating the Weyl transform to the eigenvalues to obtain the generalized quantization rules. Of course, it may happen that one can easily determine the generalized quantization rules and thereby proceed to find the eigenvalues, as was done in the old quantum theory. To cite an example on how this concept underlies some of the calculations in solid-state theory, we should like to point out the paper by Roth,[16] on the theory of magnetic energy levels and magnetic susceptibility. Roth assumes a generalized form of the quantization rules, in a self-consistent manner, to the transverse canonical conjugate momentum appearing in $\mathcal{H}(K)$, Eq. (38) of Ref. (16), which has been recently shown by the author[9,10] to be the Weyl transform of the Hamiltonian quantum operator. Thus, in Eq. (9), without the impurity potential the replacement of $H(p,q)$ by the energy eigenvalue is the same as applying the Roth quantization rules to the canonical conjugate variables, transverse to the magnetic field, entering in $H(p,q)$ and the second-(and higher-) order terms in Eq. (9) automatically drops out, i.e., all quantum effects are taken care of by the Roth quantization condition, with the integral over p and q replaced by proper counting of states, including degeneracy. Equation (9) thereby leads to the exact way of calculating $\mathrm{Tr}F(\mathcal{K})$ as used by Roth[16] and by Lifshitz and Kosevich.[17]

Now we are ready to discuss the quasiclassical approximation for the impurity shielding by quantum plasma, as first used by Das and de Alba and later investigated by Horing by the use of RPA dielectric-function formalism.[3] The QCA is based on equating $H(p,q)$, the Weyl transform of $\mathcal{H}$, to a discrete set of energy values obtained by applying the Roth, Lifshitz, and Kosevich type of quantization to the canonical conjugate momentum appearing in $H(p,q)$. As the degeneracy is determined mainly by the commutation relation of the canonical conjugate momentum operator,[17] the summation over p is replaced by summation over the degenerate energy values with factor of degeneracy the same as that of the susceptibility calculation without the impurity potential. We will refer to the QCA scheme as a modified Weyl correspondence. This procedure is believed to be exact, from the point of view of Eq. (6), for very high magnetic field where the effect of the potential on the transverse quantization due to the magnetic field can be neglected; this conjecture is verified in Appendix A. Since $H(p,q)$ is not equated to the exact eigenvalues, even for very high magnetic field, of the Hamiltonian operator Eq. (5), one expects that the second term of Eq. (9), and of course higher-order terms in Eq. (6), will give quantum corrections. The QCA as used by Das and de Alba[1] completely neglects these quantum corrections. The defect of the QCA is that it does not show any spatial anisotropy in the screening. We will show that it is these quantum corrections which produce the desired spatial anisotropy in the screening length.

Following the principle which we have outlined above for cases where quantization due to the magnetic field is very important, we can write Eq. (11) by using the modified Weyl correspondence as

$$H(p,q)=(N+\tfrac{1}{2})\hbar\omega_c+\frac{p_z^2}{2m}-eV(q)+g\mu_B s_z B\,. \qquad (34)$$

Substituting this in Eq. (10), taking proper account of the degeneracy, we have the expression for $n(q)$ given by

$$n(q)=\frac{eB}{4\pi^2\hbar^2 c}\sum_{s_z=\pm 1/2}\sum_{N=0}^{\infty}\Bigg\{\int dp_z\Big[f((N+\tfrac{1}{2})\hbar\omega_c+p_z^2/2m-eV(q)+g\mu_B s_z B)$$
$$+\frac{\hbar^2 e}{12m}\nabla_z^2 V(q) f''((N+\tfrac{1}{2})\hbar\omega_c+p_z^2/2m-eV(q)+g\mu_B B s_z)$$
$$-\frac{\hbar^2 e^2}{24m}|\nabla_z V(q)|^2 f'''((N+\tfrac{1}{2})\hbar\omega_c+p_z^2/2m-eV(q)+g\mu_B s_z B)\Big]\Bigg\}, \qquad (35)$$

where only $\nabla_z^2 V(q)$ remains in $n(q)$. The self-consistent equation for the potential is given, as before, by the Poisson equation in electrostatics, Eq. (4). In what follows, we will neglect the last term of Eq. (10). This is justified for $T=0$ and probably negligible for $k_B T \ll \mu$.

The quantum correction to the QCA is indeed due to quantum effects associated with the direction along the magnetic field, owing to the presence of the impurity potential. In what follows we will derive the screening for the following two cases: (a) intermediate field strength, $T\neq 0$ and (b) quantum limit, $T=0$.

a. Intermediate field strength, $k_B T\ll\mu$. We will write Eq. (4) as

$$\nabla^2 V(q)=\sum_{s_z=\pm 1/2} F(\mu+eV(q)-g\mu_B s_z B)+\frac{\hbar^2 e}{12m}\nabla_z^2 V(q)\frac{\partial^2}{\partial\mu^2}\sum_{s_z=\pm 1/2} F(\mu+eV(q)-g\mu_B s_z B)$$
$$+\frac{\hbar^2 e^2}{24m}|\nabla_z V(q)|^2\frac{\partial^3}{\partial\mu^3}\sum_{s_z=\pm 1/2} F(\mu+eV(q)-g\mu_B s_z B)-4\pi e n_0-4\pi Z e\delta(q)\,, \qquad (36)$$

where

$$F(\mu+eV(q)-g\mu_B s_z B)=4\pi e\frac{eB}{4\pi^2\hbar^2 c}\sum_{N=0}^{\infty}\int dp_z f((N+\tfrac{1}{2})\hbar\omega_c+p_z^2/2m-eV(q)+g\mu_B s_z B)\,. \qquad (37)$$

For low temperature ($k_B T\ll\mu$), $F(\mu+eV(q)-g\mu_B s_z B)$ has been given by Das and Hebborn.[2] The result in our notation and including spin is

$$F(\mu+eV(q)-g\mu_B s_z B)=\frac{m^{3/2}(k_BT)(\hbar\omega_c)^{1/2}4\pi e}{2\pi\hbar^3}\sum_{l=1}^{\infty}(-1)^l l^{-1/2}\frac{\cos[(2\pi l/\hbar\omega_c)(\mu+eV(q)-g\mu_B s_z B)-\frac{3}{4}\pi]}{\sinh(2\pi^2 lk_BT/\hbar\omega_c)}$$

$$-\frac{\sqrt{2m}\,(\hbar\omega_c)^{1/2}eB(4\pi e)}{2\pi^2\hbar^2 c}\int_0^{\infty}\frac{2}{3}\left(\frac{\epsilon+eV(q)}{\hbar\omega_c}\right)^{3/2}\frac{\partial}{\partial\epsilon}f(\epsilon+g\mu_B s_z B-\mu)\,d\epsilon\ . \quad (38)$$

The self-consistent equation for $V(q)$ is

$$\left[\nabla_x^2+\nabla_y^2+\left(1-\frac{\hbar^2 e}{12m}\frac{\partial^2}{\partial\mu^2}\sum_{s_z=\pm1/2}F(\mu+eV(q)-g\mu_B s_z B)\right)\nabla_z^2\right]V(q)$$

$$=\left(1+\frac{\hbar^2e^2}{24m}\,|\nabla_z V(q)|^2\frac{\partial^3}{\partial\mu^3}\right)\sum_{s_z=\pm1/2}F(\mu+eV(q)-g\mu_B s_z B)-4\pi e n_0-4\pi Ze\delta(q)\ . \quad (39)$$

It is clear from the last equation that screening in the direction along the magnetic field is different from screening in the transverse direction. To exhibit the important spatial anisotropy in the screening length contained in Eq. (39), we linearize the equation in the potential and thus neglect the linear terms in $V(q)$ occurring in S in the left-hand side. Then we obtain

$$(\nabla_x^2+\nabla_y^2+S\nabla_z^2)\,V(q)=\lambda^2V(q)-4\pi Ze\delta(q)\ , \quad (40)$$

where

$$\lambda^2=e\sum_{s_z=\pm1/2}\frac{\partial}{\partial\mu}F(\mu-g\mu_B s_z B)\ ,$$

$$S=1-\frac{\hbar^2 e}{12m}\frac{\partial^2}{\partial\mu^2}\sum_{s_z=\pm1/2}F(\mu-g\mu_B s_z B)\ .$$

If we define $z'=z/\sqrt{S}$, then we get

$$\nabla^2V(q')=\lambda^2V(q')-4\pi Ze\delta(q')\ , \quad (41)$$

and the spherically symmetric solution in terms of $(x,\ y,\ z')$ is

$$V(q')=(Ze/|q'|)\exp(-\lambda|q'|)\ . \quad (42)$$

By converting to $(x,\ y,\ z)$ coordinates, $(x,\ y,\ z)=(x',\ y',\ \sqrt{S}z')$, we find that the screening is anisotropic with constant potential coordinates scaled in the direction along the magnetic field and the potential ceases to be spherically symmetric in (x,y,z) space. We find[18]

$$\lambda^2=\lambda_0^2\,[1-\tfrac{1}{48}(\hbar\omega_c/\mu)^2-O((k_BT/\mu)^2)]-\frac{8\pi k_BT}{(\hbar\omega_c)^{1/2}}\left(\frac{1}{a_0}\right)^{3/2}\frac{1}{e}\sum_{l=1}^{\infty}l^{1/2}\frac{\sin(2\pi l\mu/\hbar\omega_c-\frac{3}{4}\pi)}{\sinh(2\pi^2lk_BT/\hbar\omega_c)}\ , \quad (43)$$

$$S=1-\frac{1}{12\pi}\left(\frac{2e^2}{a_0}\right)^{1/2}\sum_{s_z=\pm1/2}\left((\mu-g\mu_B s_z B)^{-1/2}+\frac{(\pi k_BT)^2}{8}(\mu-g\mu_B s_z B)^{-5/2}\right)$$

$$+\frac{4\pi^2}{3}\left(\frac{e^2}{a_0}\right)^{1/2}\frac{k_BT}{(\hbar\omega_c)^{3/2}}\sum_{l=1}^{\infty}l^{3/2}\frac{\cos(2\pi l\mu/\hbar\omega_c-\frac{3}{4}\pi)}{\sinh(2\pi^2lk_BT/\hbar\omega_c)}\ . \quad (44)$$

b. Quantum limit, $T=0$. The features of the screening in the quantum limit is of especial interest in connection with the transverse and longitudinal magnetoresistance data for GaAs at 2 °K with 4×10^{16} carriers cm^{-3} measured by Askenazy, Ulmet, and Leotin[19] at very high magnetic field. They found the usual rapid B^2 rise in $\Delta\rho/\rho$ followed by an unusual equally rapid decrease beyond 80 kG. This decrease was attributed to screening effects as the $N=0$ Landau level approaches the Fermi level. Recently, Wallace[20] investigated the features of the screening in this regime using linear-response theory by the use of dielectric response function, and concluded that the range of the potential decreases in the quantum limit, more rapidly in the transverse than in the longitudinal direction. In the transverse direction the screening length decreases with the cyclotron radius. We will show that essentially equivalent results can be obtained by the distribution-function method; furthermore, we will include spin in our analysis and indicate the critical field at which the screening length goes to the Thomas-Fermi value. This result may suggest the possibility for an increase in the number of carriers for fields beyond the critical value. For $T=0$ we immediately obtain, from Eq. (36), the following:

$$\nabla^2 V(q) = 4\pi e \left\{ \frac{eB(2m)^{1/2}}{4\pi^2\hbar^2 c} \left[\sum_{s_z=\pm 1/2} \sum_{N=0}{}' \left(2[\mu + eV(q) - g\mu_B s_z B - (N+\tfrac{1}{2})\hbar\omega_c]^{1/2} - \frac{1}{24}\frac{\hbar^2 e}{m} \nabla_z^2 V(q)[\mu + eV(q) - g\mu_B s_z B - (N+\tfrac{1}{2})\hbar\omega_c]^{-3/2} + \frac{3}{4}\frac{\hbar^2 e^2}{24m} |\nabla_z V(q)|^2 [\mu + eV(q) - g\mu_B s_z B - (N+\tfrac{1}{2})\hbar\omega_c]^{-5/2} \right) \right] \right\} - 4\pi e n_0 - 4\pi Z e \delta(q) , \tag{45}$$

where the summation over N is restricted to real values for the summand. For our present purpose we will consider the ultra quantum limit for which only $N=0$ and $s_z = -\frac{1}{2}$ contributes, i.e., all spins are aligned. Denoting by $\alpha = (\frac{1}{2}m/m^* - \frac{1}{4}g)$, where g is the spin g factor and m^* is the effective mass, we have

$$(\nabla_x^2 + \nabla_y^2 + \{1 + 4\pi e\gamma\delta[\mu - \alpha\hbar\omega_c + eV(q)]^{-3/2}\}\nabla_z^2)V(q) = 4\pi e\gamma \left\{ [\mu - \alpha\hbar\omega_c + eV(q)]^{1/2} + \frac{3}{8}\frac{\hbar^2 e^2}{24m^*} |\nabla_z V(q)|^2 [\mu - \alpha\hbar\omega_c + eV(q)]^{-5/2} \right\} - 4\pi e n_0 - 4\pi Z e \delta(q) , \tag{46}$$

where

$$\gamma = \frac{eB(2m^*)^{1/2}}{\pi^2\hbar^2 c} , \quad \delta = \frac{1}{2}\frac{\hbar^2 e}{24m^*} .$$

To linearize the above equation we make the assumption that $\mu - \alpha\hbar\omega_c \gg eV(q)$, which is certainly not valid at the impurity site, but turns out to be a self-consistent assumption since for the most part in q space the potential is highly screened. Since we are only interested in the features of the spatial anisotropy of the screening length, we again neglect the $V(q)$ term in the left-hand side, resulting in the simple scaling of the z axis as in the intermediate-field case.

We therefore have

$$\nabla^2 V(q') = \lambda^2 V(q') - 4\pi Z e \delta(q') , \tag{47}$$

where

$$z' = z \left[1 + \frac{1}{6\pi}\left(\frac{2e^2}{\hbar\omega_c^* a_0}\right)^{1/2}\left(\frac{\hbar\omega_c^*}{\mu - \alpha\hbar\omega_c}\right)^{3/2} \right]^{-1/2} , \tag{48}$$

$$\lambda^2 = \frac{2\pi e^2 n_0}{\mu - \alpha\hbar\omega_c} = \frac{4}{\pi^3}\frac{1}{a_0}\left(\frac{1}{l}\right)^4 \frac{1}{n_0} , \tag{49}$$

$$n_0 = \frac{eB(2m^*)^{1/2}}{\pi^2\hbar^2 c}(\mu - \alpha\hbar\omega_c)^{1/2} . \tag{50}$$

l is the cyclotron radius and a_0 is the Bohr radius, using an effective mass. The spherically symmetric potential in (x, y, z') space is of the form of Eq. (42) and, transforming to $(x, y, z) = (x, y, \sqrt{S}\, z')$ space, we find that the screening length in the direction along the magnetic field is larger than the screening length in the transverse direction since S, determined from Eq. (48), is greater than one and increases with the magnetic field strength. Thus the screening length in the transverse direction decreases with the cyclotron radius while the screening length in the longitudinal direction can eventually increase[21] with magnetic field strength. We can estimate the critical field at which the transverse screening length is equal to the Thomas-Fermi value by writing λ^2 as

$$\lambda^2 = \lambda_0^2 \frac{E_F/3}{\mu - \alpha\hbar\omega_c} , \tag{51}$$

where E_F is the Fermi energy in the absence of the field. Thus, at field strength where $\mu - \alpha\hbar\omega_c = \frac{1}{3}E_F$, $\lambda^2 = \lambda_0^2$, and the screening length in the transverse direction is equal to the Thomas-Fermi value. For fields beyond the critical value, $\lambda^2 > \lambda_0^2$. These results may be a clue to the explanation of some high-field experiments[19] mentioned at the beginning of this section.

V. CONCLUDING REMARKS

In this paper, we have laid down the quantum-mechanical basis of the distribution-function method in impurity screening first used by Thomas. In the process, we have obtained a finite temperature and magnetic-field-dependent generalization of previous nonlinear results.[7] We have introduced quantum corrections to the quasiclassical approximation introduced by Das and de Alba by adding the desired spatial anisotropy in the screening. The results of the calculation for the screening at low field, intermediate field, and in the quantum limit can be summarized as follows: The effect of the magnetic field is to increase the screening length from the Thomas-Fermi value with oscillatory component at intermediate fields and finally decreases the transverse screening length back to the Thomas-Fermi value in the quantum limit. Further increase in the magnetic field results in the transverse screening length less than the Thomas-Fermi value. The screening length along the magnetic field changes less rapidly than the transverse screening at intermediate fields; the spatial anisotropy increases,[21] more significantly, as the quantum limit is approached. In the calculation presented, the spatial anisotropy in the screening is determined very simply by the z-coordinate scaling factor S.

We would like to clarify the limitation of the formalism used here in regards to the accurate calculation of $n(q)$. It is clear that the distribution-function method depends on being able to express the free energy as a volume integral which then automatically defines $n(q)$.[8] In principle, the formalism can be carried to all orders in accuracy; however, going beyond the $\hbar^2$ term in Eq. (9) becomes very tedious. In Sec. IV, we have taken care of the important quantization effects caused by the magnetic field, to all orders, by applying the correspondence principle. Theoretically if one is just interested in the accurate calculation or $\mathrm{Tr}F(\mathcal{H})$ one can apply the correspondence principle using the exact eigenvalue of $\mathcal{H}$ in the presence of the magnetic field and impurity potential with proper accounting of states. This method, however, is incapable of defining $n(q)$. Another method of defining $n(q)$ through the free energy is, of course, through the explicit use of wave functions. This method employs the density matrix.[22] The distribution-function method is, however, much simpler and straightforward in getting approximate results.[23] The distribution-function method can easily be applied to particles of arbitrary dispersion law, at all temperatures, and can include multiband effects.[9,10]

Finally, the formalism used in deriving the particle density does not contain any formal approximations beyond the expansion to order $\hbar^2$. The basic physical assumption that independent particles move in a self-consistent potential is, of course, common to all theories. The results presented here are all rooted in the exact expression, given by Eq. (9) to order $\hbar^2$, for obtaining the trace as a volume integral. In principle, all the results can be obtained to all orders in $\hbar^2$ and present no difficulties except that the calculations become very tedious. The calculations make use of the Weyl-Wigner formulation of quantum mechanics.[9] In Sec. II, the treatment is straightforward since no approximations at all are involved and the treatment in Sec. IV is physically meaningful and very enlightening through the use of Weyl correspondence.

ACKNOWLEDGMENTS

I would like to thank Professor P. R. Wallace for helpful discussions and for the hospitality extended to me at Eaton Electronics Research Laboratory, McGill University, where this work was carried out. I would also like to thank Dr. J. C. Jones for some helpful comments.

APPENDIX A: COMPARISON WITH LINEAR-RESPONSE THEORY

Horing's work is based on linear-response theory and Green-function techniques using the random-phase approximation. The self-consistent potential is written as, Eq. (1) of Ref. 3,

$$V(q)=\bar{F}^{-1}\{4\pi Ze[p^2-4\pi e^2 \mathrm{Im} I(p,\omega=0+i\delta)]^{-1}\}, \tag{A1}$$

where F^{-1} is the operation of taking the inverse Fourier transform. To compare with the present results, we construct the Poisson equation from (A1),

$$\nabla^2 V(q)=4\pi e[-\mathrm{Im} I(i\nabla)eV(q)]-4\pi Ze\delta(q). \tag{A2}$$

Thus we have, up to terms linear in $V(q)$,

$$n(q)-n_0=PK(i\nabla)eV(q), \tag{A3}$$

where

$$P=\int_0^\infty d\omega\,\frac{f_0(\omega)}{\hbar^3}\int_{-\infty+\delta}^{i\infty+\delta}\frac{ds}{2\pi i}e^{s\omega}\frac{\pi^{3/2}}{(2\pi)^3}\times\left(\frac{2m}{s}\right)^{1/2}\frac{m\hbar\omega_c}{\tanh(\hbar\omega_c s/2)}, \tag{A4}$$

$$K(p)=s\int_{-1}^{1}dT\exp\left(\frac{\hbar^2p_z^2}{8m}s(T^2-1)\right)\exp\left(\frac{\hbar(p_x^2+p_y^2)}{2m\omega_c}\;\frac{\cosh(\frac12\hbar\omega_c sT)-\cosh(\frac12\hbar\omega_c s)}{\sinh(\frac12\hbar\omega_c s)}\right). \tag{A5}$$

We will evaluate the function K, to order p^2, for the following two cases: zero-magnetic-field limit and very high magnetic field.

a. Zero field.

$$K(p)=s\int_{-1}^{1}dT\left(1+\frac{\hbar^2p_z^2}{8m}s(T^2-1)+\cdots\right)\times\left(1+\frac{\hbar^2}{8m}(p_x^2+p_y^2)s(T^2-1)+\cdots\right)=2s\left(1-\frac{s\hbar^2p^2}{12m}+\cdots\right). \quad (A6)$$

Substituting in (A3) we have[3]

$$n(q)=n_0+\left(\frac{\partial}{\partial\mu}\rho\right)eV(q)+\frac{\hbar^2e}{12m}\nabla^2V(q)\frac{\partial^2}{\partial\mu^2}\rho\,, \quad (A7)$$

where $n_0=\rho$. This expression is the same as the $n(q)$ term in Eq. (13) linearized in $V(q)$.

b. Very high field. At very high field K becomes

$$K=s\int_{-1}^{1}dT\left(1+\frac{\hbar^2p_z^2}{8m}s(T^2-1)+\cdots\right)\times\left(1+\hbar\frac{(p_x^2+p_y^2)}{2m\omega_c}\frac{e^{1/2\hbar\omega_c sT}-e^{1/2\hbar\omega_c s}}{e^{1/2\hbar\omega_c s}}+\cdots\right)=2s\left(1-\frac{\hbar^2p_z^2}{12m}+\cdots\right). \quad (A8)$$

By the use of (A3) we have

$$n(q)=n_0+\left(\frac{\partial}{\partial\mu}\rho\right)eV(q)+\frac{\hbar^2e}{12m}\nabla_z^2V(q)\frac{\partial^2}{\partial\mu^2}\rho\,. \quad (A9)$$

This expression is the expression for $n(q)$ in Eq. (35) linearized in $V(q)$. Indeed, the high-field approximation, which gives the quasiclassical approximation as the leading term, assumes that the potential of the impurity does not affect the quantization of the canonical conjugate momentum transverse to the magnetic field, a situation that is analogous to the phenomenon of complete magnetic breakdown in solids.

We would like to comment on some features of Horing's result for $V(q)$ which is given in the form

$$V(q)=Ze\exp(-\lambda|q'|)(A|q'|)^{-1}\,, \quad (A10)$$

where A is a function independent of q. The presence of A seems to suggest that a renormalization of the impurity charge occurs. However, we believe the appearance of A in $V(q)$ is spurious and is essentially due to the approximation of linear response, inherent in Horing's work. To see how this would arise here is to linearize, for example, Eq. (13) instead of (15), one then obtains a multiplying factor for the impurity at the origin which actually goes to 1 had we not made linearization at the early stage of the calculation [refer to statement below Eq. (16)].

APPENDIX B: COMPARISON WITH OTHER NONLINEAR THEORY

In this Appendix, we will take the generalization of nonlinear Thomas-Fermi theory, at zero temperature in the absence of magnetic field, given by DuBois and Kivelson.[7] We take Eqs. (4.30), (6.3), (6.5), and (7.4) of their paper and neglect correlation, anomalous and exchange contributions. We will show that their result is compatible with the result presented in this paper. Equation (7.4) of their paper may be written, with $\hbar$ restored, as

$$\nabla^2(\phi_0+\phi_2)=-4\pi e^2\left[\frac{[P_F^0(q)]^3}{3\pi^2}-\frac{m}{\pi^2\hbar^2}P_F^0(q)\phi_2-\frac{m\hbar^2}{24\pi^2\hbar^4P_F^0(q)}\left(2\nabla^2\phi_0+\frac{m}{\hbar^2[P_F^0(q)]^2}\nabla\phi_0\cdot\nabla\phi_0\right)\right]+4\pi Ze^2\delta(q), \quad (B1)$$

where $P_F^0(q)=[(2m/\hbar^2)(\mu-\phi_0)]^{1/2}$. They have split ϕ into $\phi_0+\phi_2$, where ϕ_0 is the solution of the Thomas-Fermi theory (zero order in $\hbar$) and ϕ_2 is a correction of order $\hbar^2$ [note that the operator used by DuBois and Kivelson, Eq. (3.7) of their paper, is the same as that defined by Baraff and Borowitz and can be rigorously characterized[9,10] as an operator which, upon acting on a product of the respective Weyl transform of two operators, yields the Weyl transform of the product of the same two operators]. The iterative nature of their treatment is in fact evident since Eq. (B1) determines a differential equation for ϕ_2 in terms of the known ϕ_0, the local Thomas-Fermi potential to zero order in $\hbar$. Equation (B1) is in fact the same as

$$\nabla^2\phi=-4\pi e^2\left[\frac{[P_F(q)]^3}{3\pi^2}-\frac{m\hbar^2}{24\pi^2\hbar^4P_F(q)}\times\left(2\nabla^2\phi+\frac{m}{\hbar^2[P_F(q)]^2}(\nabla\phi)^2\right)\right]+4\pi Ze^2\delta(q), \quad (B2)$$

where $P_F(q)=[(2m/\hbar^2)(\mu-\phi)]^{1/2}$, if the above equation is written up to order $\hbar^2$ in both sides. Iterative solution to this equation is represented by (B1). However, instead of solving (B1), a differential equation for ϕ_2, we may solve (B2) self-consistently for ϕ. The expression in the large square bracket of (B2) is in fact the expression for the particle density, to order $\hbar^2$, originally given by Golden.[6] To apply to our case, we must also add the potential due to positive background charges resulting in adding a $4\pi e^2 n_0$ term on the right-hand side of (B2). Equation (B2) is exactly Eq. (13) of this paper since from Eq. (6.3) of Ref. 7,

$$\rho(q)=\frac{1}{3\pi^2}[P_F(q)]^3. \quad \text{(B3)}$$

Thus substituting $\phi=-eV(q)$ we obtain Eq. (13),

$$\nabla^2 V(q)=4\pi e\left\{\rho(q)+\frac{\hbar^2 e}{12m}\nabla^2 V(q)\frac{\partial^2}{\partial\mu^2}\rho(q)+\frac{\hbar^2 e^2}{24m}|\nabla V(q)|^2\frac{\partial^3}{\partial\mu^3}\rho(q)\right\}-4\pi e n_0-4\pi Ze\,\delta(q). \quad \text{(B4)}$$

Finally, we like to point out that the linear-response RPA result of Lindhard and Horing can in fact be regained by linearizing (B2) in ϕ.

APPENDIX C: NONDEGENERATE ZERO-MAGNETIC-FIELD LIMIT OF THE THERMODYNAMIC POTENTIAL

Let us take the expression for the thermodynamic potential determined from Eqs. (2) and (9). We obtain

$$\mathrm{Tr}F(\mathcal{K})=\frac{\tilde{\mathrm{Tr}}}{h^3}\int d^3p\,d^3q\left(F(K(p,q))+\frac{\hbar^2 e}{24m}F''(K(p,q))\nabla^2V(q)\right), \quad \text{(C1)}$$

where we have used $H(p,q)$ given by Eq. (11) with $A(q)=0$. Now in a nondegenerate Maxwell-Boltzman distribution, we have

$$F''(K(p,q))=-\frac{1}{k_BT}\exp\{[\mu-H(p,q)]/k_BT\}. \quad \text{(C2)}$$

Thus

$$\mathrm{Tr}F(\mathcal{K})=\frac{2}{h^3}\int d^3p\,d^3q\,F(K(p,q))+\frac{\hbar^2}{24m}\frac{1}{k_BT}\frac{2}{h^3}\int d^3p\,d^3q\,\exp\{[\mu-H(p,q)]/k_BT\}\nabla^2(-eV(q)),$$

which can also be written

$$\mathrm{Tr}F(\mathcal{H})=F_{cl}+\frac{\hbar^2}{24m}\frac{N}{k_BT}\langle\nabla^2-eV(q)\rangle. \quad \text{(C3)}$$

This is essentially the Landau and Lifshitz result.[12] Note the inclusion of spin in Landau and Lifshitz analysis simply results in a multiplier 2 as it occurs here and can be absorbed in F_{cl} and N in the last equation.

APPENDIX D: MAGNETIC SUSCEPTIBILITY OF FREE ELECTRONS FROM EQ. (9)

Let us again take the expression of the thermodynamic potential, determined from Eq. (9), with $H(p,q)$ given by Eq. (11) but with $V(q)$ set equal to zero. Let us assume the magnetic field in the z direction and use the symmetric gauge for the vector potential, $A(q)=\frac{1}{2}B\times q$. It is easy to verify the following:

$$\frac{\partial^2K}{\partial p_i\partial p_j}\frac{\partial^2K}{\partial q_i\partial q_j}=\frac{1}{2}\left(\frac{eB}{c}\right)^2\left[\frac{\partial H}{\partial p_x^2}\frac{\partial H}{\partial p_y^2}-\left(\frac{\partial H}{\partial p_x\partial p_y}\right)^2\right], \quad \text{(D1)}$$

$$\frac{\partial^2K}{\partial p_i\partial q_j}\frac{\partial^2K}{\partial p_j\partial q_i}=\frac{1}{2}\left(\frac{eB}{c}\right)^2\left[\left(\frac{\partial^2H}{\partial p_x\partial p_y}\right)^2-\frac{\partial^2H}{\partial p_x^2}\frac{\partial^2H}{\partial p_y^2}\right], \quad \text{(D2)}$$

and these substituted in the expression of the thermodynamic potential, we obtain

$$\mathrm{Tr}F(\mathcal{K})=\frac{\tilde{\mathrm{Tr}}}{h^3}\int d^3p\,d^3q\left\{F(K(p,q))-\frac{\hbar^2}{24}F''(K(p,q))\left(\frac{eB}{c}\right)^2\left[\frac{\partial^2H}{\partial p_x^2}\frac{\partial^2H}{\partial p_y^2}-\left(\frac{\partial^2H}{\partial p_x\partial p_y}\right)^2\right]\right\}. \quad \text{(D3)}$$

Denoting by $\hbar k=p-(e/c)A(q)$, we can write

$$\mathrm{Tr}F(\mathcal{K})=\frac{\tilde{\mathrm{Tr}}}{(2\pi)^3}\int d^3k\;d^3q\left\{F(K(k))-\frac{1}{24}\left(\frac{eB}{\hbar c}\right)^2F''(K(k))\left[\frac{\partial^2H}{\partial k_x^2}\frac{\partial H}{\partial k_y^2}-\left(\frac{\partial H}{\partial k_x\partial k_y}\right)^2\right]\right\}, \quad \text{(D4)}$$

where $H(k)=\hbar^2k^2/2m+g\mu_Bs_zB$. Expanding $F(K(k))$ in powers of B up to second order, we obtain

$$\mathrm{Tr}F(\mathcal{K})=\frac{1}{(2\pi)^3}\sum_{s_z=\pm 1/2}\int d^3k\,d^3q\left\{F(K^0(k))+F'(K^0(k))(g\mu_B s_z B)+\frac{1}{2!}F''(K^0(k))(\mu_B B)^2\right.$$
$$\left.-\left(\frac{eB}{\hbar c}\right)^2\frac{1}{24}F''(K^0(k))\left[\frac{\partial^2 H^0}{\partial k_x^2}\frac{\partial^2 H^0}{\partial k_y^2}-\left(\frac{\partial H^0}{\partial k_x\partial k_y}\right)^2\right]\right\},\quad \text{(D5)}$$

where $H^0(k)=\hbar^2k^2/2m$. The magnetic susceptibility is now given by

$$\chi=-\frac{1}{V}\frac{\partial^2}{\partial B^2}\mathrm{Tr}F(\mathcal{K})\bigg|_{B\to 0},\quad \text{(D6)}$$

which yields

$$\chi=-\frac{2}{V(2\pi)^3}\int d^3k\,d^3q\,f'(K^0(k))\mu_B^2$$
$$+\frac{1}{3}\frac{2}{V(2\pi)^3}\int d^3k\,d^3q\,f'(K^0(k))\mu_B^2.\quad \text{(D7)}$$

The first term gives the Pauli spin paramagnetism χ_P and the second term gives the Landau-Peierls orbital diamagnetism χ_{LP}. We have for free electrons[9]

$$\chi_{\mathrm{LP}}=-\frac{1}{12\pi^2}\frac{e^2}{mc^2}k_F,\quad \text{(D8)}$$

$$\chi_P=\frac{1}{4\pi^2}\frac{e^2}{mc^2}k_F.\quad \text{(D9)}$$

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*Work supported by the National Research Council of Canada.

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[8]Some caution will have to be exercised in obtaining $n(q)$. To clarify Eqs. (2) and (3), note that $n(q)$ is also the diagonal matrix element of the thermodynamic Green function (see, for example, Ref. 7) in the q representation. Thus integration by part on the right-hand side of Eq. (2) is not permitted, as this may change the integrand resulting in an incorrect $n(q)$ as obtained from Eq. (3).

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[11]For one-band nonrelativistic quantum dynamics the eigenfunction for position and momentum operators are, respectively, a Dirac delta function and plane waves.

[12]L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, New York, 1968), pp. 93–97.

[13]Any doubts as to the validity of the expansion in $\hbar$ and B jointly used in this section can be dismissed if one realizes that at very low fields our manipulation is such that singularities associated with sharp magnetic energy levels are averaged out. It is precisely through the use of Weyl-Wigner formalism that difficulties caused by singularities are avoided. The results can only be expected to be valid in the asymptotic sense.

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[23]To obtain the Friedel-Kohn-type "wiggle" would necessitate evaluation of $n(q)$ to all orders in $\hbar^2$.