Relation between current and density profiles of interacting electronic systems in a magnetic field

G. Vignale and P. Skudlarski
Department of Physics and Astronomy, University of Missouri-Columbia, Columbia, Missouri 65211
(Received 3 June 1992)

An exact formal relationship between the equilibrium orbital-current and density profiles of a nonuniform electronic system in the presence of a magnetic field is derived from current-density-functional theory. In the local-density approximation we obtain an explicit formula, including exchange and correlation effects, for the equilibrium current in terms of the gradient of density. This formula is shown to reduce to exact asymptotic results in the limit of very large magnetic fields or in the linear-response regime. A surprising consequence of our formula is that in three dimensions, the direction of circulation of the current, relative to the gradient of the density, can have either sign, depending on the local value of the density. A nonlocal linear relationship between current and density for rapidly varying density profiles and/or weak magnetic fields is also derived.

I. INTRODUCTION

It is a remarkable fact of quantum mechanics that a stationary electronic system at thermodynamic equilibrium in a magnetic field can support persistent orbital currents. In classical statistical mechanics the average equilibrium current vanishes identically at every point in space, no matter what the potential energy is. This is because, classically, the distribution of velocities is not affected by either the potential or the magnetic field. In quantum mechanics, however, the noncommutativity of positions and velocities leads to an intertwining of their distributions, resulting in the appearance of orbital currents in nonuniform systems. A prime example of nondissipative orbital currents is provided, of course, by the Hall current in the quantum Hall effect[1] at $T=0$.

The problem of calculating the equilibrium current distribution in an interacting electronic system subjected simultaneously to an external magnetic field and a nonuniform potential is presently receiving a great deal of attention. This problem arises in various different contexts, for instance: (1) in understanding the distribution of currents in quantum Hall systems, including the effects of impurities and edge states;[2,3] (2) in determining the magnetic field associated with the formation of certain nonuniform structures, such as the Wigner crystal in the two-dimensional electron gas;[4] and (3) in the physics of mesoscopic systems.[5] In this paper, we limit ourselves to macroscopic systems, for which the effect of the boundary conditions is negligible.

An important step toward the solution of this problem is the exact result obtained by Girvin and MacDonald,[6] which relates the exact orbital current distribution $\mathbf{j}(\mathbf{r})$ of a two-dimensional electron gas to the gradient of its density $n(\mathbf{r})$:

$$\mathbf{j}(\mathbf{r})=\frac{\hbar}{2m}\nabla n(\mathbf{r})\times\hat{\mathbf{z}}\ , \tag{1}$$

where $\hat{\mathbf{z}}$ is the unit vector in the direction of the (uniform) magnetic field. This result holds only when the magnetic field is so strong that the many-electron wave function lies entirely within the lowest Landau level. It is in fact a special case of a powerful identity[6] expressing the one-particle density matrix in terms of the density. Equation (1) can be straightforwardly extended to a three-dimensional (3D) electronic system, provided that the many-body wave function lies within the lowest Landau subband. In this case, the density determines completely the elements of the one-particle density matrix which are diagonal with respect to the z coordinate, parallel to the magnetic field. But since the current lies in a plane perpendicular to the magnetic field, it can be calculated using precisely these matrix elements—hence the result (1) still holds in 3D. (A detailed derivation of this result is presented in the Appendix.)

The conditions of applicability of Eq. (1) are obviously very restrictive. However, the existence of a relationship between orbital current and density *independent of the form of the external potential* for a given magnetic field can be derived rigorously from current-density functional theory[7] (CDFT). According to this theory, the exact density and orbital current distributions of an interacting electronic system in the presence of external scalar and vector potentials $V_0(\mathbf{r})$ and $\mathbf{A}_0(\mathbf{r})$ ($\mathbf{B}_0=\nabla\times\mathbf{A}_0$) are obtained by minimizing the functional

$$E[n(\mathbf{r}),\mathbf{s}(\mathbf{r}),\mathbf{j}_p(\mathbf{r})]=T_s[n(\mathbf{r}),\mathbf{s}(\mathbf{r}),\mathbf{v}p(\mathbf{r})]+E_{\rm xc}[n(\mathbf{r}),\mathbf{s}(\mathbf{r}),\mathbf{v}_p(\mathbf{r})]+E_H[n(\mathbf{r})]$$
$$+\frac{e}{c}\int d^3r\,\mathbf{j}_p(\mathbf{r})\cdot\mathbf{A}_0(\mathbf{r})+\int d^3r\,n(\mathbf{r})\left[V_0(\mathbf{r})+\frac{e^2}{2mc^2}A_0^2(\mathbf{r})\right]+g\frac{e\hbar}{2mc}\int d^3r\,\mathbf{s}(\mathbf{r})\cdot\mathbf{B}_0(\mathbf{r}) \tag{2}$$

with respect to density, spin density $\mathbf{s}(\mathbf{r})$, and canonical current density $\mathbf{j}_p(\mathbf{r})$. T_s, E_{xc}, and E_H are the pseudokinetic, exchange-correlation, and Hartree energy functionals, respectively, and g is the magnetic moment Landé g factor. The *physical* orbital current density is given by

$$\mathbf{j}(\mathbf{r})=\mathbf{j}_p(\mathbf{r})+\frac{e}{mc}n(\mathbf{r})\mathbf{A}_0(\mathbf{r}) , \tag{3}$$

and $\mathbf{v}(\mathbf{r})$ is the vorticity field defined as

$$\mathbf{v}(\mathbf{r})=\nabla\times\frac{\mathbf{j}_p(\mathbf{r})}{n(\mathbf{r})} . \tag{4}$$

In addition, the *full* current density includes a contribution $\mathbf{j}_{spin}=(ge\hbar/2mc)\nabla\times\mathbf{s}(\mathbf{r})$. This is explicitly known in terms of the spin density, and therefore does not require any further treatment.

The minimization of the energy functional can be carried out in two steps. In a first step, we fix the density profile and minimize with respect to $\mathbf{j}_p(\mathbf{r})$ and $\mathbf{s}(\mathbf{r})$. This yields the equations

$$\frac{\delta F[n(\mathbf{r}),\mathbf{s}(\mathbf{r}),\mathbf{j}_p(\mathbf{r})]}{\delta\mathbf{j}_p(\mathbf{r})}=-\frac{e}{c}\mathbf{A}_0(\mathbf{r}) , \tag{5a}$$

and

$$\frac{\delta F[n(\mathbf{r}),\mathbf{s}(\mathbf{r}),\mathbf{j}_p(\mathbf{r})]}{\delta\mathbf{s}(\mathbf{r})}=-g\frac{e\hbar}{2mc}\mathbf{B}_0(\mathbf{r}) . \tag{5b}$$

We have introduced the internal energy functional $F\equiv T_s+E_{xc}+E_H$. Now, according to the Hohenberg-Kohn theorem of CDFT,[7] the F functional is universal, i.e., independent of $V_0(\mathbf{r})$ and $\mathbf{A}_0(\mathbf{r})$. Thus, Eqs. (5a) and (5b) give us an exact formal relationship between orbital current and density profiles, which depends only on the magnetic field but not on the scalar potential. Substituting the solutions $\mathbf{j}_p(\mathbf{r})$ and $\mathbf{s}(\mathbf{r})$ of Eqs. (5) into (2) we obtain an effective functional which must be minimized only with respect to n, in order to find the actual ground-state density.

The focus of this paper is on the relationship between orbital-current and density profiles. We shall provide an explicit form for this relationship, using the local-density approximation to the internal energy functional F. We shall prove that Eqs. (5), in the limit of strong magnetic field or slowly varying density (that is, when the local-density approximation is expected to be valid), yield an expression for the current which differs from Eq. (1) only by a density and magnetic-field-dependent factor $\gamma(n,B_0)$. This factor is directly proportional to the derivative of the chemical potential μ of an interacting uniform electron gas with respect to magnetic field at a fixed density n, or, equivalently, to the derivative of the magnetization with respect to density at a fixed magnetic field. Only in the limit $B_0\to\infty$, γ reduces to 1. In fact, we shall see that in three-dimensional systems γ can have an either positive or negative sign, depending on the local value of the density.

II. LOCAL RELATIONSHIP BETWEEN DENSITY AND CURRENT

In this section we consider physical systems in which the density profile varies slowly on the scale of the magnetic length $l=(\hbar c/eB_0)^{1/2}$. Since $l\cong 252/B_0^{1/2}$ Å, where B_0 is expressed in T, we see that even for the largest attainable magnetic fields l remains of the order of several tens of Å. Therefore, we are talking of density variations that take place on a scale of hundreds of Å. This length scale is characteristic of many low-density systems such as doped semiconductors and semimetals, and can also be realized in artificial microstructures. In this regime, the local-density approximation to the energy functional is expected to be valid. The local-density approximation to the exchange-correlation energy functional in current-density-functional theory has the form[8]

$$E_{xc}[n(\mathbf{r}),\mathbf{v}(\mathbf{r}),\mathbf{s}(\mathbf{r})]=\int d^3r\, n(\mathbf{r})\epsilon_{xc}[n(\mathbf{r}),s(\mathbf{r}),|\mathbf{B}(\mathbf{r})|] . \tag{6}$$

where $\epsilon_{sc}[n(\mathbf{r}),s(\mathbf{r}),B(\mathbf{r})]$ is the exchange-correlation energy (per particle) of a uniform electron liquid of density $n(\mathbf{r})$ and spin density $s(\mathbf{r})$, in a uniform effective magnetic field

$$\mathbf{B}(\mathbf{r})=-\frac{mc}{e}\mathbf{v}(\mathbf{r}) \tag{7}$$

which couples only to the orbital degrees of freedom. The exchange part of the uniform energy has been calculated by Danz and Glasser.[9] Recently, we have calculated the correlation part within the random-phase approximation.[10] Thus, the ϵ_{xc} function can be regarded as known with reasonably good accuracy.

The approximation of the pseudokinetic energy functional $T_s[n,\mathbf{j}_p,\mathbf{s}]$ is more delicate. For a given local value of $\mathbf{j}_p$ we construct a fictitious vector potential $\mathbf{A}(\mathbf{r})$, which produces $\mathbf{j}_p$ in a uniform electron gas of density n and spin density s. The fictitious vector potential couples only to the orbital degrees of freedom (current and density); it does not, in particular, produce any additional Zeeman splitting. Since $\mathbf{j}(\mathbf{r})=0$ everywhere within the uniform electron gas, we find

$$\mathbf{A}(\mathbf{r})=-\frac{mc}{e}\frac{\mathbf{j}_p(\mathbf{r})}{n(\mathbf{r})} . \tag{8}$$

The fictitious magnetic field corresponding to the fictitious vector potential is, of course, the vorticity defined in Eq. (4). Now the pseudo-kinetic-energy functional can be expressed as

$$\begin{aligned}T_s[n(\mathbf{r}),\mathbf{j}_p(\mathbf{r}),\mathbf{s}(\mathbf{r})]=&\int d^3r\, n(\mathbf{r})\epsilon_k[n(\mathbf{r}),s(\mathbf{r}),|\mathbf{B}(\mathbf{r})|]\\&-\frac{e}{c}\int d^3r\,\mathbf{j}_p(\mathbf{r})\mathbf{A}(\mathbf{r})\\&-\frac{e^2}{2mc^2}\int d^3r\, n(\mathbf{r})A^2(\mathbf{r}) ,\end{aligned} \tag{9}$$

where $\epsilon_k[n(\mathbf{r}),s(\mathbf{r}),|\mathbf{B}(\mathbf{r})|]$ is the full (gauge-invariant) kinetic energy (per particle) of the uniform noninteracting electron gas, and the last two terms subtract the part of the kinetic energy that pertains to the interaction with the fictitious field $\mathbf{A}$.

Combining Eqs. (7), (8), and (9) we obtain, for the total-energy functional,

$$E[n(\mathbf{r}),\mathbf{j}_p(\mathbf{r}),\mathbf{s}(\mathbf{r})]=\int d^3r\, n(\mathbf{r})\epsilon[n(\mathbf{r}),s(\mathbf{r}),|\mathbf{B}(\mathbf{r})|]+\frac{m}{2}\int d^3r\frac{|\mathbf{j}(\mathbf{r})|^2}{n(\mathbf{r})}+E_H[n(\mathbf{r})]$$
$$+\int d^3r\, n(\mathbf{r})V_0(\mathbf{r})+\frac{ge\hbar}{2mc}\int d^3r\,\mathbf{s}(\mathbf{r})\cdot\mathbf{B}_0(\mathbf{r})\ , \tag{10}$$

where $\epsilon=\epsilon_k+\epsilon_{xc}$ is the total energy of the uniform electron gas in the fictitious magnetic field. Next, we minimize the functional with respect to $\mathbf{s}(\mathbf{r})$ and $\mathbf{j}_p(\mathbf{r})$ or, equivalently, since n and $\mathbf{A}_0$ are held constant, with respect to $\mathbf{j}(\mathbf{r})$. This leads to the following set of Euler-Lagrange equations for the orbital current:

$$\mathbf{j}(\mathbf{r})=-\frac{c}{e}\nabla\times\mathbf{M}(\mathbf{r})\ , \tag{11a}$$

$$\mathbf{M}(\mathbf{r})=-n(\mathbf{r})\frac{\partial\epsilon}{\partial B}[n(\mathbf{r}),B(\mathbf{r})]\hat{z}\ , \tag{11b}$$

where

$$\mathbf{B}(\mathbf{r})=\mathbf{B}_0-\frac{mc}{e}\nabla\times\frac{\mathbf{j}(\mathbf{r})}{n(\mathbf{r})}+\frac{e}{c}\int d^3r'\frac{\mathbf{j}(\mathbf{r}')\times(\mathbf{r}'-\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|^3}\ . \tag{11c}$$

In these equations, the function $\epsilon(n,B)$ is defined to be the *minimum* of the previous function $\epsilon(n,s,B)$ with respect to spin density. Notice that the derivative of $\epsilon(n,B)$ with respect to the fictitious field has to be calculated *at constant Zeeman splitting,* as explained above.

Equation (11a) shows that the current does obey the continuity equation $\nabla\cdot\mathbf{j}(\mathbf{r})=0$ as required. Equation (11b) says that the local magnetization is obtained by taking the thermodynamic derivative of the local energy density with respect to the local magnetic field. Finally, Eq. (11c) tells us how to compute the effective magnetic field from the local intensive variables of the system. In writing Eq. (11c) we have also included (last term) the additional magnetic field generated by the currents according to Ampère's law of classical electromagnetism. This term follows from reinterpreting the "external" vector potential A_0 in Eq. (2) as a "screened" vector potential, which includes the self-consistent contribution of the orbital currents according to Ampère's law. Notice that Eqs. (11) are derived for an arbitrary magnetic field $\mathbf{B}_0(\mathbf{r})$, not necessarily a uniform one. The functional relationship between $\mathbf{j}$ and n depends, of course, on the local value of B_0.

Equations (11) take a considerably simpler form in the physical regime of slowly varying density described at the beginning of this section. In this limit, neglecting the small Ampere's contribution, we can set $B(r)\cong B_0$ in Eq. (11b), so that the $\mathbf{r}$ dependence of M arises entirely from the density profile. Taking the curl of M we obtain

$$\mathbf{j}(\mathbf{r})=\frac{\hbar}{2m}\gamma[n(\mathbf{r}),B_0(\mathbf{r})]\nabla n(\mathbf{r})\times\hat{z}\ , \tag{12}$$

where

$$\gamma(n,B_0)\equiv\frac{2mc}{e}\left[1+n\frac{\partial}{\partial n}\right]\frac{\partial\epsilon}{\partial B_0}[n(\mathbf{r}),B_0]$$
$$=\frac{2mc}{\hbar e}\frac{\partial\mu(n,B_0)}{\partial B_0}\ , \tag{13}$$

and $\mu(n,B)$ is the chemical potential of the uniform interacting electron liquid, and its partial derivative is taken at constant density and Zeeman splitting. One can show that including the variation of the Zeeman splitting with B_0 in Eq. (13) amounts to including the spin-current contribution, discussed after Eq. (4) with a local relationship between spin and density.

Equation (12) is the main result of this paper. It establishes a local relationship between the orbital current and the density profile of a nonuniform, interacting electronic system. In contrast to Eq. (1), which holds only for systems confined to the lowest Landau level or subband, Eq. (12) holds for a broader range of densities and magnetic fields, provided the conditions of applicability of the local-density approximation are met. In addition, as shown in the next section, Eq. (12) reduces to Eq. (1) in the limit of large magnetic field. The validity of Eq. (12) presupposes the existence of finite thermodynamic derivatives of the energy of the uniform electron gas with respect to density and magnetic field. In the case of *incompressible* systems $\partial\mu/\partial n\to\infty$, and one can show that $\gamma\to\infty$ (see the next section). Thus Eq. (12) is violated for incompressible systems—for example a noninteracting two-dimensional electron gas with an integer number of fully occupied Landau levels. In that case, one can have a finite current even in the bulk of the system, where the density gradient is zero. Another restriction to the validity of Eq. (12) is that it becomes completely inapplicable in the case of spontaneous orbital currents, i.e., when $B_0=0$, but $\mathbf{j}\neq 0$ due to a spontaneous symmetry breaking. In this case one may still consider using the local-density approximation to calculate the current, but it is then necessary to revert to the full self-consistent Eqs. (11), with $B_0=0$.

III. EXACT LIMITING CASES

In this section we prove that Eq. (12) yields the *exact* orbital current in several limiting cases.

(i) *Strong uniform magnetic field.* The chemical potential of the uniform electron gas in a uniform magnetic field can be written as

$$\mu=\frac{\hbar\omega_c}{2}+\frac{\hbar^2k_F^2}{2m}+\mu_{\rm xc}\ , \tag{14}$$

where $\omega_c=(eB_0/mc)$ is the classical cyclotron frequency, k_F is the Fermi momentum in the lowest Landau subband, and $\mu_{\rm xc}$ is the exchange-correlation contribution to μ. In the limit $B_0\to\infty$ the second and third term become negligible with respect to the first one, which is proportional to B_0. Thus, using Eq. (13) we immediately verify that $\gamma(n,B_0)\to 1$, in agreement with the exact result, Eq. (1).

(ii) *Linear-response regime.* We start from a uniform electron gas of density n in a uniform magnetic field B_0. We apply a *small* external potential $V(\mathbf{r})$. In the linear-response approximation, the Fourier transform of the induced density variation is

$$\delta n(\mathbf{q})=\chi_{00}(\mathbf{q})V_{\rm sc}(\mathbf{q})\ , \tag{15}$$

where $V_{\rm sc}(\mathbf{q})$ is the Fourier transform of the self-consistent potential, i.e., the external potential plus the Hartree contribution, and $\chi_{00}(\mathbf{q})$ is the static screened density-density response function.[13] The induced orbital current, in the same linear approximation, is given by

$$\delta j_\alpha(\mathbf{q})=\chi_{\alpha,0}(\mathbf{q})V_{\rm sc}(\mathbf{q})\ , \tag{16}$$

where $\chi_{\alpha,0}(\mathbf{q})$ is the static screened current-density response function, which vanishes for $\alpha=z$ or for $B_0=0$. Eliminating $V_{\rm sc}(\mathbf{q})$ between Eqs. (15) and (16) we obtain an exact, nonlocal relationship between density and current:

$$\delta j_\alpha(\mathbf{q})=\frac{\chi_{\alpha,0}(\mathbf{q})}{\chi_{00}(\mathbf{q})}\delta n(\mathbf{q})\ . \tag{17}$$

In the limit of slowly varying density we can replace the response functions by their $q\to 0$ limit, and we recover a local relationship. From the definition of the linear response functions and the fact that $\mathbf{j}(\mathbf{r})=-(c/e)\nabla M(\mathbf{r})\times\hat{z}$, it is easy to see that

$$\chi_{00}(\mathbf{q})\to\frac{\partial n}{\partial\mu}\ , \tag{18a}$$

and

$$\chi_{\alpha,0}(\mathbf{q})\to i(\mathbf{q}\times\hat{\mathbf{z}})_\alpha\frac{c}{e}\frac{\partial M}{\partial\mu}\ , \tag{18b}$$

where $M=-n(\partial\epsilon/\partial B)$ (at constant Zeeman splitting) is the orbital magnetization. Substituting Eqs. (18) in Eq. (17), and assuming that $\partial\mu/\partial n$ is finite, i.e., that the system is not incompressible, we obtain our Eq. (12) for the current density, with γ given by Eq. (13). On the other hand, for an incompressible system $\partial\mu/\partial n\to\infty$, we obtain $\chi_{00}(\mathbf{q})\sim q^2$ for $q\to 0$, and therefore $\gamma\to\infty$, showing that one can have finite current even when the density gradient vanishes.

(iii) *Widom-Streda formula.* We can also show that our formula for the current is equivalent, in the linear response regime, to the well-known Widom-Streda formula[11] for the off-diagonal conductivity in the quantum Hall effect. To prove this we begin by observing that the gradient of the density in the presence of a slowly varying potential is given, according to Eq. (15), by

$$iq_\alpha\delta n(\mathbf{q})=\chi_{00}(\mathbf{q})E_\alpha(\mathbf{q})\ , \tag{19}$$

where $E_\alpha(\mathbf{q})$ is a component of the electric field $\mathbf{E}=-\nabla V_{\rm sc}$. The left-hand side of Eq. (19) can be expressed in terms of the orbital current, according to Eq. (12). Taking the limit $q\to 0$ and combining Eqs. (13) and (18a) for $\gamma(n,B_0)$ and the small-q limit of the density-density response function, respectively, we obtain

$$\mathbf{j}(\mathbf{q}=0)=c\frac{\partial n}{\partial B_0}\hat{\mathbf{z}}\times\mathbf{E}(\mathbf{q}=0)\ , \tag{20}$$

which agrees with the Widom-Streda expression for the nondissipative current in the quantum Hall effect.

IV. CALCULATION OF γ AND DISCUSSION

In this section we present our calculations of the density- and magnetic-field-dependent factor $\gamma(n,B_0)$, which determines the orbital current according to Eq. (12). Naturally, $\gamma(n,B_0)$ is divided in two parts: a kinetic contribution γ_k and an exchange-correlation contribution $\gamma_{\rm xc}$. γ_k can be calculated exactly from the noninteracting part of the chemical potential, i.e., the first two terms of Eq. (14). In three dimensions, the Fermi momentum k_F in the lowest Landau subband is related to the density by

$$n=\frac{1}{2\pi^2l^2}\sum_N k_{FN\sigma}(k_F)\ , \tag{21}$$

where the sum runs over the occupied Landau subbands, and $k_{FN\sigma}$, the Fermi momentum in the Nth Landau subband ($\sigma=1$ for spin up and $\sigma=0$ for spin down) is given by

$$k_{FN\sigma}=\left[k_F^2-\frac{2m\omega_c}{\hbar}\left[N+(1-\sigma)\frac{g}{2}\right]\right]^{1/2}\ . \tag{22}$$

Using these formulas, we easily obtain

$$\gamma_k=1-2\frac{\sum_{N,\sigma}[k_{FN\sigma}l-N(k_{FN\sigma}l)^{-1}]}{\sum_{N,\sigma}(k_{FN\sigma}l)^{-1}} \tag{23}$$

in three dimensions. The results of the numerical evaluation of $\gamma(n,B_0)$ in three dimensions are shown in Fig. 1. The upper panel shows the noninteracting contribution, calculated according to Eq. (23) for different values of g corresponding to spinless ($g=\infty$—one spin component only), nonpolarized ($g=0$—no Zeeman splitting), and ideal ($g=2$) electrons. The first two cases do not differ in the noninteracting case. They also give the same exchange contribution and only slightly differ in correlation. The lower panel shows the exchange and correlation contributions, the latter calculated in the random-phase approximation for spinless ($g=\infty$) electrons. Two things are remarkable. First we observe that the nonin-

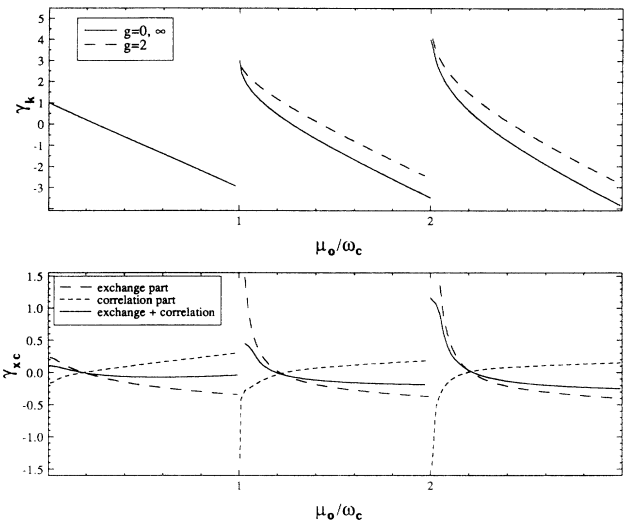

FIG. 1. Upper panel: kinetic contribution to $\gamma(n,B_0)$, as a function of noninteracting chemical potential μ_0/ω_c. Solid line represents results for spinless ($g=\infty$) and nonpolarized ($g=0$) electrons, while dashed line represents results for spin-polarized ($g=2$) electrons. Lower panel: exchange (dashed line) and correlation (dotted line) contribution to $\gamma(n,B_0)$, for spinless electrons ($g=\infty$). Notice the strong cancellation of exchange and correlation effects.

teracting γ_k (and hence the full γ) exhibits a strong oscillatory behavior as a function of density. In brief, γ_k is positive when the noninteracting Fermi level is close to the bottom of a Landau subband; it decreases into negative values as the Landau subband becomes increasingly populated, and finally it reverts discontinuously to a (larger) positive value when the next Landau subband begins to be populated. While the discontinuous jump of γ_k at each Landau subband edge crossing is probably an artifact of the local-density approximation due to the nondifferentiability of the energy functional at the subband crossings, the change in sign of γ_k that occurs when the noninteracting Fermi level is far from band edges is a genuine and interesting effect. It predicts, for example, that if we measure the current in the surface region of an electron-hole droplet[12] we can find a reversal in the direction of circulation of the current as we move from the inner region, where the density is high, to the outer region, where the density is low. Mathematically it can be shown that the sign reversal of γ is caused by the off-diagonal matrix elements of the (kinetic) angular momentum operator between states in different Landau subbands. It is, therefore, a subtle and purely quantum-mechanical phenomenon.

Our second observation concerns the role of the exchange-correlation effects. Far from the band edge these give a very small contribution not only because they are individually small, but because they have opposite signs and largely cancel each other in the final result. Near the Landau subband edges, we find that both exchange and correlation contributions have a logarithmic singularity when the bottom of a subband is approached from above, but those singularities cancel against each other and the total exchange-correlation contribution is finite. From the knowledge of the asymptotic form of the exchange-correlation energy per electron for barely populated subbands we obtain the exact form of the limit of the exchange-correlation contribution to γ when the occupation of the highest subband tends to zero, and find that it has a sizeable discontinuity at the band edge shown in the lower panel of Fig. 1. It must be pointed out that this conclusion has been reached by assuming that the Landau subband distribution of electrons is the same as in the noninteracting gas. Recently we have discovered[10] that this is not the case. In the interacting system Landau subbands are repopulated in such a way as to avoid having a *very small* number of electrons in any one subband. This effect is expected to modify the behavior of γ near the subband edge and possibly further decrease its discontinuity.

V. NONLOCAL RELATION BETWEEN CURRENT AND DENSITY

Figure 1 is paradoxical in that it suggests that the absolute magnitude of oscillations of γ, and hence of the current, increases at a given density with decreasing magnetic field. The paradox is resolved by observing that, with decreasing magnetic field, the magnetic length l increases, and thus we abandon the regime of "slowly varying density" in which the local-density approximation is valid. We can study the crossover from local to nonlocal behavior in the current-density relation within the frame of linear-response theory. Judging from our experience with the local regime, exchange-correlation effects are not too important except near the band edges, and thus we are left with the simple problem of evaluating the noninteracting density-density and current-density correlation functions for a uniform electron gas in a uniform magnetic field [see Eqs. (15)–(17)]. This is readily done by using standard Green's-function techniques.[13] We start from Eq. (17) and observe that $\chi_{\alpha,0}(\mathbf{q})$ must be a vector perpendicular to $\mathbf{q}$, so that the continuity equation is satisfied. Thus we can define a scalar response function $\chi^{j-n}(\mathbf{q})$ by

$$\frac{\chi_{\alpha,0}(\mathbf{q})}{\chi_{0,0}(\mathbf{q})}=\chi^{j-n}(\mathbf{q})\cdot(-i\mathbf{q}\times\hat{z})_\alpha \ . \tag{24}$$

From this we obtain

$$\chi_{j-n}(\mathbf{q})=-\frac{\chi_{+,0}(\mathbf{q})}{\chi_{0,0}q_+} \ , \tag{25}$$

where $q_\pm=q_x\pm iq_y$, $\chi_{\pm,0}(\mathbf{q})=\chi_{x,0}(\mathbf{q})\pm i\chi_{y,0}(\mathbf{q})$, and

$$\chi_{00}(\mathbf{q})=\frac{-1}{2\pi^2\omega_c q_z l^4}\sum_{N,M}|F_{NM}(\mathbf{q}_\perp)|^2\ln\left|\frac{(N-M)\omega_c-\frac{q_z^2}{2m}-k_{FN}\frac{q_z}{m}}{(N-M)\omega_c-\frac{q_z^2}{2m}+k_{FN}\frac{q_z}{m}}\right| \ , \tag{26}$$

$$\chi_{\pm,0}(\mathbf{q})=q_{\pm}\frac{\omega_c l^2}{2}\chi_{00}(\mathbf{q})-\frac{i\sqrt{2}}{4\pi^2 l^2 q_z}\sum_{N,M}\sqrt{N+1}F_{N+1,M}(\mathbf{q}_\perp)F^*_{N,M}(\mathbf{q}_\perp)\left\{\ln\left|\left|\frac{(N-M)\omega_c-\frac{q_z^2}{2m}-k_{FN}\frac{q_z}{m}}{(N-M)\omega_c-\frac{q_z^2}{2m}+k_{FN}\frac{q_z}{m}}\right|\right|-\ln\left|\left|\frac{(N-M)\omega_c+\frac{q_z^2}{2m}-k_{FM}\frac{q_z}{m}}{(N-M)\omega_c+\frac{q_z^2}{2m}+k_{FM}\frac{q_z}{m}}\right|\right|\right\}. \quad (27)$$

Here $F_{NM}(\mathbf{q}_\perp)$ is the matrix element of the density-fluctuation operator for Landau subbands N,M defined as

$$F_{MN}(\mathbf{q}_\perp)=\left[\frac{N!}{M!}\right]^{1/2}\left[\frac{(-q_y+iq_x)l}{\sqrt{2}}\right]^{M-N}\times\exp\left[\frac{-q_\perp^2 l^2}{4}\right]L_N^{M-N}\left[\frac{q_\perp^2 l^2}{2}\right], \quad (28)$$

where $L_N^{\alpha}(x)$ is the generalized Laguerre polynomial.

The nonlocal relation between the current and the density gradient is given by

$$\delta\mathbf{j}(\mathbf{r})=\int d^3r'\,\chi^{j-n}(\mathbf{r}-\mathbf{r}')\nabla n(\mathbf{r}')\times\hat{z}\ . \quad (29)$$

In Fig. 2 we plot $\chi^{j-n}(\mathbf{q})$ as a function of $q_\perp l$ perpendicular to the magnetic field [$\mathbf{q}=(\mathbf{q}_\perp,q_z)$, here $q_z=0$]. This determines the nonlocal relationship between current and density in the linear-response regime. We see that the "local" regime $\chi^{j-n}(\mathbf{q})\sim\gamma$ holds up to a wave vector $q_\perp$ of the order of l^{-1}, then the response function begins to decrease to zero, which means that equilibrium orbital currents disappear in the absence of magnetic field. Comparing the plots of $\chi_{j-n}(\mathbf{q})$ at different magnetic fields we may notice that when the magnetic field is reduced, at a fixed density profile the region of validity of $\chi_{j-n}(\mathbf{q})\sim\gamma$ decreases, even in terms of $q_\perp l$. Equations (27) and (28) are useful to determine the size of the "local" regime and to calculate the equilibrium current in nonuniform systems where the magnetic length is large compared to the other length scales, and a nonlocal connection between current and density is expected.

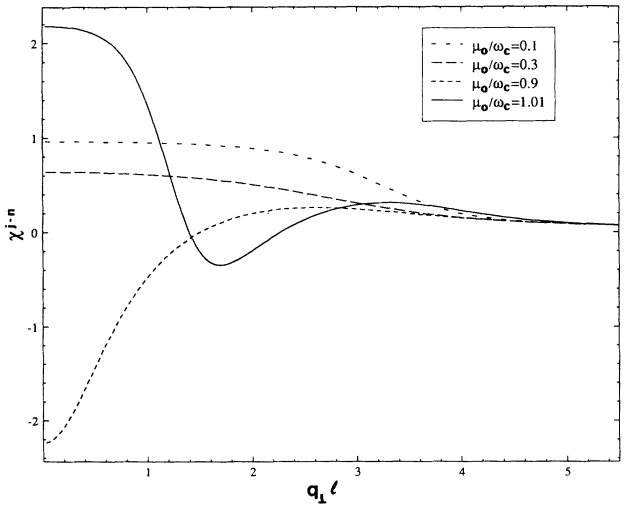

FIG. 2. Linear, nonlocal current-density response kernel $\chi_{j-n}(\mathbf{q})$ as a function of $\mathbf{q}_\perp l$ for a noninteracting electron gas, with $q_z=0$. Different curves where obtained for different values of the noninteracting chemical potential μ_0 in units of the cyclotron energy $\hbar\omega_c$. Notice that in the $\mathbf{q}\to 0$ limit χ_{j-n} reduces to the value of γ appropriate for this value of μ_0/ω_c (see Fig. 1).

VI. CONCLUSION

This paper has presented a study of the relationship between current and density in an interacting nonuniform electronic system in a more general frame than previously considered. Using current-density-functional theory we have shown the existence of such a relation in a form independent of the scalar potential. In the limit in which the local-density approximation is valid we have obtained an explicit form of the current-density relation. This form is shown to generalize previously known exact results, to which it reduces in the appropriate limits. We have found that the current-density relation in three-dimensional systems exhibits interesting and unexpected behavior, entailing a reversal in the direction of circulation of current at certain values of density. A remarkable cancellation of exchange-correlation effects on the current far from band edges has been demonstrated. Near band edges, the logarithmic singularity of the exchange contribution to γ is exactly cancelled by the correlation correction, and a finite discontinuity is left. This discontinuity may be modified by repopulation of Landau subbands. Finally, we have considered the nonlocal linear connection between current and density for rapidly varying densities and/or weak magnetic fields. An explicit expression for the nonlocal linear current-density kernel of a noninteracting electron gas has been presented.

ACKNOWLEDGMENTS

We wish to thank Dr. Mark Rasolt and Professor A. H. MacDonald for some useful discussions. This work was supported in part by the National Science Founda-

tion Grant No. DMR-9100988 and by the Donors of the Petroleum Research Fund administered by the American Chemical Society.

APPENDIX

Here we prove the relation (1) for a three-dimensional system. The Fourier transform of the current operator is given by

$$\mathbf{j}(\mathbf{q})=\frac{1}{2m}\sum_i(\mathbf{\Pi}_i e^{i\mathbf{q}\mathbf{r}_i}+e^{i\mathbf{q}\mathbf{r}_i}\mathbf{\Pi}_i)\ , \tag{A1}$$

where

$$\mathbf{\Pi}_i\equiv\mathbf{p}_i+\frac{e}{c}\mathbf{A}(\mathbf{r}_i)\ ,$$

$\mathbf{A}$ is a vector potential of the uniform magnetic field and i is a particle label.

Using the standard commutation rules, we rewrite

$$j_+(\mathbf{q})=\frac{1}{m}\sum_i \Pi_{+i}e^{i\mathbf{q}\mathbf{r}_i}-q_+n(\mathbf{q})\frac{\hbar}{2m}\ , \tag{A2}$$

$$j_-(\mathbf{q})=\frac{1}{m}\sum_i e^{i\mathbf{q}\mathbf{r}_i}\Pi_{-i}-q_-n(\mathbf{q})\frac{\hbar}{2m}\ , \tag{A3}$$

where: $q_\pm=q_x\pm iq_y$, $j_\pm(\mathbf{q})=j_x(\mathbf{q})\pm ij_y(\mathbf{q})$, $\Pi_\pm=\Pi_x\pm i\Pi_y$ are the usual Landau-level rising $(+)$ and lowering $(-)$ operators, and $n(\mathbf{q})=\sum_i e^{i\mathbf{q}\mathbf{r}_i}$ is the Fourier transform of the density operator.

When taking the matrix element of $j_\pm(\mathbf{q})$ between states belonging to the lowest Landau subband the terms containing Π_+, Π_- vanish, and we are left with

$$j_+(\mathbf{q})\cong -q_+n(\mathbf{q})\frac{\hbar}{2m}\ , \tag{A4}$$

$$j_-(\mathbf{q})\cong -q_-n(\mathbf{q})\frac{\hbar}{2m}\ , \tag{A5}$$

which leads to

$$\mathbf{j}(\mathbf{r})=\frac{\hbar}{2m}\nabla n(\mathbf{r})\times\hat{z}$$

and ends our proof.

[1] *The Quantum Hall Effect,* edited by R. E. Prange and S. M. Girvin (Springer-Verlag, New York, 1987).

[2] O. Heinonen, in *Physical Phenomena at High Magnetic Field,* edited by E. Manousakis *et al.* (Addison-Wesley, New York, 1991), p. 112; see also O. Heinonen and P. L. Taylor, Phys. Rev. B **32**, 633 (1985); A. H. MacDonald, T. M. Rice, and W. F. Brinkman, *ibid.* **28**, 3648 (1983).

[3] Ch. Simon *et al.*, Phys. Rev. B **33**, 1190 (1986); B. E. Kane, D. C. Tsui, and G. Weinmann, Phys. Rev. Lett. **59**, 1353 (1987).

[4] Tin-Lun Ho and Joughyun Kahng (unpublished).

[5] L. P. Levy, G. Dolan, J. Dunsmiur, and H. Bouchiat, Phys. Rev. Lett. **64**, 2074 (1990); V. Chandrashekhar *et al.*, *ibid.* **67**, 3578 (1991).

[6] A. H. MacDonald and S. M. Girvin, Phys. Rev. B **38**, 6295 (1988).

[7] G. Vignale and M. Rasolt, Phys. Rev. Lett. **59**, 2360 (1987); Phys. Rev. B **37**, 10 685 (1988); M. Rasolt and G. Vignale, Phys. Rev. Lett. **65**, 1498 (1990).

[8] G. Vignale, M. Rasolt, and D. J. Geldart, Adv. Quantum Chem. **21**, 235 (1990).

[9] R. W. Danz and M. L. Glasser, Phys. Rev. B **4**, 94 (1971).

[10] P. Skudlarski and G. Vignale (unpublished).

[11] P. Streda, Solid State Phys. **15**, L717 (1982); **15**, L1299 (1982).

[12] For a current-density-functional treatment of the surface structure of electron-hole droplets in high magnetic field, see G. Vignale, P. Skudlarski, and M. Rasolt, Phys. Rev. B **45**, 8494 (1992).

[13] P. Noziéres, *The Theory of Interacting Fermi Systems* (Benjamin, New York, 1964).