Density-functional theory of two-dimensional electron gas in a magnetic field

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An explicit form for the density matrix of a two-dimensional electron gas in a transverse magnetic field is obtained as a function of the Fermi energy and the field strength. The high- and low-field limits of this generalized expression lead to known results derived earlier. Expressions for the kinetic and exchange energies are derived from the density matrix and are recast as density functionals in terms of the density and the current density as basic variables. The scheme for a density-functional calculation using these energy functionals is outlined.

Two-dimensional (2D) electron gas (i.e., a system of electrons confined to a plane) subjected to a transverse magnetic field has been of interest[1] since the early days of quantum mechanics and is associated with a number of interesting consequences[2] of quantum origin. One such important example that was predicted long ago by Landau[3] and has played a major role ever since is the de Haas–van Alphen (dHvA) effect,[4] which is concerned with the oscillation in the magnetic moment with increasing magnetic field. Recent experimental realization of a 2D electron gas at the semiconductor-oxide interface of a Si MOSFET and the discovery of newer phenomena such as the quantum Hall effect[5,6] (QHE) has provided renewed impetus to the study of this system.

The present work is concerned with the formulation of a density-functional theory[7–9] (DFT) for the 2D electron gas in a magnetic field using the single-particle density quantities as basic variables. After the recent works have established[10,11] that electrons in magnetic field are amenable to a density based description, the crux of the problem is to have explicit expressions for the energy density functionals in terms of the electron density and the current density. In what follows, the density matrix is first evaluated using the states of noninteracting electrons in a uniform perpendicular magnetic field. We thereby obtain explicit expressions of the kinetic and the exchange energy functionals in terms of the Fermi energy and the field strength, which can be evaluated using the density and current density. These energy density functionals are valid also for inhomogeneous systems within the local-density approximation. Oscillations, characteristic of the dHvA effect, are shown to be inherent in the energy density functionals.

Consider an electron of charge e and mass m in a uniform magnetic field $\mathbf{B}$. Assuming the z axis to indicate the field direction and the xy plane the plane of confinement of the motion of the electron, the Hamiltonian can be written as

$$\hat{H}=(1/2m)[\hat{p}_x+(e/c)By]^2+\hat{p}_y^{\,2}/2m \ , \tag{1}$$

using the Landau gauge[3] for the vector potential, i.e., $\mathbf{A}=(-By,0,0)$. The corresponding wave function is given by

$$\psi_{n,p_x}=\exp(ip_x x/\hbar)\phi_n(y-y_0) \ ; \tag{2}$$

$$\phi_n(y-y_0)=C_n\exp[-(\beta/2)(y-y_0)^2] \times H_n(\beta^{1/2}(y-y_0)) \ , \tag{3}$$

where

$$C_n=[(\beta/\pi)^{1/2}/(2^n n!)]^{1/2}, \quad \beta=m\omega/\hbar \ , \quad \omega=eB/mc, \quad y_0=-(cp_x)/(eB) \ , \tag{4}$$

and the energy eigenvalues are

$$\varepsilon_n=(n+1/2)\hbar\omega \ . \tag{5}$$

If the motion is confined to an area L_xL_y, the values of y_0 and p_x are restricted by

$$-L_y/2\le y_0\le L_y/2, \quad -p_x^F\le p_x\le p_x^F \ , \quad p_x^F=m\omega L_y/2 \ , \tag{6}$$

and the degeneracy of each Landau level is given by

$$g_n=L_xL_y m\omega/(2\pi\hbar) \ . \tag{7}$$

If there are N electrons and the Fermi energy ε_F corresponds to the (n_F-1)th energy level, the (spin-averaged) density ρ and the first-order density matrix $\rho(\mathbf{r};\mathbf{r}')$ are given by

$$\rho=(N/L_xL_y)=[m\omega/(\pi\hbar)]n_F =[m/(\pi\hbar^2)](\varepsilon_F+\hbar\omega/2) \ , \tag{8}$$

$$\rho(\mathbf{r};\mathbf{r}')=(2/L_x)\sum_{p_x}\sum_{n}\exp[i(p_x/\hbar)(x-x')] \times\phi_n(y-y_0)\phi_n^*(y'-y_0) \ . \tag{9}$$

Now, using the recurrence relation for the harmonic-oscillator wave functions, one can obtain the simple summation formula

$$2^{1/2}(q-q')\sum_{n=0}^{n_F-1}\phi_n(q)\phi_n^*(q') = n_F^{1/2}[\phi_{n_F}(q)\phi_{n_F-1}^*(q')-\phi_{n_F-1}(q)\phi_{n_F}^*(q')] \ . \quad (10)$$

Substituting Eq. (10) into Eq. (9) and replacing the summation by integration, the density matrix can be written as

$$\rho(\mathbf{r};\mathbf{r}')=(1/\pi\hbar)\int_{-p_x^F}^{p_x^F}dp_x\exp[i(p_x/\hbar)(x-x')] \times(n_F/2)^{1/2}[1/(q-q')] \times[\phi_{n_F}(q)\phi_{n_F-1}^*(q') -\phi_{n_F-1}(q)\phi_{n_F}^*(q')] \ , \quad (11)$$

where q and q' denote $\beta^{1/2}(y-y_0)$ and $\beta^{1/2}(y'-y_0)$, respectively. Considering now the area (L_xL_y) to be large corresponding to a large N (but finite density), one can replace p_x^F, appearing in the limits of integration in Eq. (11), by infinity. Using standard integration tables[12] and after some straightforward algebra, one obtains the simplified expression

$$\rho(\mathbf{r};\mathbf{r}')=(\beta/\pi)\exp[-(\beta/4)|\mathbf{r}-\mathbf{r}'|^2] \times L_{n_F-1}^1((\beta/2)|\mathbf{r}-\mathbf{r}'|^2) \times\exp[-i(\beta/2)(x-x')(y+y')] \ , \quad (12)$$

where $L_n^1(x)$ denotes the associated Laguerre polynomial. The density matrix is, however, gauge dependent and for the choice of the symmetric gauge, i.e., $\mathbf{A}=(-By/2,Bx/2,0)$, Eq. (12), on gauge transformation, leads to the expression

$$\rho(\mathbf{r};\mathbf{r}')=\rho(z;z')=(\beta/\pi)\exp[-(\beta/4)|z-z'|^2] \times L_{n_F-1}^1((\beta/2)|z-z'|^2) \times\exp[-(\beta/4)(z^*z'-zz'^*)] \ , \quad (13)$$

with $z=x+iy$. Equations (12) and (13) express the first-order density matrix of a 2D electron gas (noninteracting) in a transverse magnetic field and when evaluated at $\mathbf{r}=\mathbf{r}'$, yield the density expression of Eq. (8). The special cases of this general expression are as follows. For large magnetic field, only the lowest Landau level is occupied and the density matrix of Eq. (13) simplifies to

$$\rho(\mathbf{r};\mathbf{r}')|_{\omega\to\infty}=(\beta/\pi)\exp[-(\beta/4)|z-z'|^2] \times\exp[-(\beta/4)(z^*z'-zz'^*)] \ , \quad (14)$$

which has recently been obtained by MacDonald and Girvin.[13] For very small field, however, n_F would be large and one can employ the asymptotic limit of the Laguerre polynomial.[14] The zero magnetic field limit of the density matrix is thus given by

$$\rho(\mathbf{r};\mathbf{r}')|_{\omega\to 0}=(1/\pi)|\mathbf{r}-\mathbf{r}'|^{-1}k_FJ_1(k_F|\mathbf{r}-\mathbf{r}'|) \ , \quad (15)$$

with $k_F=(2m\varepsilon_F/\hbar^2)^{1/2}$, and is identical to the density matrix of a free-electron gas in two dimensions. Using the density matrix of Eq. (12) and the expression

$$\varepsilon_{\text{kin}}=\left\{\left[\frac{1}{2m}\right]\left[-i\hbar\left[\frac{\partial}{\partial x}\right]+\left[\frac{e}{c}\right]By\right]^2 -\left[\frac{\hbar^2}{2m}\right]\left[\frac{\partial^2}{\partial y^2}\right]\right\}\rho(\mathbf{r};\mathbf{r}')\Big|_{r=r'} \ , \quad (16)$$

one obtains the kinetic energy density

$$\varepsilon_{\text{kin}}=(1/\pi)(\hbar^2/2m)\beta^2n_F^2 \ , \quad (17)$$

which can also be arrived at by directly summing over the energy levels.

The exchange energy density can now be evaluated from the density matrix using the relation

$$\varepsilon_x=-(e^2/4)\int d\mathbf{r}'|\rho(\mathbf{r};\mathbf{r}')|^2/|\mathbf{r}-\mathbf{r}'| \ . \quad (18)$$

Substituting Eq. (12) into Eq. (18) and using expansion of $(L_n^1)^2$ in terms of the Laguerre polynomials $\{L_k^2\}$ and standard integrals,[12] one obtains the result

$$\varepsilon_x=-(e^2/\pi)(\beta/2)^{3/2}n_F\sum_{k=0}^{n_F-1}\{\Gamma(n_F+k+1)\Gamma(2k+\tfrac{1}{2})/[\Gamma(n_F-k)\Gamma(2k+2)\Gamma(k+2)\Gamma(k+1)]\} \times F(-(n_F-k-1),(2k+\tfrac{1}{2});(2k+2);2) \ . \quad (19)$$

Here, the hypergeometric series $F(\alpha,\beta;\gamma;z)$ reduces to a polynomial since α is a negative integer.

We now consider the limiting cases for the energy densities at high and low magnetic fields. In the high-field limit, only the lowest level is occupied and the kinetic and exchange energy densities are given by

$$\varepsilon_{\text{kin}}|_{\omega\to\infty}=(1/2\pi)m\omega^2 \ , \qquad \varepsilon_x|_{\omega\to\infty}=-(e^2/2)(\beta^3/2\pi)^{1/2} \ . \quad (20)$$

At zero magnetic field, Eq. (15) is obeyed and the energy densities reduce to the 2D free-electron-gas results

$$\varepsilon_{\text{kin}}|_{\omega\to 0}=(1/4\pi)(\hbar^2/2m)k_F^4 \qquad \varepsilon_x|_{\omega\to 0}=-(\tfrac{2}{3})e^2(1/\pi^2)k_F^3 \ . \quad (21)$$

At intermediate field strengths, however, it would be of interest to study the behavior of the energy density quantities as the field strength is varied. In Fig. 1, the kinetic and exchange energy densities, evaluated using the general expressions given by Eqs. (17) and (19), respectively, are plotted against the field strength. [Note that n_F is the

integer part of $[\varepsilon_F/\hbar\omega+1).]$ The abcissa is $\varepsilon_F/\hbar\omega$ and the ordinate chosen is $\bar{\varepsilon}(\omega)/\bar{\varepsilon}(0)$, which denotes the mean-energy density per electron ($\bar{\varepsilon}=\varepsilon/\rho$) at finite ω relative to the free-electron-gas result ($\omega=0$). The oscillations are characteristic of the dHvA-type effect; however, here closed shell has been assumed in obtaining the expressions and hence the interpretation is somewhat different.

Equations (8), (17), and (19) express the density, kinetic energy density, and the exchange energy density, respectively, in terms of the parameters n_F and ω. Another quantity of importance is the current density j defined as

$$\mathbf{j}=\mathbf{j}_p+\mathbf{j}_d,\quad \mathbf{j}_p=(\hbar/m)\mathrm{Im}[\nabla\rho(\mathbf{r},\mathbf{r}')|_{r=r'}]\ ,$$
$$\mathbf{j}_d=(e/mc)\mathbf{A}\rho\ , \tag{22}$$

where $\mathbf{j}_p$ and $\mathbf{j}_d$ denote, respectively, the paramagnetic and diamagnetic contributions. In the present case of uniform magnetic field, one has the relations

$$\nabla\times\mathbf{j}_p=-\nabla\times\mathbf{j}_d=-\omega\rho,\quad \omega=-\nabla\times(\mathbf{j}_p/\rho)\ . \tag{23}$$

Using Eqs. (8) and (23), one can express n_F (or ε_F) and ω in terms of the density variables ρ and $\mathbf{j}_p$. The quantity $\nabla\times(\mathbf{j}_p/\rho)$ has appeared earlier in the recent work of Vignale and Rasolt;[10] but its significance as the cyclotron frequency ω is now evident from Eq. (23). One thus obtains the kinetic energy density functional

$$\varepsilon_{\mathrm{kin}}=(\hbar^2/2m)\pi\rho^2\ , \tag{24}$$

which is identical to that of a 2D free-electron gas [see Eq. (21) with $k_f=(2\pi\rho)^{1/2}$] but is determined here by a density that depends on the magnetic field.

The exchange energy can be calculated using Eq. (19), by substituting n_F obtained by retaining the integer part of its magnitude evaluated from densities, with a minimum value of unity. Alternatively, one can replace the sum in Eq. (19) by an integral using the Poisson summation formula (Euler-McLaurin formula)[15] given by

$$\sum_{k=0}^{n_F} f(k)=\int_0^{n_F} f(x)dx+2\sum_{s=1}^{\infty}\int_0^{n_F} f(x)\cos(2\pi sx)dx\ , \tag{25}$$

where $f(k)$ is the function to be summed over k.

While the functionals derived here are exact for a homogeneous electron gas in a uniform magnetic field, they can be used also for inhomogeneous electron systems within the local-density approximation, which assumes the validity of these expressions locally and the actual kinetic and exchange energies are to be evaluated by integrating the energy densities after replacing ρ and j by actual position dependent $\rho(\mathbf{r})$ and $\mathbf{j}(\mathbf{r})$ at the point $\mathbf{r}$. This is in the spirit of the Thomas-Fermi Dirac theory where one obtains the energy density functionals by considering plane waves corresponding to a homogeneous electron gas at constant scalar potential. The present results, however, correspond to a constant scalar potential and a uniform magnetic field. For an actual many-electron system (2D) characterized by a scalar potential $v(\mathbf{r})$ and a vector potential $\mathbf{A}(\mathbf{r})$, the net energy density

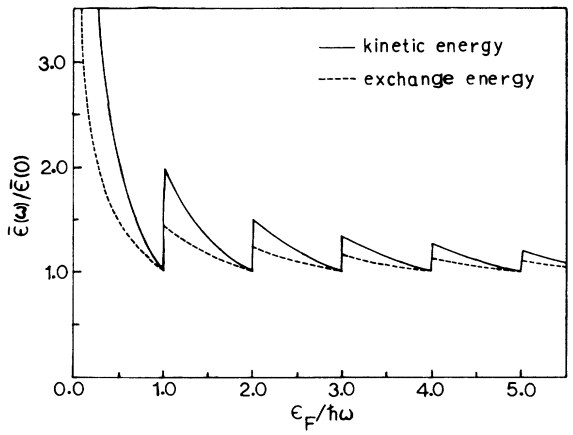

FIG. 1. Magnetic field dependence of the mean kinetic energy and mean exchange energy of a 2D electron gas relative to the free-electron-gas results (see text).

functional is given by

$$E[\rho,\mathbf{j}]=\int d\mathbf{r}\,v(\mathbf{r})\rho(\mathbf{r})+(e/c)\int d\mathbf{r}\,\mathbf{A}(\mathbf{r})\cdot\mathbf{j}(\mathbf{r})$$
$$-(e^2/2mc^2)\int d\mathbf{r}\,\mathbf{A}^2(\mathbf{r})\rho(\mathbf{r})+\int d\mathbf{r}\,\varepsilon_{\mathrm{kin}}(\mathbf{r})$$
$$+U_{\mathrm{int}}[\rho,\mathbf{j}]+\int d\mathbf{r}\,\varepsilon_x(\mathbf{r})\ , \tag{26}$$

which consists of a potential-dependent (the first three terms) and a universal functional part (the last three terms, viz., the kinetic, exchange, and the internal Coulomb energy contributions), and assumes a minimum value for correct ρ and j. The resulting Euler equations $(\delta E/\delta\rho)=\mu$ and $(\delta E/\delta\mathbf{j})=0$, where μ is the Lagrange multiplier for the normalization of density, provide a scheme for the calculation of the density and current density. The exchange energy expression can, however, be used in a Kohn-Sham-type calculation as well.

For the time-dependent case, the expressions for the density functionals can be evaluated using time-dependent densities as variables. The extension to spin polarized and finite temperature cases is also straightforward. The Coulomb correlation energy, which has not been discussed here, is also of interest.

In conclusion, we emphasize that the expression for the density matrix derived here is general and exact. It yields the lowest-Landau-level result of MacDonald and Girvin[13] in the strong-field limit and the free-electron result in the zero-field limit. The kinetic and exchange energy densities are obtained here in terms of the Fermi energy ε_F and the field strength parameter ω. Their evaluation using the density quantities has also been outlined. The present work thus provides the energy functionals to be used in a density functional calculation involving magnetic fields. In view of recent interest in DFT for 2D systems[13,16] involving magnetic fields,[10,11] there is scope of wide applicability of these results.

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