Local-density approximation to the energy density functionals in a magnetic field

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For an electron gas in a uniform magnetic field, explicit expressions of the electron density, current density, and the density matrix are derived as functions of the Fermi energy and the field strength, using plane waves and the Landau energy levels. The local-density approximations for the kinetic and the exchange energy functionals for an inhomogeneous many-electron system are thereby suggested using the density quantities as basic variables. A practical scheme for the density-functional calculation involving the magnetic field in the spirit of Thomas-Fermi-Dirac theory is outlined.

I. INTRODUCTION

Density-functional theory[1-4] (DFT) is well established as an important tool for the study of static as well as dynamic properties of many-electron systems. A density-functional description in presence of a magnetic field has however formally been developed for both static[5,6] and time-dependent[7-9] situations only recently. This formulation is strongly motivated by a desire to obtain density-based approaches to several phenomena of current interest, viz., the quantum Hall effect,[10] high-temperature superconductivity,[11] etc.

The proof that the scalar and vector potentials characterizing a many-electron system are uniquely determined by the single-particle electron density and the current density, has established that problems involving magnetic fields are amenable to density based descriptions. The crux of the problem now is to have explicit expressions for the energy density functionals in terms of the electron density and the current density.

While in the Kohn-Sham-like single-particle prescription, only the exchange-correlation functional is unknown, in a statistical model in the spirit of the Thomas-Fermi-Dirac (TFD) theory,[4] the additional unknown quantity is the kinetic energy functional. The present work aims at deriving expressions for the kinetic and the exchange energy functionals for a many-electron system in presence of electric and magnetic fields.

As has been proved elsewhere,[7] these functionals are universal and are expressible in terms of the density quantities alone. In absence of this formal proof, in the earlier works on the statistical theory in magnetic fields,[12-17] however, the external magnetic field strength has appeared explicitly in the expressions and also only the electron density has been employed[17] to define the functionals. Some of the results are restricted to strong magnetic field regime alone. In this work, we proceed to derive explicit schemes for obtaining the energy functionals (whose existence is already assured) from the single-particle density quantities alone. We resort to a local density approximation (LDA) in the spirit of TFD theory. This amounts to using a locally homogeneous approximation where for systems involving scalar potential alone, one derives the functional forms by using plane waves, i.e., solutions for electrons moving in a constant potential or zero electric field. In LDA, one evaluates the energy quantities from this functional form using the position-dependent density $\rho(\mathbf{r})$. The LDA result for magnetic field should follow analogously. The solutions for a constant vector potential are again plane waves; however, we assume the electrons to move in a very weak uniform magnetic field and employ the corresponding energy levels for filling the electrons in the momentum space up to the Fermi level. The zeroth-order wave function (i.e., plane waves) is still used to evaluate the density matrix and the modified energy levels only incorporate the correct symmetry properties in presence of magnetic field.

In what follows, we derive expressions for the single-particle density matrix in Sec. II and the corresponding energy functionals in Sec. III. Discussion on the gauge invariance and the density-functional formalisms is presented in Sec. IV. Illustrative numerical results are discussed in Sec. V and finally we offer a few concluding remarks in Sec. VI.

II. DENSITY MATRIX OF A HOMOGENEOUS ELECTRON GAS IN A UNIFORM MAGNETIC FIELD

Consider a system of N electrons subjected to a uniform magnetic field $\mathbf{B}$ $(=\nabla\times\mathbf{A})$ in the z direction, for which the energy levels are given by

$$\varepsilon_{n,k_z}=(n+\tfrac{1}{2})\hbar\omega+(\hbar^2/2m)k_z^2=\varepsilon_\perp+\varepsilon_\parallel\ , \tag{1}$$

where $\omega=|eB/mc|$. The discrete quantum number n $(=0,1,2,\ldots)$ quantizes the energy in the perpendicular xy plane whereas k_z characterizes the continuous energy component from the motion in the z direction.

Electrons occupy the various energy states up to the Fermi energy ε_F. The values of k_z range from $-k_z^F$ to

k_z^F, where k_z^F depends on the value of n and is given by

$$k_z^F(n)=\{(2m/\hbar^2)[\varepsilon_F-(n+\tfrac{1}{2})\hbar\omega]\}^{1/2} . \tag{2}$$

If the electron is restricted to a parallelopiped of volume $V(=L_xL_yL_z)$, the degeneracy of the Landau levels is independent of n and is given by

$$g_n=(L_xL_y/2\pi)(m\omega/\hbar) . \tag{3}$$

If the electrons occupy the levels up to $n=n_F$ with the corresponding k_z levels filled, one has the result

$$N=2\sum_{n=0}^{n_F}(L_xL_y/2\pi)(m\omega/\hbar)(L_z/2\pi)2k_z^F(n)$$
$$=2(V/4\pi^2)(m\omega/\hbar)2(2m/\hbar^2)^{1/2}\times\sum_{n=0}^{n_F}[\varepsilon_F-(n+\tfrac{1}{2})\hbar\omega]^{1/2} . \tag{4}$$

The summation in Eq. (4) can be evaluated using the Poisson summation formula[18,19] (Euler-McLaurin formula) given by

$$\sum_{n=0}^{n_F}f(n)=\int_0^{n_F}f(x)dx+2\sum_{s=1}^{\infty}\int_0^{n_F}f(x)\cos(2\pi sx)dx , \tag{5}$$

and the result leads to the expression for density[20]

$$\rho=(N/V)=[(2m\varepsilon_F)^{3/2}/(3\pi^2\hbar^3)]\{1+(3/8\pi)2^{1/2}(\hbar\omega/\varepsilon_F)^{3/2}\sum_{s=1}^{\infty}[(-1)^{(s+1)}/s^{3/2}]\cos[(2\pi s\varepsilon_F/\hbar\omega)+\pi/4)\} . \tag{6}$$

The same expression also follows through the diagonal element of the first-order density matrix which we now proceed to calculate using the plane waves. This is justified since the field considered is small and we employ the zeroth-order orbitals with correct energy levels for occupation. The density matrix is then given by

$$\rho(\mathbf{r};\mathbf{r}')=(2/V)\sum_{\mathbf{k}}\exp[i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')] , \tag{7}$$

where the sum extends up to the Fermi level and the degeneracy of the levels are taken into account.

Since the Landau levels of Eq. (1) indicate that the momentum space would consist of coaxial cylinders whose heights correspond to k_z^F of Eq. (2) and the radii correspond to the energy $(n+\frac{1}{2})\hbar\omega$, it would be natural to switch over to the cylindrical coordinates (R,φ,z). Equation (7) can thus be written as

$$\rho(\mathbf{r};\mathbf{r}')=(2/V)\sum_{\mathbf{k}_R}\sum_{k_z}\exp[i\mathbf{k}_R\cdot(\mathbf{R}-\mathbf{R}')]\exp[ik_z(z-z')] , \tag{8}$$

which simplifies to

$$\rho(\mathbf{r};\mathbf{r}')=(2/V)(L_z/2\pi)\sum_{k_R}J_0(k_R|\mathbf{R}-\mathbf{R}'|)\times 2\sin[k_z^F(n)|z-z'|]/|z-z'| , \tag{9}$$

after carrying out the integration over k_z and φ, the angle between $\mathbf{k}_R$ and $\mathbf{R}-\mathbf{R}'$. Since k_R is defined by

$$(\hbar^2/2m)k_R^2=(n+\tfrac{1}{2})\hbar\omega , \tag{10}$$

characterizing the energy arising from the motion in the xy plane, quantized by the quantum number n, the sum of Eq. (9) can be replaced by summation over n with appropriate degeneracy factor. Equation (9) can thus be written as

$$\rho(\mathbf{r};\mathbf{r}')=(2/V)(L_z/2\pi)(L_xL_ym\omega/2\pi\hbar)2\sum_{n=0}^{n_F}J_0(k_R|\mathbf{R}-\mathbf{R}'|)\sin[k_z^F(n)|z-z'|]/|z-z'|$$
$$=(m\omega/\pi^2\hbar)\sum_{n=0}^{n_F}J_0(k_R|\mathbf{R}-\mathbf{R}'|)\sin(k_z^F(n)|z-z'|)/|z-z'| , \tag{11}$$

where k_R and k_z^F are functions of n given by Eqs. (10) and (2), respectively.

Applying the Poisson summation formula (5) to Eq. (11), one obtains the density matrix

$$\rho(\mathbf{r};\mathbf{r}')=\rho^0(\mathbf{r};\mathbf{r}')+\Delta\rho(\mathbf{r};\mathbf{r}') . \tag{12a}$$

where

$$\rho^0(\mathbf{r};\mathbf{r}')=(m\omega/\pi^2\hbar)\int_0^{n_F}dn[\sin(k_z^F|z-z'|)/|z-z'|]J_0(k_R|\mathbf{R}-\mathbf{R}'|) \tag{12b}$$

and

$$\Delta\rho(\mathbf{r};\mathbf{r}')=(m\omega/\pi^2\hbar)2\sum_{s=1}^{\infty}\int_0^{n_F} dn\,\cos(2\pi sn)[\sin(k_z^F|z-z'|)/|z-z'|]J_0(k_R|\mathbf{R}-\mathbf{R}'|)\ , \tag{12c}$$

with the n-dependent k_z^F and k_R given by Eqs. (2) and (10), respectively. The integration in Eq. (12b) is straightforward and leads to the result

$$\rho^0(\mathbf{r};\mathbf{r}')=(1/\pi^2)k_F^3[(\sin x - x\cos x)/x^3]\ , \tag{13}$$

where

$$k_F=[(2m/\hbar^2)(n_F+\tfrac{1}{2})\hbar\omega]^{1/2}=[(2m/\hbar^2)\varepsilon_F]^{1/2}\ , \tag{14}$$

and

$$x=k_F|\mathbf{r}-\mathbf{r}'|\ . \tag{15}$$

Equation (12c) after some algebraic manipulations leads to the result

$$\Delta\rho(\mathbf{r};\mathbf{r}')=(1/\pi^{7/2})(m\omega/\hbar)^{3/2}J_0(k_F|\mathbf{R}-\mathbf{R}'|)\times\sum_{k=0}^{\infty}A_k(z-z')^{2k}\ , \tag{16}$$

where

$$A_k=[\Gamma(k+\tfrac{3}{2})/(2k+1)!](-1)^k(m\omega/\pi\hbar)^k\times\sum_{s=1}^{\infty}[(-1)^{(s+1)}/s^{k+3/2}]\times\cos[(2\pi s\varepsilon_F/\hbar\omega)+(1-2k)\pi/4]\ . \tag{17}$$

The diagonal elements from Eqs. (13) and (16) clearly correspond to the density given by Eq. (6).

Making use of the asymptotic (large-ε_F) expansion of the Bessel functions, and after some algebra, Eq. (16) can be further simplified to obtain the closed form:

$$\Delta\rho(\mathbf{r};\mathbf{r}')=(2\pi^3)^{-1}(m\omega/\hbar)^{3/2}J_0[(2m\varepsilon_F/\hbar^2)^{1/2}|\mathbf{R}-\mathbf{R}'|]\sum_{s=1}^{\infty}[(-1)^{(s+1)}/s^{3/2}][1+m\omega^2(z-z')^2/(4\pi^2s^2\varepsilon_F)]^{-3/4}\times\cos\{\pi/4+(2\pi s\varepsilon_F/\hbar\omega)[1+m\omega^2(z-z')^2/(4\pi^2s^2\varepsilon_F)]^{1/2}\}\ . \tag{18}$$

Equations (12a), (13), and (18) together define the single-particle reduced density matrix in terms of the Fermi energy ε_F and the cyclotron frequency ω, while the corresponding expression for density is given by Eq. (6) and can easily be recovered by substituting $|\mathbf{R}-\mathbf{R}'|=0$ and $|z-z'|=0$ in these equations.

III. KINETIC AND EXCHANGE ENERGY DENSITIES IN PRESENCE OF MAGNETIC FIELD

We define the kinetic energy density as

$$\varepsilon_{\rm kin}=-(\hbar^2/2m)\nabla^2\rho(\mathbf{r};\mathbf{r}')|_{r=r'}\ , \tag{19a}$$

which can easily be calculated from the density matrix. After some algebra, the final expression for the kinetic energy is given by

$$\begin{aligned}\varepsilon_{\rm kin}&=(\hbar^2/m)(1/10\pi^2)k_F^5\\&\quad+(\hbar^2/2m)(m\omega/\hbar)^{3/2}(1/2\pi^3)\{k_F^2\sum_{s=1}^{\infty}[(-1)^{(s+1)}/s^{3/2}]\cos[(2\pi s\varepsilon_F/\hbar\omega)+\pi/4]\\&\qquad+(1/2\pi)(m\omega/\hbar)\sum_{s=1}^{\infty}[(-1)^s/s^{5/2}]\cos[(2\pi s\varepsilon_F/\hbar\omega)-\pi/4]\}\\&=(\hbar^2/m)(1/10\pi^2)k_F^5\{1+(5/2\pi)(2\varepsilon_F/\hbar\omega)^{-3/2}\sum_{s=1}^{\infty}[(-1)^{(s+1)}/s^{3/2}]\cos[(2\pi s\varepsilon_F/\hbar\omega)+\pi/4]\\&\qquad+(5/4\pi^2)(2\varepsilon_F/\hbar\omega)^{-5/2}\sum_{s=1}^{\infty}[(-1)^s/s^{5/2}]\cos[(2\pi s\varepsilon_F/\hbar\omega)-\pi/4]\}\ .\end{aligned} \tag{19b}$$

The other energy density functional of interest is the exchange energy which can now be evaluated from the definition

$$\varepsilon_x=-(e^2/4)\int d\mathbf{r}'|\rho(\mathbf{r};\mathbf{r}')|^2/|\mathbf{r}-\mathbf{r}'|\ , \tag{20}$$

and the density matrix of Eqs. (12), (13), and (18). The exchange energy density can be written as

$$\varepsilon_x=\varepsilon_x^0+\varepsilon_x^{(1)}+\varepsilon_x^{(2)}\ , \tag{21a}$$

where

$$\varepsilon_x^0 = -(e^2/4)\int d\mathbf{r}'|\rho^0(\mathbf{r};\mathbf{r}')|^2/|\mathbf{r}-\mathbf{r}'| \ , \tag{21b}$$

$$\varepsilon_x^{(1)} = -(e^2/2)\int d\mathbf{r}'\rho^0(\mathbf{r};\mathbf{r}')\Delta\rho(\mathbf{r};\mathbf{r}')/|\mathbf{r}-\mathbf{r}'| \ , \tag{21c}$$

$$\varepsilon_x^{(2)} = -(e^2/4)\int d\mathbf{r}'|\Delta\rho\mathbf{r};\mathbf{r}')|^2/|\mathbf{r}-\mathbf{r}'| \ . \tag{21d}$$

Using Eq. (14) for $\rho^0(\mathbf{r};\mathbf{r}')$, one obtains ε_x^0 as the conventional Dirac exchange expression

$$\varepsilon_x^0 = -(e^2/4\pi^3)k_F^4 \ . \tag{22}$$

The evaluation of $\varepsilon_x^{(1)}$ is also straightforward. Using the expression for $\Delta\rho(\mathbf{r};\mathbf{r}')$ given by Eq. (16), one obtains after performing the angular integration the result

$$\varepsilon_x^{(1)} = -(e^2)\pi^{-4}(m\omega/\hbar)^{3/2}k_F \sum_{k=0}^{\infty}[\Gamma(k+\tfrac{3}{2})\Gamma(k+\tfrac{1}{2})/\Gamma(2k+2)](-1)^k(m\omega/\pi\hbar)^k(2^k/k_F^{2k})$$
$$\times \sum_{s=1}^{\infty}[(-1)^{(s+1)}/s^{k+3/2}]\cos[(2\pi s\varepsilon_F/\hbar\omega)+\pi/4-k\pi/2]$$
$$\times \int_0^{\infty} dx\, x^{k-1}J_{k+1/2}(x)J_{3/2}(x) \ . \tag{23}$$

From the properties of Γ functions and Bessel functions, one can obtain a result

$$\sum_{k=0}^{\infty}[\Gamma(k+3/2)\Gamma(k+1/2)/\Gamma(2k+2)](-1)^k y^k J_{k+1/2}(x)$$
$$= (\pi^{1/2}/2)\int_0^{\infty} dt\, t^{-1/2}\exp(-t)J_{1/2}[x(1+yt/2x)^{1/2}]/(1+yt/2x)^{1/4} \ . \tag{24}$$

Using Eq. (24) and Eq. (23) and carrying out the integration over x, one obtains

$$\varepsilon_x^{(1)} = \varepsilon_x^0(4/3\pi)(2\varepsilon_F/\hbar\omega)^{-1}\sum_{s=1}^{\infty}[(-1)^s/s]\int_0^{\infty} dt\, t^{-1/2}(1+t)^{-1}\sin[(2\pi s\varepsilon_F/\hbar\omega)(1-t)]\,{}_2F_1(1,\tfrac{1}{2};\tfrac{5}{2};1/(1+t)) \ , \tag{25}$$

where the hypergeometric series ${}_2F_1(1,\frac{1}{2};\frac{5}{2};1/(1+t))$ can be evaluated using the expression

$${}_2F_1(1,\tfrac{1}{2};\tfrac{5}{2};z) = 3\sum_{n=0}^{\infty}(2n+1)^{-1}(3n+1)^{-1}z^n \tag{26}$$

with ${}_2F_1(1,\frac{1}{2};\frac{5}{2};1)=\frac{3}{2}$. The expression of $\varepsilon_x^{(2)}$ given by Eq. (21d) can also be simplified, but since ω considered here is small, we retain terms up to first order and neglect $\varepsilon_x^{(2)}$ for obtaining ε_x.

IV. ENERGY DENSITY FUNCTIONALS AND THE GAUGE TRANSFORMATIONS

While Eq. (6) expresses the electron density as a function of ε_F and ω, another quantity of importance in systems involving magnetic field is the current density $\mathbf{j}$ defined as

$$\mathbf{j} = \mathbf{j}_p + \mathbf{j}_d \ , \tag{27a}$$

where the paramagnetic current $\mathbf{j}_p$ and the diamagnetic contribution $\mathbf{j}_d$ are given, respectively, by

$$\mathbf{j}_p = (\hbar/m)\mathrm{Im}[\nabla\rho(\mathbf{r};\mathbf{r}')|_{r=r'}] \tag{27b}$$

$$\mathbf{j}_d = (e/mc)\mathbf{A}\rho \ . \tag{27c}$$

In order to obtain the energy quantities as density functionals, the parameters ε_F and ω are to be expressed in terms of the density-related quantities.

It is, however, important to note that the expressions for $\rho(\mathbf{r};\mathbf{r}')$, $\varepsilon_{\mathrm{kin}}$, and ε_x derived here are exact in the limit $\mathbf{B}\to\mathbf{0}$. The corresponding vector potential, for example, $\mathbf{A}=(-By,0,0)$ within the Landau gauge, also vanishes in the same limit. The density matrix given by Eq. (18) has been obtained for this limit and does not contain $\mathbf{A}$ explicitly. We now discuss the gauge transformation properties of this density matrix under the gauge transformations

$$\mathbf{A}\to\mathbf{A}' = \mathbf{A}+\nabla\lambda(\mathbf{r},t) \ , \tag{28a}$$

$$\phi\to\phi' = \phi-(1/c)(\partial/\partial t)\lambda(\mathbf{r},t) \ , \tag{28b}$$

where ϕ is the scalar potential. The proper gauge transformation of the density matrix is given by

$$\rho(\mathbf{r};\mathbf{r}')\to\rho'(\mathbf{r};\mathbf{r}')$$
$$= \rho(\mathbf{r};\mathbf{r}')\exp\{-(ie/\hbar c)[\lambda(\mathbf{r},t)-\lambda(\mathbf{r}',t)]\} \ , \tag{28c}$$

which demands that the kinetic energy density of Eq. (19) should accordingly transform as

$$\varepsilon_{\mathrm{kin}}\to\varepsilon'_{\mathrm{kin}} = \varepsilon_{\mathrm{kin}}-(e/c)\nabla\lambda\cdot\mathbf{j}_p+(e^2/2mc^2)(\nabla\lambda)^2\rho \ . \tag{29}$$

The exchange energy, however, is gauge invariant and would not change under the transformation (28). This leaves the total energy expression gauge invariant as expected.

For the gauge transformation of the density matrix given by Eq. (28c), the paramagnetic current density also transforms as

$$\mathbf{j}_p\to\mathbf{j}'_p = \mathbf{j}_p-(e/mc)(\nabla\lambda)\rho \ . \tag{30}$$

The net current density $\mathbf{j}$ defined in Eq. (27a) is, however,

gauge invariant and vanishes in the limit of zero magnetic field. The exact current density for an electron gas in a uniform magnetic field vanishes as well. We therefore demand $\mathbf{j}=0$ in Eq. (27) and express ω in terms of the density variables ρ and $\mathbf{j}_p$ by

$$\omega=-\nabla\times(\mathbf{j}_p/\rho)\ , \tag{31}$$

where $\mathbf{j}_p$ is related to $\mathbf{j}$ by $\mathbf{j}_p=\mathbf{j}-(e/mc)\mathbf{A}\rho$ and therefore $\omega=-\nabla\times(\mathbf{j}/\rho)+(e/mc)\mathbf{B}$. Also by inverting Eq. (6), one can obtain ε_F as a function of the density ρ. Equations (19), (22), and (25) that express the kinetic and exchange energy functionals in terms of ε_F and ω, can therefore be evaluated through the density quantities ρ and $\mathbf{j}_p$. The quantity $\nabla\times(\mathbf{j}_p/\rho)$ has appeared earlier in the recent work of Vignale and Rasolt,[5,6] but its significance as the cyclotron frequency ω is now evident from Eq. (31).

Although the functionals obtained here correspond to a homogeneous electron gas in a constant scalar potential and uniform weak magnetic field, they can be used also for an inhomogeneous many-electron system as an approximation. This local-density approximation amounts to assuming 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 $\mathbf{j}$ by actual position dependent $\rho(\mathbf{r})$ and $\mathbf{j}(\mathbf{r})$ at the point $\mathbf{r}$.

For an actual many-electron system characterized by a scalar potential $v(\mathbf{r})$ and a vector potential $\mathbf{A}(\mathbf{r})$, the net energy density functional is given by

$$\begin{aligned}E[\rho,\mathbf{j}]=&\int d\mathbf{r}\, v(\mathbf{r})\rho(\mathbf{r})+(e/c)\int d\mathbf{r}\ \mathbf{A}(\mathbf{r})\cdot\mathbf{j}(\mathbf{r})\\&-(e^2/2mc^2)\int d\mathbf{r}\ \mathbf{A}^2(\mathbf{r})\rho(\mathbf{r})\\&+\int d\mathbf{r}\,\varepsilon_{\rm kin}(\mathbf{r})+U_{\rm int}[\rho,\mathbf{j}]\int d\mathbf{r}\,\varepsilon_x(\mathbf{r})\ ,\end{aligned} \tag{32}$$

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). Equation (32), as has already been mentioned, can easily be shown to be gauge invariant under the gauge transformation (28) and the corresponding transformation of $\varepsilon_{\rm kin}$ given by Eq. (29). The energy can be minimized with respect to the variations of ρ and $\mathbf{j}$, and the resulting Euler equations would provide a scheme for the calculation of the density and the current density. This defines the Thomas-Fermi-Dirac-type statistical theory in the presence of a magnetic field. The exchange energy density expression can be used in a Kohn-Sham type calculation as well.

V. ILLUSTRATIVE RESULTS AND DISCUSSION

It would be of interest to study the behavior of the density quantities discussed here as the magnetic field strength is varied. In Fig. 1, we have plotted the calculated values of the electron density ρ, the mean kinetic energy per electron $\bar{\varepsilon}_{\rm kin}$ $(=\varepsilon_{\rm kin}/\rho)$, and the mean exchange energy per electron $\bar{\varepsilon}_x$ $(=\varepsilon_x/\rho)$ relative to the corresponding free-electron gas results under zero field.

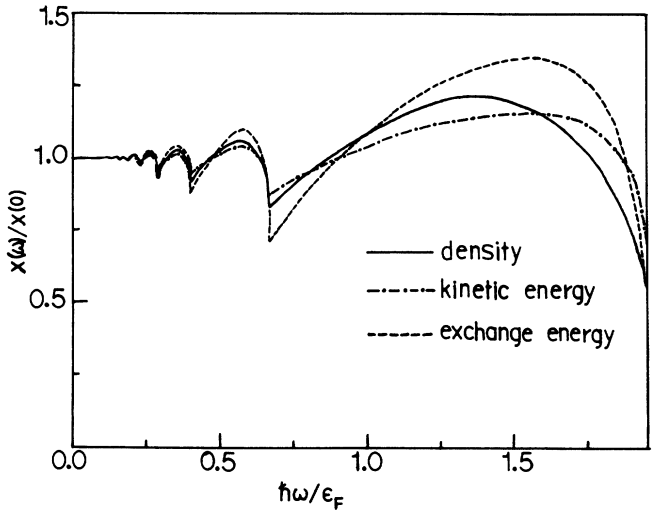

FIG. 1. Magnetic field dependence of the electron density (——), the mean kinetic energy (—·—·—·), and the mean exchange energy (— — —) relative to the corresponding free-electron gas results (see text).

The oscillations are characteristic of the de Haas–van Alphen type effect;[21] however, here closed shell has been assumed in deriving the expressions and therefore the interpretation is somewhat different.

The density ρ as well as the mean energy quantities $\bar{\varepsilon}_{\rm kin}$ and $\bar{\varepsilon}_x$ oscillate around the corresponding field free results and the periodic rise is observed at identical values of the parameter $\hbar\omega/\varepsilon_F$. Another interesting aspect is that both $\bar{\varepsilon}_{\rm kin}$ and $\bar{\varepsilon}_x$ attain the free-electron results at identical values of this parameter. Also, the period as well as the amplitude of the oscillations exhibit an increase with the magnetic field strength. These aspects arise from the field dependence of the magnitude and the degeneracy of the quantized Landau energy levels.

VI. CONCLUDING REMARKS

We have derived here expressions for the density matrix, kinetic, and exchange energies for a system of electrons subjected to a weak uniform magnetic field and the de Haas–van Alphen type oscillations are demonstrated. A density functional scheme in the spirit of Thomas-Fermi-Dirac-type statistical theory for a magnetic field is outlined. The energy functionals are shown to be expressible in terms of ε_F or ρ and the quantity $\omega=-\nabla\times(\mathbf{j}_p/\rho)$. The latter combination has been first introduced by Vignale and Rasolt in their recent work[5,6] and now finds the interpretation of an effective local cyclotron frequency in the density-functional description of an inhomogeneous many-electron system in arbitrary magnetic field. For the case of time-dependent magnetic field, the expressions for the density functionals can be evaluated using time-dependent densities as variables. As has been proved elsewhere,[7,9] the important quantity in such situations for obtaining the energy density functionals is the current density $\mathbf{j}$ (or $\mathbf{j}$ and ρ for convenience).

The present work, for simplicity, is developed using the

spin-averaged densities at zero temperature. The extension to spin polarized as well as finite temperature cases is straightforward. The Coulomb correlation energy which has not been discussed here is also of interest.

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