Exchange and Correlation Effects in the 3D Electron Gas in Strong Magnetic Fields and Application to Graphite*

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The self-consistent theory for obtaining the spin-dependent local-field correction $G_{\pm}(\mathbf{q})$ due to Singwi, Toi, Land, and Sjölander is extended to investigate the exchange and correlation effects in the three-dimensional electron gas in strong magnetic fields. We find that $G_{\pm}(\mathbf{q})$ barely changes with H as long as it is weak enough for the ratio of ℓ, the magnetic length, to r_0, the average interelectron spacing, to be larger than about 0.7. With this information, we calculate the self-energy in a self-consistent way to obtain the electronic structure of graphite in strong magnetic fields. The result obtained is in agreement with experiment.

I. INTRODUCTION

Graphite, a typical layered semimetal, exhibits an interesting electronic phase transition at temperatures T around 1K in magnetic fileds H above 25T applied perpendicular to the layer plane (the z-direction) (Tanuma *et al.* 1981, Iye *et al.* 1982, Iye and Dresselhaus 1985). Due to the smallness of the effective mass m^* in the xy-plane combined with the small carrier concetration n_e, a semi-magnetic quantum limit is realized for H of this order. By 'semi-magnetic quantum limit' we mean that the electrons and holes occupy only the Landau subbands specified by $n = -1$ and 0. To be precise, there are eight relevant Landau subbands due to the small spin-Zeeman splitting and the band degeneracy accounting for the existence of H-K-H and H'-K'-H' edges in the Brillouin zone. Further experiments have been done concerning this phenomenon by increasing H (Ochimizu *et al.* 1992, Yaguchi *et al.* 1993). In particular, the electronic structure has been measured recently by the infrared magneto-spectroscopy with H up to 400T (Miura *et al.* 1997).

In the (semi-)magnetic quantum limit, the electronic polarization function evaluated in the random-phase approximation (RPA) $\Pi_0(\mathbf{q}, \omega)$ has logarithmic divergences at $\omega = 0$ and the values of q_z connecting the Fermi-surface points in the z-direction in momentum space. These divergences may bring about some electronic phase transition. In fact, Yoshioka and Fukuyama (YH 1981) claimed that the experimentally observed phase transition was connected with the formation of charge-density wave (CDW) associated with the instability in the $n = 0$ subband. Sugihara (1984) claimed the occurrence of CDW in the $n = -1$ subband with a different treatment of the screening effect from YH. Takahashi and Takada (1994) attributed the phenomenon to the spin-density wave (SDW) in the $n = 0$ subband by taking account of the spatial separation of carriers in the H-K-H and H'-K'-H' edges in strong magnetic fields.

All those calculations were done in the RPA based on the electronic structure in the one-body approximation (Nakao 1976). However, the RPA is not supposed to be valid in the actual situation. For example, the magnetic length ℓ is 36$\mathring{A}$ at $H = 50$T, while the mean intercarrier distance r_0 is about 30$\mathring{A}$ for $n_e \approx 3 \times 10^{18}\mathrm{cm}^{-3}$, indicating that ℓ is about the same as r_0 and that the ratio ℓ/r_0 may become 0.6 for H around 200T. This is the case similar to the two-dimensional (2D) electron gas in which the fractional quantum Hall effect (FQHE) is observed (Tsui *et al.* 1982). As Laughlin (1983) has shown, the FQHE can be explained only by the consideration of strong correlation.

It may be argued that the present 3D system is fundamentally different from the 2D electron gas in a strong magnetic field due to the absence of complete degeneracy in the kinetic energy, a peculiar feature of the 2D system, but if we estimate the conventional density parameter r_s by the relation $r_0 = r_s a_{\mathrm{B}}^*$ with the effective Bohr radius a_{B}^*, we obtain r_s in the range $4-15$, suggesting a strongly-correlated electronic system which cannot be treated in the RPA. Note that m^* changes with H due to nonparabolicity of the bands. A rough estimate for m^* can be obtained by regarding the Landau-level splitting between $n = -1$ and 0 subbands at the K (or K') point as the cyclotron energy $\omega_c = eH/m^*c$. The splitting is 20meV (61meV) for at $H = 50$T (200T), leading to $m^* = 0.3m_e$ ($0.4m_e$) with m_e the mass of a free electron. There is an ambiguity about the static dielectric constant ϵ_0, depending on how much polarization effects of valence electrons will be included faithfully in the micro-

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scopic Hamiltonian, but it is less than 5. Those values for m^* and ϵ_0 provide an estimate for $a_{\rm B}^*$ in the range $2-8\mathring{A}$.

The ground state of the 3D electron gas without magnetic fields has been a subject of intense interest for more than half a century and by now the virtually exact result for the correlation energy ε_c is known as a function of r_s thanks to the Green's function Monte Carlo (GFMC) calculation of Ceperley and Alder (1980). The result for ε_c, with similar accuracy, together with important information about the effective electron-electron interaction is also obtained by the self-consistent effective-local-potential approach proposed by Singwi, Tosi, Land and Sjölander (STLS 1968). To the authors' knowledge, however, the correlation effect in the 3D electron gas in the presence of a high magnetic field has never been treated seriously. Skudlarski and Vignale (1993) addressed the problem in some detail, but they employed the RPA in the actual calculation of ε_c.

In view of this theoretical situation, we investigate the exchange and correlation effects in the 3D electron gas in a strong magnetic field in Sec. 2 in order to obtain an indispensable information to consider physics in graphite. We point out that the STLS theory can be extended to the system in magnetic fields without any difficulty as regards its concept. By implementing a numerical self-consistent procedure to obtain the static structure factor, we provide the result for ε_c as a function of r_s as well as ℓ/r_0 in the STLS formalism. The local-field correction $G_{\pm}(\mathbf{q})$, a central quantity in the effective-local-potential approach, is also given for both charge (G_+) and spin (G_-) fluctuation channels in comparison with the results at $H=0$. In Sec. 3, we calculate the electronic structure in graphite in strong magnetic fields with the inclusion of many-body self-energy correction in which the effective electron-electron interaction is evaluated with the use of $G_{\pm}(\mathbf{q})$. The results obtained are compared favourably with experiment. A summary and a discussion on the related problems are given in Sec. 4. In this paper, we employ units in which $\hbar=1$.

II. THREE-DIMENSIONAL ELECTRON GAS

A. Formulation

The electron gas is a system consisting of N electrons embedded in a positive-charge background. The electrons interact with one another through the Coulomb interaction. Thus, by using $\psi_\sigma(\mathbf{r})$ the electron field operator of spin σ, we can write the Hamiltonian H as

$$H = H_0 + H_1, \tag{1}$$

with

$$H_0 = \sum_\sigma \int d\mathbf{r}\psi_\sigma^\dagger(\mathbf{r})\left[\frac{1}{2m^*}\Big(\mathbf{p}+\frac{e}{c}\mathbf{A}(\mathbf{r})\Big)^2 + V(\mathbf{r}) + \frac{g^*}{2}\mu_{\rm B}\sigma\cdot\mathbf{H}\right]\psi_\sigma(\mathbf{r}), \tag{2}$$

and

$$H_1 = \frac{1}{2}\sum_{\sigma\sigma'}\int d\mathbf{r}\int d\mathbf{r}'\psi_\sigma^\dagger(\mathbf{r})\psi_{\sigma'}^\dagger(\mathbf{r}')\frac{e^2}{\epsilon_0|\mathbf{r}-\mathbf{r}'|}\psi_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r}), \tag{3}$$

where $\mathbf{A}(\mathbf{r})$ is the vector potential satisfying $\mathbf{H}=\mathrm{rot}\mathbf{A}$, g^* is the effective g-factor characterizing the Zeeman splitting, $\mu_{\rm B}$ is the Bohr magneton and $V(\mathbf{r})$ is the potential accounting for the interaction between an electron and the positive-charge background. We take the volume of the system to be unity.

In an effective-potential approach to the many-electron problem, a basic assumption is that each electron responds to a perturbing potential as if it were a free particle. The many-body aspect is included by the construction of the induced potential $V_{\rm eff}(\mathbf{q})$ which arises from the charges induced by an external disturbance. The RPA amounts to the evaluation of induced charges in the mean-field approximation. The exchange and correlation change the actual effect of the induced charges on the induced potential. A procedure to describe the change is to reduce $V_{\rm eff}(\mathbf{q})$ from the bare Coulomb potential $V_0(\mathbf{q})\equiv 4\pi e^2/\epsilon_0\mathbf{q}^2$ in such a way as

$$V_{\rm eff}^{\sigma\sigma'}(\mathbf{q}) = [1-G_{\sigma\sigma'}(\mathbf{q})]V_0(\mathbf{q}), \tag{4}$$

for the potential of an electron with spin σ with the induced electrons with spin σ'. This is an approximate procedure, but it is physically appealing and it turns out to be very useful in the 3D electron gas without the magnetic field.

A very successful scheme to obtain the local-field correction $G_{\sigma\sigma'}(\mathbf{q})$ was proposed by STLS. In the scheme, we first introduce $\rho_{\mathbf{q}\sigma}$, the density fluctuation operator of spin σ, defined by

$$\rho_{\mathbf{q}\sigma} \equiv \int d\mathbf{r}e^{-i\mathbf{q}\cdot\mathbf{r}}\psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r}). \tag{5}$$

The induced potential can be obtained by considering the restoring-force part in the equation of motion for $\rho_{\mathbf{q}\sigma}$. The part is included in the double commutator $[H_1,[H,\rho_{\mathbf{q}\sigma}]]$. A straightforward calculation gives

$$\begin{aligned}\big[H_1,[H,\rho_{\mathbf{q}\sigma}]\big] &= \sum_{\mathbf{q}'\neq\mathbf{0}}\sum_{\sigma'}V_0(\mathbf{q}')\Big(-\frac{\mathbf{q}'\cdot\mathbf{q}}{m^*}\Big)\rho_{-\mathbf{q}'\sigma'}\rho_{\mathbf{q}+\mathbf{q}'\sigma}\\ &= \frac{4\pi e^2N_\sigma}{\epsilon_0 m^*}\sum_{\sigma'}\Big(\rho_{\mathbf{q}\sigma'}\\ &\quad -\frac{1}{N_\sigma}\sum_{\mathbf{q}'\neq\mathbf{0},-\mathbf{q}}\frac{\mathbf{q}\cdot\mathbf{q}'}{q'^2}\rho_{-\mathbf{q}'\sigma'}\rho_{\mathbf{q}+\mathbf{q}'\sigma}\Big),\end{aligned} \tag{6}$$

where $\rho_{\mathbf{0}\sigma}=N_\sigma$ is the total number of spin-σ electrons.

An ingenious trick due to STLS at this stage is to replace $\rho_{-\mathbf{q}'\sigma'}\rho_{\mathbf{q}+\mathbf{q}'\sigma}$ in the second term of the last equation of (6) by $\rho_{\mathbf{q}\sigma'}\langle\rho_{-\mathbf{q}-\mathbf{q}'\sigma'}\rho_{\mathbf{q}+\mathbf{q}'\sigma}\rangle/N_{\sigma'}$. With this replacement, we can see easily that the local-field correction is given by

$$G_{\sigma\sigma'}(\mathbf{q})=\frac{1}{\sqrt{N_\sigma N_{\sigma'}}}\sum_{\mathbf{q}'\neq\mathbf{0},-\mathbf{q}}\frac{\mathbf{q}\cdot\mathbf{q}'}{q'^2}\Big[S_{\sigma\sigma'}(\mathbf{q}+\mathbf{q}')-\delta_{\sigma\sigma'}\Big], \tag{7}$$

where the spin-dependent static structure factor $S_{\sigma\sigma'}(\mathbf{q})$ is defined as

$$S_{\sigma\sigma'}(\mathbf{q})\equiv\frac{1}{\sqrt{N_\sigma N_{\sigma'}}}\langle\rho_{\mathbf{q}\sigma}\rho_{-\mathbf{q}\sigma'}\rangle. \tag{8}$$

According to the fluctuation-dissipation theorem, $S_{\sigma\sigma'}(\mathbf{q})$ is related to the coupled charge-spin response functions (Marinescu and Quinn 1997). In particular, in the paramagnetic phase in which we assume that g^* is negligibly small to give $N_\uparrow=N_\downarrow=N/2$, the charge and spin parts, $S_+(\mathbf{q})$ and $S_-(\mathbf{q})$, are decoupled to each other to give, respectively, at $T=0$

$$\begin{aligned}S_+(\mathbf{q})&=S_{\uparrow\uparrow}(\mathbf{q})+S_{\uparrow\downarrow}(\mathbf{q})\\&=\frac{1}{\pi N}\int_0^\infty d\omega\frac{\Pi_0(\mathbf{q},i\omega)}{1+[1-G_+(\mathbf{q})]V_0(\mathbf{q})\Pi_0(\mathbf{q},i\omega)},\end{aligned} \tag{9}$$

and

$$\begin{aligned}S_-(\mathbf{q})&=S_{\uparrow\uparrow}(\mathbf{q})-S_{\uparrow\downarrow}(\mathbf{q})\\&=\frac{1}{\pi N}\int_0^\infty d\omega\frac{\Pi_0(\mathbf{q},i\omega)}{1-G_-(\mathbf{q})V_0(\mathbf{q})\Pi_0(\mathbf{q},i\omega)},\end{aligned} \tag{10}$$

with $G_\pm(\mathbf{q})\equiv[G_{\uparrow\uparrow}(\mathbf{q})\pm G_{\uparrow\downarrow}(\mathbf{q})]/2$. By solving the coupled equations, (7), (9) and (10), self-consistently, we obtain the local-field corrections $G_\pm(\mathbf{q})$ and the structure factors $S_\pm(\mathbf{q})$ simultaneously. We confine ourselves to this paramagnetic situation in the rest of this section, though a spin-polarized situation is also considered in Sec. 3.

In rederiving the STLS formalism with the Hamiltonian in (1), we find a very important point: The equation (6) holds irrespective of $\mathbf{A}(\mathbf{r})$. This indicates that the essential framework of STLS remains the same even if it is considered in the presence of the magnetic field. Its presence reflects only in the evaluation of $\Pi_0(\mathbf{q},i\omega)$, the response function of a free electron. For example, in the 3D electron gas in a magnetic field $\mathbf{H}=(0,0,H)$, $\Pi_0(\mathbf{q},i\omega)$ is written as

$$\begin{aligned}\Pi_0(\mathbf{q},i\omega)=\frac{1}{4\pi^2\omega_c\ell^3}\sum_\sigma\sum_{nn'}\frac{|F_{nn'}(\mathbf{q}_\perp)|^2}{q_z\ell}\\ \times\ln\left(\frac{\omega^2+[(n-n')\omega_c-q_z^2/2m^*-k_{\mathrm{F}n\sigma}q_z/m^*]^2}{\omega^2+[(n-n')\omega_c-q_z^2/2m^*+k_{\mathrm{F}n\sigma}q_z/m^*]^2}\right),\end{aligned} \tag{11}$$

where $\mathbf{q}=(\mathbf{q}_\perp,q_z)$, n and n' represent indices for the Landau subband and $k_{\mathrm{F}n\sigma}$ is the Fermi momentum in the z-direction for the subband characterized by n and spin σ. The effect of the cyclotron motion manifests itself in the form factor $F_{nn'}(\mathbf{q}_\perp)$, given by

$$\begin{aligned}F_{nn'}(\mathbf{q}_\perp)=\left(\frac{n!}{n'!}\right)^{1/2}\left[\frac{(-q_y+iq_x)\ell}{\sqrt{2}}\right]^{n'-n}\\ \times\exp(-\mathbf{q}_\perp^2\ell^2/4)L_n^{(n'-n)}(\mathbf{q}_\perp^2\ell^2/2),\end{aligned} \tag{12}$$

with $L_n^{(\alpha)}(x)$ the generalized Laguerre polynomial. Because $\Pi_0(\mathbf{q},i\omega)$ shows a different response for $\mathbf{q}$ in the xy-plane from that for $\mathbf{q}$ in the z-direction, $G_\pm(\mathbf{q})$ as well as $S_\pm(\mathbf{q})$ will have an anisotropic behavior in this case.

We also note that (6) holds irrespective of $V(\mathbf{r})$. Since (1) represents the first-principles Hamiltonian in solid state physics if m^* is replaced by m_e and $V(\mathbf{r})$ describes the electron-ion interaction in a crystal, this fact suggests that the STLS scheme is applicable as it is to a material with such a complicated band structure as in the case of graphite.

B. Numerical results in the paramagnetic phase

Two parameters specifies the present system. One is the density parameter r_s, characterizing the strength of the Coulomb correlation. The other is ℓ/r_0, specifying the strength of the magnetic field. The magnetic quantum limit is obtained for ℓ/r_0 less than $(4\sqrt{2}/3\pi)^{1/3}\approx 0.84$ and the semi-magnetic quantum limit (in which two lowest Landau subbands are occupied) appears as long as it is in the range from 0.84 to $[4(2+\sqrt{2})/3\pi]^{1/3}\approx 1.13$.

In Fig. 1, $G_\pm(\mathbf{q})$ is plotted as a function of q_x or q_z depending on the direction of $\mathbf{q}$ for several values of ℓ/r_0 at $r_s=1$. Those $\mathbf{q}$'s are scaled by the Fermi momentum p_{F} at $H=0$. We find that $G_\pm(\mathbf{q})$ hardly changes from that at $H=0$ for ℓ/r_0 larger than about 0.7. This remains true for larger values of r_s. Qualitatively we can understand easily that $G_\pm(\mathbf{q})$ does not change much for r_0 smaller than ℓ, because it describes the short-range repulsive nature of electrons and such a nature does not change if the length scale for the cycloron motion is larger than that for correlation. Quantitatively we find that the exchange-correlation hole is very robust against the magnetic field in the sense that it hardly changes up to the point of $\ell/r_0\approx 0.7$. We also find that the charge part is more robust than the spin part.

The effect of the magnetic field becomes apparent for $\ell/r_0<0.7$ and $G_\pm(\mathbf{q})$ shows an anisotropic behavior. For small $|\mathbf{q}|$ in the charge channel, larger deviation is seen in $G_+((0,0,q_z))$ from the corresponding values at $H=0$ than that in $G_+((q_x,0,0))$, while for large $|\mathbf{q}|$, the opposite is the case. This indicates that the deformation of the exchange-corelation hole occurs in such a way as the deformation extends in a rather long range in the z-direction, while in the xy-plane the deformation appears

only in a short range. Thus the exchange-correlation hole is elongated in the z-direction in the charge channel. A completely opposite situation is found for the spin channel. For small $|\mathbf{q}|$, $G_-((q_x,0,0))$ deviates more than $G_-((0,0,q_z))$, but for large $|\mathbf{q}|$, we find a reverse situation. A detailed study will be given in the future, to clarify the physical reason for these complicated behaviors.

The exchange and correlation energies per electron, ε_x and ε_c, can be calculated through the relations

$$\varepsilon_x = \frac{1}{2}\sum_{\mathbf{q}} V_0(\mathbf{q})[S_{\rm HF}(\mathbf{q})-1], \tag{13}$$

and

$$\varepsilon_c = \frac{1}{2}\int_0^1 d\lambda \sum_{\mathbf{q}} V_0(\mathbf{q})[S_+(\mathbf{q}:\lambda)-S_{\rm HF}(\mathbf{q})], \tag{14}$$

where $S_{\rm HF}(\mathbf{q})$ is the static structure factor in the Hartree-Fock approximation and $S_+(\mathbf{q}:\lambda)$ is the charge part of the static structure factor for the system described by the Hamiltonian $H_0+\lambda H_1$. In the magnetic quantum limit, $S_{\rm HF}(\mathbf{q})$ is given by

$$S_{\rm HF}(\mathbf{q}) = 1-\exp(-\mathbf{q}_\perp^2\ell^2/2)\Big(1-\frac{|q_z|}{2k_{\rm F0}\ell}\Big)\theta(2k_{\rm F0}-|q_z|), \tag{15}$$

with $\theta(x)$ the Heaviside step function. Note that the cusp at $|q_z|=2k_{\rm F0}$ in the curve of $S_{\rm HF}(\mathbf{q})$ reflects the logarithmic divergence in $\Pi_0(\mathbf{q},0)$.

The results for ε_x and ε_c are given in Fig. 2 as a function of r_s for $\ell/r_0=0.7$ in (a) and 0.4 in (b), respectively. Due to the robustness of $G_\pm(\mathbf{q})$, ε_c does not change much from that at $H=0$ for $\ell/r_0=0.7$. However, at $\ell/r_0=0.4$, a considerable change is seen. Note that for low values of ℓ/r_0 and/or large values of r_s, $|\varepsilon_c|$ exceeds $|\varepsilon_x|$, which never occurs at $H=0$. This suggests that the correlation effect becomes more important than the exchange effect in a high magnetic field. This fact might have some connection with the occurrence of FQHE in the 2D electron gas in which the the radial density distribution function $g(\mathbf{r})$ behaves not in the way as $g(\mathbf{r})\propto|\mathbf{r}|^2$ (as expected from the Pauli principle) but as $g(\mathbf{r})\propto|\mathbf{r}|^{2/\nu}$ for the occupation rate $\nu=1/3,1/5,\cdots$.

To summarize this section, we find that the effect of the magnetic field on $G_\pm(\mathbf{q})$ is small as long as ℓ/r_0 is larger than 0.7, which corresponds to $H=150$T in graphite.

III. GRAPHITE

A. Brief description of our formalism

In the case of graphite, the electron field operator $\psi_\sigma(\mathbf{r})$ is expanded in terms of the basis functions $\{\phi_{nXdk_ztσ}(\mathbf{r})\}$ as

$$\psi_\sigma(\mathbf{r}) = \sum_{nX}\sum_{dk_z}\sum_t\sum_\sigma \phi_{nXdk_ztσ}(\mathbf{r})c_{nXdk_ztσ} \equiv \sum_N \phi_N(\mathbf{r})c_N, \tag{16}$$

where N represents a set of quantum indices, $\{n,X,d,k_z,t,\sigma\}$, in which n and X specify the magnetic wave function in the xy-plane in the Landau gauge, d and k_z describe the nature of the Bloch function in the z-direction with $d=B$ (B') for electrons in the H-K-H (H'-K'-H') edge and k_z in the first Brillouin zone, and $t=1,\cdots,4$ corresponds to the bands E_1, E_2, E_3, and E_3' in the Slonczewski-Weiss (SW) model for graphite (Slonczewski and Weiss 1958, McClure 1960). Note that n starts at -1 in graphite conventionally. Since the bands E_3 and E_3' appear near the Fermi level, we will be mainly concerned with these bands in the following.

The one-body part of the Hamiltonian H_0 in (2) is diagonal in this expansion and it is written as

$$H_0 = \sum_N \varepsilon_N c_N^\dagger c_N. \tag{17}$$

The matrix elements of the Coulomb interaction in (3), $V_0(N_1,N_2:N_3,N_4)$, can be evaluated with the use of those basis functions to obtain

$$H_1 = \frac{1}{2}\sum_{N_1N_2N_3N_4} V_0(N_1,N_2:N_3,N_4)c_{N_1}^\dagger c_{N_2}^\dagger c_{N_3}c_{N_4}. \tag{18}$$

With the information on ε_N and $V_0(N_1,N_2:N_3,N_4)$, the calculation of the polarization function in the RPA, $\Pi_0(\mathbf{q},i\omega)$, is straightforward, though it is tedius.

Since all the ingredients are now in hand, we can implement the STLS scheme in order to determine the local-field correction $G_\pm(\mathbf{q})$. As for the change with the increase of the magnetic field, however, we can skip this implementation for H less than about 150T because of the robustness of $G_\pm(\mathbf{q})$ against the magnetic field. If we can assume further that the effect of the crystal potential on $G_\pm(\mathbf{q})$ is weak, we need not perform the STLS procedure even at $H=0$. The validity of this assumption is not checked at present, but we just consider it to be the case and employ $G_\pm(\mathbf{q})$ obtained in the 3D electron gas without the magnetic field.

With those values of $G_\pm(\mathbf{q})$, the effective electron-electron interaction in the electron gas is given by (Kukkonen and Overhauser 1979)

$$V_{\sigma\sigma'}(\mathbf{q},i\omega) = V_0(\mathbf{q}) - V_+(\mathbf{q})^2\frac{\Pi_0(\mathbf{q},i\omega)}{1+[1-G_+(\mathbf{q})]V_0(\mathbf{q})\Pi_0(\mathbf{q},i\omega)} -\sigma\sigma' V_-(\mathbf{q})^2\frac{\Pi_0(\mathbf{q},i\omega)}{1-G_-(\mathbf{q})V_0(\mathbf{q})\Pi_0(\mathbf{q},i\omega)}, \tag{19}$$

with $V_+(\mathbf{q}) \equiv [1-G_+(\mathbf{q})]V_0(\mathbf{q})$ and $V_-(\mathbf{q}) \equiv -G_-(\mathbf{q})V_0(\mathbf{q})$. By attaching the form factors associated with the basis functions $\{\phi_{nXdk_ztσ}(\mathbf{r})\}$ to $V_{\sigma\sigma'}(\mathbf{q},i\omega)$ in

(19) appropriately, we can obtain the effective electron-electron interaction $V(N_1, N_2; N_3, N_4 : i\omega)$ pertinent for the electrons in graphite. This effective interaction can be used to calculate the self-energy in just the same way as done for the 3D electron gas (Takada 1993). Specifically, the self-energy for an electron specified by N, Σ_N, is evaluated in the static approximation at $T = 0$ as

$$\Sigma_N = \sum_{N'} \theta(\mu - \varepsilon_{N'} - \Sigma_{N'})[V_H(N, N'; N', N : 0) - V(N, N'; N, N' : 0)\delta_{\sigma\sigma'}\delta_{dd'}]. \quad (20)$$

The first term is "the Hartree-type" contribution and due care is necessary to avoid double counting of the screening effect. Namely, the effective interaction is composed of ring, ladder, and exchange diagrams, but the ring contribution should be excluded here. Such a procedure is indicated by the suffix 'H'. The second term is the screened-Fock contribution.

Since the chemical potential μ as well as the self-energy $\Sigma_{N'}$ is included in its righthand side (and therefore $\Pi_0(\mathbf{q}, i\omega)$ should be recalculated with the renormalized electronic structure), (20) provides a nontrivial self-consistent way of obtaining the self-energy Σ_N, but it can be solved by a numerical iteration method to determine the electronic structure of graphite in strong magnetic fields.

As for the choice of ϵ_0, there is an ambiguity as mentioned in Sec. 1. Since the polarization effect due to valence electrons is included faithfully in $\Pi_0(\mathbf{q}, i\omega)$, we need to consider only the core polarization in ϵ_0. Thus it must be small and we tentatively take $\epsilon_0 = 1$ here. This choice of ϵ_0 combined with $m^* = 0.3m_e$ provides $a_{\rm B}^* \approx 1.7\mathring{A}$. Because n_e is expected to increase in proportion to $(2\pi\ell^2)^{-1}$ or H in high magnetic fields, r_0 decreases, but the decrease is very slow, namely, $r_0 \propto H^{-1/3}$. Therefore, as compared to the case of $H \approx 5$T at which we consider that n_e is about the same as that for $H = 0$, r_0 at $H \approx 50$T is about the half of that at $H = 0$. This amounts to $r_0 \approx 15\mathring{A}$ and consequently $r_s \equiv r_0/a_{\rm B}^* \approx 9$. This value of r_s will be used in the following calculation at $H \approx 50$T.

B. Calculated results for the electronic structure

In Fig. 3(b), calculated results for the electronic structure are given for $H = 50$T and 55T. For comparison, the corresponding results in the noninteraction case (the SW model) are plotted in Fig. 3(a). It is noteworthy that the many-body effect makes the subband specified by $n = 0$ and $\sigma = \uparrow$ empty for $H > 53$T. This is never expected either in the SW model or in the RPA as shown in Fig. 3(c) in which $G_{\pm}(\mathbf{q})$ is taken to be zero, but experimentally this phenomenon is observed to occur at $H = 52 - 54$T (Miura *et al.* 1997, Yaguchi 1998). Thus we can get a reasonable electronic structure for graphite only with the inclusion of the exchange and correlation effects. Physically, this evacuation of minority carriers due to the many-body self-energy effect arises for the same reason as the occurrence of ferromagnetism in the electron gas. In fact, a very large enhancement of the Zeeman splitting is obtained in our many-body calculation compared to the one-body calculation, indicating a tendency towards ferromagnetism.

We note that fine tuning of r_s is not necessary to obtain this phenomenon at H around 55T, as illustrated in Fig. 3(d) in which the result with $r_s = 10$ instead of $r_s = 9$ is given. Although the absolute value of Σ_N changes much, the critical magnetic field increases only a little bit (about 2T) with this change of r_s.

Another interesting point in Fig. 3 is that the dispersion curve for the $n = 0$ subbands along the z-direction changes quite dramatically near $k_z = \pm\pi/c$ (the H or H' point). This is due to the fact that the magnitude of the self-energy correction depends on k_z, reflecting the spatial location of electrons in the crystal. The conduction electrons in the $n = 0$ subbands near the K and K' points in momentum space are mainly in the B and B' sites of carbon atoms in real space, but those electrons near the H and H' points reside in the A and A' sites of carbon atoms. This indicates that the self-energy correction becomes small for those minority electrons at the A and A' sites, leading to a large deformation of the dispersion relation.

This change of the dispersion curve may bring about an interesting phase in stronger magnetic fields. In Fig. 4, as an example, the calculated result for the electronic structure at $H = 200$T is given. In the SW model shown in (a), the state is (semi-)metallic, because the Fermi level crosses the dispersion curves of the Landau subbands. The many-body effect changes the situation completely and the semiconducting behavior is expected, because no states are available at the Fermi level. This absence of the states at the Fermi level prevents a further transition to ferromagnetism in the state obained; this is substantiated by the fact that no enhancement of the Zeeman splitting is seen here, although we have adopted the formalism that allows spin polarization to any degree.

In order to obtain the result in Fig. 4, we have used the r_s value of 12 due to the increase of the effective mass m^* as mentioned in Sec. 1, but this result is less accurate compared to the case in Fig. 3, because we cannot neglect the effect of the magnetic field on the local-field correction $G_{\pm}(\mathbf{q})$ at this value of H. However, we believe that the qualitative nature of Fig. 4(b) would be preserved even if we improved on the values of $G_{\pm}(\mathbf{q})$ or if we took the value of r_s a little different from 12.

IV. SUMMARY AND DISCUSSION

We have proposed a theoretical framework for the correlation problem in the electron gas in strong magnetic fields. The framework is an extension of the STLS for-

malism and it goes far beyond the RPA. On the basis of this theory, we have considered the electronic structure of graphite in a magnetic field up to a few hundred teslas. We have found that the effect of the self-energy correction is so large that the subband specified by $n = 0$ and $\sigma = \uparrow$ becomes unoccupied at $H \approx 53$T, a fact observed experimentally but never be expected in the one-body approximation. We have also speculated the occurrence of a semiconducting phase for H larger than about 200T.

In principle, the present theory can be employed to the 2D electron gas as well, but it is not known yet whether the FQHE can be described or not in the present approach. We guess that some indication for the FQHE will probably be obtained, but it may be difficult to get an incommpressible fluid state at some special values of the occupation rate ν. In any case, this is an important future problem.

As for graphite, the nature of the electronic phase transition for H less than 52T remains undecided, but it is clear that the phase transition has connected with the subband with $n = 0$ and $\sigma = \uparrow$, because the tansition disappears for $H > 52$T at which the subband becomes unoccupied (Yaguchi 1998). Thus the proposal of Sugihara has to be rejected, but it is not decided yet whether the state is a CDW or a SDW or even perhaps some other unknown state.

ACKNOWLEDGMENTS

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[1] Ceperley D M and Alder B J 1980 Phys. Rev. Lett. **45** 566
[2] Iye Y, Tedrow P, Timp G, Dresselhaus M S, Dresselhaus G, Furukawa A and Tanuma S 1982 Phys. Rev. B **25** 5478
[3] Iye Y and Dresselhaus G 1985 Phys. Rev. Lett. **54** 1182
[4] Kukkonen C A and Overhauser A W 1979 Phys. Rev. B **20** 550
[5] Laughlin R B 1983 Phys. Rev. Lett. **50** 1395
[6] Marinescu D C and Quinn J J 1997 Phys. Rev. B **56** 1114
[7] McClure J W 1960 Phys. Rev. **119** 606
[8] Miura N, Shimamoto Y, Nakagawa H, Takamasu T and Nojiri H 1997 *Proc. Int. Conf. High Magnetic Fields in the Physics of Semiconductors II* (World Scientific, Singapore), eds. G. Landwehr and W.Ossau, p. 939
[9] Nakao K 1976 J. Phys. Soc. Jpn. **40** 761
[10] Ochimizu H, Takamasu T, Takeyama S, Sasaki S and Miura N 1992 Phys. Rev. B **46** 1986
[11] Singwi K S, Tosi M P, Land R H and Sjölander A 1968 Phys. Rev. **176** 589
[12] Skudlarski P and Vignale G 1993 Phys. Rev. B **48** 8547
[13] Slonczewski J C and Weiss P R 1958 Phys. Rev. **109** 272
[14] Sugihara K 1984 Phys. Rev. B **29** 975
[15] Takada Y 1993 Phys. Rev. B **47** 5202
[16] Takahashi K and Takada Y 1994 *Physica* B **201** 384
[17] Tanuma S, Inada R, Furukawa A, Takahashi O, Iye Y and Onuki Y 1981 *Physics in High Magnetic Fields* (Springer, Berlin) p 316
[18] Tsui D C, Störmer H L and Gossard A C 1982 Phys. Rev. Lett. **48** 1559
[19] Yaguchi H, Iye Y, Takamasu T and Miura N 1993 *Physica* B **184** 332
[20] Yaguchi H 1998 private communication
[21] Yoshioka D and Fukuyama H 1981 J. Phys. Soc. Jpn. **50** 725

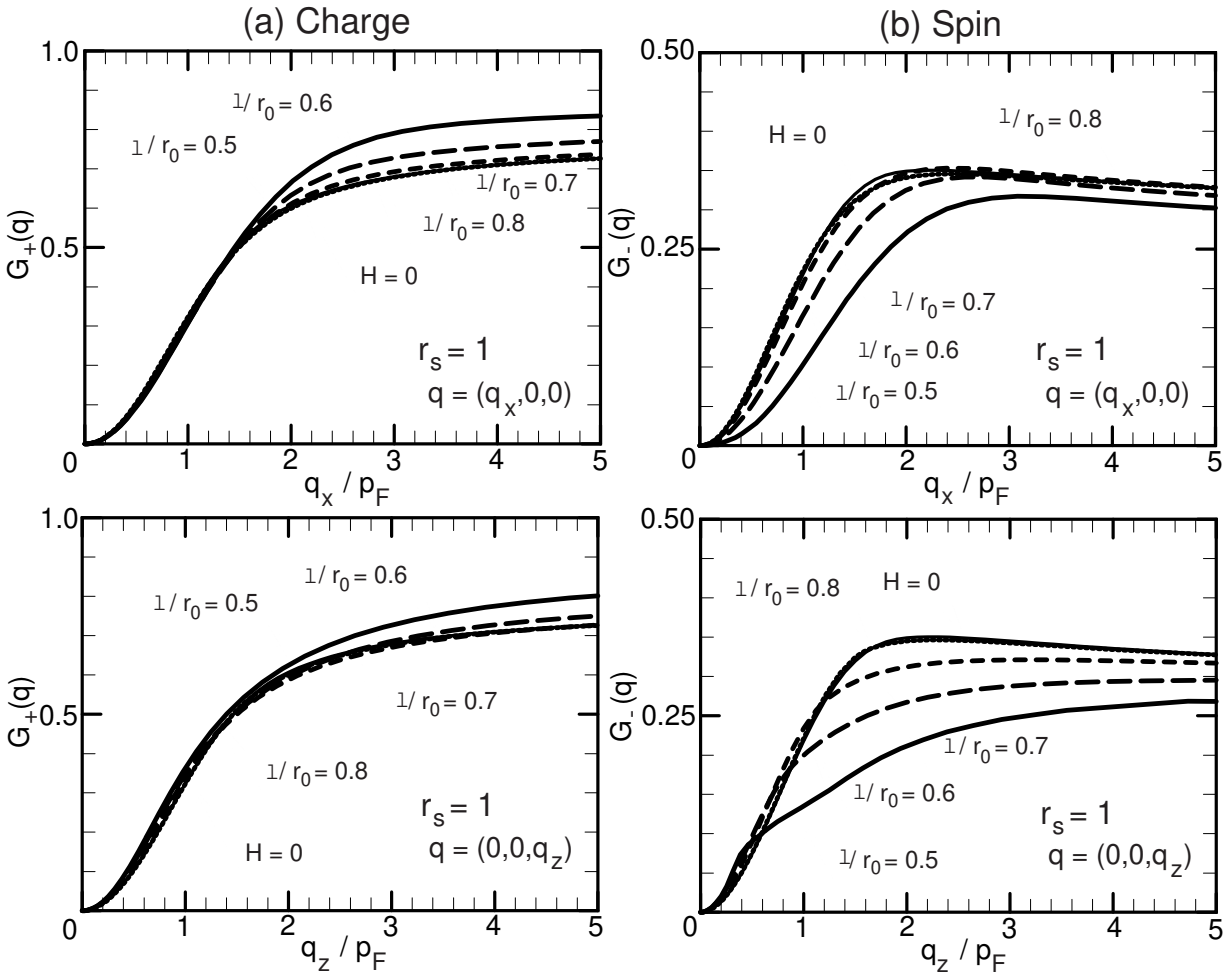

FIG. 1. The local-field correction in the 3D electron gas in a magnetic field.

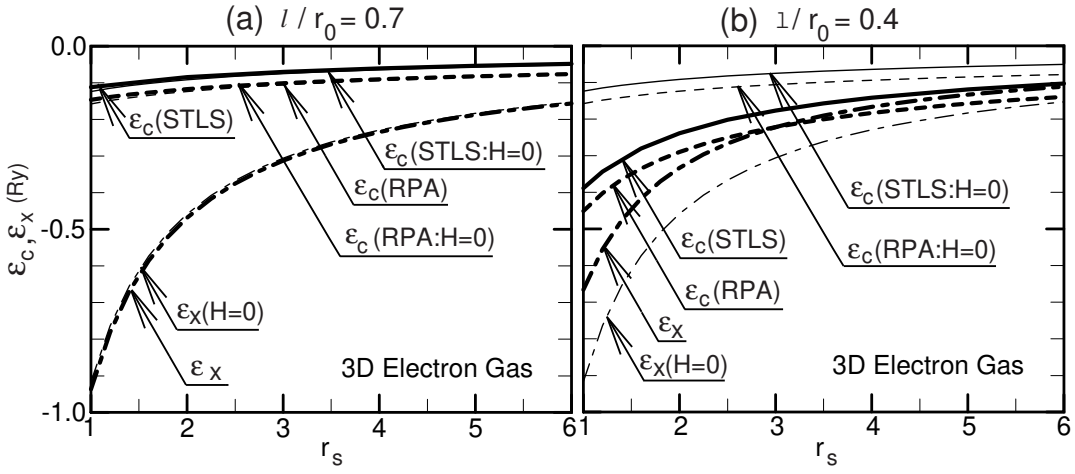

FIG. 2. Exchange and correlation energies in the 3D electron gas in a magnetic field.

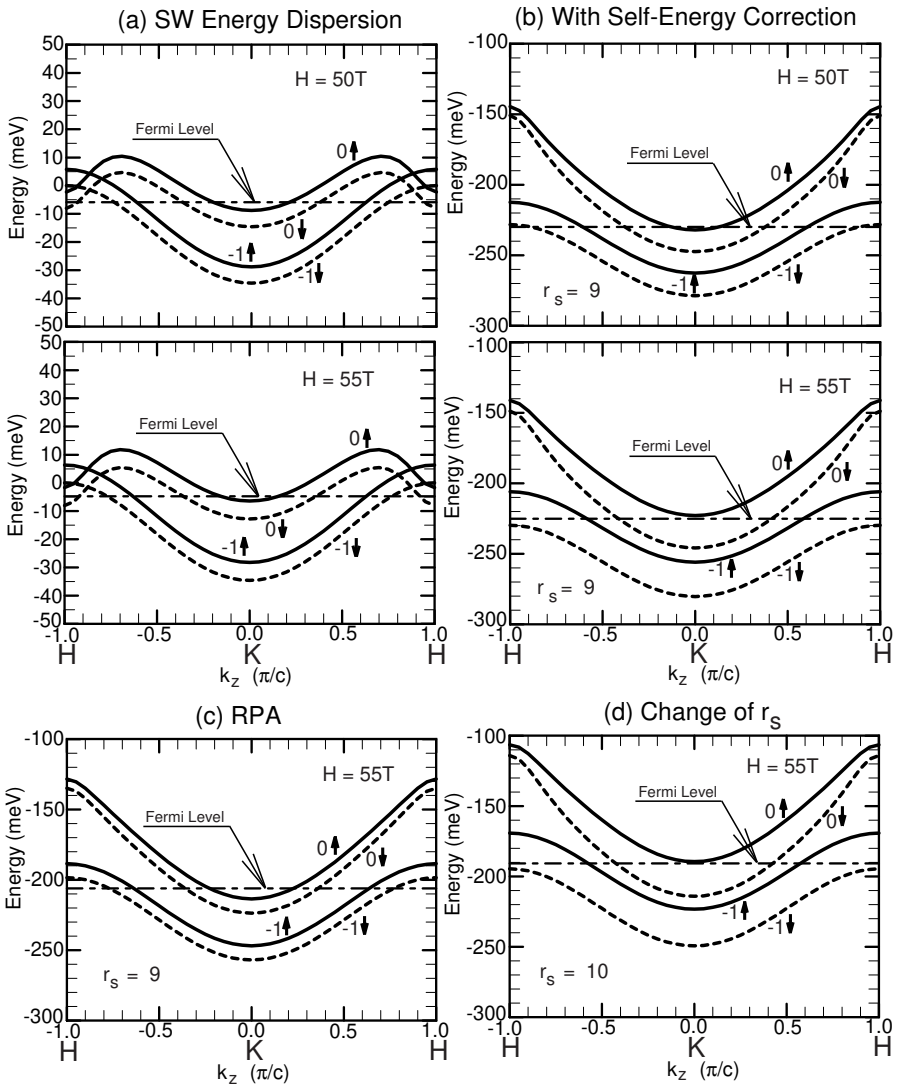

FIG. 3. The electronic structure of graphite at $H = 50$T and 55T. In (a), no many-body effect is considered, while in (b), the self-energy correction is included self-consistently. For comparison, the RPA result is given in (c) and the result of the self-consistent many-body calculation with $r_s = 10$ in (d).

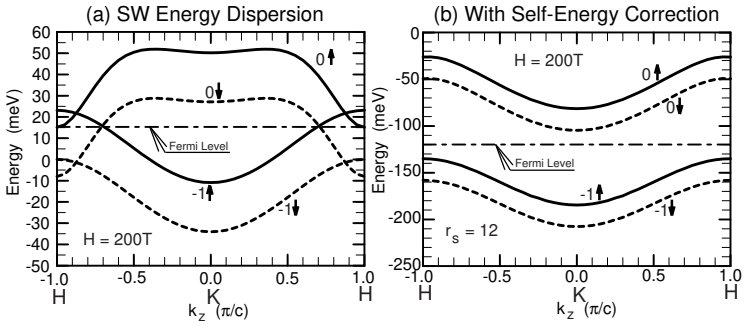

FIG. 4. Electronic structure of graphite at $H = 200$T.