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Ground-state energy of a two-dimensional charge-density-wave state in a strong magnetic field

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The charge-density-wave state of two-dimensional electrons which occupy only the lowest Landau level is investigated. The previous Hartree-Fock calculation by Yoshioka and Fukuyama [J. Phys. Soc. Jpn. 47, 394 (1979)] is extended to include the higher harmonics of the density wave. The correction to the Hartree-Fock ground-state energy is calculated by second-order perturbation theory. Effects of higher Landau levels are also estimated. It is found that the ground-state energy is a smooth function of ν, the filling factor of the lowest Landau level.

I. INTRODUCTION

Two-dimensional electrons form a Wigner crystal at low density at low temperatures.[1] Such a crystalline state has been observed for electrons on a liquid-helium surface.[2] However, when the electron density becomes higher the cost of the kinetic energy to form the crystal becomes larger than the gain of the Coulomb interaction between the electrons, and the crystal is not formed. The two-dimensional electron systems realized in Si metal-oxide-semiconductor (MOS) and GaAs-AlGaAs heterojunction have rather high density, $n \gtrsim 10^{11}$ cm^{-2}. Hence the Wigner crystal is not expected to be formed in these systems.

The situation is different when a strong magnetic field is applied perpendicular to the two-dimensional plane.[3] In a strong magnetic field the electrons are localized within the order of the Larmor radius $l=\sqrt{c/eH}$. Even at high densities, as long as the field is strong enough so that l is much smaller than $r_s=(\pi n)^{-1/2}$, the mean distance between the nearest electrons, a Wigner crystal can form without the cost of the kinetic energy.

In the experimentally realized system of $n \gtrsim 10^{11}$ cm^2 and $H \simeq 10$ T, l and r_s are of the same order, so if the Wigner crystal is formed, the overlap of the wave functions is not negligible. It will be better to describe such a state as a charge-density-wave (CDW) state. Fukuyama *et al.*[4] considered a system where only the lowest Landau level is partially filled (i.e., $2\pi l^2 n < 1$), and calculated the transition temperature to CDW states by the Hartree-Fock approximation. They obtained a rather high transition temperature ($T_c \simeq 30$ K for Si MOS in $H=10$ T) and found that the CDW state with the highest T_c has a periodicity which is different from that of the Wigner crystal of the same density. Later Yoshioka and Fukuyama[5] showed that the CDW state has the expected periodicity in the ground state and that it can be considered as a Wigner crystal of electrons or holes with overlapping wave function. While the Hartree-Fock approximation grossly overestimates the transition temperature, these calculations indicate the possibility of realizing the Wigner crystal or CDW state in Si-MOS or GaAs-AlGaAs heterojunction in a magnetic field of the order of 10 T.

Several attempts to detect this CDW state have been made on Si MOS,[6-9] and a number of unusual behaviors have been found. However, in Si MOS the effect of the random potential makes it difficult to interpret the experiments. In this respect the GaAs-AlGaAs heterojunction is a more favorable system for the investigation of the CDW state, since electron mobility is higher than in Si MOS. The experiments on GaAs-AlGaAs became possible quite recently, and the experiments have been done mainly to investigate the quantized Hall effect.[10] Two recent experiments[11,12] have led to the suggestion that the CDW state may be realized in these systems.

Paalanen *et al.*[11] measured the resistivity tensor at temperatures down to 50 mK, and observed vanishingly small ρ_{xx} and steplike behavior of ρ_{xy} as a function of the magnetic field, namely, ρ_{xy} seems to take only the quantized value. Fukuyama and Platzman[13] suggested a possible interpretation of the data based by assuming the formation of the CDW state. The magnetic field in this experiment was not very high, $H<8$ T, and several Landau levels are occupied by electrons. Another experiment[12] done at higher magnetic field, $H<20$ T, revealed very strange behavior of ρ_{xx} and ρ_{xy}. Tsui *et al.* observed a dip in ρ_{xx} and a plateau in ρ_{xy} at $\rho_{xy}=3h/e^2$ as a function of the magnetic field, when the lowest Landau level is about $\frac{1}{3}$ filled, i.e., the filling factor $\nu \equiv 2\pi l^2 n \simeq \frac{1}{3}$. They suggested the following interpretation of this phenomenon. If the CDW state at $\nu=\frac{1}{3}$ is energetically favorable, the filling factor

may be pinned at $\frac{1}{3}$ in a finite region of the magnetic field. The sliding of the CDW ground state may explain the plateau at $\rho_{xy}=3h/e^2$. The purpose of this paper is to investigate whether the CDW state at $\nu=\frac{1}{3}$ is energetically favorable or not.

Yoshioka and Fukuyama[5] (YF) have already calculated the ground-state energy of the CDW state as a function of ν. They took into account only the lowest Landau level (strong magnetic field approximation) and applied the Hartree-Fock theory. They further simplified the problem by neglecting the higher harmonics of the CDW. The CDW state was found to have the same periodicity as the Wigner crystal. The ground-state energy is a smooth function of the filling factor ν except at $\nu=\frac{1}{2}$, where the phase transition between the electron Wigner crystal and hole Wigner crystal occurs.

In this paper we improve the approximation used by YF. For simplicity we keep the strong magnetic field approximation, even though for GaAs-AlGaAs in a field of 15 T, $\hbar\omega_c\simeq 300$ K and $e^2/\epsilon l=200$ K. We solve the Hamiltonian obtained by this approximation by the Hartree-Fock theory in Sec. II. The calculation is the same as YF except now we consider the higher harmonics of the CDW. The derivation of the Hartree-Fock Hamiltonian is repeated for convenience. We solve this Hamiltonian by the same method as YF but in a different representation. We will see that the conclusion by YF is essentially correct: The energy is a smooth function of ν, and the CDW state can be considered as a Wigner crystal. In Sec. III we improve the Hartree-Fock approximation by calculating the effect of the difference between the original Hamiltonian and the Hartree-Fock Hamiltonian using second-order perturbation theory. Effects of the higher Landau levels are also estimated. We will see that the correction to the energy is only a few percent and is also a smooth function of ν. Finally, discussion is given in Sec. IV.

II. HARTREE-FOCK THEORY

A. Derivation of the Hartree-Fock Hamiltonian

In a magnetic field the energy spectrum of a two-dimensional free electron is quantized into Landau levels. The Coulomb interaction between the electrons causes broadening of each Landau level and mixes different Landau levels. However, when the energy difference between the nearest Landau levels, $\hbar\omega_c$, is much larger than the typical order of the Coulomb interaction, $e^2/\epsilon l$, where ϵ is the dielectric constant and $l=(c/eH)^{1/2}$, the Larmor radius, the mixing of the different Landau levels will be negligible. In this case we can consider only one Landau level, which is partially filled by electrons, and investigate the effect of the Coulomb interaction. In this paper we assume $\hbar\omega_c \gg e^2/\epsilon l$ and consider the situation when only the lowest Landau level is partly filled. In this strong magnetic field approximation the Hamiltonian is given by

$$H=\frac{1}{2L^2}\sum_q v(q)\rho(q)\rho(-q)\ , \tag{2.1}$$

where

$$v(q)=\frac{2\pi e^2}{\epsilon q}\ , \tag{2.2}$$

$$\rho(q)=\sum_x \exp\left[-iq_x X-\frac{(ql)^2}{4}\right]a^\dagger_{X_+}a_{X_-}\ , \tag{2.3}$$

$$X_\pm=X\pm\tfrac{1}{2}l^2q_y,\quad 0\le X=\frac{2\pi l^2}{L}j\le L\ . \tag{2.4}$$

In these equations $\rho(q)$ is the density operator expressed in terms of the creation (annihilation) operator $a^\dagger_X$ (a_X) of the electron wave function in the Landau gauge, L is the linear dimension of the system, and j is an integer. In this model the number of states are finite and given by $L^2/2\pi l^2$. In the following we express the electron density $n=N/L^2$ in terms of the filling factor ν ($=2\pi l^2 n$) of the total states. It should be noted that the Hamiltonian has an electron-hole symmetry: The Hamiltonian has the same form after the transformation $a^\dagger_X \leftrightarrow a_X$. Hence the ground state at filling factor ν is equivalent to that at $\nu'=1-\nu$. Hereafter, we consider only the system with $\nu\le\frac{1}{2}$.

We obtain the Hartree-Fock Hamiltonian assuming the following triangular charge-density-wave state:

$$\langle\rho(r)\rangle=\frac{1}{2\pi l^2}\sum_Q \Delta(Q)\exp(i\vec{Q}\cdot\vec{r}-\tfrac{1}{4}l^2Q^2) \tag{2.5}$$

or

$$\Delta(\vec{Q})=\frac{2\pi l^2}{L^2}\sum_X \langle a^\dagger_{X_+}a_{X_-}\rangle\exp(iQ_xX)\ , \tag{2.6}$$

where

$$Q=\left[\left(j+\frac{k}{2}\right)Q_0,\frac{\sqrt{3}}{2}kQ_0\right]\ , \tag{2.7}$$

$$X_\pm=X\pm\tfrac{1}{2}l^2Q_y\ . \tag{2.8}$$

Here $\Delta(0)=\nu$, Q_0 gives the fundamental periodicity of the CDW state, which should be determined to minimize the energy, and j and k are integers. Then the Hamiltonian is decoupled to give the following

Hartree-Fock Hamiltonian:

$$H_{\rm HF}=\sum_Q\sum_X U(Q)\Delta(-Q)\exp(-iQ_xX)a^\dagger_{X_+}a_{X_-}-\frac{1}{2}\frac{L^2}{2\pi l^2}\sum_Q U(Q)\,|\,\Delta(Q)\,|^2\,, \tag{2.9}$$

$$U(Q)=\frac{e^2}{\epsilon l}\left[\frac{1}{Ql}\exp\left[-\frac{Q^2l^2}{2}\right](1-\delta_{Q,0})-\left[\frac{\pi}{2}\right]^{1/2}\exp\left[-\frac{Q^2l^2}{4}\right]I_0\left[\frac{Q^2l^2}{4}\right]\right]. \tag{2.10}$$

B. Diagonalization of the Hartree-Fock Hamiltonian

The Hartree-Fock (HF) Hamiltonian is diagonalized by unitary transformations. We diagonalize it in three steps. First we transform operator a_X into $b_{X,Y}$:

$$b_{X,Y}=\frac{1}{\sqrt{s_m}}\sum_{s=0}^{s_m}\exp\left[-i\frac{\sqrt{3}}{2}sQ_0Y\right]a_{X+(\sqrt{3}/2)sl^2Q_0}\,, \tag{2.11}$$

where s is an integer, $s_m=2L/(\sqrt{3}l^2Q_0)$, $0\le X\le\frac{1}{2}\sqrt{3}l^2Q_0$, Y is the integral multiple of $2\pi l^2/L$, and $b_{X,Y+4\pi l^2/\sqrt{3}Q_0}=b_{X,Y}$. Then $H_{\rm HF}$ is rewritten as follows:

$$H_{\rm HF}=\sum_Q\sum_X\sum_Y U(Q)\Delta(-Q)\exp[-i(Q_xX+Q_yY+\tfrac{1}{2}l^2Q_xQ_y)]b^\dagger_{X,Y}b_{X,Y+l^2Q_x}-\frac{1}{2}\frac{L^2}{2\pi l^2}\sum_Q U(Q)\,|\,\Delta(Q)\,|^2\,, \tag{2.12}$$

where the summation over Y is restricted to $0\le Y<4\pi l^2/\sqrt{3}Q_0$. We note that Y is defined modulo $4\pi l^2/\sqrt{3}Q_0$ and Y is coupled to $Y+l^2Q_x$. So we define integers M and N such that

$$\tfrac{1}{2}NQ_0l^2=\frac{4\pi}{\sqrt{3}}\frac{1}{Q_0}M \tag{2.13}$$

or

$$\frac{M}{N}=\frac{\sqrt{3}}{8\pi}Q_0^2l^2\,, \tag{2.14}$$

and replace $b_{X,Y}$ by $c_{X,Y,j}$,

$$c_{X,Y,j}=b_{X,Y+1/2jl^2Q_0}\,, \tag{2.15}$$

where $1\le j\le N$ and Y is restricted to $0\le Y<l^2Q_0/2M$. Then $H_{\rm HF}$ is rewritten as

$$H_{\rm HF}=\sum_X\sum_Y\sum_j\sum_k M_{j,k}(X,Y)c^\dagger_{X,Y,j}c_{X,Y,k}-\frac{1}{2}\frac{L^2}{2\pi l^2}\sum_Q U(Q)\,|\,\Delta(Q)\,|^2\,, \tag{2.16}$$

$$M_{j,k}(X,Y)=\sum_Q U(Q)\Delta(-Q)\exp\{-i[Q_xX+Q_yY+\tfrac{1}{4}(j+k)l^2Q_0Q_y]\}\delta_{k,j+2Q_x/Q_0}\,. \tag{2.17}$$

The matrix $M_{j,k}(X,Y)$ is Hermitian, so $H_{\rm HF}$ is diagonalized by a unitary matrix $U_{j,k}(X,Y)$,

$$H_{\rm HF}=\sum_X\sum_Y\sum_j\alpha^\dagger_{X,Y,j}E_j(X,Y)\alpha_{X,Y,j}-\frac{1}{2}\frac{L^2}{2\pi l^2}\sum_Q U(Q)\,|\,\Delta(Q)\,|^2\,, \tag{2.18}$$

where

$$[U^{-1}(X,Y)M(X,Y)U(X,Y)]_{j,k}=\delta_{j,k}E_j(X,Y)\,, \tag{2.19}$$

$$\alpha_{X,Y,j}=\frac{1}{\sqrt{s_m}}\sum_k\sum_s U^{-1}_{j,k}(X,Y)\exp\left[-i\frac{\sqrt{3}}{2}sQ_0Y-2\pi isk\frac{M}{N}\right]a_{X+(\sqrt{3}/2)sl^2Q_0}\,. \tag{2.20}$$

C. Hartree-Fock ground state

In the ground state the amplitude of the CDW or the order parameter $\Delta(Q)$ is given as follows:

$$\Delta(Q)=\frac{2\pi l^2}{L^2}\sum_X \langle a^\dagger_{X_+} a_{X_-}\rangle \exp(-iQ_xX)$$

$$=\frac{2\pi l^2}{L^2}\sum_X\sum_Y\sum_j\sum_k U_{k+2Q_x/Q_0,j}(X,Y)\Theta(\mu-E_j(X,Y))U^{-1}_{j,k}(X,Y)$$

$$\times\exp[-i(Q_xX+Q_yY+\tfrac{1}{2}l^2Q_xQ_y+\tfrac{1}{2}kl^2Q_0Q_y)]\,, \tag{2.21}$$

where μ is the chemical potential and Θ is the step function. This is the self-consistent equation. To find the ground state for a given value of ν, we first assume some Q_0, solve Eq. (2.21) for $\Delta(Q)$ and μ, and minimize the expectation value of the Hamiltonian $E_{\rm HF}(Q_0,\nu)$ with respect to Q_0, where $E_{\rm HF}(Q_0,\nu)$ is given as follows:

$$E_{\rm HF}(Q_0,\nu)=\tfrac{1}{2}\sum_X\sum_Y\sum_j E_j(X,Y)\Theta(\mu-E_j(X,Y))=\frac{1}{2}\frac{L^2}{2\pi l^2}\sum_Q U(Q)\,|\,\Delta(Q)\,|^2\,. \tag{2.22}$$

However, this procedure cannot be done as it is, firstly, because there are an infinite number of order parameters, and secondly, an arbitrary choice of Q_0 may make the order of the matrix $M_{j,k}(X,Y)$ too large. YF avoided this difficulty by considering only the order parameters with $|Q|=Q_0$ and noting that the energy spectrum $E_j(X,Y)$ has a large gap between lower $2M$ and $2M+1$ bands, where $M/N=\sqrt{3}Q_0^2l^2/8\pi$, and that the choice of Q_0 such that $\nu=2M/N$ should give the lowest energy, since the Fermi level lies in the large gap. In this paper we also assume that the same choice of Q_0 gives the lowest energy. We choose several ν given by a ratio of small integers $2M$ and N, thereby avoiding diagonalization of a large matrix. We solve Eq. (2.21) only by taking into account a finite number of order parameters whose Q satisfies $|Q|\le Q_M$. We increase Q_M until the results converge.

We performed this procedure for $\nu=2M/N$ with $N\le 13$ and $0.1818\le\nu\le 0.5$. The values of ν, M, and N are shown in Table I. For $\nu=\frac{1}{3}$ and $\frac{1}{2}$ we took into account the order parameters up to $Q_M=7Q_0$. We found that it was adequate to take Q_M to be $4Q_0$: The difference of the ground-state energy for $Q_M=7Q_0$ and $Q_M=4Q_0$ was less than $10^{-3}\%$, and the difference of the energy spectrum

TABLE I. Values of $\nu=2M/N$ for which calculations are done.

ν	M	N
0.1818	1	11
0.2	1	10
0.2222	1	9
0.25	1	8
0.2857	1	7
0.3077	2	13
0.3333	1	6
0.3636	2	11
0.4	1	5
0.4444	2	9
0.4615	3	13
0.5	1	4

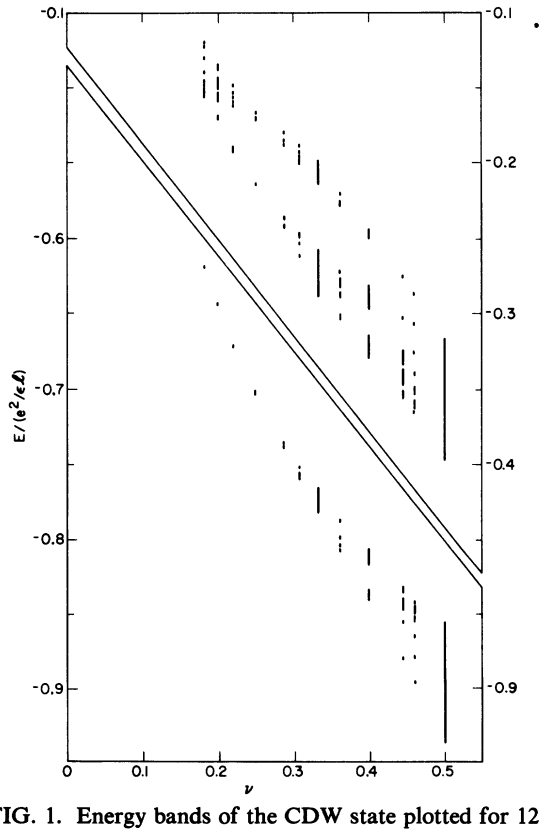

FIG. 1. Energy bands of the CDW state plotted for 12 choices of ν. At each ν the vertical lines show the range of energy E where there is a state with $E=E_j(X,Y)$.

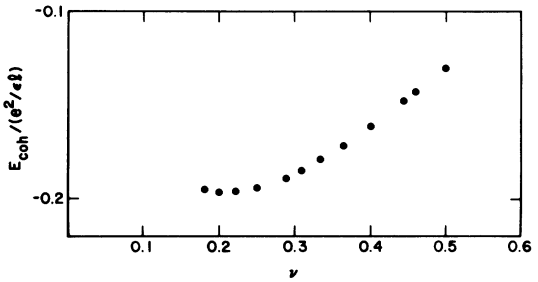

FIG. 2. Cohesive energy per particle $E_{\rm coh}(\nu)$ for the 12 choices of ν.

was less than 0.7%. So for the other choice of ν we took Q_M to be $4Q_0$.

Figure 1 shows the energy bands for each ν. We plot the allowed value of $E_j(X,Y)$ for each ν. We note that the energy bands split into two parts, one below $-0.6e^2/\epsilon l$ and the other above $-0.4e^2/\epsilon l$. The lower bands (valence bands) consist of $2M$ bands which are completely filled. The upper $N-2M$ bands (conduction bands) are empty. The energy gap between these two groups are roughly independent of the choice of N and M, i.e., $\nu=\frac{1}{2}$ has the nearly same energy gap as $\nu=\frac{6}{13}=0.462$. We can safely assume that this large gap continues to exist for larger values of N and M in this range of ν. This large gap at the Fermi level ensures the choice of Q_0 for a given ν.

It is interesting to recall that YF have found that the bottom of the conduction band and the top of the valence band show cusplike behavior at $\nu=\frac{1}{3}$. When higher harmonics are included we see from Fig. 1 that while the cusp is considerably reduced, it is still visible.

Figure 2 shows the cohesive energy per particle,

$$E_{\rm coh}(\nu)=\frac{1}{2}\frac{1}{\nu}\sum_{Q\neq 0}U(Q)\,|\,\Delta(Q)\,|^2\,, \tag{2.23}$$

which is the difference of the ground-state energy per particle between the CDW state and the uniform state appropriate at very high temperature, whose ground-state energy per particle is given by $\frac{1}{2}U(0)\nu$. Again $E_{\rm coh}(\nu)$ seems to be a smooth function of ν: $E_{\rm coh}(\frac{1}{3})$ is approximately given by linear interpolation of $E_{\rm coh}(\frac{4}{13})$ and $E_{\rm coh}(\frac{4}{11})$. Apparently, contributions from the cusp at the top of the valence band are canceled by the presence of gaps in the valence band for $\nu\neq\frac{1}{3}$.

We also compared the present ground-state energy with the previous calculation by YF and with the ground-state energy of the classical Wigner crystal, namely, the Coulomb energy of the triangular lattice of point electrons. Figure 3 shows this comparison. We plot the ground-state energy per particle. The

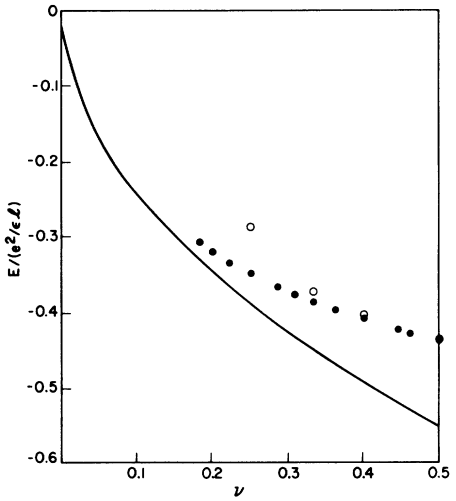

FIG. 3. Ground-state energy per particle of the CDW state and the classical Wigner crystal. The closed circles show the present calculation, the open circles show the results of YF, and the solid line shows the result for the classical Wigner crystal.

uniform Fock energy $\frac{1}{2}U(0)\nu$ is included for the CDW state here. The ground-state energy per particle for the classical Wigner crystal is given by Bonsall and Maradudin[14] to be $-1.9605e^2\sqrt{n}/\epsilon$ $-0.782\sqrt{\nu}e^2/\epsilon l$. This value gives a lower bound of the energy for the present system. The spread of the electron wave function increases the energy for the CDW state.

Figure 4 shows the first three order parameters: $\Delta(Q_0)$, $\Delta(\sqrt{3}Q_0)$, and $\Delta(2Q_0)$. They are also a smooth function of ν. In this figure the order

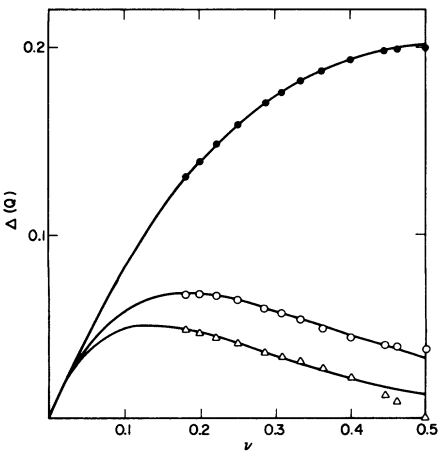

FIG. 4. First three order parameters. The closed circles show $\Delta(Q_0)$, the open circles show $\Delta(\sqrt{3}Q_0)$, and the open triangles show $\Delta(2Q_0)$. The solid lines show $\Delta_W(Q_0)$, $\Delta_W(\sqrt{3}Q_0)$, and $\Delta_W(2Q_0)$, where Δ_W is the overlapping Gaussian approximation [Eq. (2.25)].

parameters of the hypothetical Wigner crystal $\Delta_W(Q)$ are also shown by solid lines. These $\Delta_W(Q)$ are calculated from the following density pattern[5]:

$$\langle\rho(r)\rangle=\frac{1}{2\pi l^2}\sum_{R_n}\exp[-(r-R_n)^2/2l^2]$$
$$=\frac{1}{2\pi l^2}\sum_{Q}\Delta_W(Q)\exp(i\vec{Q}\cdot\vec{r}-\tfrac{1}{4}l^2Q^2)\ , \tag{2.24}$$

where it is assumed that each electron has the Gaussian density distribution of the lowest Landau level around the lattice point R_n, and that the total density pattern is given by simple summation. This equation gives the following $\Delta_W(Q)$:

$$\Delta_W(Q)=\nu\exp(-\tfrac{1}{4}l^2Q^2)\ . \tag{2.25}$$

We find that the difference between $\Delta(Q)$ and $\Delta_W(Q)$ is smaller than 0.01. This means that the density pattern given by Eq. (2.24) gives a good approximation to the actual density pattern of the CDW state. If we calculate $E_{\rm coh}(\nu)$, Eq. (2.23), using $\Delta_W(Q)$ for $\Delta(Q)$, the result reproduces the actual $E_{\rm coh}(\nu)$ within 0.1% for $\nu<0.4$. This agreement shows that the CDW state can be interpreted as the Wigner crystal and gives a strong support for the smoothness of the ground-state energy.

There is more proof which supports the smoothness of the ground-state energy. We can verify that the order parameter $\Delta(Q)$ satisfies the following sum rule:

$$\sum_{Q}|\Delta(Q)|^2=\nu\ . \tag{2.26}$$

The proof is given in Appendix A. If $\Delta(Q)$ at each pair of (j,k), where $Q=[(j+\frac{1}{2}k)Q_0,(\sqrt{3}/2)kQ_0]$, is a continuous function of ν, it follows from Eqs. (2.23) and (2.26) that $E_{\rm coh}(\nu)$ is also a smooth function of ν. Incidentally, in the one-harmonic approximation, Eqs. (2.26) and (2.23) give simple analytic form for $E_{\rm coh}(\nu)$. This sum rule also means that there is a lower bound for the Hartree-Fock cohesive energy $E_{\rm coh}(\nu)$,

$$E_{\rm coh}(\nu)\geq\frac{1}{2\nu}U_{\rm min}\sum_{Q\neq0}|\Delta(Q)|^2$$
$$=\tfrac{1}{2}(1-\nu)U_{\rm min}\ , \tag{2.27}$$

where $U_{\rm min}$ is the minimum value of $U(Q)$, which is $-0.557e^2/\epsilon l$. At $\nu=\frac{1}{3}$ the actual cohesive energy is about 97% of this lower bound.

The results we get thus far are qualitatively the same as those of YF. The CDW state can be interpreted as the Wigner crystal, and there is a large energy gap at the Fermi level. One of the effects of taking into account many order parameters is that both the conduction bands and the valence band narrow. The band narrowing is a consequence of better localization of the electron density. This effect becomes larger at small ν where the higher harmonics become more important. The narrowing is particularly striking for the conduction band. Another effect of the higher harmonics, lowering of the ground-state energy, is also larger at smaller ν.

Finally, we remark that the above interpretation of the CDW state as a Wigner crystal of electrons is appropriate only for $\nu<\frac{1}{2}$. For $\nu>\frac{1}{2}$ the electron-hole symmetry of the Hamiltonian tells us that the CDW state looks like a Wigner crystal of holes. There is a phase transition at $\nu=\frac{1}{2}$ between an electron and hole Wigner crystal when we change ν.

III. SECOND-ORDER PERTURBATION

In this section we calculate the correction to the Hartree-Fock ground-state energy by the second-order perturbation. We are motivated by the observation that the present problem has no small expansion parameter. Without explicit calculation it is not obvious whether the higher-order corrections will be small. Furthermore, while the Hartree-Fock energy is a smooth function of ν, it is conceivable that the cusp in the band structure discussed in the preceding section might appear in the second-order energy.

The Hamiltonian is written in the following way:

$$H=H_{\rm HF}+(H-H_{\rm HF})\ . \tag{3.1}$$

We treat $(H-H_{\rm HF})$ as a perturbation Hamiltonian. The Hartree-Fock ground state $|\Phi\rangle$ is given as

$$|\Phi\rangle=\prod_{j}{}'\prod_{X}\prod_{Y}\alpha^{\dagger}_{X,Y,j}|0\rangle\ , \tag{3.2}$$

where the product over j is done for occupied states only and $|0\rangle$ is the vacuum. The first-order correction is zero, since

$$\langle\Phi|H|\Phi\rangle=\langle\Phi|H_{\rm HF}|\Phi\rangle=E_{\rm HF}\ , \tag{3.3}$$

the second-order correction is given as

$$E_2=\langle\Phi|(H-H_{\rm HF})\frac{1}{E_{\rm HF}-H}(H-H_{\rm HF})|\Phi\rangle$$
$$=\sum_i\langle\Phi|H-H_{\rm HF}|\Phi_i\rangle\frac{1}{E_{\rm HF}-E_i}$$
$$\times\langle\Phi_i|H-H_{\rm HF}|\Phi\rangle$$
$$=\sum_i\frac{1}{E_{\rm HF}-E_i}\langle\Phi|H|\Phi_i\rangle\langle\Phi_i|H|\Phi\rangle\ , \tag{3.4}$$

where $H|\Phi_i\rangle=E_i|\Phi_i\rangle$, and $|\Phi_i\rangle$ is a state where two electrons and two holes are excited from $|\Phi\rangle$. Let us express the state where one electron is added to $|\Phi\rangle$ by $|\phi_k\rangle$ and one hole is added to $|\Phi\rangle$ by $|\psi_k\rangle$, namely,

$$|\phi_k\rangle=\alpha^{\dagger}_{X_k,Y_k,j_k}|\Phi\rangle\ , \tag{3.5}$$

$$|\psi_k\rangle=\alpha_{X_k,Y_k,j_k}|\Phi\rangle\ . \tag{3.6}$$

Then E_2 is written as follows:

$$\begin{aligned}E_2=\sum_k\sum_j\sum_m\sum_n\frac{1}{4L^4}\sum_{q_1}\sum_{q_2}\sum_{X_1}\cdots\sum_{X_4}v(q_1)v(q_2)\exp[-iq_{1x}(X_1-X_2)-iq_{2x}(X_3-X_4)]\\ \times\exp(-\tfrac{1}{2}l^2q_1^2-\tfrac{1}{2}l^2q_2^2)\frac{1}{E_m+E_n-E_j-E_k}\\ \times(\langle\Phi|a^{\dagger}_{X_1+l^2q_{1y}/2}|\psi_m\rangle\langle\psi_m|a_{X_3-l^2q_{2y}/2}|\Phi\rangle\langle\Phi|a^{\dagger}_{X_2-l^2q_{1y}/2}|\psi_n\rangle\\ \times\langle\psi_n|a_{X_4+l^2q_{2y}/2}|\Phi\rangle-\langle\Phi|a^{\dagger}_{X_1+l^2q_{1y}/2}|\psi_m\rangle\\ \times\langle\psi_m|a_{X_4+l^2q_{2y}/2}|\Phi\rangle\\ \times\langle\Phi|a^{\dagger}_{X_2-l^2q_{1y}/2}|\psi_n\rangle\langle\psi_n|a_{X_3-l^2q_{2y}/2}|\Phi\rangle)\\ \times(\langle\Phi|a_{X_2+l^2q_{1y}/2}|\phi_k\rangle\langle\phi_k|a^{\dagger}_{X_4-l^2q_{2y}/2}|\Phi\rangle\langle\Phi|a_{X_1-l^2q_{1y}/2}|\phi_j\rangle\\ \times\langle\phi_j|a^{\dagger}_{X_3+l^2q_{2y}/2}|\Phi\rangle\\ -\langle\Phi|a_{X_2+l^2q_{1y}/2}|\phi_k\rangle\langle\phi_k|a^{\dagger}_{X_3+l^2q_{2y}/2}|\Phi\rangle\\ \times\langle\Phi|a_{X_1-l^2q_{1y}/2}|\phi_j\rangle\langle\phi_j|a^{\dagger}_{X_4-l^2q_{2y}/2}|\Phi\rangle)\ ,\end{aligned} \tag{3.7}$$

where $E_k=E_{j_k}(X_k,Y_k)$, etc. This summation cannot be done analytically. Even the numerical computation is difficult, since we must sum over many variables. However, we can overcome this difficulty in the following way. We note that the energy denominator is nearly constant, roughly twice the energy gap. We expand the deviation from this constant up to second order: We define the mean energy of the occupied bands E_v and the mean energy of the empty bands E_c,

$$E_v=\frac{2\pi l^2}{\nu L^2}\sum_X\sum_Y\sum_j E_j(X,Y)\Theta(\mu-E_j(X,Y))\ , \tag{3.8}$$

$$E_c=\frac{2\pi l^2}{(1-\nu)L^2}\sum_X\sum_Y\sum_j E_j(X,Y)\Theta(E_j(X,Y)-\mu)\ . \tag{3.9}$$

E_c and E_v are related to each other,

$$(1-\nu)E_c+\nu E_v=U(0)\nu\ , \tag{3.10}$$

since

$$\sum_j E_j(X,Y)=\sum_j M_{jj}(X,Y)\ . \tag{3.11}$$

Then we express the deviation from E_c and E_v as follows, and expand the energy denominator:

$$E_j=E_c+e_j,\quad E_m=E_v+e_m\ ,$$
$$(E_m+E_n-E_k-E_j)^{-1}\simeq[2(E_v-E_c)]^{-1}-(e_m+e_n-e_k-e_j)[2(E_v-E_c)]^{-2}+(e_m+e_n-e_k-e_j)^2[2(E_v-E_c)]^{-3}+\cdots\ . \tag{3.12}$$

We define $\Delta_c^{(n)}(Q),\Delta_v^{(n)}(Q)$ as follows:

$$\sum_i \langle\Phi\,|\,a_{X_1}^\dagger\,|\,\psi_i\rangle\frac{e_i^n}{[2(E_c-E_v)]^n}\langle\psi_i\,|\,a_{X_2}\,|\,\Phi\rangle\equiv\sum_Q\Delta_v^{(n)}\exp[\tfrac{1}{2}Q_x(X_1+X_2)]\delta_{X_1-X_2,l^2Q_y}\ , \tag{3.13}$$

$$\sum_i \langle\Phi\,|\,a_{X_1}\,|\,\phi_i\rangle\frac{e_i^n}{[2(E_c-E_v)]^n}\langle\phi_i\,|\,a_{X_2}^\dagger\,|\,\Phi\rangle\equiv\sum_Q\Delta_c^{(n)}\exp[\tfrac{1}{2}Q_x(X_1+X_2)]\delta_{X_2-X_1,l^2Q_y}\ , \tag{3.14}$$

or

$$\Delta_v^{(n)}(Q)=\frac{2\pi l^2}{L^2}\sum_X\sum_Y\sum_j\sum_k U_{k+2Q_x/Q_0,j}(X,Y)\left[\frac{E_j(X,Y)-E_c}{2(E_c-E_v)}\right]^n\Theta(\mu-E_j(X,Y))\times U_{j,k}^{-1}(X,Y)\exp[-i(Q_xX+Q_yY+\tfrac{1}{2}l^2Q_xQ_y+\tfrac{1}{2}kl^2Q_0Q_y)]\ , \tag{3.15}$$

$$\Delta_c^{(n)}(Q)=\frac{2\pi l^2}{L^2}\sum_X\sum_Y\sum_j\sum_k U_{k+2Q_x/Q_0,j}(X,Y)\left[\frac{E_j(X,Y)-E_v}{2(E_c-E_v)}\right]^n\Theta(E_j(X,Y)-\mu)\times U_{j,k}^{-1}(X,Y)\exp[-i(Q_xX+Q_yY+\tfrac{1}{2}l^2Q_xQ_y+\tfrac{1}{2}kl^2Q_0Q_y)]\ . \tag{3.16}$$

We use such notation because $\Delta_v^{(0)}(Q)=\Delta(Q)$ and $\Delta_c^{(0)}(Q)=\delta_{Q,0}-\Delta(Q)$. Moreover, $\Delta_v^{(1)}$ and $\Delta_c^{(1)}$ are related to each other,

$$\Delta_c^{(1)}(Q)+\Delta_v^{(1)}(Q)=\frac{1}{2(E_c-E_v)}\{[U(Q)-E_v+E_c]\Delta(Q)-E_c\delta_{Q,0}\}\ . \tag{3.17}$$

We insert Eqs. (3.12)–(3.14) into (3.7), then we can sum over X and Y and we obtain the following expression for E_2:

$$\begin{aligned}E_2=-\frac{1}{4}\frac{1}{E_c-E_v}\sum_q\sum_Q\sum_{Q_1}\sum_{Q_2}U\left[q+\frac{Q}{2}\right]U\left[q-\frac{Q}{2}\right]\exp\{-il^2[q_x(Q_x+Q_{1x}-Q_{2x})-q_y(Q_y+Q_{1y}-Q_{2y})]\}\\ \times\{[\Delta_v^{(0)}(Q+Q_1)+\Delta_v^{(1)}(Q+Q_1)+\Delta_v^{(2)}(Q+Q_1)]\\ \times[\Delta_v^{(0)}(Q-Q_2)+\Delta_v^{(1)}(Q-Q_2)+\Delta_v^{(2)}(Q-Q_2)]\\ \times[\Delta_c^{(0)}(Q_1)-\Delta_c^{(1)}(Q_1)+\Delta_c^{(2)}(Q_1)][\Delta_c^{(0)}(Q_2)-\Delta_c^{(1)}(Q_2)+\Delta_c^{(2)}(Q_2)]\\ +\Delta_v^{(0)}(Q+Q_1)\Delta_v^{(0)}(Q-Q_2)\Delta_c^{(1)}(Q_1)\Delta_c^{(1)}(Q_2)\\ +\Delta_v^{(1)}(Q+Q_1)\Delta_v^{(1)}(Q-Q_2)\Delta_c^{(0)}(Q_1)\Delta_c^{(0)}(Q_2)\\ -\Delta_v^{(1)}(Q+Q_1)\Delta_v^{(0)}(Q-Q_2)\Delta_c^{(1)}(Q_1)\Delta_c^{(0)}(Q_2)\\ -\Delta_v^{(0)}(Q+Q_1)\Delta_v^{(1)}(Q-Q_2)\Delta_c^{(1)}(Q_1)\Delta_c^{(0)}(Q_2)\\ -\Delta_v^{(1)}(Q+Q_1)\Delta_v^{(0)}(Q-Q_2)\Delta_c^{(0)}(Q_1)\Delta_c^{(1)}(Q_2)\\ -\Delta_v^{(0)}(Q+Q_1)\Delta_v^{(1)}(Q-Q_2)\Delta_c^{(0)}(Q_1)\Delta_c^{(1)}(Q_2)\}\ .\end{aligned} \tag{3.18}$$

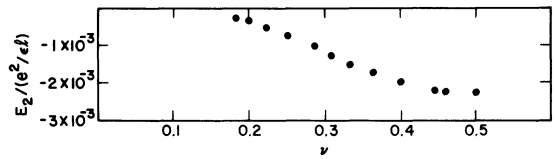

FIG. 5. Correction to the cohesive energy per particle by the second-order perturbation theory E_2 for the 12 choices of ν.

The effective potential $U(q)$ diverges at $q=0$ as q^{-1}. It may seem that the term with $Q=0$ gives a divergent contribution to E_2. However, we can show that the other factor vanishes at $q\to 0$ as q^2 due to the sum rule Eq. (2.26) and the relation between $\Delta_c^{(1)}(Q)$ and $\Delta_v^{(1)}(Q)$, Eq. (3.17); hence the divergence of $[U(q)]^2$ does not give a divergence of E_2.

Now we can evaluate E_2 numerically. We calculated $\Delta_v^{(n)}(Q)$ and $\Delta_c^{(n)}(Q)$ at the values of ν chosen in Sec. II, and calculated E_2. It turns out that the expansion of the energy denominator is a good approximation. The values of $\Delta_v^{(1)}(Q)$ and $\Delta_c^{(1)}(Q)$ are smaller than 10^{-2} and the values of $\Delta_v^{(2)}(Q)$ and $\Delta_c^{(2)}(Q)$ are smaller than 10^{-3}. About 95% of E_2 comes from the terms with $\Delta_v^{(0)}(Q)$ and $\Delta_c^{(0)}(Q)$ only.

The result is shown in Fig. 5 as a correction to the cohesive energy, $\Delta E_{\rm coh}=E_2/N$, where N is the total number of electrons. Again $\Delta E_{\rm coh}$ seems to be a smooth function of ν. Moreover, the absolute value of $\Delta E_{\rm coh}$ is very small compared to $E_{\rm coh}$, only 2% at $\nu=\frac{1}{2}$. Therefore, the Hartree-Fock approximation seems to be a very good approximation for the ground-state energy.

IV. DISCUSSION

In this paper we investigated the CDW ground state of a two-dimensional electron in a strong magnetic field. We assumed that the cyclotron energy $\hbar\omega_c$ is much larger than the order of the Coulomb interaction energy $e^2/\epsilon l$ and considered only the lowest Landau level (strong magnetic field approximation). This model has been investigated in the Hartree-Fock approximation before by YF. Since they considered only a single harmonic of the order parameter, it was not an exact Hartree-Fock theory. In this paper we considered all the important order parameters, and solved the Hartree-Fock self-consistent equations. We found that the conclusion reached by YF was essentially correct: The CDW state is a Wigner crystal of electrons ($\nu\le\frac{1}{2}$) or a Wigner crystal of holes ($\frac{1}{2}\le\nu<1$) and there is a large energy gap at the Fermi level for any value of ν. We found that the width of the occupied bands is very narrow, which means the electrons are well localized. The ground-state energy looks like a smooth function of ν; $\nu=\frac{1}{3}$ seems to have no special feature.

Then we calculated the correction to the ground-state energy by the second-order perturbation theory. We found that the correction is a smooth function of ν and that it is less than 2% of the Hartree-Fock ground-state energy. It seems that the Hartree-Fock theory is a good approximation for the ground-state energy which appears to be a smooth function of ν.

We have also estimated the effect of the higher Landau levels by the second-order perturbation. The calculation is given in Appendix B. The correction to the energy depends on the ratio of $\hbar\omega_c$, cyclotron energy, and $e^2/\epsilon l$, the Coulomb energy. If we use $H=15$ T, at which the anomaly is observed in GaAs-AlGaAs, $m^*=0.07m_0$ and $\epsilon=13$, $\hbar\omega_c$ is about 300 K and $e^2/\epsilon l$ is about 200 K. Then the correction to the ground-state energy is less than 0.8%. Hence the neglect of the higher Landau levels is a good approximation.

In conclusion, the Hartree-Fock theory and its improvements did not produce a commensurability energy at $\nu=\frac{1}{3}$. Thus an explanation of the observed Hall step at $\nu=\frac{1}{3}$ must await a more sophisticated treatment of the problem.

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APPENDIX A

Here we verify the sum rule $\nu=\sum_Q |\Delta(Q)|^2$. The order parameter $\Delta(Q)$ is given as follows:

$$\Delta(Q)=\frac{2\pi l^2}{L^2}\frac{1}{s_m}\sum_X\sum_Y\sum_j\sum_{k_1}\sum_{k_2}\sum_s U^{-1}_{j,k_1}(X,Y)U_{k_2,j}(X,Y)\Theta(\mu-E_j(X,Y))$$
$$\times\exp\left[-iQ_x\left[X+\frac{\sqrt{3}}{2}sl^2Q_0\right]-iQ_y(Y+\tfrac{1}{2}l^2k_2Q_0-\tfrac{1}{2}l^2Q_x)\right.$$
$$\left.+s(k_1-k_2)\frac{\sqrt{3}}{4}l^2Q_0^2\right]. \qquad \text{(A1)}$$

If we perform the summation over s, we get Eq. (2.21). However, here we leave the s summation and perform the Q summation first,

$$\begin{aligned}\sum_Q |\Delta(Q)|^2 = \sum_Q \left[\frac{2\pi l^2}{s_m L^2}\right]^2 \sum_{X_1}\sum_{X_2}\sum_{Y_1}\sum_{Y_2}\sum_{j_1}\sum_{j_2}\sum_{k_1}\cdots\sum_{k_4}\sum_{s_1}\sum_{s_2}\Theta(\mu-E_{j_1}(X_1,Y_1))\Theta(\mu-E_{j_2}(X_2,Y_2)) \\ \times U^{-1}_{j_1,k_1}(X_1,Y_1)U_{k_2,j_1}(X_1,Y_1) \\ \times U_{k_3,j_2}(X_2,Y_2)U^{-1}_{j_2,k_4}(X_2,Y_2) \\ \times\exp\left[-iQ_x\left[X_1-X_2+(s_1-s_2)\frac{\sqrt{3}}{2}l^2Q_0\right]\right. \\ -iQ_y[Y_1-Y_2+(k_2-k_4)\tfrac{1}{2}l^2Q_0] \\ +i[s_1(k_1-k_2)-s_2(k_3-k_4)] \\ \left.\times\frac{\sqrt{3}}{4}l^2Q_0^2\right] \\ = \left[\frac{2\pi l^2}{s_m L^2}\right]\sum_{X_1}\sum_{X_2}\sum_{Y_1}\sum_{Y_2}\sum_{j_1}\sum_{j_2}\sum_{k_1}\cdots\sum_{k_4}\sum_{s_1}\sum_{s_2}\delta_{s_1,s_2}\delta_{X_1,X_2}\delta_{Y_1,Y_2}\delta_{k_2,k_4}\Theta(\mu-E_{j_1}(X_1,Y_1)) \\ \times\Theta(\mu-E_{j_2}(X_1,Y_1))U^{-1}_{j_1,k_1}(X_1,Y_1) \\ \times U_{k_2,j_1}(X_1,Y_1)U_{k_3,j_2}(X_1,Y_1) \\ \times U^{-1}_{j_2,k_2}(X_2,Y_2)\exp\left[-is_1(k_1-k_3)\frac{\sqrt{3}}{4}l^2Q_0^2\right].\end{aligned} \tag{A2}$$

Now we perform the s_1 summation which gives δ_{k_1,k_3}, hence

$$\begin{aligned}\sum_Q |\Delta(Q)|^2 = \frac{2\pi l^2}{L^2}\sum_X\sum_Y\sum_{j_1}\sum_{j_2}\sum_{k_1}\sum_{k_2}U^{-1}_{j_1,k_1}(X,Y)U_{k_2,j_1}(X,Y)U_{k_1,j_2}(X,Y) \\ \times U^{-1}_{j_2,k_2}(X,Y)\Theta(\mu-E_{j_1}(X,Y))\Theta(\mu-E_{j_2}(X,Y)) \\ = \frac{2\pi l^2}{L^2}\sum_X\sum_Y\sum_j\Theta(\mu-E_j(X,Y))=\nu\,.\end{aligned} \tag{A3}$$

APPENDIX B

Here we estimate the effect of the higher Landau levels. The main effect of the higher Landau levels will be taken into account by the Hartree-Fock theory. The approximate Hamiltonian is now given as

$$\begin{aligned}H_{\rm HF} = \sum_Q\sum_X U(Q)\Delta(Q)\exp(-iQ_xX)a^\dagger_{X_+}a_{X_-} - \frac{1}{2}\frac{L^2}{2\pi l^2}\sum_Q U(Q)|\Delta(Q)|^2 + \sum_{n=1}^{\infty}\sum_X n\omega_c a^\dagger_{n,X}a_{n,X} \\ + \sum_Q\sum_X\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}U_{nm}(Q)\Delta(-Q)\exp(-iQ_xX)a^\dagger_{n,X_+}a_{m,X_-}\,.\end{aligned} \tag{B1}$$

The first two terms in Eq. (B1) are the same as Eq. (2.9), and the notations are the same as in Sec. II. The other terms come from the higher Landau levels. The annihilation operator in the nth Landau level is written as

$a_{n,X}$, where $a_{0,X}\equiv a_X$. The effective potential $U_{nm}(Q)$ is given by

$$U_{00}(Q)=0\ , \tag{B2}$$

$$U_{nm}(Q)=U^*_{mn}(-Q)$$
$$=\frac{e^2}{\epsilon l}\left[\frac{i}{\sqrt{2}}lQ_x+\frac{1}{\sqrt{2}}lQ_y\right]^{n-m}\left[\frac{1}{Ql}\exp(-\tfrac{1}{2}l^2Q^2)\left[\frac{m!}{n!}\right]^{1/2}L_m^{(n-m)}(\tfrac{1}{2}l^2Q^2)\right.$$
$$\left.-\frac{1}{\sqrt{2}}\frac{\Gamma(n+\frac{1}{2})}{\Gamma(n-m+\frac{1}{2})}{}_1F_1(n+\tfrac{1}{2},n-m+\tfrac{1}{2};-\tfrac{1}{2}l^2Q^2)\right]. \tag{B3}$$

In this equation it is assumed without the loss of generality that $n>m$, $L_m^{(n)}(X)$ is the Laguerre function, $\Gamma(n)$ is the gamma function, and ${}_1F_1(\alpha;\beta;X)$ is the hypergeometric function.

The unperturbed state is given by $|\Phi\rangle$, Eq. (3.2). The correction to the ground-state energy in the second-order perturbation is given by

$$\Delta E=\sum_{Q_1}\sum_{Q_2}\sum_{X_1}\sum_{X_2}\sum_{n=1}^{\infty}U_{0n}(Q_1)U_{n0}(Q_2)\Delta(-Q_1)\Delta(-Q_2)$$
$$\times\exp(-iQ_{1x}X_1-iQ_{2x}X_2)\left\langle\Phi\left|a^\dagger_{0X_{1+}}a_{nX_{1-}}\frac{1}{E_{\rm HF}-H_{\rm HF}}a^\dagger_{n,X_{2+}}a_{0X_{2-}}\right|\Phi\right\rangle, \tag{B4}$$

where

$$X_{1\pm}=X_1\pm\tfrac{1}{2}l^2Q_{1y}\ , \tag{B5}$$

$$X_{2\pm}=X_2\pm\tfrac{1}{2}l^2Q_{2y}\ . \tag{B6}$$

The energy denominator $E_{\rm HF}-H_{\rm HF}$ can be approximated by $-n\omega_c$. Then ΔE is expressed as follows:

$$\Delta E=-\frac{L^2}{2\pi l^2}\sum_{n=1}^{\infty}\sum_{Q_1}\sum_{Q_2}\frac{1}{n\omega_c}U_{0n}(Q_1)U_{n0}(Q_2)\Delta(Q_1+Q_2)\Delta(-Q_1)\Delta(-Q_2)\exp\left[\frac{i}{2}l^2(Q_{2x}Q_{1y}-Q_{1x}Q_{2y})\right], \tag{B7}$$

where we have used Eq. (3.13) and the following relation:

$$\langle\Phi\,|\,a_{n,X_1}a^\dagger_{n,X_2}\,|\,\Phi\rangle=\delta_{X_1,X_2},\quad n\geq 1\ . \tag{B8}$$

The value of ΔE depends on the ratio of ω_c and $e^2/\epsilon l$. When ω_c is $1.5e^2/\epsilon l$, ΔE is about 0.8% of $E_{\rm HF}$ at $\nu=\frac{1}{3}$.

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