Charge-density-wave states in the fractional quantum Hall regime

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We show that within the Hartree-Fock approximation, self-consistent solutions exist for the two-dimensional electron gas in the extreme quantum limit which show energy cusps at filling factors of odd denominator only. The associated gaps are larger for rational factors represented by simple fractions. One such state holding 0.5 electrons in the charge-density-wave unit cell is discussed in detail.

I. INTRODUCTION

The understanding of how a two-dimensional electron gas behaves in the presence of a large magnetic field has gained primary attention since the discovery of the quantum Hall effect.[1,2] In particular the role of interactions among the electrons has been studied using various approaches in order to explain the effect in the extreme quantum limit, where only the lowest Landau level is occupied and it is not filled. It is a general belief that at a very low concentration of electrons the system forms a Wigner crystal with the electrons well localized at the lattice sites of a triangular lattice.[3-5] As electrons are added and the occupation of the level approaches 1 some controversy remains as to whether the charge density in the ground state has space fluctuations or not.[6-12] If the latter is the case and the electrons form an homogeneous liquid in some regime, a transition to the Wigner solid or, more generally, to a charge-density wave (CDW), must occur.

The Hartree-Fock theory predicts that at zero temperature such a transition takes place when the Landau level is exactly full. At fractional filling ν the exchange interaction stabilizes a CDW solution of the self-consistent equations. These solutions are constructed assuming a lattice symmetry for the charge density characterized by a unit cell that holds γ electrons. Both the shape of the cell and the size of γ are input parameters in the Hartree-Fock scheme. It is known that the lowest-energy solution in the case of a unidirectional wave occurs for a large γ of the order of the ratio between the linear dimensions of the system L and the magnetic length l.[13] In contrast, the choice $\gamma=1$ minimizes the energy when a square or an hexagonal cell is assumed, with the latter giving the lowest energy of all.[14,15]

A serious objection raised against this theory is that it fails to provide a state with the proper features to account for the presence of a gap when den(ν) is odd and its absence when den(ν) is even.[15] By den(x) we denote the denominator of the fraction x. The existence of such a gap is at the basis of our current understanding of the zero-resistance Hall states found in experiment. It has been suggested recently however that such a state exists within Hartree-Fock theory and that actually there is an infinite number of them possible.[16] They are constructed by choosing a CDW cell holding a fractional number of electrons γ, with den(γ) a power of 2.

In this work we study in detail the state with $\gamma=0.5$ electrons per CDW cell. We show that a gap is present when den(ν) is odd and evaluate its energetics. In Sec. II we review briefly the Hartree-Fock theory and show that in the extreme quantum limit a liquid state is possible only if the Landau level is full. In Sec. III the properties of the $\gamma=0.5$ state are presented and in Sec. IV our results and possible implications are discussed.

II. THE HARTREE-FOCK EQUATIONS

We consider N interacting electrons confined to move in a plane normal to an external magnetic field $\mathbf{B}$. In the Hartree-Fock approximation the single-particle states $|\alpha\rangle$ obey the equation

$$\left[\frac{1}{2m}(\mathbf{p}-e\mathbf{A}/c)^2+\sum_{\alpha'} n_{\alpha'}\langle\alpha'|V|\alpha'\rangle\right]|\alpha\rangle-\sum_{\alpha'} n_{\alpha'}\langle\alpha'|V|\alpha\rangle|\alpha'\rangle=\varepsilon_\alpha|\alpha\rangle\ . \tag{1}$$

The label α represents orbital and spin quantum numbers. V is the Coulomb potential between electrons. We are interested in spin-polarized states where all spins are aligned with the external field so that we shall ignore the spin degree of freedom as well as the Zeeman energy.[12,17] We use the Landau gauge $\mathbf{A}=B(0,x,0)$ throughout, in which the noninteracting ($V=0$) solutions of (1) are

$$\langle r|nk\rangle=\frac{1}{(2^n n!\pi^{1/2}lL)^{1/2}}e^{iky}\times\exp\left[-\frac{(x-l^2k)^2}{2l^2}\right]H_n(x/l-lk)\ , \tag{2}$$

$$\varepsilon_n=\frac{\hbar^2}{2ml^2}(2n+1)\ ,$$

with $H_n(z)$ the Hermite polynomial. There are two length scales in the problem: the linear dimensions L of the plane the electrons move in, and the magnetic length $l=(\hbar c/eB)^{1/2}$. States are characterized by the quantum numbers n,k and energies are degenerate in k with degeneracy $D=L^2/(2\pi l^2)$. We are interested in the case of a large magnetic field with an energy-level filling factor $\nu=N/D\leq 1$ (quantum limit) so that even in the presence of the mutual interaction between the electrons only the states with $n=0$ (lowest Landau level) are relevant. Mixing of the states with higher unperturbed energy states will be ignored in our treatment.

An important result of the Hartree-Fock approximation is that in the quantum limit a uniform (liquid) spin-polarized state can only exist if the lowest Landau level is full. To prove this statement consider the sum rule (Appendix A)

$$\sum_{\mathbf{q}} |\rho_{\mathbf{q}}|^2 e^{l^2q^2/2}=N_0^2/\nu\ , \tag{3}$$

where $N_0=N/L^2$ is the electron density and

$$\rho_{\mathbf{q}}=\frac{1}{L^2}\sum_{\alpha} n_\alpha \langle \alpha | e^{i\mathbf{q}\cdot\mathbf{r}} | \alpha\rangle \tag{4}$$

is a Fourier component of the electron distribution. For a uniform density $\rho_{\mathbf{q}}=N_0\delta_{\mathbf{q},0}$, which replaced in (3) shows that the liquid state is consistent only if $\nu=1$. At lower values of ν all self-consistent Hartree-Fock solutions have space fluctuations.

Charge-density-wave states are solutions of (1) obeying the condition

$$\rho_{\mathbf{q}}=\sum_{\mathbf{G}}\rho_{\mathbf{G}}\delta_{\mathbf{G},\mathbf{q}}\ . \tag{5}$$

The charge density has the symmetry of a lattice whose reciprocal-lattice vectors are the set $\mathbf{G}$. In order to solve Eq. (1) for these ansatz states it is convenient to write this equation in the representation defined by the basis (2). Only the interaction-energy matrix elements are of interest in this representation since the kinetic energy terms are diagonal and independent of k and may be handled in a trivial way. Taking the inner product of (1) with the state $\langle k |$ and evaluating the matrix elements of the Coulomb potential in this representation we obtain, using (5)

$$\left[\varepsilon_\alpha-\frac{\hbar^2}{2ml^2}\right]\langle k|\alpha\rangle-\sum_{\mathbf{G}} V_{\mathbf{G}} e^{-i(k+G_y/2)l^2G_x} e^{-l^2G^2/4}\langle k+G_y|\alpha\rangle=0\ , \tag{6}$$

where

$$V_{\mathbf{G}}=\frac{\nu\rho_{\mathbf{G}}}{N_0}\left[\frac{1-\delta_{\mathbf{G},0}}{lG}-\sqrt{\pi/2}I_0\left[-\frac{l^2G^2}{4}\right]e^{l^2G^2/4}\right]\frac{e^2}{\varepsilon l}\ , \tag{7}$$

is the effective potential of the Coulomb interaction. The first and second terms in the square bracket represent the direct and exchange contributions, respectively. $I_0(x)$ is a modified Bessel function. The potential depends on the charge density as determined from the solutions of Eq. (6),

$$\rho_{\mathbf{G}}=\frac{1}{L^2}\sum_{\alpha} n_\alpha \sum_{k}\langle k|\alpha\rangle\langle\alpha|k+G_y\rangle \times e^{-l^2G^2/4} e^{il^2(k+G_y/2)G_x}\ . \tag{8}$$

Equations (6)–(8) must be solved self-consistently to obtain the CDW state. The total energy is then given by

$$E=\tfrac{1}{2}\sum_{\alpha} n_\alpha\left[\varepsilon_\alpha+\frac{\hbar^2}{2ml^2}\right]$$

or

$$\varepsilon=\frac{\hbar^2}{2ml^2}-\sqrt{\pi/2}\frac{\nu}{2}\frac{e^2}{\varepsilon l}+\frac{1}{2N_0}\sum_{\mathbf{G}(\neq 0)}\rho_{\mathbf{G}}^* V_{\mathbf{G}}\ , \tag{9}$$

where $\varepsilon=E/N$ is the energy per particle. The first term is the kinetic energy, the second arises from exchange in the average electron distribution, and the third gives the contribution due to space fluctuations.

The CDW state is possible thanks to the exchange interaction, which, as is apparent in (7), has the sign opposite to the direct Coulomb term. It assures that the potential minima will occur where the electron is most likely to be found. This can be clearly appreciated if one uses the Gaussian approximation

$$\rho_{\mathbf{G}}=N_0 e^{-l^2G^2/2}\ , \tag{10}$$

which is known to reproduce quite accurately the self-consistent solution of Eqs. (6)–(8) if $\gamma=1$ and $\nu\leq 0.4$.[15] In this approximation the charge density at the origin and any other lattice point is

$$\rho(0)=\sum_{\mathbf{G}}\rho_{\mathbf{G}}=N_0\sum e^{-l^2G^2/2}\ .$$

This sum may be evaluated with the aid of (5) and (3) and gives $\rho(0)=\nu^{-1}$. The electrons form a lattice of Gaussians whose height grow as the system is made more dilute at constant magnetic field. The Fourier components of the potential in this approximation as given by (7) approach those of a lattice of positive charge in a negative uniform background (Appendix B). This remarkable result is entirely due to exchange and provides for the attractive wells at the lattice sites needed to achieve self-consistency.

III. STATES WITH FRACTIONAL γ

Some general results concerning the spectrum of Eq. (6) are well known.[18,19] Its structure is completely deter-

mined by the number of flux quanta ϕ traversing the unit cell of the effective crystalline potential. If this number is a rational $\phi=p/q$ then the eigenvalues are grouped into a set of exactly p bands. This results from the fact that the coefficients of the set of linear equations (6) depend on the index k through the argument of circular functions only and the equations can therefore be closed and made a finite set, p in number. The coefficients are Hermitian so that there are p solutions for each value of the quantum numbers α, yielding p bands as these numbers are varied. Another known result is that bands do not overlap and hold an equal number of states D/p.

A theory of the fractional quantum Hall effect can be constructed with the use of just these facts. It involves the usual language of bands and gaps of solid-state physics. Take for instance a CDW holding $\gamma=0.5$ of an electron per cell. Then one can show that of the p bands composing the Hartree-Fock orbital spectrum an integral number is filled and the rest empty if den(ν) is odd, whereas a half-filled band occurs if den(ν) is even, as in a metal. To see this we write $\nu=(N/N_c)/(D/N_c)$, where N_c is the number of CDW cells in the sample. In this fraction the numerator is the number of electrons per cell that we fix at the value 0.5, and the denominator is the degeneracy per cell which is just our parameter ϕ, so that $\nu=(q/2)/p$. Thus, of the p bands available, $q/2$ are filled. In order that this number be an integer, q must be even implying that p which is prime to q, must be odd. Thus it is a necessary condition for the existence of a gap that den(ν)$=p$ be odd. One can easily check that when den(ν) is even there is always a half-filled band so there is no gap above the last occupied state. All other fractional values of γ of denominator 2^k have the same property only that if the positive integer $k\neq 1$ the occupancy of the partially occupied band is a fraction in general different from $\frac{1}{2}$.

It remains to be shown that a gap is actually present in the many body system. Such a gap is manifest through downward cusps in the energy function as the parameters

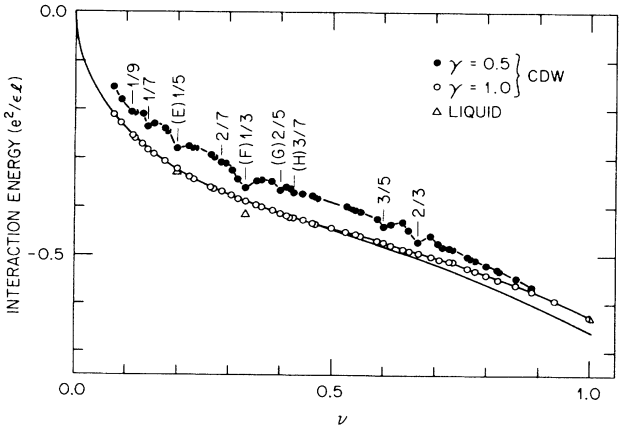

FIG. 1. Interaction energy per particle $\varepsilon-\hbar^2/2ml^2$ for the Hartree-Fock charge-density-wave states with 0.5 electrons (closed circles) and 1.0 electrons (open circles) per cell. The solid line is the Gaussian approximation and triangles are for the liquid state of Ref. 6.

are varied.[20] We present results for the case $\gamma=0.5$ and a triangular lattice.[21] Equations (6)—(8) were solved self-consistently keeping up to 11 shells of Fourier components in the potential. The accuracy of a solution was checked through the sum rule (3) and found the best values to obey it to within six significant figures. Figure 1 shows the interaction energy per particle at several rational values of ν in the interval 0—1. Self-consistent solutions (open circles) for the $\gamma=1$ case, as well as the Gaussian approximation (solid line) are included for comparison. Results for odd values of den(ν) up to 19 and accuracy within the resolution of the figure only are shown. The triangles are the energies of the correlated Jastrow function proposed by Laughlin.[6] It is apparent from the figure that our sample state with $\gamma=0.5$ exhibits the appropriate cusps at simple fractions of ν and that the $\gamma=1.0$ state does not. This selective behavior may be understood with the aid of Fig. 2 which shows the dimensionless eigenvalues

$$\lambda=(\varepsilon_\lambda-\hbar^2/2ml^2-V_0)\exp(\pi/\sqrt{3}\phi)/2V_1$$

of (6) as a function of the flux parameter ϕ. Fourier coefficients up to the first shell of reciprocal-lattice vectors were retained in the potential when obtaining this plot only. Higher-order coefficients do not change the graph qualitatively. Note that the number of bands equals the numerator of ϕ in all cases as expected, and that these bands never overlap. Other properties of this plot were discussed in Ref. 19. A diagonal AB has been drawn through the main gap to separate its lower (L) from its upper (U) portion. It is known that the number of states in L equals D/ϕ. Now, since $D/\phi=\nu D/\gamma=N/\gamma$ when $\gamma=1$, all these states are occupied while all states in U are empty. A large gap separates occupied from unoccupied states and the Fermi energy may be associated with a λ value somewhere near the line AB for all values of $0<\nu<1$. As more particles are added to the system at constant magnetic field, just as many new states appear in the lower portion L so that as γ (or ϕ) is changed the extra electrons exactly keep this portion filled while U remains empty. This makes the energy per particle smooth. When $\gamma=0.5$, on the contrary, L has twice as many states as there are electrons. States below point E, for example, are those occupied at $\nu=\frac{1}{5}$, while states above points F, G, and H are the filled ones for $\nu=\frac{1}{3}$, $\frac{2}{5}$, and $\frac{3}{7}$, respectively. To see how the cusps arise we look at the case $\nu=\frac{1}{3}$ more closely. The number of states above F is $D(1-1/\phi)=D-2N$ so that as the number of particles N is increased (moving to the right in the figure), less states are available and any additional electron above $\nu=\frac{1}{3}$ must occupy a state in the lower portion L separated from the rest by a gap. A similar situation occurs at points G, H, and E. This is the origin of the cusps appearing in the curve $\gamma=0.5$ in Fig. 2. Notice that the acuteness of a cusp is associated with the size of the corresponding gap and this in turn depends on how large the integers p,q are in the rational $\nu=q/2p$. As a rule the cusp becomes less prominent as the integers increase. Because of the self-similarity of the plot one actually expects a cusp everywhere in the curve $\varepsilon(\nu)$, for den(ν) odd, only that just those for low p,q integers will be visible.

A discontinuity in $\partial\varepsilon/\partial\nu$ implies an energy gap $\Delta(\nu)$ in the spectrum of elementary excitations. There are two inequivalent ways of taking this derivative, however, since the CDW cell size is an additional variable in the energy. The curves in Fig. 2 assume the cell size to change as ν is varied so that as more electrons are added to the system the number of electrons per cell γ stays the same. This criterion gives a gap for $\gamma=0.5$ and no gap in the $\gamma=1$ case as discussed previously. One may instead choose to keep the cell size fixed (ϕ constant) in computing the derivative, in which case by Koopman's theorem the energy gap is just the gap in the Hartree-Fock orbital spectrum. This procedure yields a gap both for $\gamma=1$ at all ν, and for $\gamma=0.5$ whenever den(ν) is odd. It turns out that in the latter case this gap is smaller than the one obtained using the first method. Values for selected filling factors are $\Delta(\frac{1}{3})=0.379$, $\Delta(\frac{2}{3})=0.265$, $\Delta(\frac{2}{5})=0.243$, and $\Delta(3/7)=0.172$, all in units of $e^2/\varepsilon l$.

IV. DISCUSSION

We have shown that the Hartree-Fock CDW state with 0.5 electrons in the unit cell has gaps whenever den(ν) is odd. The associated elementary excitations are electron-

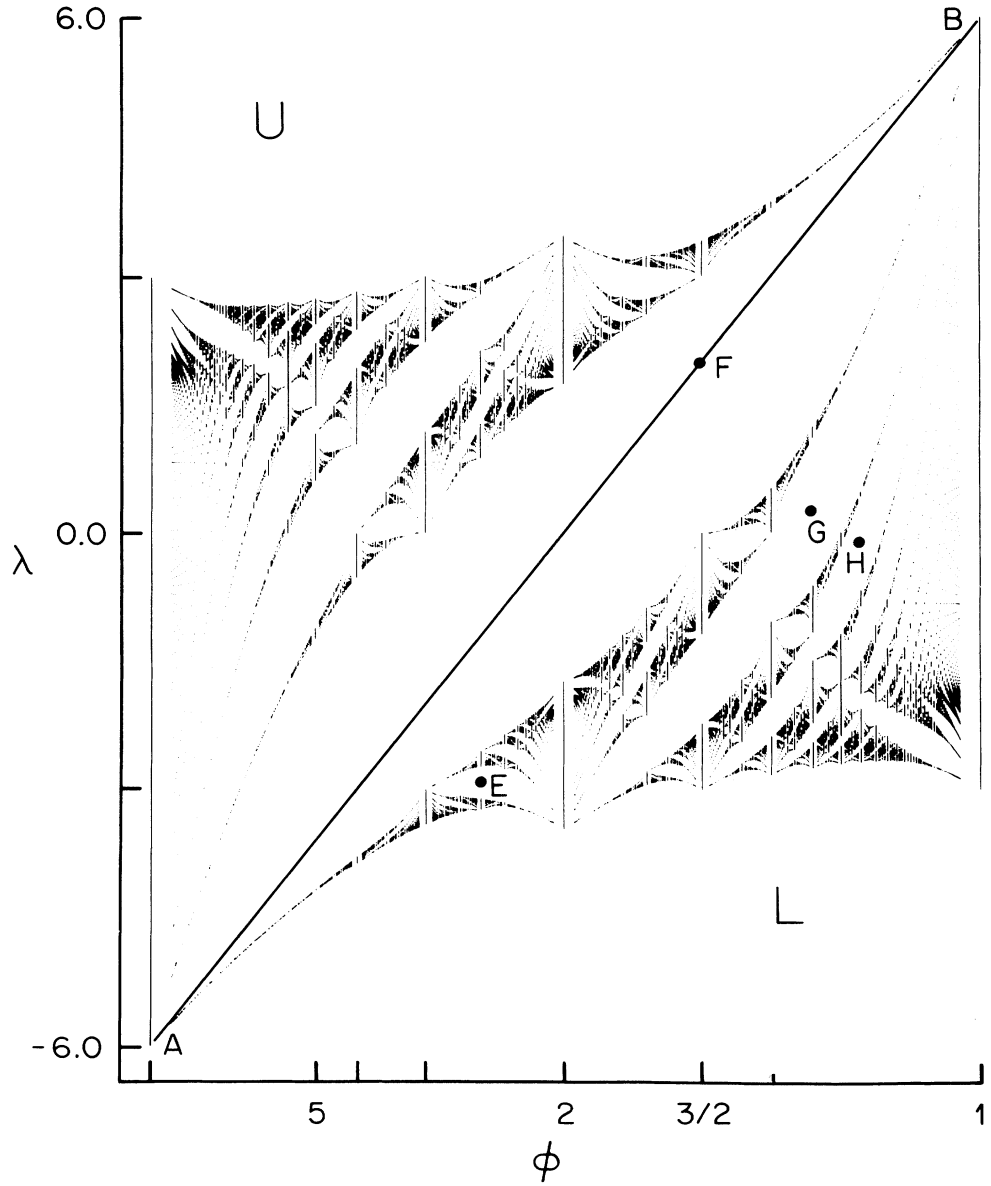

FIG. 2. Eigenvalues of Eq. (6) with one shell of Fourier components in the self-consistent potential retained. λ is a dimensionless energy parameter (see text). The variable ϕ is the number of flux quanta traversing a unit cell and is proportional to the external magnetic field. For purposes of discussion the plot has been divided by the diagonal AB into an upper (U) and lower (L) sections and gaps have been labeled (E—H) at certain values of ϕ.

hole pairs and the size of the gaps decreases as the integers characterizing the rational ν grow. Thus for instance, the gap at $\nu=\frac{1}{3}$ is larger than the gap at $\nu=\frac{2}{5}$. This state shows therefore all the qualitative features demanded by the current interpretation of the fractional quantum-Hall-effect data. The case studied here is part of a family of states characterized by a unit cell holding a fraction $m/2^k$ electrons. In spite of its success, our state, although variationally optimized in the Hartree-Fock sense, is not the lowest energy state even within Hartree-Fock theory. It could still be the best approximation to the true ground state given by this theory since electron correlations are known to be important[6–8] and the correlation energy is likely to affect differently the Hartree-Fock states with $\gamma=1$ and $\gamma=0.5$ electrons per cell. This is suggested by the fact that for a given value of ν these states have quite different order parameters, as one might expect. In the former case the charge density is concentrated in Gaussian peaks at sites of hexagonal symmetry in the lattice, whereas in the latter the density profile has a honeycomb structure with gentle peaks at points of triangular symmetry.[22] The effect of correlations in the $\gamma=0.5$ state is presently unknown. Yoshioka and Lee have used second-order perturbation theory to estimate the correlation energy in the $\gamma=1$ state and found a correction of about 0.5% over the interaction energy at $\nu=\frac{1}{3}$, a value an order of magnitude smaller than the improvements brought about by strongly correlated ansatz wave functions represented by the triangles in Fig. 1.

Even if the liquid transition at $T=0$ occurs at a value $\nu_c<1$ it is an important question what is the nature of the ground state with space fluctuations in the charge density at $\nu<\nu_c$. We hope our results will stimulate further studies of the CDW state, keeping in mind that the $\gamma=0.5$ state or other states in its class contain different physical properties than the $\gamma=1$ state.

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APPENDIX A

In order to prove the sum rule (3) we insert twice over the completeness relation of the states (2) into (4) and obtain

$$\rho_{\mathbf{q}}=\frac{1}{L^2}\sum_{\alpha} n_\alpha \sum_{k}\sum_{k'}\langle\alpha\,|\,k'\rangle\langle k\,|\,\alpha\rangle\langle k'\,|\,e^{i\mathbf{q}\cdot\mathbf{r}}\,|\,k\rangle\ ,$$

where the assumption that the states $|\alpha\rangle$ are in the lowest Landau level has been used. Using

$$\langle k'\,|\,e^{i\mathbf{q}\cdot\mathbf{r}}\,|\,k\rangle=\delta_{k',k+q_y}e^{-l^2q^2/4}e^{il^2(k+q_y/2)q_x}\ , \tag{A1}$$

we obtain

$$\rho_{\mathbf{q}}=\frac{1}{L^2}\sum_{\alpha} n_\alpha \sum_{k}\langle\alpha\,|\,k+q_y\rangle\langle k\,|\,\alpha\rangle \times e^{-l^2q^2/4}e^{il^2(k+q_y/2)q_x}\ . \tag{A2}$$

We next form the sum

$$S=\sum_{\mathbf{q}}|\rho_{\mathbf{q}}|^2e^{l^2q^2/2}=\frac{1}{L^4}\sum_{\alpha,\alpha'} n_{\alpha'}n_\alpha \sum_{k,k',q_y}\langle\alpha'\,|\,k'\rangle\langle k\,|\,\alpha\rangle\langle\alpha\,|\,k+q_y\rangle\langle k'+q_y\,|\,\alpha'\rangle\sum_{q_x}e^{il^2(k-k')qx}\ .$$

The last sum equals $D\delta_{kk'}$. Using the completeness relation twice and the orthonormality of the orbital states we obtain

$$S=\frac{D}{L^4}\sum_{\alpha} n_\alpha^2\ .$$

The sum equals the total number of electrons N so noting that $\nu=N/D$ we obtain $S=(N^2/L^4)/(N/D)=N_0^2/\nu$, which is the desired result. A version of this sum rule applicable to CDW states was first derived by Yoshioka and Lee.[15]

APPENDIX B

In the Gaussian approximation the effective CDW potential is

$$V_{\mathbf{G}}=\nu\left[\frac{1-\delta_{\mathbf{G},0}}{lG}e^{-l^2G^2/2} -\sqrt{\pi/2}I_0\left[-\frac{l^2G^2}{4}\right]e^{-l^2G^2/4}\right]\frac{e^2}{\varepsilon l}\ .$$

The second term within the square brackets has the asymptotic form

$$\sqrt{\pi/2}I_0(x)e^{-x}\sim\frac{1}{2x^{1/2}}+\frac{0.0624}{x^{3/2}}+\cdots\ ,$$

so that for lG sufficiently large,

$$V_{\mathbf{G}}\sim-2\pi N_0\frac{e^2}{\varepsilon G}\ , \tag{B1}$$

where we have used the equality $\nu=2\pi N_0 l^2$. This is just the Fourier component of the potential due to a lattice of positive point charges of charge $e/\sqrt{\varepsilon}$.

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