Phonons as Collective Modes: The Case of a Two-Dimensional Wigner Crystal in a Strong Magnetic Field

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We present a fully quantum-mechanical theory for the phonon modes of a two-dimensional Wigner crystal in the strong-magnetic-field limit. Our theory is based on a time-dependent Hartree-Fock approximation for the density-density response function χ which is exact in the harmonic limit but allows for arbitrarily large anharmonicity. Our calculation is facilitated by identities, valid in the strong-magnetic-field limit, which allow χ to be expressed *solely* in terms of the ground-state electron density.

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The usual description of phonon modes in a crystal is based on a harmonic approximation which assumes that displacements from lattice sites are small. For crystals formed from light particles this approximation can be poor even at zero temperature because of quantum-mechanical zero-point motion. A number of different techniques,[1] most based in different ways on the exact solution to the harmonic approximation, have been developed which can deal successfully with the anharmonicities of quantum solids. Nevertheless, it is clear that for extremely quantum solids a formulation in which expansions in displacements from lattice sites do not appear at all is desirable. It has long been recognized[2] that one such formulation is provided by a theory which treats the density fluctuations of a quantum solid in a time-dependent Hartree-Fock approximation (TDHFA). In this theory, the phonon modes appear as poles in the density-density response function and it is possible to show[2] that the familiar facts of harmonic lattice dynamics are recovered in the appropriate limit. The phonon modes are seen as collective excitations entirely analogous to the plasmon or zero-sound modes which occur when the ground state is a fluid and whose excitation energies are usually determined in the same way. The utility of this approach to the study of lattice dynamics in quantum solids has been limited by practical difficulties associated with the broken translational symmetry of the crystalline ground state. In this Letter we present its first successful application.

Because of the quantization of kinetic energy in units of $\hbar\omega_c=\hbar eB/m^*c$, electrons in two dimensions are expected to form a Wigner crystal in a strong magnetic field. The Wigner-crystal states are in competition with the incompressible fluid states[3] responsible for the fractional quantum Hall effect[4] which are especially stable when the filling factor of the lowest Landau level ($\nu\equiv 2\pi l^2 n\equiv n\Phi_0/B=nhc/eB$) is a fraction with an odd denominator. (We use l as our unit of length.) Recent experimental evidence[5] suggests that the crystal state becomes stable for $\nu\lesssim\frac{1}{4}$ except for ν near $1/m$ for $m=5,7$ and possibly[6] larger *odd* integers. Anomalies seen in sound propagation,[7] which are not yet fully understood, might indicate that the ground state is also crystalline for ν near $\frac{1}{2}$.

In the strong-field limit of the harmonic approximation to the crystal lattice dynamics[8] the phonon frequencies are given by

$$\omega_-=\frac{\sqrt{\det(D)}}{\omega_c}\equiv\frac{\omega_0^2}{\omega_c}\sqrt{\det(\tilde{D})} \tag{1}$$

and

$$\omega_+=\omega_c+\frac{1}{2}\frac{\operatorname{tr}(D)}{\omega_c}=\omega_c+\frac{\omega_0^2}{2\omega_c}\operatorname{tr}(\tilde{D}), \tag{2}$$

where D is the dynamical matrix in the absence of a magnetic field, $\tilde{D}=\omega_0^{-2}D$ is a dimensionless quantity, $\omega_0^2=8e^2/ma_0^3$, and a_0 is the triangular crystal lattice constant. Since $\omega_0^2/\omega_c=(e^2/\hbar l)(\nu\sqrt{3}/\pi)^{1.5}$ is independent of the electron mass, we see that the lower phonon frequency corresponds to an excitation of the Wigner crystal in which the quantized kinetic energy is not changed while the upper phonon frequency corresponds to an excitation in which an electron is promoted to a higher Landau level. We show below that this quantization of kinetic energy and the absence of Landau-level mixing in the strong-field limit of the Wigner crystal allows the density-density response function to be evaluated in a remarkably simple way.

In the strong-field limit of the Hartree-Fock approximation (HFA) for the crystalline ground state,[9] the single-particle HF Hamiltonian is given by $H=\sum_{\mathbf{G}}W(\mathbf{G})\bar{\rho}(\mathbf{G})$, where $\bar{\rho}(\mathbf{k})$ is the density operator projected onto the lowest Landau level. Each electron sees an identical periodic potential W with Fourier transform

$$\begin{aligned}W(\mathbf{G})&=\frac{1}{A}\left[\frac{2\pi e^2}{|\mathbf{G}|}(1-\delta_{G,0})-e^{G^2/2}\int d^2q\,\frac{e^2}{q}e^{i(q_xG_y-q_yG_x)}e^{-q^2/2}\right]\rho_{\mathrm{HF}}(\mathbf{G})\\&\equiv\frac{1}{A}[V_c(\mathbf{G})-I(\mathbf{G})]\rho_{\mathrm{HF}}(\mathbf{G})\equiv\frac{U(\mathbf{G})\rho_{\mathrm{HF}}(\mathbf{G})}{A},\end{aligned} \tag{3}$$

where $V_c(\mathbf{G})=2\pi e^2/|\mathbf{G}|$ is the 2D Coulomb interaction, $\rho_{\rm HF}(|\mathbf{G}|)$ is the Fourier transform of the ground-state density, A is the system area, and $-I(\mathbf{G})$ is the exchange contribution to the effective electron-electron interaction. (The **G**'s are reciprocal-lattice vectors of the crystal.) The fact that the exchange contribution to $W(\mathbf{G})$ is proportional to $\rho_{\rm HF}(\mathbf{G})$ is a consequence of the analyticity of the single-particle wave functions in the lowest Landau level which allows the one-particle density matrix to be expressed in terms of its diagonal elements.[10] The static HFA cannot account for the correlations between the motions of electrons on different lattice sites which are responsible for the low excitation energies of long-wavelength phonons, and in the harmonic limit ($\nu \ll 1$) reduces to an optimal Einstein oscillator approximation in which the zero-point energy of the lattice is overestimated[11] by about 15%. The TDHFA describes the correlated density fluctuations around the HFA mean-field approximation.

In the strong-field limit the TDHFA density-density response function is given by

$$\chi(\mathbf{r}_1,\mathbf{r}_2;\omega_n)=\chi^0(\mathbf{r}_1,\mathbf{r}_2;\omega_n)+\hbar^{-1}\int d^2r_3\int d^2r_4\,\chi^0(\mathbf{r}_1,\mathbf{r}_3;\omega_n)U(\mathbf{r}_3-\mathbf{r}_4)\chi(\mathbf{r}_3,\mathbf{r}_4;\omega_n)\,, \tag{4}$$

where $\chi^0(\mathbf{r}_1,\mathbf{r}_2;\omega_n)$ is the density-density response functions for noninteracting electrons in the HFA effective periodic potential and $U(\mathbf{r})$, the Fourier transform of $U(\mathbf{q})$, describes the Coulombic and exchange fields seen by the responding electrons. Diagrammatically, Eq. (4) corresponds to the usual summation of bubble and ladder diagrams for χ. This simple form results from the analyticity of the Landau-level wave functions which allows[10,12] the interaction lines in ladder diagrams to be converted to interaction lines between bubbles (χ^0) with $V_c(\mathbf{q})$ replaced by $I(\mathbf{q})$.

In general, the evaluation of

$$\chi^0(\mathbf{r}_1,\mathbf{r}_2;\omega_n)=\frac{1}{\beta\hbar}\sum_{\omega_p}G(\mathbf{r}_1,\mathbf{r}_2;\omega_n+\omega_p)G(\mathbf{r}_2,\mathbf{r}_1;\omega_p) \tag{5}$$

requires a knowledge of the eigenvalues and eigenvectors of the one-particle HF Hamiltonian. This process is very cumbersome and time consuming, especially in light of the intricate electronic structure of electrons in a periodic potential and a constant magnetic field.[13] We have found, however, that in the strong-magnetic-field limit it is possible to express χ^0 in terms of the ground-state density alone. This property follows from using the commutation relation for the density operator projected onto the lowest Landau level,[14]

$$[\bar\rho(\mathbf{k}_1),\bar\rho(\mathbf{k}_2)]=2i\exp\left(\frac{\mathbf{k}_1\cdot\mathbf{k}_2}{2}\right)\sin\left(\frac{(\mathbf{k}_1\times\mathbf{k}_2)\cdot\hat{\mathbf{z}}}{2}\right)\bar\rho(\mathbf{k}_1+\mathbf{k}_2)\,, \tag{6}$$

in the equation of motion for χ^0. Using the periodicity of the crystalline state it is sufficient to consider

$$\begin{aligned}\chi^0_{\mathbf{G},\mathbf{G}'}(\mathbf{k};\omega_n)&=\int d\mathbf{r}\int d\mathbf{r}'\,e^{-i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}\chi^0(\mathbf{r},\mathbf{r}';\omega_n)e^{i(\mathbf{k}+\mathbf{G}')\cdot\mathbf{r}'}\\&=\int_0^{\beta\hbar}d\tau\,e^{-i\omega_n\tau}\{-\langle T\bar\rho(\mathbf{k}+\mathbf{G},\tau)\bar\rho(-\mathbf{k}-\mathbf{G}',0)\rangle\}\,,\end{aligned} \tag{7}$$

where

$$\frac{\hbar\,\partial\bar\rho(\mathbf{k},\tau)}{\partial\tau}=[H_{\rm HF},\bar\rho(\mathbf{k},\tau)]=\sum_{\mathbf{G}}W(\mathbf{G})[\bar\rho(\mathbf{G},\tau),\bar\rho(\mathbf{k},\tau)]\,, \tag{8}$$

and **k** is in the crystalline Brillouin zone. Differentiating the quantity in curly brackets in Eq. (7) with respect to τ using Eqs. (8) and (6) gives, after analytically continuing to real frequencies,

$$\sum_{\mathbf{G}''}[(\omega+i\delta)\delta_{\mathbf{G},\mathbf{G}''}-A_{\mathbf{G},\mathbf{G}''}(\mathbf{k})]\chi^0_{\mathbf{G}'',\mathbf{G}'}(\mathbf{k};\omega)=-B_{\mathbf{G},\mathbf{G}'}(\mathbf{k})\,, \tag{9}$$

where

$$B_{\mathbf{G},\mathbf{G}'}(\mathbf{k})=2ie^{-(\mathbf{k}+\mathbf{G})\cdot(\mathbf{k}+\mathbf{G}')/2}\sin\left(\frac{[(\mathbf{k}+\mathbf{G})\times(\mathbf{k}+\mathbf{G}')]\cdot\hat{\mathbf{z}}}{2}\right)\rho_{\rm HF}(\mathbf{G}-\mathbf{G}') \tag{10}$$

and

$$A_{\mathbf{G},\mathbf{G}'}(\mathbf{k})=2ie^{-(\mathbf{k}+\mathbf{G})\cdot(\mathbf{G}-\mathbf{G}')/2}\sin\left(\frac{[(\mathbf{k}+\mathbf{G})\times(\mathbf{k}+\mathbf{G}')]\cdot\hat{\mathbf{z}}}{2}\right)\frac{\rho_{\rm HF}(\mathbf{G}-\mathbf{G}')U(\mathbf{G}-\mathbf{G}')}{\hbar}\,. \tag{11}$$

Comparing Eqs. (4) and (9) it follows that, in an obvious matrix notation,

$$[(\omega+i\delta)I-A(\mathbf{k})+B(\mathbf{k})U(\mathbf{k})]\chi(\mathbf{k};\omega)=-B(\mathbf{k})\,, \tag{12}$$

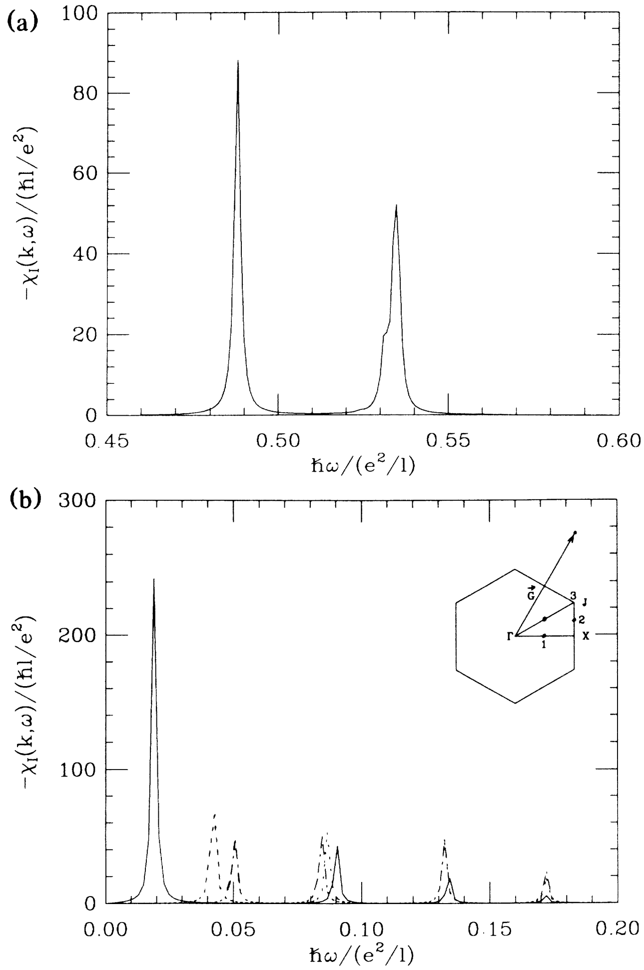

FIG. 1. (a) $\mathrm{Im}(\chi^0_{G,G})$ as a function of ω for filling factor $\nu=\frac{1}{4}$ and at a given $\mathbf{k}$ showing the transitions between the one occupied and the three unoccupied subbands of the first Landau level. (b) $\mathrm{Im}(\chi_{G,G})$ at filling factor $\nu=\frac{1}{4}$ for $\mathbf{k}$'s at the points labeled 1–3 in the inset. [A solid line is used for point 1, a dashed line for point 2, and a dash-dotted line for point 3. The inset also shows the $\mathbf{G}$ used in (a) and (b).] The strong peaks at low frequencies reflect the magnetophonon excitations. The intersubband excitations of (a) have disappeared in $\mathrm{Im}(\chi)$, being replaced by new anharmonic effects (see text).

where $U_{G,G'}(\mathbf{k})=\delta_{G,G'}U(\mathbf{k}+\mathbf{G})$.

Using Eqs. (9) and (12), $\chi^0(\mathbf{k};\omega)$ and $\chi(\mathbf{k};\omega)$ can be evaluated simply by inverting a matrix once $\rho_{\mathrm{HF}}(\mathbf{G})$ is known.[15] Since $\rho_{\mathrm{HF}}(\mathbf{G})$ decreases rapidly with $|\mathbf{G}|$, an accurate approximation to $\chi^0(\mathbf{k};\omega)$ and $\chi(\mathbf{k};\omega)$ can be obtained when the infinite matrices are truncated to a relatively small number of shells of reciprocal-lattice vectors. $\mathrm{Im}[\chi^0(\mathbf{k};\omega)]$ is plotted in Fig. 1(a) at a given wave vector $\mathbf{k}$ (χ^0 has a very weak $\mathbf{k}$ dependence) and for $\nu=\frac{1}{4}$. It shows peaks associated with transitions between the one occupied and the three unoccupied Hofstader subbands[13] of the Landau level which occur at this filling factor. (The gap between the third and fourth subbands is smaller than the width of the lowest subband.) We have compared χ^0's evaluated from Eq. (9) with those obtained from brute force evaluation of Eq. (5) and find excellent agreement. It is remarkable that the detailed spectral features in χ^0 are captured without reference to the single-particle density of states. $\mathrm{Im}(\chi)$ is plotted in Fig. 1(b). The lowest-energy peak in $\mathrm{Im}(\chi)$ is strongly $\mathbf{k}$ dependent and it traces out the dispersion relation of the magnetophonon branch which is associated with intra-Landau-level excitations. Anharmonic effects described by the TDHFA are clearly reflected in the remaining structure of $\mathrm{Im}(\chi)$ and also in the finite width (i.e., finite lifetime) of the magnetophonon excitations. The positions of the multiphonon peaks seen in Fig. 1(b) are more weakly $\mathbf{k}$ dependent, indicating that these excitations are quite localized. We see that including correlations qualitatively alters the density fluctuations. In particular, $\mathrm{Im}(\chi)$ has essentially no structure at frequencies higher than those of Fig. 1(b); i.e., no trace remains in the TDHFA of the transitions between Landau-level subbands which occur in the independent-electron approximation.

The dispersion relation of the magnetophonon modes obtained from the peaks of $\mathrm{Im}(\chi)$ is plotted in Fig. 2 for different filling factors and compared with that obtained in the harmonic approximation and in a partially[16] self-consistent harmonic approximation in which the electrons are given a form factor $(2\pi l^2)^{-1}\exp(-|\mathbf{r}-\mathbf{R}_i|^2/2l^2)$ corresponding to the quantized cyclotron orbits of the lowest Landau level. At small filling factors the form-factor approximation accounts reasonably well for the anharmonic corrections to the magnetophonon dispersion but at larger filling factors the corrections are substantially overestimated. We find that the TDHFA

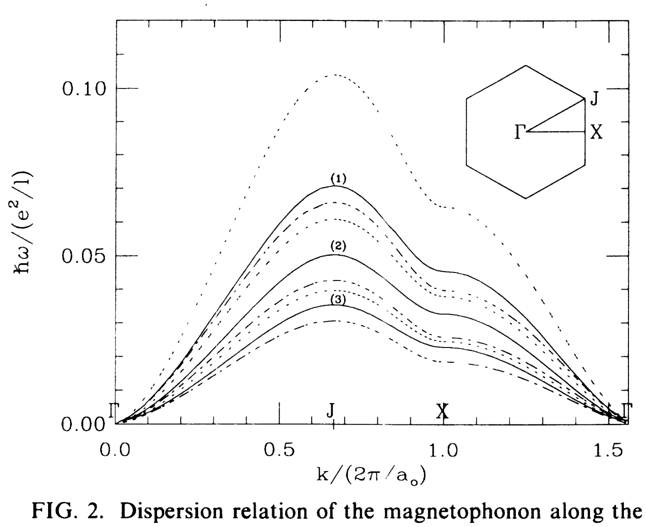

FIG. 2. Dispersion relation of the magnetophonon along the edges of the irreducible Brillouin zone (see inset) for filling factors (1) $\nu=\frac{1}{3}$, (2) $\nu=\frac{1}{4}$, (3) $\nu=\frac{1}{5}$, and for the TDHFA (solid line), the harmonic approximation (dash-dotted line), and the form-factor approximation (dashed line). At a given filling factor, the TDHFA result lies between the other results.

dispersion relation can be phenomenologically approximated by setting $l \rightarrow \alpha l$ in the form factor, where $\alpha = \alpha(\nu)$ decreases with ν and approaches 1 at small filling factors.

In summary, although the dispersion relation of the magnetophonons obtained in the TDHFA is remarkably similar to that obtained by other methods, the TDHFA results do contain qualitatively new features due to anharmonicity. We have used the equation-of-motion method described in this Letter to study the dispersion relation of the magnetoplasmon modes which occur at energies near $\hbar\omega_c$ by allowing for transitions between the $n=0$ and $n=1$ Landau levels. Generalization to transitions from $n=0$ to $n>1$ identify excitation modes with no classical analog.[17] In addition, we are presently studying the effect of pinning on the Wigner-crystal ground state and on its excitations. In closing, we remark that the equation-of-motion method presented here suggests a new approach to the study of localization in the strong-field limit.

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[15]A similar analysis using the equation of motion for the one-particle Green's function allows $\rho_{\mathrm{HF}}(\mathbf{G})$ to be determined by inverting a matrix dependent only on the crystal type and the Landau-level filling factor.

[16]This type of approximation has been employed by Kazumi Maki and Xenophen Zotos, Phys. Rev. B **28**, 4349 (1983). It can be regarded as a self-consistent phonon approximation in which the change in the effective potential due to the zero-point motion of the cyclotron orbit centers is neglected.

[17]This result, along with a more detailed account of the results presented here, will be published separately. R. Côté and A. H. MacDonald (to be published).