Self-consistent phonon and magnetophonon and cubic anharmonic corrections of the 2D electron lattice

Self-consistent phonon and magnetophonon and cubic anharmonic corrections of the 2D electron lattice

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Abstract. Anharmonic corrections to the phonon and magnetophonon spectrum of the two-dimensional electron solid at zero temperature are investigated. A self-consistent phonon theory is used and the cubic anharmonic correction coming from second order perturbation theory is included. This correction is larger than the self-consistent one, and yields a decrease in the phonon spectrum. Lindemann's ratio and corrections to the total energy of the solid are calculated as well.

1. Introduction

There has recently been great interest in the quantum two-dimensional electron solid and its melting properties, with and without a perpendicular magnetic field. Willett *et al* [1] found that, in the low-density limit, the conductivity of GaAs heterojunctions in a strong external magnetic field is activated in character and interpreted this as the presence of a solid phase. Jiang *et al* [2] observed re-entrant melting behaviour close to a filling factor of 1/5. Andrei *et al* [3] observed anomalies in long-wavelength acoustic wave absorption around the same filling factor. Goldman *et al* and Williams *et al* [4] observed non-linear conductivity behaviour at low filling factors. All these experiments in high magnetic fields suggest the existence of a two-dimensional quantum electron solid. Tanatar *et al* [5] performed fixed node Green function Monte Carlo simulations on the 2D quantum electron fluid and solid. They found a solid–fluid transition at $r_s = 37$ with a mean square displacement of about $\gamma = 0.25$. This compares favourably with earlier variational Monte Carlo calculations by Ceperley [6], who found the transition at $r_s = 33$ with the same Lindemann ratio. Experiments at zero field were performed about ten years ago on the surface of liquid helium, but these experiments were probing the Wigner crystal in the classical or finite temperature regime where there is no long-range order present in the system.

To understand and assess the anharmonicity that may become important near melting, we studied the self-consistent phonons of the electron lattice together with their cubic-anharmonic corrections.

Let us introduce some definitions and notations first. The kinetic energy of the 2D electron system, measured in units of Rydberg, is proportional to $1/r_s^2$ where $\pi a_0^2 r_s^2 = 1/n_s$ and $a_0 = \hbar^2/me^2$ is the Bohr radius and n_s the electron density. The potential energy is proportional to $1/r_s$ and therefore at low densities or large r_s the kinetic energy becomes negligible, and since correlations between electrons become

important, the lowest energy state will be realized by electrons sitting on a regular lattice. This was Wigner's original argument [7] that predicted the solid phase at low densities. When r_s is lowered, the kinetic energy tends to delocalize electrons more, and anharmonic effects will become important near the melting point.

For a solid with Lindemann ratio γ, the exchange correction to the energy at melting is of the order of $\exp(-1/2\gamma^2)$. For $\gamma \sim 30\%$, this is about 4×10^{-3} and is negligible compared to the direct interaction. Therefore, statistics do not affect the energy of the solid and will be neglected in this work.

In the next section, we describe the self-consistent phonon theory and its generalization to the case of a magnetic field, as well as a derivation of the cubic correction. In section 3 we discuss the results and show dispersion graphs of phonon and magnetophonons of the electron crystal at different densities and filling factors.

2. Theory

We first recapitulate the formalism at zero field. In a real system the Hamiltonian is a sum of the kinetic energy of the particles and their potential energy. In a solid where the average position R_i of the particles is on a regular lattice, one usually expands the potential energy about the equilibrium position of the particles as:

$$H = \sum_i \frac{P_i^2}{2m} + \frac{1}{2}\sum_{i,j}' v(r_i - r_j) = \sum_i \frac{P_i^2}{2m} + \frac{1}{2}\sum_{i,j}' v(R_i - R_j + \xi_i - \xi_j) = H_0 + \delta H \quad (1)$$

where

$$H_0 = \sum_i \frac{P_i^2}{2m} + \frac{1}{2}\sum_{i,j}' \left\{ v(R_{ij}) + \xi_{ij} \cdot \nabla v(R_{ij}) + \frac{1}{2}\xi_{ij}\xi_{ij} : \nabla^{(2)}v(R_{ij}) \right\} \quad (2)$$

$$\delta H = H_3 + H_4 = \frac{1}{2}\sum_{ij}' \left\{ \frac{1}{3!}\xi_{ij}\xi_{ij}\xi_{ij} \vdots \nabla^{(3)}v(R_{ij}) + \frac{1}{4!}\xi_{ij}\xi_{ij}\xi_{ij}\xi_{ij} \vdots \nabla^{(4)}v(R_{ij}) + \cdots \right\} \quad (3)$$

H_0 is the harmonic Hamiltonian and δH the anharmonic one. The force on particle i, $\sum_j' \nabla v(R_{ij})$, is zero. Thus the linear term $\sum \xi \cdot \nabla v$ is zero. Here $\nabla^{(2)}v(R_{ij})$ represents the tensor $(\partial^2/\partial R_\alpha \partial R_\beta)\, v(R = R_{ij})$ where $v(r)$ is the pair potential. : represents the double contraction of the latter tensor with the vectors ξ_{ij}. R_i refers to the lattice sites and $\xi_i = \xi(R_i)$ to the dynamical displacements about these sites. In terms of the normal modes of H_0, we have:

$$\xi(R_i) = \sum_{q\lambda} \left(\frac{\hbar}{2mN\omega^0_{q\lambda}} \right)^{1/2} e_{q\lambda}\, (a_{q\lambda} + a^\dagger_{-q\lambda})\, e^{iq\cdot R_i}. \quad (4)$$

Here the operator $a_{q\lambda}$ $(a^\dagger_{q\lambda})$ annihilates (creates) a phonon of wavevector q, polarization λ and frequency $\omega^0_{q\lambda}$. $e_{q\lambda}$ is the direction of the polarization.

Keeping only H_0 constitutes the harmonic approximation and it is an exactly solvable problem. This approximation works well in the case where the average displacements of the atoms about their equilibrium position do not exceed 5%. However, since the mean square displacements are inversely proportional to the square root of

the mass, the deviations will be large for light particles, and therefore anharmonic terms will be important.

In addition to the self-consistent treatment, we will also calculate the third-order term H_3, in second-order perturbation theory. This cubic anharmonic correction is known, from previous studies [8,9], to provide for a correction comparable to that from the self-consistent phonon results.

2.1. Self-consistent anharmonic corrections

A self-consistent phonon calculation for the two-dimensional Wigner solid was performed by Platzman and Fukuyama [10] in order to find the melting point of the system. This calculation uses the Debye approximation so that sums can be done analytically. The Ewald sum technique [11] was not implemented to deal with the long-range Coulomb potential, in that sense it was not an exact treatment. The self-consistent phonon theory has been successfully applied to rare gas solids and also to the 3D Wigner solid [8], where the Ewald summation technique was used. This calculation has been generalized recently to 2D rare gas solids [9]. The phonon dispersion for Ne was found to display a large correction due to the quantum zero point vibration. This suggests the importance of quantum fluctuations in the melting of lighter elements such as He^4, [12] H$_2$, [13] and He^3 [14]. We now describe and apply this theory to the 2D Wigner crystal. The only difference in the case of the Coulomb interaction is its long range, and one has to properly take care of the summations over the lattice sites. Using this theory, one can calculate the self-consistent second-order vertex $\langle \nabla^{(2)} v(R + \xi) \rangle$ and more generally the ground state average of any function of the dynamical variable ξ.

The ground state self-consistent phonon wavefunction is a Gaussian which involves frequencies that are calculated from an averaged dynamical matrix $D_{\alpha\beta}^{\text{SCP}}$.

$$\Psi(\xi_1, \ldots, \xi_N) \propto \exp\left(- \sum_{q\lambda} \left(\frac{\hbar}{2m\omega_{q\lambda}} \right) \xi_{q\lambda} \xi_{-q\lambda} \right)$$

where $\xi_{q\lambda} = \sum_i 1/\sqrt{N}\, e^{-iqR_i}\, \xi_i \cdot e_{q\lambda}$ is the normal mode coordinate.

This dynamical matrix itself is evaluated in the ground state of the system.

$$D_{\alpha\beta}^{\text{SCP}}(q) = \sum_R \langle \nabla_{\alpha\beta}^{(2)} v(R + \xi) \rangle (1 - e^{iqR}). \tag{5}$$

The ground state average is the average over $\xi_{q\lambda}$ having a Gaussian distribution of width $(\hbar/2m\omega_{q\lambda})^{1/2}$ which is the mean square displacement of a 1D harmonic oscillator; more precisely, the average of any function F of the variable ξ is given by:

$$\langle F(\xi(R)) \rangle = \frac{\det(\Lambda_R)^{1/2}}{2\pi} \int d^2\xi\, F(\xi(R))\, e^{-\xi \cdot \Lambda_R \cdot \xi/2} \tag{6}$$

where

$$\left(\Lambda_R^{-1} \right)^{\alpha\beta} = \langle (\xi^\alpha(R) - \xi^\alpha(0))(\xi^\beta(R) - \xi^\beta(0)) \rangle = \frac{\hbar}{mN} \sum_{q\lambda} \frac{e_{q\lambda}^\alpha e_{q\lambda}^\beta}{\omega_{q\lambda}^0} (1 - \cos qR). \tag{7}$$

So one can start from the set of quasi-harmonic frequencies of the solid, $\omega_{q\lambda}^0$ (obtained from (5) with $\xi = 0$), use them in (7) to get $\Lambda^{\alpha\beta}$ to do the average in (5), and diagonalize the self-consistent dynamical matrix to obtain new frequencies; these frequencies can themselves be used as input in (7) and so on, until convergence of this iteration process. In (6), the average of any odd function of ξ is zero, and in an expansion in powers of ξ only even powers contribute. These SCP frequencies can be expanded in power series of $r_s^{-1/2}$; the leading-order term which is the harmonic frequency, is proportional to $r_s^{-3/2}$, and each higher-order term has an additional power of $r_s^{-1/2}$.

We can also deduce the correction to the total energy by summing all SCP frequencies over the first Brillouin zone and subtracting off the harmonic total energy.

Because of the long-range nature of the Coulomb potential, the sum in (5) is formed of terms like $\langle 1/(R + \xi)^3 \rangle$, and hence is slowly convergent. The usual SCP procedure needs to be modified. The bare Coulomb interaction ($\xi = 0$) can be summed exactly by use of the Ewald sum technique. We therefore Fourier transform only the difference between the renormalized and the bare second-order vertex, to which we add the bare dynamical matrix.

$$D^{\text{SCP}}(q) = D^{\text{Ewald}}(q) + \sum_R{}'(1 - e^{iqR}) \left\{ \langle \nabla^{(2)}v(R + \xi) \rangle - \nabla^{(2)}v(R) \right\}.$$

The same trick is used to compute the third-order vertex needed for the cubic-anharmonic correction.

$$w_3(k_1, k_2, k_3) = \sum_R{}' (e^{ik_1R} + e^{ik_2R} + e^{ik_3R}) \, \nabla^{(3)}v(R) \tag{8}$$

$$w_3^{\text{SCP}} = w_3^{\text{Ewald}} + \sum_R{}' (e^{ik_1R} + e^{ik_2R} + e^{ik_3R}) \left\{ \langle \nabla^{(3)}v(R + \xi) \rangle - \nabla^{(3)}v(R) \right\}. \tag{9}$$

Although w_3 has terms proportional to $1/R^4$, the difference in curly brackets is proportional to $1/R^6$ and converges much faster.

2.1.1. The case of a magnetic field. In a magnetic field the harmonic Hamiltonian H_0 is changed to:

$$H_{0B} = \sum_i \frac{(P_i - qA_i)^2}{2m} + \tfrac{1}{2}\sum_{i,j}{}' \left\{ v(R_{ij}) + \xi_{ij} \cdot \nabla v(R_{ij}) + \tfrac{1}{2}\xi_{ij}\xi_{ij} : \nabla^{(2)}v(R_{ij}) \right\}. \tag{10}$$

It is still a quadratic function of ξ and can be exactly diagonalized [15]. The normal modes are given by:

$$\xi_q = \sum_\lambda \left(\frac{\hbar}{2m\omega_{q\lambda}} \right)^{1/2} e_{q\lambda} \, (r_{q\lambda\mu}b_{q\mu} + r_{q\lambda\mu}^* b_{-q\mu}^\dagger) \tag{11}$$

where $b_{q\mu}$ ($b_{q\mu}^\dagger$) is the magnetophonon annihilation (creation) operator of wavevector q and polarization μ (longitudinal or transverse), r_q is a 2×2 matrix:

$$r_q = \begin{pmatrix} \cos\theta_q & -i\sin\theta_q \\ -i\sin\theta_q & \cos\theta_q \end{pmatrix} \qquad \cos 2\theta_q = \frac{\omega_{ql} - \omega_{qt}}{u_q} \qquad \sin 2\theta_q = \frac{\omega_c G_q}{u_q}$$

$$u_q = \sqrt{(\omega_{ql} - \omega_{qt})^2 + \omega_c^2 G_q^2} \qquad G_q = \frac{-2\sqrt{\omega_{ql}\omega_{qt}}}{\omega_{ql} + \omega_{qt}} \qquad \omega_{q\lambda} = \omega_{q\lambda}^0 \left[1 + \frac{\omega_c^2}{(\omega_{ql}^0 + \omega_{qt}^0)^2} \right]^{1/2} \tag{12}$$

where $\omega_{q\lambda}^0$ are the phonon frequencies of the Wigner crystal in absence of a magnetic field and ω_c is the cyclotron frequency, given by $\omega_c = eB/m$. The magnetophonon energies are given by:

$$E_{k\mu} = \frac{\hbar}{2}\left[\sqrt{\omega_c^2 + (\omega_{kl}^0 + \omega_{kt}^0)^2} \pm \sqrt{\omega_c^2 + (\omega_{kl}^0 - \omega_{kt}^0)^2}\right]$$

+ for μ = longitudinal, − for μ = transverse.

In the zero field limit, one can see that $\omega \to \omega^0$, $r_{\lambda\mu} \to \delta_{\lambda\mu}$ and $E_{k\mu} \to \hbar\omega_{k\mu}^0$, and the usual normal modes and dispersion relations are recovered.

The procedure will be therefore the same as before, only the matrix Λ_R has to be redefined properly as a function of the new normal modes:

$$(\Lambda_R^{-1})^{\alpha\beta} = \frac{\hbar}{mN} \sum_{q\lambda\mu_1\mu_2} \frac{e_{q\mu_1}^\alpha e_{q\mu_2}^\beta}{(\omega_{q\mu_1}\omega_{q\mu_2})^{1/2}} r_{q\lambda\mu_1} r_{q\lambda\mu_2}^* (1 - \cos qR). \tag{13}$$

Note that Λ^{-1} satisfies $(\Lambda^{-1})^{\alpha\beta} = (\Lambda^{-1})^{\beta\alpha*}$, but since we have $\sum_\lambda r_{q\lambda\mu_1} r_{q\lambda\mu_2}^* = \delta_{\mu_1\mu_2}$, Λ is real and therefore symmetric.

So the set of equations that are iterated in this case are: (13) to define Λ, (5) and the use of (6) to define the dynamical matrix, then the latter diagonalized yields $\omega_{q\lambda}^0$. The equation (12) defines the new frequencies that will be reused in (13) and now the process is iterated until convergent.

2.2. The cubic anharmonic correction

As its name indicates, this term comes from the third-order term in (3) and will be evaluated in second-order perturbation theory. Let us first give the expression for the correction to the total energy:

$$\Delta E_{33} = \sum_j{}' \frac{|\langle 0 | H_3 | j \rangle|^2}{E_0 - E_j}. \tag{14}$$

This energy is easily evaluated by use of equations (3), (4) and (8). One finally finds

$$\Delta E_{33} = -\frac{1}{6N} \sum_{k_i} \Delta\left(\sum_{i=1,3} k_i\right) \prod_{i=1,3}\left(\frac{\hbar}{2m\omega_{k_i}}\right) \frac{|V(k_1,k_2,k_3)|^2}{\omega_{k_1}^0 + \omega_{k_2}^0 + \omega_{k_3}^0} \tag{15}$$

where

$$V(k_1,k_2,k_3) = \sum_R{}' (e^{ik_1R} + e^{ik_2R} + e^{ik_3R})\, e_{k_1}^\alpha e_{k_2}^\beta e_{k_3}^\gamma\, \nabla_\alpha \nabla_\beta \nabla_\gamma v(R) \tag{16}$$

k_i represents the mode (k_i, λ_i) and the sum is over the vectors and their polarization. ΔE_{33} is obviously negative, since it is a second-order correction to the ground state energy.

The correction to the phonon frequencies can be calculated by using the following formula:

$$\Delta(q) = \sum_j{}' \frac{|\langle q | H_3 | j \rangle|^2}{E_q - E_j} - \sum_j{}' \frac{|\langle 0 | H_3 | j \rangle|^2}{E_0 - E_j} \tag{17}$$

and

$$|q\rangle = a_q^\dagger |0\rangle.$$

By definition, $\Delta(q)$ measures the difference between the correction to the energy of the crystal plus one phonon and the correction to the energy of the perfect crystal. It is therefore the correction to the energy of a single phonon of momentum q and polarization λ. Using the same formulas as above, we get:

$$\Delta(q) = -\frac{1}{2N} \sum_{k_1,k_2} \Delta(k_1 + k_2 + q) \left(\frac{\hbar}{2m}\right)^3$$

$$\times \frac{|V(k_1,k_2,q)|^2}{\omega_{k_1}\omega_{k_2}\omega_q} \left(\frac{1}{\omega_{k_1} + \omega_{k_2} + \omega_q} + \frac{1}{\omega_{k_1} + \omega_{k_2} - \omega_q}\right). \tag{18}$$

This expression is identical to the shift $\Delta(q,\omega)$ obtained by Green function techniques [16,9], where ω is replaced by the on-shell frequency ω_q. The first denominator in the above expression, where the three frequencies are added, corresponds to intermediate states having 4 phonons $|k_1,k_2,q,q\rangle$; and the second denominator corresponds to 2-phonon states $|k_1,k_2\rangle$.

2.2.1. The case of a magnetic field. In a magnetic field, only the normal modes have changed. The rest of the calculation is the same as before. From (17) we get:

$$\Delta(q) = -\frac{1}{2N} \sum_{k_1,k_2,\lambda_1,\lambda_2} \Delta(k_1 + k_2 + q) \left(\frac{\hbar}{2m}\right)^3$$

$$\times \left\{ \left| \sum_{\mu\mu_1\mu_2} \frac{V(k_1\mu_1,k_2\mu_2,q\mu) r_{k_1\lambda_1\mu_1} r_{k_2\lambda_2\mu_2} r_{q\lambda\mu}^*}{(\omega_{k_1\mu_1}\omega_{k_2\mu_2}\omega_{q\mu})^{1/2}} \right|^2 \left(\frac{1}{E_{k_1\lambda_1} + E_{k_2\lambda_2} - E_q}\right) \right.$$

$$\left. + \left| \sum_{\mu\mu_1\mu_2} \frac{V(k_1\mu_1,k_2\mu_2,q\mu) r_{k_1\lambda_1\mu_1} r_{k_2\lambda_2\mu_2} r_{q\lambda\mu}}{(\omega_{k_1\mu_1}\omega_{k_2\mu_2}\omega_{q\mu})^{1/2}} \right|^2 \left(\frac{1}{E_{k_1\lambda_1} + E_{k_2\lambda_2} + E_q}\right) \right\}. \tag{19}$$

Unless explicitly mentioned, the label k specifies both the wavevector and the polarization; i.e. $k_i = (k_i, \lambda_i)$.

The results for the shift mentioned above include only the shift due to the cubic term H_3 where only $\nabla^{(3)}v(R)$ appears. Since we are dealing with the SCP theory that sums terms to all orders, instead of the bare cubic vertex, we will use the SCP vertex given by $\langle\nabla^{(3)}v(R+\xi)\rangle$ and calculated from (9). In order to avoid divergence problems due to the second denominator in $\Delta(q)$, we will replace ω_q by zero; this means that we calculate the *static* shift of the single particle energies $\Delta(q,\omega = 0)$. The results, are not very different from $\Delta(q,\omega_q)$.

3. Numerical results

If one wants to expand quantities like the Lindemann ratio or the total energy in powers of some expansion parameter, one can basically consider the two following limits.

(a) The high field limit defined by $\omega_c \gg \omega_0 = (8e^2/ma^3)^{1/2}$ or $r_s\nu^2 \ll 3.4$. In this case ν is the only relevant expansion parameter and one can write all dimensionless physical variables as a function of ν, and expand them in powers of ν; the $\nu \to 0$ limit being the classical limit of point particles.

(b) The low field limit defined by $\omega_c \ll \omega_0$ or $r_s\nu^2 \gg 3.4$: In this case all physical quantities can be expanded in powers of $1/r_s$ only. The limit $r_s \to \infty$ being the classical case.

In both cases (a) and (b) anharmonicity can be measured by the Lindemann ratio $\gamma = (\langle \xi^2 \rangle/a^2)^{1/2}$ which has the following expression in the harmonic approximation. Case (a): $\gamma = 0.60\nu^{1/2}$. Case (b): $\gamma = 0.71r_s^{-1/4}$.

In figures 1–5 we display the phonon and magnetophonon dispersion relations of the 2D electron crystal from zero to high fields and at different densities. The self-consistent correction increases the phonon frequencies, and the cubic correction decreases frequencies to even below the harmonic values. These corrections increase with the filling factor and decrease with r_s in both the high and the low magnetic field limit.
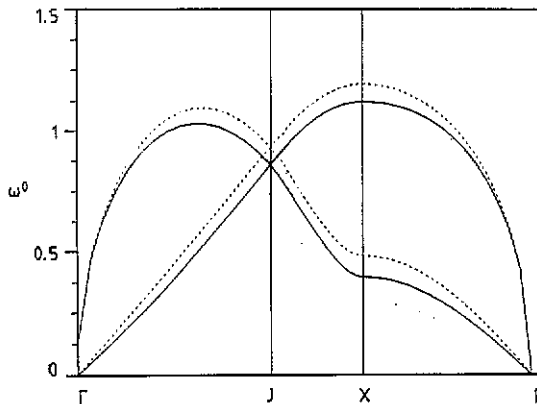

Figure 1. Phonon dispersion relations for $r_s = 41$ and $B = 0$. ω is in units of $\omega_0 = (8e^2/ma^3)^{1/2}$. The harmonic, self-consistent and cubic phonons are represented respectively by the solid, the broken and the dotted curves.

Figure 1 shows the zero field case at $r_s = 41$, a density close to the melting of the Wigner crystal. Even close to melting, the anharmonic correction is only around ten per cent and quite small. This is a characteristic of soft potentials. In figures 2 and 3 we show the two magnetophonon branches in the high field limit: $r_s = 10, \nu = 0.2$ ($r_s\nu^2 = 0.4$); the system is presumably in the solid phase but near melting. Again the anharmonic corrections are small. The frequencies are measured in units of ω_0^2/ω_c, therefore if the y-intercept is approximately 9, then the cyclotron frequency divided by ω_0 is equal to 3. The case of intermediate fields where $r_s\nu^2 \sim 3.4$ is shown in figure 4: $r_s = 32$ and $\nu = 0.32$. Figure 5 corresponds to $\nu = 0.5$ and $r_s = 10$, parameters presumably characterizing the liquid phase. Anharmonic corrections become more important at this larger filling factor.

3.1. Calculation of the total energy

We have also calculated the total energy of the system in the following two
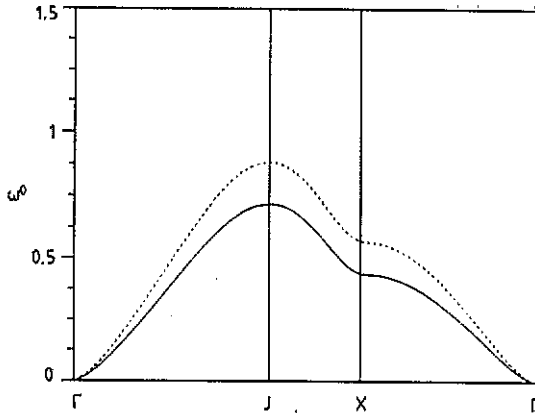
Figure 2. Transverse magnetophonon dispersion relations in the high field limit. $r_s = 10, \nu = 0.2$. ω is in units of ω_0^2/ω_c. The harmonic, self-consistent and cubic phonons are represented respectively by the solid, the broken and the dotted curves.

Figure 3. Longitudinal magnetophonon dispersion relations in the high field limit. $r_s = 10, \nu = 0.2$. ω is in units of ω_0^2/ω_c. The harmonic, self-consistent and cubic phonons are represented respectively by the solid, the broken and the dotted curves.
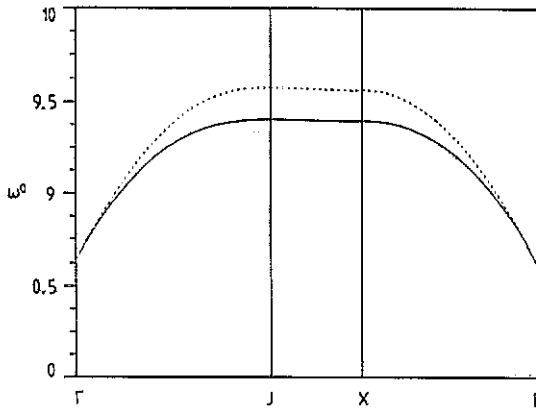
different ways.

(i) By using a perturbation expansion in powers of $1/r_s$ (or ν in the high field limit). These results are displayed below.

(ii) By using the self-consistent method. The corresponding results are shown in tables 1 and 2.

In the zero field limit (or case (b)), the total energy per particle, expressed in units of Rydberg= $e^2/2a_0$, has an apparently convergent Taylor expansion in a power series in $1/r_s^{(1/2)}$:

$$\frac{E}{N} = \frac{e^2}{2a_0} \left(-\frac{2.212205}{r_s} + \frac{1.62744}{r_s^{3/2}} + \frac{0.0824}{r_s^2} + \cdots \right). \tag{20}$$

The first term is just the configuration energy of an electron hexagonal lattice, (see Bonsall and Maradudin [11]) where the energy of a uniform background has been
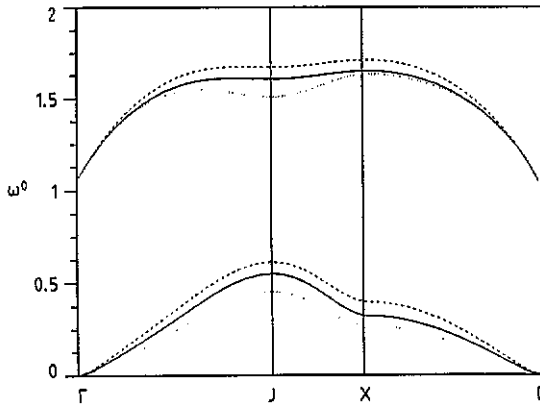
Figure 4. Magnetophonon dispersion relation in the intermediate field limit. $r_s = 32, \nu = 0.32$. ω is in units of ω_0^2/ω_c. The harmonic, self-consistent and cubic phonons are represented respectively by the solid, the broken and the dotted curves.

Figure 5. Magnetophonon dispersion relation in the intermediate field limit. $r_s = 10, \nu = 0.5$ (liquid phase). ω is in units of ω_0^2/ω_c. The harmonic, self-consistent and cubic phonons are represented respectively by the solid, the broken and the dotted curves.

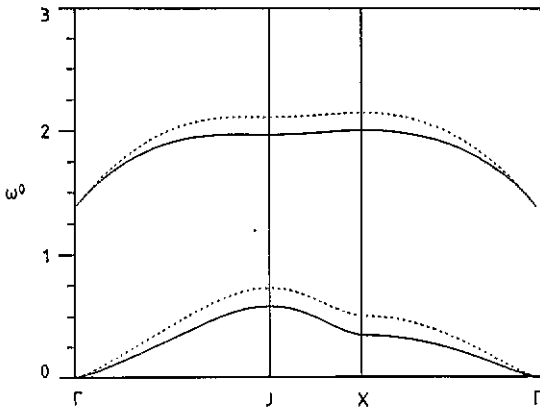subtracted. The second term is the zero point energy (harmonic approximation); and the third term is the sum of a positive quartic energy of 0.4086 (H_4 evaluated in the harmonic ground state), and a negative cubic energy of -0.3262 (H_3 evaluated in second-order perturbation theory). All these three terms can be evaluated as accurately as one wants; within the given significant figures they are all accurate. The remaining terms in the expansion, corresponding to higher-order corrections, can be estimated by using a fit to the self-consistent energies discussed below and shown in tables 1 and 2, but in higher orders the SCP calculation does not include all diagrams and hence one can only get an estimate of the next terms.

Equation (20) compares well with the results obtained by a non-linear least-squares fit to the Green function Monte Carlo data [5].

$$\frac{E_{\text{GFMC}}}{N} = \frac{e^2}{2a_0} \left(-\frac{2.2122}{r_s} + \frac{1.6284}{r_s^{3/2}} + \frac{0.0508}{r_s^2} + \cdots \right). \tag{21}$$

In the high field limit (or case (a)), the total energy per particle, expressed in units of e^2/l_c can be expanded in powers of ν in the following way [17,18]:

$$\frac{E}{N} = \frac{e^2}{l_c} \left(-0.782133\nu^{1/2} + 0.24101\nu^{3/2} + 0.087\nu^{5/2} + \cdots \right).\tag{22}$$

The same definitions apply for the three terms. Only the second term is just the potential part of the zero point energy (the kinetic energy being quenched to $\hbar\omega_c/4$) or, in other words, it is the ground state average of the following term:

$$\frac{1}{2}\sum_{i,j}{}' \frac{1}{2}\xi_{ij}\xi_{ij} : \nabla^{(2)}v(R_{ij}).\tag{23}$$

The last term is the sum of a positive contribution of 0.16 [17] and a negative contribution of -0.073 [18].

In our perturbation expansion the quartic and the cubic terms are of the same order, i.e. they both have the same power dependence in r_s or ν. The quartic term confining more the harmonic oscillator wavefunction increases the harmonic energy. On the other hand the cubic term being a second-order correction to the ground state energy is always negative. As for the self-consistent corrections one can say that at least the correction after the *first* iteration leads to an increase in the harmonic energy, however the sign of the iterated result is not predictable. The same arguments apply of course to the magnetophonon dipersion relation: the self-consistent correction is usually positive whereas the cubic one is negative since it is a second-order correction to the ground state.

Table 1. Self-consistent total energies per particle in units of $e^2/2a_0$ at zero field as a function of r_s.

r_s	E^{SCP}	$(E^{SCP} - E^{har})r_s^2$	$E^{cubic}r_s^2$
41	0.3395×10^{-2}	0.4672	-0.4061
50	0.2505×10^{-2}	0.4754	-0.4034
55	0.2161×10^{-2}	0.4665	-0.4012
82	0.1170×10^{-2}	0.4539	-0.3798
200	0.3003×10^{-3}	0.4388	-0.3551
20000	0.2904×10^{-6}	0.4322	-0.3281

Table 2. Self-Consistent total energies per particle in units of e^2/l_c for $r_s = 20$ as a function of ν.

ν	E^{SCP}	$(E^{SCP} - E^{har})\nu^{-5/2}$	$E^{cubic}\nu^{-5/2}$
0.5	0.6394×10^{-1}	0.0530	-0.0220
0.32	0.3980×10^{-1}	0.0985	-0.0379
0.2	0.2215×10^{-1}	0.1638	-0.0583
0.1	0.8072×10^{-2}	0.2082	-0.0709
0.01	0.2449×10^{-3}	0.2168	-0.0733
0.001	0.7686×10^{-5}	0.2625	-0.0730

The self-consistent total energies are displayed in table 1 in the zero field case for different values of r_s ranging from 41 to 20000, and in the high field case at $r_s = 20$ and for ν ranging from 0.5 to 0.001 (table 2). At very high r_s or very low filling factors our numerical results are not as accurate due to the subtraction of two big numbers.

4. Conclusion

The static Hartree–Fock theory used by Yoshioka and Lee [19] predicted a gap in the excitation spectrum of the 2D electron system considered as a charge density wave. This can be interpreted as an effective Einstein frequency of the solid. Recently Côté and MacDonald [20] improved this calculation by using a time-dependent Hartree–Fock theory which yields a gapless dispersion relation very close to the magnetophonon spectrum. This calculation is useful pedagogically, in that it clarifies the limitations of the Hartree–Fock calculation. Their energies are always slightly above the harmonic values whereas the present calculation indicates a lowering when the cubic anharmonic correction is included. The TDHF is a different approximation, in that, the anharmonic terms are weighted by the direction and magnitude of the wavevector q. In addition, the energy denominators of the intermediate states are different. Thus the cubic anharmonic correction discussed here occurs with a negative energy denominator whereas in the TDHF approximation the corresponding energy denominator is dominated by the harmonic values of the one phonon state. In other words, the TDHF does not yield the correct perturbation expansion for small displacements especially for the cubic term, and therefore it does not give the correct anharmonic correction for very low fillings. It is this cubic correction that provides the lowering of the phonon energy in the present context.

Another limitation of this calculation is its applicability only to very high fields ($\nu \ll 1$) whereas the SCP + cubic treatment can be done for all values of r_s and ν.

One can generally say that, unlike in a HF theory, a phonon wavefunction contains correlations between the particles and is therefore a better approximation for the solid as confirmed by the calculation by Lam and Girvin [17] which yields a lower energy than the HF theory.

It is well known that for quantum systems the melting occurs for a value of the Lindemann ratio about three times larger than the classical value of 0.1 [21,22]. Using the following criterion for zero temperature melting one can get an estimate for the critical values of r_s and ν.

For $\gamma_{melting} = 0.3$ one finds, within the harmonic approximation, that in the zero field limit $r_s^* = 31.4$ and at high fields $\nu^* = 0.25$. These values are very close to recent estimates [5,6,21] and experimental values [2,4].

To summarize, using the SCP theory, we have calculated anharmonic corrections to the single particle and total energies of the 2D electron solid with and without a magnetic field. In the experimental situation corresponding to $2 \leqslant r_s \leqslant 3$ and $0.1 \leqslant \nu \leqslant 0.5$ the SCP correction to the phonon frequencies is roughly about 10% and the cubic correction about −20% of the harmonic values. However for the total energies the SCP corrections are slightly larger. One can notice that even near melting the anharmonicity of the solid, although causing the melting, is a small correction.

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