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Three-dimensional Wigner crystal in a magnetic field

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We solve the quantum problem of the oscillations of a Wigner lattice in a strong magnetic field in the harmonic approximation, taking into account the transverse radiation field. We calculate the energy of the zero-point oscillations of the lattice and the dependence of the mean squared displacement of the particles from the lattice sites on the temperature and on the magnetic field. We consider the specific heat, the magnetic moment, and the dielectric constant of the lattice in a strong magnetic field, and discuss the stability of the lattice as a function of the particle density in the limit of a strong magnetic field.

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1. INTRODUCTION

The question of the ground state of an electron–hole plasma in a semi-conductor or semimetal in the limit of a strong magnetic field ($\hbar\omega_c \gg \mathrm{Ry}$, ω_c is the cyclotron frequency of the carriers and Ry is the exciton ionization potential) has attracted considerable interest recently. Babichenko and Onishchenko[1] have shown that if the carriers of different type have comparable mass, the homogeneous state of the system in a strong magnetic field is unstable to formation of a charge-density wave (CDW). Rakhmanov[2] has analyzed the case of carriers with strongly differing masses (for example, electrons and holes in bismuth) and determined the conditions under which the heavier particles (holes) form a Wigner lattice (WL) against an approximately homogeneous compensating background of lighter particles (electrons). The possibility of formation of a WL in a magnetic field was investigated earlier in Refs. 3 and 4, where it was shown that in a strong magnetic field the WL (CDW in the case of high density[5]) is energywise favored over a homogeneous ground state. We note, however, that the cited references are qualitative and variational in character, whereas the problems connected with the stability of a lattice and with the calculation of its equilibrium characteristics must be solved on the basis of quantitative analysis of the spectrum of the crystal-structure oscillations. We report here in this connection a detailed quantitative investigation of the vibrational properties of a WL in a magnetic field. We confine ourselves to the case of an immobile compensating background. In Sec. 2 we obtain the spectrum of the eigenvalues of the Hamiltonian of the WL oscillations in an arbitrary magnetic field[1)]; we calculate the energy of the ground state of the system, which turns out to depend on the orientation of the magnetic field relative to the crystallographic axes. In Sec. 3 we determine the dependence of the mean squared displacement of the particle from the WL site on the temperature and on the magnetic field, and find that the "soft mode" $\nu_1 \sim 1/\omega_c$ that appears in a strong magnetic field, just as in the two-dimensional case,[6] does not cause lattice instability. It is shown in Sec. 4 that the low-temperature heat capacity depends substantially on the magnetic field and is proportional to $T^{3/2}$ (T is the temperature), as against T^3 for ordinary phonons; we calculate also the temperature dependence of the magnetic moment of a WL and the dielectric constant of a WL, the latter being strongly anisotropic in a strong magnetic field.

In Sec. 5 we solve the problem of the coupling of the electromagnetic and vibrational modes of a WL in a magnetic field. An exact dispersion equation is obtained and the spectrum of the eigenvalues of the system is briefly investigated with account taken of the transverse radiation field. It is shown that in the limit of a strong magnetic field allowance for the transverse field does not change qualitatively the results of the preceding sections.

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2. ENERGY OF ZERO-POINT OSCILLATIONS OF A WIGNER LATTICE IN A MAGNETIC FIELD

We consider a system of N electrons moving in a volume V against the background of a homogeneous immobile compensating charge. It is well known that an important characteristic of this system is the electron density $n=N/V$, which it is convenient to characterize by the dimensionless parameter r_s with the aid of the relation $4/3\pi(r_s a_B)^3 = n^{-1}$($a_B$ is the Bohr radius). Wigner[7] has shown that in the low-density limit, $r_s \gg 1$, the ground state of the system is a bcc lattice made up of electrons. The vibrational properties of the WL were investigated in Refs. 8–10. In the present paper we consider the influence of a homogeneous magnetic field B on the vibrational properties of a WL.

It turns out that the frequencies $\nu(\mathbf{k}, j)$ of the oscillations of a WL in a magnetic field can be expressed in terms of the frequencies $\omega(\mathbf{k}, j)$ and the polarization $q(\mathbf{k}, j)$ of the WL oscillations in the absence of a magnetic field (here $\mathbf{k}$ is the wave vector; $j=1,2,3$ is the number of the mode). We recall in this connection[11] that the frequencies $\omega(\mathbf{k}, j)$, calculated in the harmonic approximation, satisfy the Kohn sum rule

$$\sum_j \omega^2(\mathbf{k}, j) = \omega_p^2,$$

where ω_p is the plasma frequency; in the long-wave limit $\mathbf{k}\to 0$ there exist a longitudinal mode, $\mathbf{q}(\mathbf{k}, l) \parallel \mathbf{k}$, for which $\omega^2(\mathbf{k}, l) \to \omega_p^2$, and two transverse modes $\mathbf{q}(\mathbf{k}, t) \perp \mathbf{k}$, whose frequencies $\omega(\mathbf{k}, t)$ are proportional to k. Along the high-symmetry directions of the bcc lattice ([100], [111]), the oscillations retain their polarization also for finite values of k, whereas for an arbitrary direction at finite $\mathbf{k}$ the vector $\mathbf{q}(\mathbf{k}, l)$ need not necessarily be parallel to $\mathbf{k}$.

Let the initial density of the electrons in the system be low enough ($r_s \gg 1$), so that in the absence of a magnetic field the ground state of the system is a WL with lattice sites $\mathbf{R}_i$ specified in a certain Cartesian coordinate system. The Hamiltonian of the system in the magnetic field $\mathbf{B}=\mathbf{n}B$ is, in the harmonic approximation,

$$\hat{H} = \sum_{i,\alpha} \frac{\hat{\pi}_{i\alpha}^2}{2m} + \frac{1}{2}\sum_{i,\alpha,j,\beta} G_{i,j}^{\alpha,\beta}\, \hat{u}_{i\alpha}\hat{u}_{j\beta} + N v_0, \tag{1}$$

where $v_0 = -1.792\mathrm{Ry}/r_s$ is the electrostatic energy per electron of the bcc lattice, $\hat{u}_{i\alpha} = r_{i\alpha} - R_{i\alpha}$ are the operators of the electron displacements from the sites, $\hat{\pi}_{i\alpha}$ are the operators of the electron momenta in the magnetic field, and $G_{ij}^{\alpha\beta}$ is the force tensor, equal to

$$G_{ij}^{\alpha\beta} = -\frac{\partial^2}{\partial r_\alpha \partial r_\beta}\frac{e^2}{r}\Big|_{r=R_{ij}}, \quad i\neq j,$$
$$G_{ij}^{\alpha\beta} = \sum_{k\neq i}\frac{\partial^2}{\partial r_\alpha \partial r_\beta}\frac{e^2}{r}\Big|_{r=R_{ik}}, \quad i=j, \tag{2}$$

with $R_{ij} = |\mathbf{R}_i - \mathbf{R}_j|$. The operators $\hat{\pi}_{i\alpha}$ and $\hat{u}_{j\beta}$ satisfy the commutation relations

$$[\hat{u}_{i\alpha}, \hat{u}_{j\beta}] = 0, \quad [\hat{u}_{i\alpha}, \hat{\pi}_{j\beta}] = i\hbar\delta_{ij}\delta_{\alpha\beta},$$
$$[\hat{\pi}_{i\alpha}, \hat{\pi}_{j\beta}] = -i(\hbar^2/\lambda^2)\, n_\gamma \delta_{ij}\hat{e}_{\alpha,\beta,\gamma}, \quad \alpha, \beta, \gamma = x, y, z. \tag{3}$$

Here $\lambda = (c\hbar/eB)^{1/2}$ is the magnetic length, δ_{ij} is the Kronecker symbol, $\hat{e}_{\alpha,\beta,\gamma}$ is a unit antisymmetrical tensor, and n_γ is the projection of the unit vector along the magnetic-field direction.

We transform the operators as follows:

$$\hat{\pi}_{i\alpha} = \left(\frac{2}{N}\right)^{1/2}\sum_{l,\mathbf{k}>0}\{\cos(\mathbf{k}\mathbf{R}_i)\hat{\Pi}_l(\mathbf{k}) + \sin(\mathbf{k}\mathbf{R}_i)\hat{\Pi}_l(-\mathbf{k})\} q_l^\alpha(\mathbf{k}),$$
$$\hat{u}_{i\alpha} = \left(\frac{2}{N}\right)^{1/2}\sum_{l,\mathbf{k}>0}\{\cos(\mathbf{k}\mathbf{R}_i)\hat{x}_l(\mathbf{k}) + \sin(\mathbf{k}\mathbf{R}_i)\hat{x}_l(-\mathbf{k})\} q_l^\alpha(\mathbf{k}). \tag{4}$$

Here $\mathbf{k}>0$ denotes the sum over half the states of the Brillouin zone of the reciprocal lattice. In addition, we choose $\mathbf{q}_l(-\mathbf{k}) = \mathbf{q}_l(\mathbf{k})$. The operators $\hat{\pi}_i$ and $\hat{x}_j$ are Hermitian and have the following commutation relations (for one and the same $\mathbf{k}$):

$$[\hat{x}_i, \hat{x}_j] = 0, \quad [\hat{x}_i, \hat{\Pi}_j] = i\delta_{ij}, \quad [\hat{\Pi}_i, \hat{\Pi}_j] = -i(\mathbf{n}\mathbf{q}_l)\hat{e}_{ijl}. \tag{5}$$

The Hamiltonian (1) reduces with the aid of the transformation (4) to a sum of independent Hamiltonians:

$$\hat{H} = \sum_{\mathbf{k}}\hat{H}_{\mathbf{k}}, \quad \hat{H}_{\mathbf{k}} = \frac{1}{2}\sum_{i=1}^{3}(\hat{\Pi}_i^2 + \omega_i^2\hat{x}_i^2). \tag{6}$$

In (5) and (6) we normalize the operators $\hat{x}$ to the magnetic length λ, the operators $\hat{\pi}$ to $\hbar/\lambda$, the frequencies ω_i to ω_c, and the energy $\hat{H}$ to $\hbar\omega_c$. It is seen from (5) and (6) that the magnetic field couples oscillation modes with one and the same vector $\mathbf{k}$, and leaves independent the oscillations with different $\mathbf{k}$. The Hamiltonian $\hat{H}_k$ coincides with the Hamiltonian of a particle in a magnetic field and in an asymmetrical harmonic potential.

We can construct for the Hamiltonian $\hat{H}_k$ a system of creation and annihilation operators, putting

$$\hat{a}^+ = \sum_i(\alpha_i\hat{\Pi}_i + \beta_i\hat{x}_i).$$

The coefficients α_i and β_i are determined from the condition $[\hat{H}, \hat{\alpha}^+] = \nu\hat{\alpha}^+$, where ν are the natural frequencies of the Hamiltonian H_k (we leave out the index $\mathbf{k}$ from now on). To determine the natural frequencies $\nu_j, j=1,2,3$, we obtain the equation

$$\Delta(\nu) = \det\begin{vmatrix}\omega_1^2-\nu^2 & -i\nu n_3 & i\nu n_2\\ i\nu n_3 & \omega_2^2-\nu^2 & -i\nu n_1\\ -i\nu n_2 & i\nu n_1 & \omega_3^2-\nu^2\end{vmatrix} = 0, \tag{7}$$

or

$$\nu^6 - (1+\omega_0^2)\nu^4 + (p+\Omega_1^2)\nu^2 - s = 0,$$
$$\omega_0^2 = \sum_{i=1}^{3}\omega_i^2, \quad \Omega_1^2 = \sum_{i=1}^{3} n_i^2\omega_i^2, \quad s = \omega_1^2\omega_2^2\omega_3^2, \tag{8}$$
$$p = \omega_1^2\omega_2^2 + \omega_1^2\omega_3^2 + \omega_2^2\omega_3^2, \quad n_i^2 = (\mathbf{n}\mathbf{q}_i)^2;$$

with $\mathbf{n}$ the unit vector along the external magnetic field.

Each natural frequency ν_j corresponds to a creation operator

$$\hat{a}_j^+ = \frac{1}{\sigma_j}\sum_{l=1}^{3}\Delta_{jl}^{(j)}\left\{\hat{\Pi}_l + i\frac{\omega_l^2}{\nu_j}\hat{x}_l\right\}, \tag{9}$$

where $\Delta_{jl}^{(j)} = \Delta jl(\nu_j)$ are the corresponding cofactors of the determinant $\Delta(\nu)$. The normalization coefficients σ_j are equal to

$$\sigma_j=\left(\frac{2\nu_j\Delta_{jj}^{(j)}}{\varkappa_j}\right)^{1/2}, \quad \varkappa_j=\frac{1}{(\nu_j^2-\nu_i^2)(\nu_j^2-\nu_s^2)}, \quad j\neq i\neq s, \; j, \; i, \; s=1, \; 2, \; 3. \tag{10}$$

With the aid of the dispersion equation (8) we can show that $\Delta_j^{(j)}\varkappa_j>0$, so that the coefficients σ_j are real. It can be verified that in the limit as $\omega_c\to 0$ Eq. (9) goes over into the usual formula for the phonon creation operator.[11] In the actual derivations it is useful to bear in mind the following relations:

$$\sum_{i=1}^{3}\varkappa_i=0, \quad \sum_{i=1}^{3}\nu_i^2\varkappa_i=0, \quad \sum_{i=1}^{3}\nu_i^4\varkappa_i=1,$$
$$\sum_{i=1}^{3}\nu_i^6\varkappa_i=1+\omega_0^2, \quad \sum_{i=1}^{3}\frac{\varkappa_i}{\nu_i^2}=-\frac{1}{s}, \tag{11}$$

which can be proved with the aid of (8).

Equations (7)–(10) solve our problem; the Hamiltonian H_k is expressed in terms of the operators $a_j^+(k)$ and $a_j(k)$:

$$\hat{H}_{\mathbf{k}}=\sum_{j=1}^{3}\nu_j(\mathbf{k})\{\hat{a}_j^+(\mathbf{k})\hat{a}_j(\mathbf{k})+{}^1/_2\},$$
$$[\hat{a}_j(\mathbf{k}), \hat{a}_i(\mathbf{k}')]=0, \quad [\hat{a}_j(\mathbf{k}), \hat{a}_j^+(\mathbf{k}')]=\delta_{ij}\delta_{\mathbf{k},\mathbf{k}'}. \tag{12}$$

Obviously, the wave functions of the Hamiltonian H_k are equal to

$$|\tilde{n}\rangle=|\tilde{n}_1, \tilde{n}_2, \tilde{n}_3\rangle=\prod_{j=1}^{3}[(a_j^+)^{\tilde{n}_j}/(\tilde{n}_j!)^{1/2}]\,|0\rangle, \tag{13}$$

where $|0\rangle$ is the ground state, so that $\hat{a}_j|0\rangle=0$.

We now investigate the dispersion equation (8) in the limit of a strong magnetic field $\omega_c\gg\omega_0$. From (8) we get

$$\nu_1\approx\sqrt{s}/\Omega_1\omega_c, \quad \nu_2\approx\Omega_1, \quad \nu_3\approx\omega_c. \tag{14}$$

Comparing this result with a solution of the problem of particle motion in a centrosymmetric potential in a magnetic field [when $\omega_1^2=\omega_2^2=\omega_3^2$) in (6)], we see that in the general case of an asymmetrical harmonic potential, in the limit of a strong magnetic field, there exists a mode ν_3 corresponding to excitation of the particle to Landay cyclotron levels, and a mode ν_1, analogous to excitations with different magnetic quantum numbers, and by virtue of the fact that $\nu_1\sim 1/\omega_c$ the strong magnetic field tends to preserve the degeneracy in the magnetic quantum number, which is characteristic of a free particle.[12] Obviously, the mode ν_2 describes the motion of the particle along the field in a harmonic potential with averaged frequency Ω_1 [see also (20)].

Knowing the WL oscillation frequencies, we can obtain the energy of the zero-point oscillations of the WL in a magnetic field. In the limit $\omega_c\gg\omega_0$ we have

$$E_0=\sum_{i,\mathbf{k}}\frac{\hbar\nu_i(\mathbf{k})}{2}\approx N\frac{\hbar\omega_c}{2}+\sum_{\mathbf{k}}\frac{\hbar\Omega_1(\mathbf{k})}{2}+O\left(\frac{1}{\omega_c}\right). \tag{15}$$

In principle, on account of the term $\hbar\omega_c/2$, the energy of the zero-point oscillations of the WL can exceed the gain in the electrostatic energy (v_0 per particle) of the WL. This, however, still does not demonstrate instability of the lattice, since in a strong magnetic field the contribution to the energy $\hbar\omega_c/2$ does not depend on the structure of the ground state of the system. The energy v_0 must therefore be compared with the quantity $N^{-1}\Sigma\hbar\Omega_1/2$, which plays the role of the energy of the zero-point oscillations. By virtue of the inequality $\Omega_1\leq\Sigma_i\omega_i$, the magnetic field only decreases the energy of the zero-point oscillations of the WL. This decrease, however, is negligible, since $\Omega_i\sim\omega_p$, and therefore the energy of the zero-point oscillations per particle in the magnetic field is $\propto r_s^{-3/2}$, i.e., of the same order as in the absence of a field.[11]

It is interesting to note also that the energy of the zero-point oscillations (15) depends on the direction of the magnetic field relative to the crystallographic axes. Consequently, neglecting surface effects (friction of the electron crystal against the sample surface), the lattice as a whole will rotate in a strong magnetic field so as to minimize $\Sigma\Omega_1(\mathbf{k})$. We shall show in Sec. 5 that rotation of the lattice is the result of the interaction of the induced magnetic moment of the WL with the external magnetic field.

In the foregoing analysis we have neglected exchange and anharmonic terms. In the absence of a magnetic field, Carr[10] has shown that at $r_s\gg 1$ the contribution to the energy of the ground state of the anharmonic terms is of the order of r_s^{-2} per particle, and the contribution of the exchange terms is exponentially small. The magnetic field only decreases the overlap of the wave functions of the electrons of the neighboring sites; in addition, a standard calculation by perturbation theory shows that the shift of the energy of the ground state on account of the anharmonic terms in a magnetic field is of the same order as without the field. Consequently, in our case, too, the contribution of the exchange and anharmonic terms can be regarded as a small perturbation.

3. INFLUENCE OF MAGNETIC FIELD ON THE STABILITY OF A WIGNER LATTICE

We discuss now the manner in which the magnetic field influences the stability of the WL. It was shown in Sec. 2 that, just as in the two-dimensional case,[6,13] in a strong magnetic field ($\omega_c\gg\omega_0$) a "soft" mode $\nu_1\sim 1/\omega_c$ is produced in a WL. This, however, still does not indicate divergence of the mean square of the electron displacements in the WL sites. In fact, expressing the operators $\hat{x}_j(\mathbf{k})$ in terms of the operators $\hat{a}_l(\mathbf{k})$ we obtain

$$\hat{x}_j=\sum_{l=1}^{3}\left\{\xi_l^j\frac{\hat{a}_l^++\hat{a}_l}{(2\nu_l)^{1/2}}+i\eta_l^j\frac{\hat{a}_l^+-\hat{a}_l}{(2\nu_l)^{1/2}}\right\}. \tag{16}$$

The coefficients ξ_l^j and η_l^j satisfy the relations

$$(\xi_l^j)^2+(\eta_l^j)^2=\varkappa_l\Delta_{jj}^{(l)}, \tag{17}$$
$$\xi_l^j\xi_l^s+\eta_l^j\eta_l^s=-n_jn_s\nu_l^2\varkappa_l, \quad j\neq s, \tag{18}$$

where $n_j=(\mathbf{n},\mathbf{q}_j)$. It can be shown that $\varkappa_l\Delta_{jj}^{(l)}>0$, so that ξ_l^j and η_l^j are real. All the quantities in (16)–(18) are dimensionless, just as in (5) and (6). With the aid of (13)–(18) we obtain

$$\left\langle\tilde{n}\left|\sum_{j=1}^{3}\hat{x}_j^2\right|\tilde{n}\right\rangle=\sum_{j=1}^{3}\{1-\varkappa_j(\Omega_1^2-\nu_j^2)\}\frac{1}{\nu_j}\left(\tilde{n}_j+\frac{1}{2}\right). \tag{19}$$

Here $\tilde{n}_j$ are the corresponding Bose occupation numbers. In the limit as $\omega_c \to 0$ we have $\varkappa_j \to 0, \nu_j \to \omega_j$, and Eq. (19) goes over into the usual expression for the mean squared Fourier component of the displacement of the particle from the site.[11] In the limit of a strong magnetic field $\omega_c \gg \omega_0$ we get from (19)

$$\left\langle \tilde{n} \left| \sum_{j=1}^{3} \hat{x}_j^2 \right| \tilde{n} \right\rangle \approx \frac{p\Omega_1^2 - s}{\Omega_1^3 s^{1/2}} \lambda^2 \left(\tilde{n}_1 + \frac{1}{2} \right) + \frac{\hbar}{m\Omega_1} \left(\tilde{n}_2 + \frac{1}{2} \right) + 2\lambda^2 \left(\tilde{n}_3 + \frac{1}{2} \right). \tag{20}$$

Thus, the contribution of the $\nu_1 \sim 1/\omega_c$ mode to the mean squared Fourier component of the displacement is of the order of λ^2 and decreases with increasing magnetic field.

For the mean square of the α component of the electron displacement from the WL site we obtain in the limit as $\lambda \to 0$

$$\langle \tilde{n} | \hat{u}_\alpha^2 | \tilde{n} \rangle = \frac{n_\alpha^2}{N} \sum_{\mathbf{k}} \frac{\hbar}{m\Omega_1(\mathbf{k})} \left\{ \tilde{n}_2(\mathbf{k}) + \frac{1}{2} \right\}. \tag{21}$$

Here n_α is the α-th component of the unit vector along the magnetic field in the original Cartesian coordinate system, and $\tilde{n}_2(\mathbf{k})$ are the occupation numbers of the second mode. As noted in Ref. 2, the magnetic field limits substantially only the motion of the electron in the site in a direction perpendicular to the field, so that the mean squared displacement of the electron in the site is determined by the averaged frequencies $\Omega_i(\mathbf{k}, \mathbf{n})$ of the oscillations of the electron along the magnetic field, which depend not on the magnetic field but on its orientation relative to the crystallographic axes of the WL. By virtue of the inequality $\Omega_1^{-1} \leq \Sigma_i \omega_i^{-1}$ the mean square of the amplitude of the zero-point oscillations of the electron in the site decreases in a magnetic field, but by virtue of $\Omega_1 \sim \omega_p$ its order of magnitude is $\langle \hat{u}^2 \rangle^{1/2} \sim \omega_p^{-1/2} \sim r_s^{3/4}$, i.e., it is of the same order as in the absence of a field.[11]

We examine now the change of the mean squared displacement of the electron in the WL site with increasing temperature. Inasmuch as in a strong magnetic field ($\omega_c \gg \omega_0$) the modes $\nu_2 \approx \omega_p$ and $\nu_3 \approx \omega_c$ are weakly excited up to a temperature $T \lesssim \hbar\omega_p$, it is clear that only the mode $\nu_1 \sim 1/\omega_c$ contributes to $\langle u^2 \rangle$. At not too low temperatures $T \gtrsim \hbar\nu_1$ we have

$$\langle u^2 \rangle \approx \langle u^2 \rangle|_{T=0} + \frac{T}{Nm} \sum_{\mathbf{k}} \left\{ \frac{1}{\omega_1^2} + \frac{1}{\omega_2^2} + \frac{1}{\omega_3^2} - \frac{1}{\Omega_1^2} \right\}, \tag{22}$$

where $\langle u^2 \rangle|_{T=0}$ is the mean square of the amplitude of the zero-point oscillations [see (20) and (21)]. Since $\omega_3 \sim \Omega_1 \sim \omega_p \gg \omega_{1,2}$, the temperature corrections to $\langle u^2 \rangle$ are practically independent of the magnetic field under the indicated conditions. We have, however, $\langle u^2 \rangle|_{\omega \gg \omega_0} \sim T$, starting with temperatures $T \gtrsim \hbar\nu_1$, whereas $\langle u^2 \rangle|_{\omega_c=0} \sim T$ at temperatures $T \gtrsim \Theta$, where Θ is the Debye temperature of the WL. It can be shown that a strong magnetic field decreases the mean squared displacement of the electron from the site at all temperatures, and this apparently increases the stability of the WL.

4. SPECIFIC HEAT, MAGNETIC MOMENT, AND DIELECTRIC CONSTANT OF A WIGNER LATTICE

We estimate the specific heat of a WL in the case of a strong magnetic field $\omega_c \gg \omega_p$. Carr has shown[10] that the Debye temperature of a WL in the absence of a magnetic field is $\Theta \sim \hbar\omega_p$. Inasmuch as in strong magnetic fields the modes $\nu_2 \sim \omega_p$ and $\nu_3 \sim \omega_c$, it is clear that at $T \lesssim \Theta$ the main contribution to the heat capacity of the WL is made by the mode $\nu_1 \approx \omega_1\omega_2/\omega_c$, where $\omega_1 \approx \omega_2 \sim k$ are the frequencies of the transverse oscillations of the WL in the absence of a magnetic field. In the Debye approximation we obtain for the specific heat of the system

$$C_V \sim \frac{N}{V} \left(\frac{T\hbar\omega_c}{\Theta^2} \right)^{3/2} \int_0^{\Theta^2/T\hbar\omega_c} \frac{z^{3/2} e^z dz}{(e^z - 1)^2}. \tag{23}$$

Thus, at $T \lesssim \Theta^2/\hbar\omega_c$ the specific heat of the system $C_V \sim T^{3/2} B^{3/2}$.

The magnetic moment of the system, which is connected with the orbital motion of the electrons, can be obtained by differentiating the free energy of the system with respect to B. In the harmonic approximation we have

$$\mathbf{M} = -\frac{\partial F}{\partial \mathbf{B}} = -\sum_{\mathbf{k}, j=1}^{3} \frac{\hbar}{2} \operatorname{cth} \frac{\hbar\nu_j(\mathbf{k})}{2T} \frac{\partial \nu_j(\mathbf{k})}{\partial \mathbf{B}}. \tag{24}$$

We calculate the magnetic moments of the different mode modes in the case of a strong magnetic field, $\omega_c \gg \omega_p$, and not too high temperatures $T \lesssim \Theta$. For the modes $\nu_3 \approx \omega_c$ and $\nu_2 \approx \omega_p$ we can neglect the temperature dependence of the magnetic moment. Therefore for the mode ν_3 we have $\mathbf{M}_3 = -N\mu_B \mathbf{n}$, where μ_B is the Bohr magneton and $\mathbf{n}$ is the direction of the external magnetic field. This term is analogous to the magnetic moment of the free electrons in the ultraquantum limit of the magnetic field. For the mode ν_2 we get

$$\mathbf{M}_2 = -\frac{\hbar}{2} \frac{\partial}{\partial \mathbf{B}} \sum_{\mathbf{k}} \Omega_1(\mathbf{k}) = -\mu_B \sum_{\mathbf{k}} \frac{1}{\omega_c \Omega_1(\mathbf{k})} \left\{ \sum_{l=1}^{3} \omega_l^2 n_l \mathbf{q}_l - \mathbf{n}\Omega_1^2 \right\}. \tag{25}$$

We note first that $\mathbf{n} \cdot \mathbf{M}_2 = 0$, so that the moment $\mathbf{M}_2$ is perpendicular to the external magnetic field. The magnetic moment of an individual **k** mode is proportional to the expression in the curly brackets in (25) and vanishes only when **n** is parallel to one of the vectors $\mathbf{q}_l(\mathbf{k})$. For a WL only the vector sum of the moments of the individual moments can be made to vanish; this corresponds to a minimum of the energy of the zero-point oscillations (15). In view of the high symmetry of the bcc lattice, we can expect the presence of several equivalent equilibrium positions. At equilibrium it is obvious that $(\mathbf{M}_2)_{eq} = 0$.

Next, at $T \approx 0$ K, we can neglect the contribution of the mode $\nu_1 \sim 1/\omega_c$, since $M_1 \omega_c^{-2}$. At not too low temperatures, $T \gtrsim \hbar\nu_1$, we have $\coth(\hbar\nu_1/2T) \sim 2T/\hbar\nu_1$, therefore

$$\mathbf{M}_1 = -T \sum_{\mathbf{k}} \left[\frac{1}{B} \left\{ \mathbf{n} - \frac{1}{\Omega_1^2} \sum_{l=1}^{3} \omega_l^2 n_l \mathbf{q}_l \right\} - \frac{2\mu_B \mathbf{n}}{\hbar\omega_c} \right]. \tag{26}$$

When the WL is at equilibrium, the term in the curly brackets vanishes, so that

$$\mathbf{M}_{eq} = (\mathbf{M}_1)_{eq} + \mathbf{M}_3 = -N\mu_B \mathbf{n} (1 - 2T/\hbar\omega_c). \tag{27}$$

We note that the characteristic linear dependence of the magnetic moment of the WL on the temperature appears already at temperatures $T \gtrsim \hbar\nu_1$, whereas the magnetic moment of the free electrons in the same magnetic field $\hbar\omega_c \gg T$ is constant in this temperature region.

The dielectric constant of the WL in the absence of a magnetic field was investigated by Bagchi.[15] We now compare the dielectric properties of the WL in a magnetic field with Bagchi's results. It is known[11] that the longitudinal dielectric constant can be expressed in terms of exact wave functions and energy levels of the system. With the aid of (17) and (18) we obtain in the harmonic approximation

$$\frac{1}{\varepsilon(\mathbf{k},\omega)} = 1 + \frac{\omega_p^2}{\mathbf{k}^2}\sum_{j=1}^{3}\frac{\tilde{\varkappa}_j}{\omega^2-\nu_j^2}\left\{\sum_{s=1}^{3}(\mathbf{k}\mathbf{q}_s)^2\tilde{\Delta}_{ss}^{(j)} - \omega_c^2(\mathbf{k}\mathbf{n})^2\nu_j^2\right\}, \quad (28)$$

where $\tilde{\Delta}_{ss}^{(j)} = \Delta_{ss}^{(j)} + \omega_c^2(\mathbf{n}\cdot\mathbf{q}_s)^2\nu_j^2$, $\tilde{\varkappa}_j = \varkappa_j/\omega_c^4$.

In the limit as $\omega_c \to 0$, this equation goes over into Bagchi's result:

$$\frac{1}{\varepsilon(\mathbf{k},\omega)} = 1 + \frac{\omega_p^2}{\mathbf{k}^2}\sum_{j=1}^{3}\frac{(\mathbf{k}\mathbf{q})^2}{\omega^2-\omega_j^2(\mathbf{k})}, \quad (29)$$

and in the limit $\omega \gg \nu_j$ it has the regular asymptotic form[11]

Next, in the static case ($\omega = 0$), as expected, the dependence of the dielectric constant on the magnetic field vanishes and the result agrees with Eq. (29) at $\omega = 0$. In this case, of course, all the conclusions of Bagchi's paper remain valid, and particularly the static dielectric constant of the WL $\varepsilon(\mathbf{k}, 0) < 0$.

In the long wave limit $\mathbf{k} \to 0$ we get from (28)

$$\frac{1}{\varepsilon(0,\omega)} = 1 + \omega_p^2\frac{\omega^2-\varepsilon^2\omega_c^2}{[\omega^2-\nu_1^2(0)][\omega^2-\nu_2^2(0)]}, \quad (30)$$

where $\varepsilon = \mathbf{n}\cdot\mathbf{k}/k$. Thus, the dielectric constant $\varepsilon(0,\omega)$ in a strong magnetic field is anisotropic.

5. ALLOWANCE FOR TRANSVERSE ELECTROMAGNETIC FIELDS

The importance of pointing out the tranverse electromagnetic fields in the analysis of long-wave transverse WL oscillations was noted in Ref. 15. In this section we consider the more general question of the coupling of the electromagnetic and vibrational modes of the WL in a constant homogeneous magnetic field. To take into account the transverse electromagnetic fields, it is necessary to replace the momentum operator $\hat{\pi}$ of the electrons in the magnetic field by the operators $\hat{\pi} + (e/c)\mathbf{A}$, where $\mathbf{A}$ is the vector potential of the transverse electromagnetic field ($\operatorname{div}\mathbf{A} = 0$), and we must add to the Hamiltonian (1) the free-field Hamiltonian[16]

$$\hat{H}_f = \int d\mathbf{r}\left\{2\pi c^2\mathbf{P}^2 + \frac{1}{8\pi}(\operatorname{rot}\mathbf{A})^2\right\}, \quad (31)$$

where $\mathbf{P}$ is the momentum canonically conjugate to the coordinate $\mathbf{A}$.

We introduce the usual transformation of the operators:

$$\mathbf{A}(\mathbf{r},t) = \left(\frac{2}{V}\right)^{1/2}\sum_{\mathbf{k}>0,\lambda=1}^{2}\{\hat{C}_{\mathbf{k},\lambda}\cos\mathbf{k}\mathbf{r} + \hat{C}_{-\mathbf{k},\lambda}\sin\mathbf{k}\mathbf{r}\}\mathbf{e}_{\mathbf{k},\lambda},$$
$$\mathbf{P}(\mathbf{r},t) = \left(\frac{2}{V}\right)^{1/2}\sum_{\mathbf{k}>0,\lambda=1}^{2}\{\hat{P}_{\mathbf{k},\lambda}\cos\mathbf{k}\mathbf{r} + \hat{P}_{-\mathbf{k},\lambda}\sin\mathbf{k}\mathbf{r}\}\mathbf{e}_{\mathbf{k},\lambda}. \quad (32)$$

Here $\mathbf{e}_{\mathbf{k},\lambda}$ are the free-field polarization vectors, so that $\mathbf{k}\cdot\mathbf{e}_{\mathbf{k},\lambda} = 0$ and $\mathbf{e}_{\mathbf{k},\lambda}\mathbf{e}_{\mathbf{k},\lambda'} = \delta_{\lambda\lambda'}$, with $\mathbf{e}_{-\mathbf{k},\lambda} = \mathbf{e}_{\mathbf{k},\lambda}$. We use henceforth also a unit vector $\mathbf{e}_3$ directed along the vector $\mathbf{k}$. The operators $\hat{C}_{\mathbf{k},\lambda}$ and $\hat{P}_{\mathbf{k},\lambda}$ satisfy the commutation relations

$$[\hat{C}_{\mathbf{k},\lambda}, \hat{C}_{\mathbf{k}',\lambda'}] = [\hat{P}_{\mathbf{k},\lambda}, \hat{P}_{\mathbf{k}',\lambda'}] = 0,$$
$$[\hat{C}_{\mathbf{k},\lambda}, \hat{P}_{\mathbf{k}',\lambda'}] = i\hbar\delta_{\lambda\lambda'}\delta_{\mathbf{k}\mathbf{k}'}. \quad (33)$$

Carrying out the transformations (4) and (32) in the total Hamiltonian (1), (31), we represent the Hamiltonian of the system, with account taken of the transverse fields, in the form of a sum of independent Hamiltonians

$$\hat{H} = \sum_{\mathbf{k}}\hat{H}_{\mathbf{k}},$$
$$\hat{H}_{\mathbf{k}} = \frac{1}{2}\sum_{s=1}^{3}\{\hat{\Pi}_s^2 + \omega_s^2\hat{x}_s^2\} + \frac{1}{2}\sum_{\lambda=1}^{2}\{\hat{P}_\lambda^2 + (1+\mathbf{k}^2)\hat{C}_\lambda^2\} + \sum_{s=1}^{3}\sum_{\lambda=1}^{2}\hat{\Pi}_s\hat{C}_\lambda(\mathbf{q}_s\mathbf{e}_\lambda). \quad (34)$$

In the derivation of (34) we used the long-wave approximation $\mathbf{k}\cdot\mathbf{R}_{ij} \ll 1$, i.e., we did not take into account the obvious effect of the periodic structure of the WL on the light-wave dispersion law. On the other hand, the interaction of the light with the lattice oscillations and of the different oscillation modes with one another is described correctly by this approximation.

In the expression for H_k, the first term coincides with (6), the second stems from the free-field Hamiltonian and A^2, and the third from the terms $\hat{\pi}A$. The operators in (34) satisfy the following commutation relations (for one and the same k):

$$[\hat{x}_\alpha, \hat{\Pi}_\beta] = i\delta_{\alpha,\beta}, \quad [\hat{C}_\lambda, \hat{P}_{\lambda'}] = i\omega_p\delta_{\lambda\lambda'},$$
$$[\hat{\Pi}_\alpha, \hat{\Pi}_\beta] = -i(\mathbf{n}\mathbf{q}_\gamma)\hat{e}_{\alpha\beta\gamma}. \quad (35)$$

All the remaining commutation relations are equal to zero. In (35) we have made k, P, and C dimensionless relative to ω_p/c, $\hbar\omega_c/4\pi c^2$, and $(4\pi\hbar\omega_c c^2/\omega_p^2)^{1/2}$, and have reduced the operators $\hat{x}$, $\hat{\pi}$, and $\hat{H}$, as well as the frequencies, to dimensionless form as in Sec. 2. The natural frequencies of the Hamiltonian (34) can be determined by the method used in Sec. 2. We then obtain the following dispersion equation for the natural frequencies of the system $\nu_j(\mathbf{k})$, $j = 1-5$:

$$(\nu^2-\omega_k^2)^2\Delta(\nu) + \nu^4\omega_p^4(\nu^2-\Omega_2^2) + \omega_p^2\nu^2(\nu^2-\omega_k^2)$$
$$\times\{-2\nu^4 + \nu^2[\omega_0^2 + \Omega_2^2 + 1 - (\mathbf{n}\mathbf{e}_3)^2] + d - p\} = 0. \quad (36)$$

In this equation $\omega_k = ck$, $\Delta(\nu)$ is the left-hand side of the dispersion equation in Sec. 2;

$$\Omega_2^2 = \sum_i \varepsilon_i^2\omega_i^2, \quad d = s\sum_i \varepsilon_i^2/\omega_i^2, \quad \varepsilon_i = \mathbf{e}_3\mathbf{q}_i;$$

and the remaining symbols are the same as in Sec. 2.

It can be verified that all the solutions of (36) are real, i.e., the interaction of the lattice oscillations with the intrinsic radiation does not make the lattice unstable. We note also that when we take formally the limit as $\omega_p \to 0$ the electromagnetic modes and the

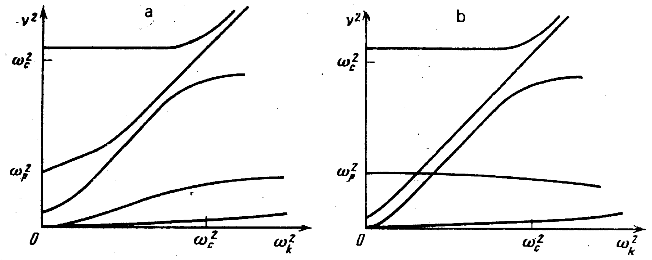

FIG. 1. Dispersion of the WL oscillations with allowance for the proper radiation field in a high-symmetry direction of a bcc lattice: a—external magnetic field perpendicular to the wave vector, b—external field parallel to the wave vector.

modes of the particle oscillations become independent.

We dwell now on the case $\omega_c \gg \omega_p$, $\omega_c \gg \omega_k$. It is easy to find from (36) that in this case the natural frequencies of the system are

$$\nu_1 = s^{1/2}/\Omega_1\omega_c, \quad \nu_2^2+\nu_3^2=\omega_k^2+\Omega_1^2+\omega_p^2(1-(\mathbf{n}\mathbf{e}_3)^2),$$
$$\nu_2^2\nu_3^2=\omega_k^2\Omega_1^2, \quad \nu_4=\omega_k, \quad \nu_5=\omega_c. \tag{37}$$

Thus, in a strong magnetic field allowance for the transverse fields leads only to corrections to the branch Ω_1 of Sec. 2. The conclusions of Secs. 3 and 4 remain qualitatively unchanged, since the asymptotic expression for the "soft" mode ν_1 remain the same as before, and in (37) the frequencies $\nu_2 \sim \omega_p$ and $\nu_3 \sim \omega_k$.

To obtain the character of the spectrum, we examine the following characteristic cases:

1. $\omega_c = 0$; direction [100] or [111]. In this case the bare polarizations are preserved: $\omega_{1,2}$ correspond to the transverse oscillations and ω_3 to the longitudinal one. From (36) at $\omega_{1,2} = \omega$ we have

$$(\nu^2-\omega_3^2)[(\nu^2-\omega_k^2)(\nu^2-\omega^2)-\omega_p^2\nu^2]^2=0. \tag{38}$$

Thus, the radiation does not influence the longitudinal oscillation, and the radiation interacts with the transverse oscillations in the region $k < \omega_p/c$. In (38) the transverse modes are doubly degenerate. When a magnetic field is applied, a nonzero right-hand side appears in (38).

2. $\mathbf{n} \perp \mathbf{k}$. The dispersion equation breaks up in this case into two: there are two roots in which the transverse oscillations are polarized along the field and which the magnetic field does not influence:

$$(\nu^2-\omega_k^2)(\nu^2-\omega^2)-\nu^2\omega_p^2=0. \tag{39a}$$

The magnetic field couples the transverse oscillations with the two transverse oscillations with polarization perpendicular to the magnetic field:

$$(\nu^2-\omega_3^2)[(\nu^2-\omega_k^2)(\nu^2-\omega^2)-\nu^2\omega_p^2]=\omega_c^2\nu^2(\nu^2-\omega_k^2). \tag{39b}$$

3. $\mathbf{n} \parallel \mathbf{k}$. In this case there is an undisplaced longitudinal oscillation $\nu^2 = \nu_3^2$. The remaining modes are coupled by the field:

$$[(\nu^2-\omega_k^2)(\nu^2-\omega^2)-\nu^2\omega_p^2]^2=\omega_c^2\nu^2(\nu^2-\omega_k^2)^2. \tag{40}$$

The qualitative form of the dispersion curves in the last two cases is shown in the figure.

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[1] The frequencies of the oscillations of a WL in a magnetic field, as well as a quasiclassical estimate of the mean squared displacement of the particle from a WL site, are given in a paper by Rakhmanov.[2]

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