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Lattice distortions in magnetic fields

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Abstract. A study is made of the stability of the possible lattice structures which result from the magnetic-field-induced lattice deformation introduced by Araujo and Khmelnitskii. The deformed lattice may either be the result of a single distortion occurring along a particular direction or of a superposition of distortions in different directions. In a noninteracting electron model the energy variation of the electron system will determine which final lattice structure is the most stable. When electron interactions are considered in the Hartree approximation we find that the energy variation of the electron system alone will not determine which final structure is the most stable. The latter is then imposed by the lattice itself. If the distortion turns out to be unidirectional then the corresponding charge-density wave should be weakly pinned even in the absence of impurities.

The problem of the motion of electrons in a uniform magnetical field and periodic electrostatic potential has been extensively studied over the years [1–4]. The electron eigenstates are characterized by a quasi-momentum $\boldsymbol{k}$ associated with translation operators which, in addition to a spatial translation of the lattice, also incorporate a guage transformation [1, 5]. These operators are defined on a magnetic lattice (ML) which is usually different from the real lattice (RL). The energy spectrum consists of Bloch bands $E(\boldsymbol{k})$. An important point is that the general properties of the spectrum (such as the distribution of the energy bands) depend only on one parameter, the magnetic field flux per unit cell ϕ/ϕ_0, where ϕ_0 denotes the flux quantum. In particular, if the flux is a rational number $\phi/\phi_0 = p/q$ then the bands are q-fold degenerate [1, 5].

It has been shown in [6] that a two-dimensional system of Bloch electrons in a perpendicular magnetic field may undergo a periodic lattice distortion (leading to a charge-density wave) if the chemical potential is located at a Van Hove singularity of the density of states and the magnetic flux per unit cell ϕ/ϕ_0 is non-integer. The energy reduction arises because the lattice deformation splits the initial Van Hove singularity into several logarithmic singularities. The existence of the singularities follows from the periodicity of the function $E(\boldsymbol{k})$. There must be saddle-points $\boldsymbol{k}^*$ and in their vicinity the dispersion relation has an expansion of the form

$$E(\boldsymbol{k}) \approx \frac{\hbar^2}{2m_+}(k_x - k_x^*)^2 + \frac{\hbar^2}{2m_-}(k_y - k_y^*)^2$$

where the effective masses $m_+ > 0$ and $m_- < 0$, for instance. Each saddle-point gives a logarithmic contribution to the density of states:

$$\frac{\sqrt{-m_+m_-}}{2\pi^2\hbar^2}\log\left|\frac{W}{E}\right| \tag{1}$$

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where W represents an energy scale which is or the order of the bandwidth. The perturbation introduced by the lattice distortion shifts the energies of different saddle-points by different amounts. This instability is a consequence of the ML and RL not having the same symmetry: when the flux per unit cell is rational and noninteger, the RL has more symmetry than the ML and this leads to the degeneracy of the energy bands. The ground state is then obtained, under certain conditions, by lifting this degeneracy. From this point of view, the phenomenon is comparable to the Jahn–Teller distortion of molecules.

The discussion in [6] concerned the case of a square lattice but it may be easily generalized to other lattice geometries: if $\phi/\phi_0 = p/q$ and the vectors $\boldsymbol{a}$, $\boldsymbol{b}$ define the RL (not necessarily square) then one may define the ML using the vectors $\boldsymbol{u}_1 = q\boldsymbol{a}$ and $\boldsymbol{u}_2 = \boldsymbol{b}$. The corresponding reciprocal lattice vectors shall be denoted by $\boldsymbol{a}^*$, $\boldsymbol{b}^*$, etc. The single-particle dispersion relation has the property [5]

$$E_0(\boldsymbol{k}) = E_0\left(\boldsymbol{k} + \frac{1}{q}\boldsymbol{u}_2^*\right).$$

A lattice distortion having period $\lambda = 2\pi q/(j|\boldsymbol{a}^*|)$ with j integer and not a multiple of q, creating the potential

$$V(\boldsymbol{r}) = V\cos(j\boldsymbol{u}_1^* \cdot \boldsymbol{r}) \tag{2}$$

would cause the energies of different saddle-points of $E_0(\boldsymbol{k})$ to shift by different amounts. Furthermore, since we could also have chosen the vectors $(\boldsymbol{a}, q\boldsymbol{b})$ to define the magnetic lattice, we see that it is also possible to have deformations with

$$V(\boldsymbol{r}) = V\cos\left(\frac{j}{q}\boldsymbol{b}^* \cdot \boldsymbol{r}\right). \tag{3}$$

The period of the distortion is chosen so as to minimize the total energy, which is proportional to $I - U^{-1}$ [6]. This would fix the value of j and the direction of the charge-density wave if $|\boldsymbol{a}| \neq |\boldsymbol{b}|$. I is a parameter which includes the electron–phonon coupling and the elastic properties of the material. The quantity U accounts for the screening of the lattice distortion due to electron interactions. In [6] it was taken to be the 2D Fourier transform of the Coulomb interaction (at the wavelength of distortion) but it may also include negative correction terms which account for exchange and correlation effects [7, 8].

While the period of the deformation is thus fixed, by the second-order (in the amplitude) contributions to the energy, the distortion can still occur along two or even three possible directions if the vectors $\boldsymbol{a}$ and $\boldsymbol{b}$, defining the lattice, have the same length [9].

In this case, the question arises whether the distortion should occur along only one of the possible directions or whether it should be a superposition of distortions in different directions. In order to solve this problem it is necessary to calculate the contributions to the energy variation to fourth order in the amplitude of distortion. It is found that in the non-interacting electron picture the variation in energy of the electron gas determines the structure of the deformed lattice. But when the electron interactions are accounted for in the spirit of Hartree theory we find that the energy variation of the electron system does not determine the final structure. The latter is then imposed by the lattice itself.

We shall consider the case $\phi = \phi_0/2$ in a square lattice of period a, as in [6]. Generally, a distortion with period, say, $2a$ would create the potential

$$V(\boldsymbol{r}) = V_1\cos\left(\frac{\pi}{\alpha}x\right) + V_2\cos\left(\frac{\pi}{a}y\right). \tag{4}$$

The expansion of the variation in energy of the system in powers of the amplitudes must be invariant under change of sign of V_1 or V_2, or under the interchange $V_1 \leftrightarrow V_2$. It follows

that it must have the form

$$\Delta E = (V_1^2 + V_2^2)A + (V_1^2 + V_2^2)^2 B + V_1^2 V_2^2 C + \cdots \tag{5}$$

which is the same as the Landau expansion of the free energy in the theory of ferroelectricity [10]. It is then seen that if $C > 0$ the distortion is unidirectional ($V_1 = V$, $V_2 = 0$), and if $C < 0$ a bidirectional distortion, with $V_1 = V_2 = V/\sqrt{2}$, is preferred. It must be noted that each of the coefficients in (5) is the sum of an electronic contribution (to be calculated below) and a lattice contribution which could be obtained from a total energy calculation of the deformed lattice (only the lattice contribution to A could be found from tabulated elastic parameters).

The potential given in (4) will be treated as a perturbation on the partially filled band. If $V_2 = 0$ and $V_1 = V$, the perturbation is diagonal in $\boldsymbol{k}$-space and its effect on the state $\boldsymbol{k} + \hat{\boldsymbol{y}}\pi/a$ is identical to its effect on the states $\boldsymbol{k}$ with V replaced by $-V$. If follows that if the energy shift of the saddle-point $\boldsymbol{k}^*$ is expanded as $\eta + b\eta^2$, with $\eta \propto V$, then the energy of the saddle-point $\boldsymbol{k}^* + \hat{\boldsymbol{y}}\pi/a$ is shifted by $-\eta + b\eta^2$. (η will be calculated in a simple model below.) Also, if the effective masses are affected by the perturbation in such a way that the prefactor of the logarithm in (1) for the point $\boldsymbol{k}^*$ is, after distortion,

$$\sqrt{-m_+ m_-}(1 + \alpha\eta + \beta\eta^2 + \cdots)$$

then we simply have to make the change $\eta \to -\eta$ for the point $\boldsymbol{k}^* + \hat{\boldsymbol{y}}\pi/a$. The other pair of saddle-points can be treated in a similar fashion. The contribution of $\boldsymbol{k}^*$ to the variation in energy is then proportional to

$$-\sqrt{-m_+ m_-}\int_{-W}^{W} \{(1 + \alpha\eta + \beta\eta^2 + \cdots)\log|E + \eta + b\eta^2| + (1 - \alpha\eta + \beta\eta^2 + \cdots) \times \log|E - \eta + b\eta^2| - 2\log|E|\} f(E) E \,\mathrm{d}E \tag{6}$$

where $f(E)$ denotes the Fermi–Dirac distribution function and W represents an energy cut-off of the order of bandwidth. At zero temperature, integrals that contain a logarithmic term have the following expansion:

$$\int_{-W}^{0} E\log|E + \xi|\,\mathrm{d}E = \int_{-W}^{0} E\log|E|\,\mathrm{d}E + W\xi - \frac{1}{2}\xi^2\log\frac{|\xi|}{W} - \frac{\xi^3}{3W} - \frac{\xi^4}{8W^2} + \cdots. \tag{7}$$

It should be kept in mind, however, that the logarithm only represents the nonanalytic part of the density of states. There is also a background regular contribution which would modify the coefficients of the simple powers in the expansion (7). This means that only the $\sim \xi^2$ term can be meaningfully retained. At finite temperature the quantity $\log|\xi|$ is replaced by $\log T$ and there are only small corrections to the coefficients of the other powers of ξ. The contribution (6) to the energy is, to logarithmic accuracy,

$$\eta^2\log\frac{T}{W} + \eta^4(b^2 + 2\alpha b + \beta)\log\frac{T}{W}. \tag{8}$$

If the distortion is bidirectional, the V_2-term will introduce matrix elements between the states $\boldsymbol{k}$ and $\boldsymbol{k} + \hat{\boldsymbol{y}}\pi/a$. From the first-order perturbation theory we obtain

$$E(\boldsymbol{k}) = E_0(\boldsymbol{k}) \pm \sqrt{|\langle\boldsymbol{k}|\hat{V}_1|\boldsymbol{k}\rangle|^2 + |\langle\boldsymbol{k} + \hat{\boldsymbol{y}}(\pi/a)|\hat{V}_2|\boldsymbol{k}\rangle|^2}. \tag{9}$$

The treatment of the saddle-points can still be done, in this case, using the method explained above. Now the changes $\eta \to -\eta$ correspond to choosing the $+$ or $-$ sign in (9) and a result analogous to (8) is obtained.

It is seen from (8) that the fourth-order term in η is large as $T \to 0$ and depends on the modifications of the effective masses introduced by the distortion as well as on the nonlinear displacements of the energy of the saddle-points.

We conclude that in the non-interacting electron picture the fourth-order terms in (5) are large and logarithmic, and the quantities b, α and β will determine the sign of C, hence the structure of the deformed lattice. The largeness of the logarithm is important because it dominates the lattice contributions to C. The quantities b, α and β should be calculated for each model of the Bloch electron system. A calculation will be given below for the case where the periodic potential can be treated as a perturbation on the Landau levels created by the magnetic field. Taking the screening into account in the spirit of the Hartree theory, we write, as in [6],

$$V = V_l + \delta n\, U \tag{10}$$

and

$$\delta n = 4w^2 V[\chi_0 + V F]. \tag{11}$$

The parameters V_1 and V_2 in equation (5) should now be replaced by V_{1l} and V_{2l}. Equation (10) expresses the fact that the potential felt by an electron is due to the lattice distortion plus the potential created by the electron density change. Equation (11) is a self-consistency condition and the quality F can be obtained, in principle, by integration of the electron density in the Brillouin zone in the neighbourhood of the saddle-points. But from the previous discussion it should be clear that F is proportional to $\log T$, at most. It has also been shown in [6] that $\chi_0 \propto \log T$. Equations (10) and (11) enable us to expand V in powers of V_l. Since $\eta \propto V$,

$$\eta = \frac{1}{1 - 4w^2 U \chi_0}\eta_\ell + \frac{4w^2 U F}{[1 - 4w^2 U \chi_0]^4}\eta_l^3 + \cdots.$$

The variation of the energy of the electron liquid is equal to $-U\delta n^2$ [6] plus the terms given in (8). Since $\chi_0 \propto \log T$, we see that, as $T \to 0$, the coefficient of the η^4 term goes to zero as $(\log T)^{-3}$. This is a small quantity, so one should expect the lattice contributions to C to dominate and determine the final structure.

We note that we have calculated ΔE to fourth order although the perturbation (4) was treated, according to (9), only to first order. The corrections to the result (9) involve matrix elements of the potential (4) between different bands. Another quantity, V/ϵ_0, where ϵ_0 is the energy separation of the bands, would then be introduced in the problem. Second-order perturbation theory in V would cause a quantitative, but not qualitative, change in the results obtained. In particular, the numbers b and β could be modified. Higher-order perturbative treatment would be unnecessary because b and β are related only to second-order ($\sim \eta^2$) effects.

For the purpose of illustration, we may use a model in which the lattice potential is a weak perturbation on the lowest Landau level and Landau level mixing can be ignored. Considering first a unidirectional distortion and allowing for a phase ϕ in the potential (4), the dispersion relation is

$$E(\boldsymbol{k}) = E_0(\boldsymbol{k}) + v\cos(ak_y + \phi) \tag{12}$$

with $v = V\exp(-\pi/4)$ [6]. The unperturbed wavefunctions, with energy $E_0(\boldsymbol{k})$, are given by

$$\Psi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{NL}}\sum_{j\in z} \mathrm{e}^{-\mathrm{i}2ajk_x}\mathrm{e}^{\mathrm{i}(k_y + 2\pi j/a)y}\phi(x + l^2k_y + 2aj)$$

where L is the linear size of the system, l is the magnetic length, $N = aL/(2\pi l^2)$ and

$$\phi(x) = \left[\frac{1}{\pi l^2}\right]^{1/4} \mathrm{e}^{-\frac{1}{2l^2}x^2}.$$

According to (12) the saddle-points ($k_x = \pm\frac{\pi}{2a}$, $k_y = 0$) of $E_0(\boldsymbol{k})$, for instance, have their energy shifted by

$$v\cos\phi - \frac{v^2\sin^2\phi}{\frac{2\hbar^2}{m+a^2} - 2v\cos\phi}.$$

So the parameter η in (6) is $\eta = v\cos\phi$. The effective mass m_- is unaffected but m_+ must be multiplied by

$$\left[1 - \eta\frac{m+a^2}{\hbar^2}\right]^{-1}$$

which is then to be expanded in powers of η. After treating the saddle-points ($k_x = 0$, $k_y = \pm\frac{\pi}{2a}$) in a similar fashion, the following result for the variation in energy of the electron gas is obtained:

$$\Delta E \propto v^2\log\frac{T}{W} + v^4\left\{(\cos^4\phi)\left(\frac{m_+a^2}{\hbar^2}\right)^2\left[\frac{1}{4}\tan^4\phi - \frac{1}{2}\tan^2\phi + \frac{3}{8}\right]\right.$$
$$\left.+(\sin^4\phi)\left(\frac{m_-a^2}{\hbar^2}\right)^2\left[\frac{1}{4}\cot^4\phi - \frac{1}{2}\cot^2\phi + \frac{3}{8}\right]\right\}\log\frac{T}{W}. \tag{13}$$

The $\sim v^4$ term shows that $\phi = 0$ is the most energetically profitable choice.

If the distortion is bidirectional then (9) gives

$$E(\boldsymbol{k}) = E_0(\boldsymbol{k}) \pm \frac{1}{\sqrt{2}}v\sqrt{\cos^2(ak_x) + \cos^2(ak_y)}.$$

The four saddle-points are displaced by the same amount, equal to $v/\sqrt{2} \equiv \eta$, and the new values M_+ and M_- if the effective masses are

$$M_+ = \frac{m_+}{1 - \eta\frac{m_+a^2}{\hbar^2}} \qquad M_- = \frac{m_-}{1 + \eta\frac{m_-a^2}{\hbar^2}}.$$

It follows that the variation of the energy of the electron gas is

$$\Delta E \propto v^2\log\frac{T}{W} + v^4\frac{a^4(3m_+^2 + 3m_-^2 - 2m_-m_+)}{16\hbar^4}\log\frac{T}{W}. \tag{14}$$

It is seen, from the results (13) and (14), that the gas would prefer a unidirectional distortion.

The electron interactions make the fourth-order terms become small $\sim (\log T)^{-3}$. If $C > 0$ and the distortion is unidirectional, it is expected that the charge-density wave will be weakly pinned because the expression (13) favours the phase $\phi = 0$. If impurities are present in the system, they should also pin these charge-density waves, in analogy with those systems which have a Peierls instability [11].

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