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Possible electron–phonon instabilities in two-dimensional Bloch-electron systems in magnetic fields

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Abstract. The spectrum of a two-dimensional electron system in a square lattice potential subject to a perpendicular magnetic field is considered. Well known symmetry considerations show that if the magnetic field flux per unit cell (measured in units of the flux quantum $hc/|e|$) is rational and non-integer, the electron energy can be expressed as a function of a generalized momentum k and the spectrum consists of translationally degenerate bands in k-space. In this work it is shown that if the chemical potential is located at a logarithmic Van Hove singularity of the density of states then it is possible that a periodic lattice distortion is energetically favourable. This instability persists when the flux is changed within a small interval. The width of this interval as well as the critical temperature marking the onset of the instability can be estimated with logarithmic accuracy. The effects of electron–electron interactions are considered in the Hartree approximation.

1. Introduction

The application of a constant magnetic field strongly modifies the band structure of electrons moving in two-dimensional periodic electrostatic potentials. The qualitative properties of the resulting spectrum depend only on a single parameter, the ratio between the magnetic field flux per unit cell (ϕ) and the flux quantum ($\phi_0 = hc/|e|$) as was shown by Brown (1964) and Zak (1964). (See also the paper by Hofstadter (1976) for a more detailed discription).

When the magnetic field flux per unit cell (ϕ/ϕ_0) is non-integer and rational it is possible to introduce a set of commuting magnetic translation operators (which commute with the Hamiltonian) defined in a lattice that has a unit cell ('magnetic cell') larger than the real unit cell of the crystal (Brown 1964, Zak 1964). From this discrete translation symmetry results a generalized quasimomentum k and the spectrum consists of several degenerate bands in k-space. So, it is seen that in this case the magnetic field introduces a periodicity additional to that of the lattice. The question this paper is addressed to is whether it is energetically profitable for the lattice to change its period and adjust the lattice translations to the magnetic translations. This tendency for, say, $\phi = \phi_0/2$, would resemble the Peierls instability (Peierls 1955) of the one-dimensional metals. It is found that there is no such instability for arbitrary electron concentrations but, if the concentration corresponds to the chemical potential being located at a logarithmic Van Hove singularity of the density of states then, in the non-interacting electron picture, there is an instability leading to a periodic lattice distortion (PLD) for arbitrarily weak electron–phonon- coupling. The PLD affects the energy spectrum by splitting originally coincident Van Hove (logarithmic) singularities and the consequent electron redistribution over the k-states in the Brillouin zone lowers the

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2DES energy by an amount that exceeds the work done by the elastic forces. For, if the singularities are split by an amount v, then, at $T = 0$, the energy of the non-interacting 2DES is lowered by $\Delta E \propto v^2 \log v$. The PLD would then always occur since the elastic energy of deformation is proportional to v^2. Electron interactions screen the lattice potential, however, and as a result the decrease in the 2DES energy becomes comparable to the elastic energy of the lattice deformation ($\propto v^2$). The sign of the net quadratic term will then determine the existence of an instability.

The model Hamiltonian for the two-dimensional system is taken as

$$\hat{H} = \frac{[p - e/cA]^2}{2m} + V(x, y) \tag{1}$$

where $\nabla \times A = B\hat{z}$ is a constant magnetic field and $V(x, y)$ describes a square lattice potential with lattice spacing a. We shall first focus on the case in which $\phi = \frac{1}{2}\phi_0$. Finite-temperature effects will be studied, as well as the behaviour of the instability for small changes in the flux. The latter must, of course, be kept within a small critical interval for the instability to exist. The width of this interval and the critical temperature of the transition to the PLD phase will be given by expressions with logarithmic accuracy.

2. Theory of the $\phi = \frac{1}{2}\phi_0$ case

The magnetic unit cell may be defined by the vectors

$$u_1 = 2a\hat{x}$$
$$u_2 = a\hat{y}$$

and the electron eigenstates ψ_k form a one-dimensional representation of the magnetic translation group:

$$T_L \psi_k(r) = e^{ik\cdot L}\psi_k(r) \tag{2}$$

with

$$-\frac{\pi}{2a} < k_x < \frac{\pi}{2a}$$
$$-\frac{\pi}{a} < k_y < \frac{\pi}{a}$$
$$T_L \equiv \exp\left[i\left(p - \frac{e}{c}A\right) \cdot L\right]$$

and L is any magnetic lattice vector. The important feature of the electron dispersion relation is its periodicity in the y-component of k (Lifshitz and Pitaevskii 1980):

$$E_0(k_x, k_y) = E_0\left(k_x, k_y + \frac{\pi}{a}\right) \tag{3}$$

which makes the magnetic Brillouin zone effectively consist of a set of two translationally degenerate 'valleys'.

We now consider the effect of a periodic lattice distortion along the direction of one of the primitive vectors (the x-axis is chosen for convenience) with period $2a$:

$$V(x) = V \cos \frac{\pi}{a} x. \tag{4}$$

The important feature of this perturbation $\hat{V}$ is that it does not couple states with different $\boldsymbol{k}$ but its diagonal matrix elements lift the above-mentioned valley degeneracy according to

$$E(\boldsymbol{k}) = E_0(\boldsymbol{k}) + \langle \boldsymbol{k} \mid \hat{V} \mid \boldsymbol{k} \rangle \tag{5}$$

($E_0(\boldsymbol{k})$ is the unperturbed dispersion relation) and this causes the valleys to exchange particles. If the chemical potential lies at a saddle point of the dispersion relation (a Van Hove singularity in the density of states) then this process will lower the energy of the electron system by an amount proportional to $-V^2 \log V$ (see below). Since this is stronger than the work done by the elastic forces ($\propto V^2$), a PLD is likely to occur. The screening of the lattice potential due to electron interactions will be considered later.

It is easy to see that the application of a flux quantum through the unit cell would not lead to a lattice distortion, for in this case a perturbation of wavelength $2a$ (for instance) would cause a gap in the k_x dependence of the energy at $k_x = \pm\pi/2a$ (which might depend smoothly on k_y) and we could then consider two possible band fillings (see figures 1 and 2). The energy change is

$$\Delta E \propto \int \mathrm{d}k_x \, \mathrm{d}k_y \Delta E(k_x, k_y) \tag{6}$$

and the main contribution to the integral comes from the shaded regions. Integration along k_x always leads to a factor of $V^2 \log V$. In the case illustrated in figure 1 the energy dependence on k_y is quadratic and since the gap is $\propto V$, the width of the integration region is $\propto \sqrt{V}$. So $\Delta E \propto V^{5/2} \log V$. In the case of figure 2 the k_y dependence is linear and therefore $\Delta E \propto V^3 \log V$. In both cases $\Delta E \ll V^2$ and V^2 is the elastic energy associated with the lattice deformation.

The following further assumptions about $E_0(\boldsymbol{k})$ are introduced. If p is an integer such that

$$-2 \leqslant p \leqslant 2$$

then there are saddle-points at $\boldsymbol{k} = (0, p\pi/2a)$ for odd p and $\boldsymbol{k} = (\pm\pi/2a, p\pi/2a)$ for even p. They all have the same energy, which is taken to be zero, so that the following expansions are valid in their vicinity:

$$\begin{aligned} E_0(k_x, k_y) &\cong \frac{\hbar^2}{2m_-}\left(k_x - \frac{\pi}{2a}\right)^2 + \frac{\hbar^2}{2m_+}\left(k_y - \frac{p\pi}{2a}\right)^2 \qquad \text{for even } p \\ E_0(k_x, k_y) &\cong \frac{\hbar^2}{2m_+}{k_x}^2 + \frac{\hbar^2}{2m_-}\left(k_y - \frac{p\pi}{2a}\right)^2 \qquad \text{for odd } p \end{aligned} \tag{7}$$

where m_- (< 0) and m_+ (> 0) denote effective masses. These assumptions are very general and not restrictive. The theory is also applicable to other saddle-points that might eventually exist.

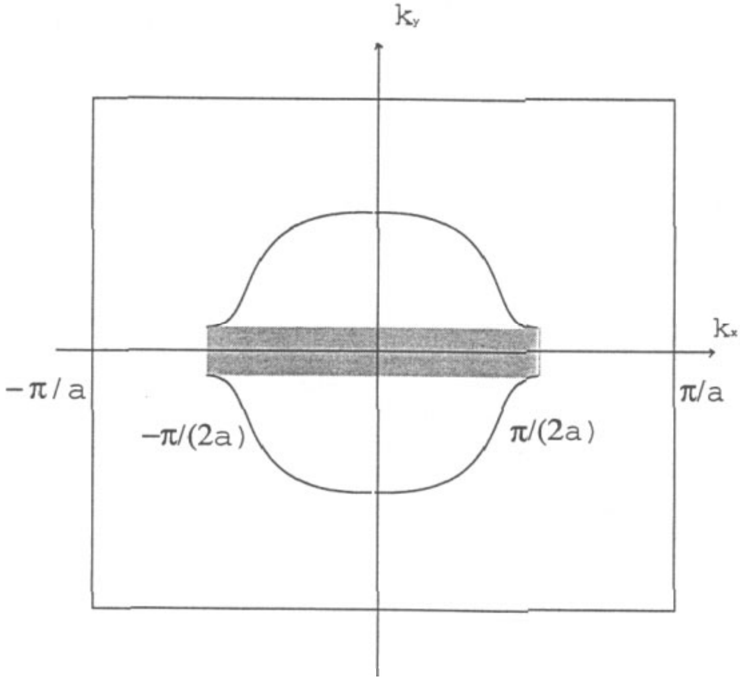

Figure 1. Possible Fermi surface for a system with a dispersion relation showing a gap at $k_x = +\pi/(2a)$ as a consequence of a periodic lattice distortion with period $2a$. The magnetic field strength is equivalent to one flux quantum per unit cell. The reduction in the 2DES energy resulting from the distortion is obtained by integration inside the shaded region.

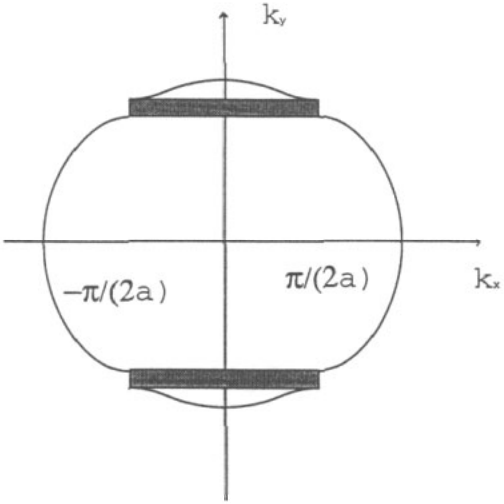

Figure 2. The same system as in figure 1 with a larger band filling.

The contribution of each saddle-point, at given k_y, to the total density of states takes the form (Van Hove 1953)

$$D(E) \approx \frac{\sqrt{-m_+ m_-}}{2\,\pi^2 \hbar^2}\ \log\left|\frac{W}{E}\right|. \tag{8}$$

Here W represents an energy scale that is of the order of the bandwidth and the total density of states for energies close to zero is given by the sum of the contributions (8) with logarithmic accuracy. The perturbation $\hat{V}$ only has diagonal matrix elements:

$$\langle \boldsymbol{k} \mid \hat{V} \mid \boldsymbol{k} \rangle = V \int \mathrm{d}^2 r\ \cos\left(\frac{\pi}{a} x\right)\ |\psi_{\boldsymbol{k}}(\boldsymbol{r})|^2 \tag{9}$$

Since the state $\psi_{\boldsymbol{k}+(\pi/a)\hat{\boldsymbol{y}}}$ is obtained by applying the translation operator along $a\hat{\boldsymbol{x}}$ (not a magnetic lattice vector) to the state $\psi_{\boldsymbol{k}}$, it is seen that the expression (9) changes sign when $\boldsymbol{k}$ is replaced by $\boldsymbol{k} + (\pi/a)\hat{\boldsymbol{y}}$. We can then assume that $\langle \boldsymbol{k} \mid \hat{V} \mid \boldsymbol{k} \rangle$ is positive for $-\pi/a < k_y < \pi/a$ passing through zero at $k_y = \pm\pi/2a$. The energy of the saddle-points with $k_y = \pm\pi/2a$ is then changed by an amount that is proportional to V^2 and the saddle-points ($\boldsymbol{k}^*$) with $k_y = 0$ and $k_y = \pi/a$ have their energy changed by v, proportional to V, defined by

$$v \equiv V \int \mathrm{d}^2 r \cos\left(\frac{\pi}{a} x\right)\ |\psi_{\boldsymbol{k}^*}(\boldsymbol{r})|^2 \equiv wV \tag{10}$$

and v is the small parameter in the problem.

We now consider $T = 0$. If the chemical potential $\mu = 0$ and the transition occurs at fixed number of particles, the equation for the changed value of the chemical potential is

$$(\mu - v)\ \log|\mu - v|\ +\ (\mu + v)\ \log|\mu + v| + 2\,(\mu - \propto v^2)\log|\mu - \propto v^2| = 0$$

and this implies $\mu \propto v^2$, which is small. Therefore, the transition occurs at practically constant chemical potential. The variation of the 2DES energy is

$$\begin{aligned}\Delta E = \frac{\sqrt{-m_+ m_-}}{2\pi^2\hbar^2}\left[\int^0 \mathrm{d}E E\ \log\left|\frac{W}{E+v}\right| + \int^0 \mathrm{d}E E\ \log\left|\frac{W}{E-v}\right| - 2\int^0 \mathrm{d}E E\ \log\left|\frac{W}{E}\right|\ \right] \\ \simeq \frac{\sqrt{-m_+ m_-}}{2\pi^2\hbar^2} v^2\ \log\left|\frac{v}{W}\right|.\end{aligned} \tag{11}$$

The logarithmic singularity that is displaced by $\propto v^2$ gives a negligible contribution and was ignored.

The effect of finite temperature is to smear the electron distribution around the logarithmic singularity in the density of states over a range of energies of order T (we take $k_{\mathrm{B}} = 1$). The splitting of the singularities will then cause a variation in the 2DES energy that is not so strong as in the zero-temperature case. If this phenomenon- only involves electron redistribution near the singularities, it is clear that the energy T will have to be much smaller than the energy scales that characterize the band shape. In particular, it is smaller than the energy range in which the density of states is logarithmic. In what follows it is assumed that the chemical potential ($\mu = 0$) lies at a Van Hove singularity of the unperturbed spectrum (changes in μ as a result of the distortion would be negligible). The energy variation is now going to be proportional to v^2, $\Delta E = v^2\chi_0$, with

$$\chi_0 = \int_{-W}^{W} D(E) \frac{\mathrm{d}^2}{\mathrm{d}E^2} \, (Ef(E)) \, \mathrm{d}E \tag{12}$$

where $f(E)$ denotes the Fermi–Dirac distribution function. Since the integral diverges logarithmically with the cut-off we obtain, with logarithmic accuracy,

$$\Delta E \simeq v^2 \, \frac{\sqrt{-m_+m_-}}{2\pi^2\hbar^2} \, \log\left|\frac{T}{W}\right|. \tag{13}$$

With the aim of studying the effect of electron interactions, which is to screen the PLD potential, we first derive the relation between χ_0 and the amplitude of the electron density wave created by the distortion. Since the perturbation caused by the PLD is diagonal we can write

$$\Delta E = \sum_j \left[\, \left(E_j^{\circ} + \langle \psi_j \mid \hat{V} \mid \psi_j \rangle \right) n_j - E_j^{\circ} \, n_j^{\circ} \, \right] \tag{14}$$

where j denotes a quantum state, n_j (n_j°) represents the thermal occupation number of the state j after (before) the PLD and E_j° is the unperturbed energy of j. Since

$$\sum_j \langle \psi_j \mid \hat{V} \mid \psi_j \rangle \, n_j^{\circ} = 0 \tag{15}$$

we have

$$\Delta E = \sum_j E_j^{\circ} \, (n_j - n_j^{\circ}) + \int \mathrm{d}^2 r \, V(\boldsymbol{r}) \, \delta n(\boldsymbol{r}). \tag{16}$$

Since the quantities $\delta n(\boldsymbol{r})$ and $V(\boldsymbol{r})$ are proportional to $\cos(2\pi/(\lambda x))$ ($\lambda = 2a$ in the present problem) with amplitudes $-\delta n$ and V respectively, we obtain

$$\delta n = \frac{2w}{v} \left| \, \Delta E - \sum_j E_j^{\circ} \, (n_j - n_j^{\circ}) \, \right| = \frac{4w}{v} \, |\Delta E \,| \equiv 4w^2 |\chi_0| V. \tag{17}$$

In the self-consistent Hartree approximation the potential in (4) represents the sum of the potential that is created by the PLD and the field created by the electron density variation:

$$V = V_l + U_{2\mathrm{D}}\left(\frac{\pi}{a}\right) \delta n \tag{18}$$

where $U_{2\mathrm{D}}(q) = 2\pi e^2/(\epsilon q)$ is the two-dimensional Fourier transform of the Coulomb potential (henceforth abbreviated by U). So the density is given by the mean-field expression

$$\delta n = \frac{4w^2\chi_0}{1 - 4w^2\chi_0 U} V_l. \tag{19}$$

Since the single-electron dispersion relation $E(\boldsymbol{k})$ now includes the effects of the field created by the other electrons, the Hartree potential must be subtracted when calculating the total energy so as to avoid the double counting of the interactions:

$$E_{\mathrm{int}} = \sum_{\boldsymbol{k}} E(\boldsymbol{k})\ \theta(\mu - E(\boldsymbol{k})) - \frac{1}{2}\int n(\boldsymbol{r})n(\boldsymbol{r}')U(\boldsymbol{r}-\boldsymbol{r}')\mathrm{d}^2\boldsymbol{r}\mathrm{d}^2\boldsymbol{r}'. \tag{20}$$

The energy change is, after Fourier transforming the Hartree term,

$$\Delta E_{\mathrm{int}} = (v^2\chi_0) - \frac{1}{2}\sum_{q}\ \delta n_q \delta n_{-q} U(q). \tag{21}$$

It is easy to see that the first term on the right-hand side is small and can be neglected. The sum over q contains only one wavelength, $q = \pm(\pi/a)\boldsymbol{x}$. Therefore,

$$\Delta E_{\mathrm{int}} \cong -\delta n^2 U. \tag{22}$$

At $T = 0$ we have $\chi_0 = \infty$ so

$$\Delta E_{\mathrm{int}}(T=0) = -\frac{\epsilon}{2\ a\ e^2} V_l^2. \tag{23}$$

Since the elastic energy of the deformation is also proportional to V_l^2,

$$E_{\mathrm{elastic}} = I\ V_l^2 \qquad I > 0 \tag{24}$$

an instability exists when

$$I - \frac{\epsilon}{2ae^2} < 0. \tag{25}$$

The critical temperature T_c of the (second-order) phase transition to the PLD state is obtained from the condition

$$\Delta E_{\mathrm{int}} = -U\ \delta n^2(T_c) = -E_{\mathrm{elastic}}. \tag{26}$$

The result is

$$\log\left(\frac{T_c}{W}\right) = \frac{\pi^2\hbar^2}{2w^2\sqrt{-m_- m_+}}\sqrt{\frac{I}{U}}\frac{1}{\sqrt{UI}-1}. \tag{27}$$

The right-hand side must be large for the logarithmic accuracy to hold.

3. Behaviour of the instability for $\phi \approx \frac{1}{2}\phi_0$

Let the total magnetic field be $(B_0 + B)\hat{\boldsymbol{z}}$ with $B_0 a^2 = \phi_0/2$. B satisfies

$$\hbar\omega \ll W \qquad \log\frac{W}{\hbar\omega} \gg 1 \tag{28}$$

with $\omega = | eB/(c\sqrt{-m_+m_-}) |$. We now need to learn how the density of states is modified near the singularity at $E = 0$. The calculation of the spectrum can be done by means of the 'Peierls substitution' (Peierls 1933):

$$E(\boldsymbol{k}) \longrightarrow E\left(\boldsymbol{K} - \frac{e}{\hbar c}\boldsymbol{A}'\right) \tag{29}$$

with $\boldsymbol{A}' = Bx\hat{\boldsymbol{y}}$, for instance. $E(\boldsymbol{k})$ is the dispersion relation used so far. The definition of the generalized momentum $\boldsymbol{K}$

$$\boldsymbol{k} = \boldsymbol{K} - \frac{e}{\hbar c}\boldsymbol{A}' \tag{30}$$

implies

$$[k_x, k_y] = \mathrm{i}\frac{eB}{\hbar c}. \tag{31}$$

It is seen that K_y is a cyclic variable ($-\pi/2a < K_y < \pi/2a$) and can be set equal to zero for the calculation of the spectrum. The principles of the calculation were established in the fifties (Zilberman 1958, Azbel 1964, Slutskin 1968). The wavefunction $\psi(K_x)$ must be an eigenstate of the operator

$$\exp\left(\mathrm{i}\frac{\hbar\pi c}{aeB}K_x\right)$$

with eigenvalue $\mathrm{e}^{\mathrm{i}\theta}$ ($0 < \theta < 2\pi$) and $\psi(K_x) = \psi(K_x + \pi/a)$. The dispersion relation is given by

$$\cos^2\frac{\theta}{2} = \cosh(\pi\varepsilon)\mathrm{Re}\left[\mathrm{i}\frac{1-\mathrm{i}\mathrm{e}^{\pi\varepsilon}}{1+\mathrm{i}\mathrm{e}^{\pi\varepsilon}}\frac{\Gamma^2(\frac{1}{4}-\mathrm{i}\varepsilon/2)}{\Gamma^2(\frac{1}{4}+\mathrm{i}\varepsilon/2)}\exp\left(\frac{\mathrm{i}}{2\hbar}\oint p\,\mathrm{d}q + 2\mathrm{i}\varepsilon\log\frac{|\varepsilon|}{2e}\right)\right] \tag{32}$$

with $\varepsilon = E/(\hbar\omega)$ and

$$\frac{1}{\hbar}\oint p\,\mathrm{d}q = \left|\frac{\hbar c}{eB}\right|\oint k_y\,\mathrm{d}k_x \tag{33}$$

is the area enclosed by the Fermi surface at energy E. If $|\varepsilon| \gg 1$ then the asymptotic expression of the gamma function for large argument can be used to show that (32) reduces to

$$\cos^2\frac{\theta}{2} \approx \mathrm{e}^{\pi|\varepsilon|}\cos\left(\frac{1}{2\hbar}\oint p\,\mathrm{d}q\right) \tag{34}$$

which describes the well known Landau levels that can be obtained from the Bohr–Sommerfeld quantization rule.

In order to obtain an expression for the case in which $|\varepsilon|$ is not large we first note that

$$\oint p\,\mathrm{d}q \approx \oint_{E=0} p\,\mathrm{d}q + 4\hbar\varepsilon\ \log\left|\frac{\Delta}{\varepsilon}\right| \tag{35}$$

(with $\Delta \equiv W/(\hbar\omega)$) and recast equation (32) in the form

$$\cos^2\frac{\theta}{2} \approx \cosh(\pi\varepsilon)\ \cos\left[\frac{1}{2\hbar}\oint_{E=0} p\,\mathrm{d}q + 2\varepsilon\log\Delta\right]. \tag{36}$$

Factors of order unity in the argument of the logarithm in (36) were neglected. So, as $|\varepsilon|$ tends to zero the spectrum consists of regularly spaced bands of slowly varying width. The first term in the argument of the cosine determines whether the chemical potential $\mu = 0$ lies in a band or in a gap and is of order Δ. It is therefore extremely sensitive to small changes in $\hbar\omega$ as it can vary by 2π if $\hbar\omega$ is varied by $\delta(\hbar\omega)$ satisfying

$$\frac{\delta(\hbar\omega)}{\hbar\omega} \approx \frac{\hbar\omega}{W}.$$

3.1. Effect of the PLD

Equation (32) shows that the electron energy spectrum exibits a somewhat complicated structure consisting of discrete bands of variable width. The expression for χ_0 is written as

$$\chi_0 = \frac{1}{2} \sum \int \rho_n(E) \, \frac{\mathrm{d}^2}{\mathrm{d}E^2}(Ef(E))_{E+E_n} \, \mathrm{d}E \tag{37}$$

where $\rho_n(E)$ is the internal density of states in the nth band and

$$\int \rho_n(E) \, \mathrm{d}E = \frac{|e \; B|}{2\pi\hbar c}.$$

The curve of critical temperatures $T_{\mathrm{c}}(B)$ is determined from the equations (19) and (26).

If $T \gg \hbar\omega$ the discreteness of the energy spectrum becomes irrelevant and the sum over n in equation (37) can be replaced with an integral over a continuous distribution of bands:

$$\chi_0 \simeq \frac{|e \; B|}{4\pi\hbar c} \int_{-W}^{W} \frac{\mathrm{d}n}{\mathrm{d}E} \left(\frac{\mathrm{d}^2}{\mathrm{d}E^2} Ef(E) \right)_{E+E_n} \mathrm{d}E \tag{38}$$

with

$$\begin{aligned} \frac{\mathrm{d}n}{\mathrm{d}E} = {} & \frac{\mathrm{d}}{\mathrm{d}E} \left(\frac{1}{2\pi\hbar} \oint p \, \mathrm{d}q \right) + \frac{2}{\pi\hbar\omega} \log \frac{|\,\varepsilon\,|}{2} + \frac{1}{\hbar\omega \cosh(\pi\varepsilon)} - \frac{1}{\pi\hbar\omega} \left(\psi\left(\frac{1}{2} - i\frac{\varepsilon}{2}\right) \right. \\ & \left. + \psi\left(\frac{1}{2} + i\frac{\varepsilon}{2}\right) \right) \end{aligned}$$

which represents the density of zeros of the right-hand side of equation (32). ψ here denotes the digamma function. The correction to the $B = 0$ result can be expanded in powers of $\hbar\omega/T$:

$$\chi_0(T, B) \simeq \frac{\sqrt{-m_+ m_-}}{2\pi^2\hbar^2} \, \log \frac{T \mathrm{e}^{f(\hbar\omega/T)^2}}{W} \tag{39}$$

with

$$f = -\frac{\psi''(\frac{1}{2})}{32\pi^2}.$$

The equation for T_{c} is

$$\log \frac{T_{\mathrm{c}} \mathrm{e}^{f(\hbar\omega/T_{\mathrm{c}})^2}}{W} = \frac{\pi^2\hbar^2}{2w^2\sqrt{-m_- m_+}} \sqrt{\frac{I}{U}} \frac{1}{\sqrt{UI} - 1}. \tag{40}$$

From here we get

$$\left(\frac{\partial^2 T_{\mathrm{c}}}{\partial B^2} \right)_{B=0} = -\frac{2\hbar^2 e^2}{m_+ m_- c^2 T_{\mathrm{c}0}} \tag{41}$$

($T_{\mathrm{c}0}$ denotes the critical temperature at $B = 0$) if the corrections due to the variability of the right-hand side of (40) with B are neglected (see next section).

At small temperature ($T \simeq \hbar\omega/\log\Delta$) the function $\mathrm{d}^2(Ef(E))/\mathrm{d}E^2$ has a sharp maximum at the chemical potential $E = \mu = 0$ and decays in an energy interval of order T. As $T \to 0$, $\chi_0(T, B)$ becomes strongly dependent on the exact position of the bands near the chemical potential and is not even a monotonic function of T. The internal density of states of the band that is close to the origin is, from (36),

$$\rho(E) = \frac{|eB|}{\pi^2\hbar c}\,\frac{\sqrt{-2m_+m_-}}{2\pi^2\hbar^2}\,(\log\Delta)\left|\frac{\cos((\log\Delta/\hbar\omega)E)}{\sqrt{\cos((2\log\Delta/\hbar\omega)E)}}\right| \tag{42}$$

if

$$|E| < \frac{\pi\hbar\omega}{4\log\Delta}$$

and $\rho(E) = 0$ outside this interval. So it is seen that $\rho(E)$ diverges at the band edges. If the band is centred at an energy E_0 satisfying (42) then, as $T \to 0$,

$$\chi_0 \;\to\; -\tfrac{1}{2}\rho(-E_0). \tag{43}$$

If $E_0 = \pm\pi\hbar\omega/(4\log\Delta)$ then χ_0 diverges with $T^{-1/2}$.

Because the behaviour of χ_0 is very sensitive to changes in $\hbar\omega$ of order $\delta\hbar\omega$, it will be here assumed that the spectrum that is 'seen' by the electron is averaged over fluctuations in $\hbar\omega$ that are not much larger than $\delta\hbar\omega$. This corresponds to taking the average of equation (43) over E_0 ranging from $-\pi\hbar\omega/(2\log\Delta)$ to $+\pi\hbar\omega/(2\log\Delta)$. Because E_0 varies (approximately) linearly with the fluctuation $d(\hbar\omega)$ then

$$\chi_0(T = 0, B) = -\frac{1}{2}\frac{\log\Delta}{\pi\hbar\omega}\int\rho(-E_0)\mathrm{d}E_0 = \frac{1}{2}\frac{\sqrt{-m_+m_-}}{2\pi^2\hbar^2}\,\log\frac{\hbar\omega}{W}. \tag{44}$$

So $T_c(B) \to 0$ at a critical magnetic field ($\hbar\omega_{cr}$) determined by

$$\frac{1}{2}\,\log\frac{\hbar\omega_{cr}}{W} = \frac{\pi^2\hbar^2}{2w^2\sqrt{-m_-m_+}}\sqrt{\frac{I}{U}}\frac{1}{\sqrt{UI}-1}. \tag{45}$$

The right-hand side depends on the magnetic field (see next section) and must be large.

4. Example

These ideas can be illustrated with a simple model in which the cyclotron energy ($\hbar\omega_0$) associated with the field B_0 is large when compared to the crystal potential caused by the lattice. The latter can then be treated as a perturbation on the lowest Landau level and will be assumed to have the simple form

$$V_\mathrm{p}(x, y) = V_\mathrm{p}(x) + V_\mathrm{p}(y). \tag{46}$$

In the gauge $\boldsymbol{A} = B_0x\hat{y}$ we can write the electron wavefunction as

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}}\sum_j \mathrm{e}^{-\mathrm{i}k_x2aj}\mathrm{e}^{\mathrm{i}(k_y+j2\pi/a)y}\phi(x + l^2k_y + 2aj) \tag{47}$$

with

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

and $l^2=\hbar c/(|e|B_0)$.The dispersion relation will then be separable in a similar fashion

$$E_0(k_x,k_y)=E_0(k_x)+E_0(k_y). \tag{48}$$

It follows from (4) and (5) that the effect of the lattice distortion is

$$E(\boldsymbol{k})=E_0(\boldsymbol{k})+v\cos(ak_y) \tag{49}$$

and

$$w=\mathrm{e}^{-(a/2l)^2}. \tag{50}$$

This follows from the fact that the unperturbed wavefunctions

$$\mathrm{e}^{\mathrm{i}k_y y}\phi(x+l^2k_y) \tag{51}$$

have their k_y-degeneracy lifted by $V_\mathrm{p}(x)$ and $V_\mathrm{p}(y)$ introduces matrix elements between states of the form (51) with k_y and k'_y satisfying

$$k_y-k'_y=\frac{2\pi}{a}j$$

where j is an integer, so that $E_0(k_x)$ is the dispersion relation in a tight-binding (TB) problem. If the magnetic field is $(B_0+B)\hat{z}$ then the energies of the 'sites' in the TB have a very slow variation is space with wavelength $\Lambda=\pi\hbar c/(B|e|a)$ and the semiclassical approximation can be used to obtain a dispersion relation identical to (32) with θ replaced by $\kappa\Lambda$ where κ is a 'Bloch momentum'. The distance between the sites is now $2\pi l^2/a$, slightly different from $2a$. Each sequence of sites in the TB problem can be labelled by k_y with $-\pi/a<k_y<\pi/a$ and this is the cyclic variable in the problem. It is then easy to see that a PLD with wavelength $\lambda=2\pi l^2/a$ will lift the k_y-degeneracy by adding a term $v\cos(ak_y)$ to the electron dispersion relation, as in (49). This is analogous to the broadening of the Landau levels of an initially free electron when a small crystal potential is applied. The changing wavelength of the PLD could not be obtained if the case $B\neq 0$ were treated just by the means of a 'Peierls substitution'.

The B dependence of the right-hand side of (40) can now be estimated. Since the elastic energy of deformation is proportional to A^2/λ^2 (A is the amplitude of the PLD) then $I\propto\lambda^{-2}$. This implies

$$\frac{1}{w}\frac{\partial w}{\partial B}\simeq\frac{1}{I}\frac{\partial I}{\partial B}\simeq\frac{1}{U}\frac{\partial U}{\partial B}\propto\frac{1}{B_0}$$

and

$$\left(\frac{\partial T_\mathrm{c}}{\partial B}\right)_{B=0}=\left((\approx 1)+\frac{\sqrt{I_0U_0}}{1-\sqrt{I_0U_0}}\right)\frac{T_{\mathrm{c}0}}{B_0}\log\frac{T_{\mathrm{c}0}}{W} \tag{52}$$

(I_0, U_0 and T_{c0} are the values of I, U and T_c at B = 0). The maximum critical temperature ($T_{\max}$) is

$$\frac{T_{\max}}{T_{c0}} = 1 + \frac{(\partial T_c/\partial B)^2}{4\,(\partial^2 T_c/\partial B^2)\,T_{c0}}. \tag{53}$$

Using (27), (41) and (52) we see that the square root of the second term in (53) is of the order of ($y \equiv \sqrt{I_0 U_0}$)

$$\frac{Wc\sqrt{-m_+m_-}}{\hbar B_0 \mid e \mid}\left((\approx 1) + \frac{\sqrt{y}}{1-\sqrt{y}}\right)\frac{Wa\,\varepsilon}{w_0{}^2e^2}\,\frac{\sqrt{y}}{1-\sqrt{y}}\,\exp\left[-\frac{Wa\,\varepsilon}{w_0^2\,e^2}\,\frac{\sqrt{y}}{1-\sqrt{y}}\right] \tag{54}$$

where

$$W \simeq \frac{\hbar^2}{\sqrt{-m_+m_-}\;a^2}$$

was used. Since

$$\frac{W\,a\,\varepsilon}{w_0{}^2e^2}\,\frac{\sqrt{y}}{1-\sqrt{y}} \simeq \log\frac{T_{0c}}{W}$$

is large in this theory we should expect (54) and, therefore, the effect of the dependence of the right-hand side of (40) on B to be small. In conclusion, we see that the method used in section 3, which was based on the Peierls substitution, gives a result that is nearly correct since the effects of the dependences of the parameter w and wavelength of distortion on the magnetic field (not taken into account in that method) cause only a small correction when the condition $\log W/T_{c0} \gg 1$ is satisfied.

5. Discussion

It is seen from (23) that the energy variation associated with a distortion at $T = 0$ does not depend on the details of the band shape (such as the effective masses m_+ and m_-) but simply on the wavelength λ of the PLD. Therefore, the role of the logarithmic form of the density of states is just to make the PLD likely to occur and the instability criterion $UI < 1$ simply depends on λ. The critical temperature T_c and critical field B_{cr} will depend on the band-shape details, however.

The analysis of the $\phi_0/2$ case together with the results of group theory and earlier investigations on the band structure (Wannier *et al* 1979, Czycholl *et al* 1988) enable us to derive the following conclusions. If the magnetic field flux per unit cell of a square lattice is non-integer and rational, $\phi/\phi_0 = p/q$, then the spectrum will consist of p subbands with q-fold degeneracy. Each of these p subbands contains a logarithmic Van Hove singularity in the density of states and the instability can then occur at p possible values of the chemical potential. The correspondent PLD has a wavelength $\lambda = qa/m$ (where m is an integer) and in those cases where several values of m are possible the PLD will choose the one that minimizes the total energy variation $\Delta E \propto -U^{-1} + I$, i.e., an expression of the form

$$-\alpha\frac{m}{q} + \beta\frac{m^4}{q^2}$$

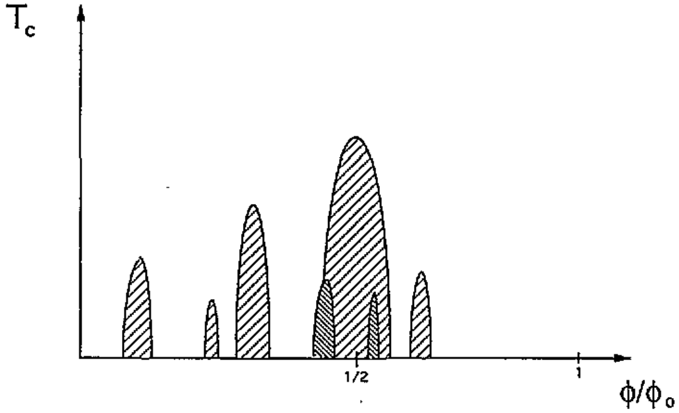

Figure 3. Phase diagrams corresponding to different rational values p/q of the flux per unit cell. The shaded regions correspond to the distorted phase. The maximum of each curve is attained for ϕ/ϕ_0 close to p/q.

(since $U \propto \lambda$ and $I \propto \lambda^{-2}$) where α and β are positive constants.

For each flux p/q we can then draw a phase diagram $T_c(B)$ (corresponding to one of the p possible chemical potentials) as was done in Section 3 for the $\frac{1}{2}$ case. The maximum of the curve is located near the field B which corresponds to $\phi/\phi_0 = p/q$ ($B = 0$ in figure 3) and its deviation from exact commensurability is small, provided $\log W/T_{c0}$ is large. Since the rational numbers in the range $B_{cr}a^2/\phi_0$ around p/q have a much larger denominator (and numerator) than q, it is expected that the corresponding bandwidths and critical temperatures are very small and therefore more difficult to observe. From here we see that the drastic changes in the analytic form of the density of states induced by small changes in the flux per unit cell make the phase diagram show the fractality just described.

We finally comment on the experimental verification of these ideas. It is beyond the current technology to apply magnetic fields equivalent to about $\phi_0/2$ per unit cell of a real crystal. It is, however, possible, with modern microfabrication techniques, to subject a 2DES to an artificially created square lattice potential with large lattice spacing, through which such magnetic-field fluxes can be applied. The instability would then correspond to a distortion of the thin layer of the material that contains the electron gas.

It is elucidating to consider a thin slab (of thickness $\simeq 10$ nm) containing the quasitwo-dimensional electron gas and a compensating positively charged background. Under the influence an externally applied square lattice potential with, say, $a = 200$ nm, the slab would make a distortion with period $2a$ (for $\phi = \phi_0/2$). Using dielectric and elastic (Young's modulus) constants of the order of those corresponding to, e.g. GaAs, we estimate $IU \simeq 10^{-3}$ and $\sqrt{I/U} \simeq 10^{34}$ J^{-1} m^{-2}. Since $\hbar^2/(\sqrt{-m_+m_-}) \simeq Wa^2$ and $w = 0.045$ we see that if $W \simeq 0.01$ meV then T_c is of the order of a few tens of millikelvin. Note that because $\log T_c/W$ is proportional to W it is convenient to choose small W so as to have $T_c \simeq W$ and make the transition occur at experimentally accessible temperatures. Here the equation (27) would not be valid because it has logarithmic accuracy. This model for the quasitwo-dimensional system is perhaps too simple to describe the real 2DEG as it is currently fabricated because the positively charged background may be far from the 2DEG. But it is worth noting that a metal gate placed near the 2DEG would induce image charge effects and reduce the screening of the lattice potential. The inequality (25) would then be replaced by a much less restrictive condition and T_c would increase. Furthermore, a material should be chosen for which the dielectric constant and the relevant elastic constants (Young's modulus) are as small as possible.

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