Variations of the electron spectrum in the neighborhood of Van Hove points, carrier localization, and structural instability in interaction with a long-wave periodic perturbation in low-dimensional systems

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We show that if the wave vector k of a periodic perturbation in one- and two-dimensional crystals satisfies the condition $k \ll \sqrt{g/t} \ll 1$, where g and t are the perturbation's magnitude and the bandwidth, a highly nonequidistant spectrum consisting of a large number of states, $n = \sqrt{g/k^2 t} \gg 1$, forms in the neighborhood of the extremal points of the spectrum over a width of $2g$. This weakens the singularity in the density of states: in one-dimensional systems a root singularity becomes logarithmic, and in two-dimensional a flat maximum is all that remains of a logarithmic singularity. The width of the logarithmic peak in the one-dimensional case and that of the maximum in the two-dimensional are values of the order of $g \ll t$. We establish the conditions for and characteristic of the instability to formation of a wave of deformation. In the one-dimensional case the system is unstable for values of the chemical potential $\mu < \mu_c \sim t(\omega_D/t)^2 \ll t$, while in the two-dimensional case the system is unstable only if the Fermi energy is exponentially close to a saddle point. In the one-dimensional case the transition to a state with spontaneous deformation at $\mu = \mu_c$ occurs suddenly, in a jump. Maximum instability occurs at $\mu = 0$, which corresponds to the bottom of the "initial" band or, which is the same, when the band $(-2g, 2g)$ is half-filled. As a result, in the one-dimensional the carriers become completely localized, while in the two-dimensional case they become localized only in one direction, which must lead to a strong anisotropy in resistance.

1. INTRODUCTION

It is well known[1,2] that the main anomalous properties of layered and quasi-one-dimensional crystals (such as the A15 compounds, dichalcogenides, and Chevrel phases) can be explained only by assuming that near the Fermi surface (FS) the density of states exhibits a narrow peak of width not exceeding several hundred degrees. In all crystals listed above there is certain to be a structural transition, which in some cases is accompanied by the formation of a superstructure.[1,2]

Perovskite-like high-T_c compounds belong to systems with a quasi-two-dimensional subsystem of carriers and, apparently, a maximum in the density of states near the FS (Ref. 3). To explain the peak in the density of states in A15 compounds, several models with one-dimensional[4–6] and anisotropic two-dimensional[7,8] carrier spectra have been suggested. In these models, however, the energy scale determining the width of the peak was generally of the order of the d-band width, which is considerably greater than required. Another feature that remained ambiguous was the relation between the peaks in the density of states and the structural transition. The polaron mechanism of peak narrowing discussed in Ref. 9 requires an unrealistically high value of the electron-phonon coupling constant. Kagan and Prokof'ev[10] discussed the mechanism of peak narrowing caused by the electron polaron effect.

At the same time it is known that the excitation spectra in the neighborhood of Van Hove points are exceptionally sensitive to perturbations. For instance, Afanas'ev and Kagan[11] discovered a qualitative transformation of the phonon spectrum caused by Van Hove singularities in the electron subsystem.

For a two-dimensional electron system with an interaction of a general type the instability to formation of charge-density and spin-density waves, when the Fermi surface passes through saddle points, was studied in Refs. 12 and 13.

This paper focuses on the fact that there is a fairly simple mechanism of formation of peaks in the density of states near the Fermi surface; and this mechanism, in the first place, yields a universal width for the peaks (much smaller than the bandwidth) and, in the second, is directly linked to the structural transition.

According to this mechanism, peak formation is caused by the quasi-classical quantization of the carrier spectrum in the neighborhood of Van Hove points under interaction with an exceptionally long-wave perturbation.

Such a perturbation can be produced either by the order parameter proper when there is a superstructure or by long-wave fluctuations of the parameter above the transition point.

We discuss below the long-wave deformation of the lattice as the order parameter, but the same results can be achieved with spontaneous magnetization or polarization. Note that the variation in a singularity in the carrier spectrum brought about by a deformation wave is, in a certain sense, an effect opposite to the one discovered by Afanas'ev and Kagan.[11]

The main results achieved in this paper may be listed as follows:

1. We show that if the wave vector k of a periodic perturbation in one- and two-dimensional crystals satisfies the condition

$$k \ll (g/t)^{1/2} \ll 1, \tag{1}$$

where g and t are the perturbation's magnitude and bandwidth, then in the neighborhood of the extremal points of the

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spectrum (Van Hove points) there forms, over a width of $2g$, a highly nonequidistant discrete spectrum, and the number of states in each well is high:

$$n_{max} \sim (g/k^2 t)^{1/2} \gg 1. \tag{1a}$$

In the neighborhood of a saddle point of the spectrum of a square lattice, the spectrum resembles a collection of Landau levels in a magnetic field, but in contrast to the latter is highly nonequidistant.

2. In the one-dimensional case this leads to a weakening of the root singularity in the density of states to a logarithmic. The logarithmic peak lies at the boundary separating the discrete spectrum from the continuous near the bottom or top of the band. The peak width is of the order of $g \ll t$.

3. Allowing for the interaction in the case of two-dimensional carriers leads to a smoothing-out of the logarithmic singularity. There remains a flat maximum approximately $\ln(t/g)$ high and g wide (Fig. 1).

4. Calculation of thermodynamic potentials at $d = 1$ and $d = 2$ (at $d = 1$ the problem can be solved exactly) shows that the system is unstable with respect to spontaneous formation of a wave of deformation. In the one-dimensional case this happens for a fairly low electron density, when

$$\mu < \mu_c \sim t(\omega_D/t)^2 \ll t \tag{2}$$

with ω_D the Debye energy. In the two dimensional-case the transition is possible only if the Fermi energy is exceptionally close to a saddle point.

As a result of such a transition in the one-dimensional case, the carriers become localized (a transition of the metal-insulator type). In the two-dimensional case the carriers become localized in a single dimension, which should lead to a sharp resistance anisotropy.

The instabilities considered below are caused by the existence of a quasiclassical discrete spectrum in the neighborhood of the extremal points of the "initial" band. The strongest instability occurs at $\mu = 0$ (corresponding to the bottom of the initial band), which corresponds to the band $(-2g, 2g)$ being half-filled. Here the number of electrons occupying discrete levels is determined by a quantity of the order of $\sqrt{g/t}$.

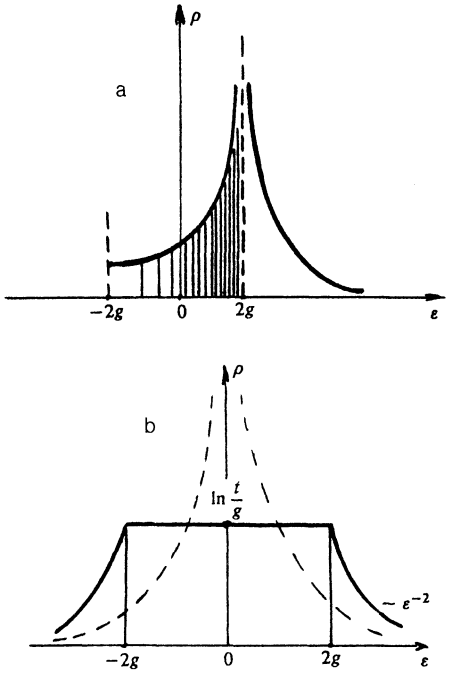

FIG. 1.

Note that at $d = 1$ the instability discussed above occurs only if the number of electrons or holes is fairly low and, therefore, does not compete with the Peierls–Fröhlich instability,[14,15] which occurs when the occupancy is one-half or close to it.

The plan of the paper is as follows. In Sec. 2 we obtain the quasiclassical spectra and the singularities in the density of states for carriers moving in the field of a long static wave directed along one of the principal axes at $d = 1$ and $d = 2$. In Sec. 3 we calculate the thermodynamic potentials and discuss the respective instabilities. Finally, in Sec. 4 we describe the quasiclassical motion when there is interaction with a periodic perturbation of a general type. We show that in the neighborhood of the extremal points of the spectrum the problem is reduced to an exactly solvable universal model. We also establish the dependence of the characteristics of the discrete spectrum on the direction of the wave.

2. QUASICLASSICAL SPECTRA AND THE DENSITY OF STATES FOR ONE- AND TWO-DIMENSIONAL CARRIERS

1. In the presence of a static wave (along the direction of the chain) the Schrödinger equation for one-dimensional carriers near the extremal points of the spectrum takes the form of the equation for a quantum rotator (or Mathieu's equation):

$$\left(-t\frac{d^2}{dx^2} + 2g\cos kx\right)\psi = \varepsilon\psi, \qquad k \ll k_c = \frac{8}{\pi}\left(\frac{g}{t}\right)^{1/2}. \tag{3}$$

For $\varepsilon > 2g$ this equation has a continuous spectrum, while for $-2g < \varepsilon < 2g$ it has narrow allowed bands. If we ignore the bandwidths, we can speak of a discrete spectrum in wells whose number is $kL/2\pi$, with L the size of the "chain."

If condition (1) is met [or, which is the same, condition (3)], the number of levels in a well, $n_{\max} = k_c/k$, is great and the discrete spectrum is specified by the Bohr–Sommerfeld formula

$$n(\varepsilon) = \frac{1}{(2\pi)}\oint dx\left(\frac{\varepsilon - 2g\cos kx}{t}\right)^{1/2} = \frac{k_c}{k}\left[E(\varkappa) - (1-\varkappa^2)K(\varkappa)\right], \tag{4}$$

where $\varkappa^2 = (\varepsilon + 2g)/4g$, and K and E are complete elliptic integrals of the first and second kinds.

The level separation in (4) is given by the following expression:

$$\omega(\varepsilon) = \frac{d\varepsilon}{dn} = \frac{\pi\omega_m}{2K(\varkappa)} = \begin{cases} \omega_m, & \varepsilon \to -2g \\ \omega_m/\ln(1-\varepsilon/2g)^{-1}, & \varepsilon \to 2g \end{cases}. \tag{5}$$

The quantity

$$\omega_m = 2k(gt)^{1/2} \ll g \tag{6}$$

determines the maximum splitting of the levels in the field of the static wave.

Combining (4) and (5), we arrive at an expression for the density of states in the discrete spectrum region:

$$\rho(\varepsilon) = \frac{kL}{2\pi}\frac{dn}{d\varepsilon} = \frac{L}{\pi^2}\frac{K(\varkappa)}{(gt)^{1/2}}. \tag{7}$$

The number of a level and the density of states in the continuous spectrum region ($\varepsilon > 2g$) are

$$n(\varepsilon) = \frac{4L}{\pi^2}\left(\frac{g}{t}\right)^{1/2}\varkappa E(\varkappa^{-1}), \quad \rho(\varepsilon) = \frac{L}{2\pi^2}\frac{\varkappa^{-1}K(\varkappa^{-1})}{(gt)^{1/2}}. \tag{8}$$

As Eqs. (4) and (7) imply, at the boundary separating the discrete and continuous spectra there emerges a new logarithmic singularity (Fig. 1a):

$$\rho(\varepsilon) = \frac{L}{2\pi^2}\frac{1}{(gt)^{1/2}}\ln\left(\frac{2g}{\delta\varepsilon}\right), \quad \delta\varepsilon = |2g - \varepsilon|. \tag{9}$$

2. Let us now study how the electron spectrum of a square lattice in the neighborhood of saddle points is transformed by a wave along one of the principal axes:

$$[-2t(\cos p_x + \cos p_y) + 2g\cos kx]\psi = \varepsilon\psi. \tag{10}$$

Near the saddle point $(0,\pi)$ Eq. (11) assumes the form

$$[(tp_x^2 + 2g\cos kx) - tp_y^2]\psi = \varepsilon\psi. \tag{11}$$

The Hamiltonian of the motion along the x axis coincides with (3). The eigenvalues of Eq. (11),

$$\varepsilon_{(0,\pi)}(n, p_y) = \varepsilon_n - tp_y^2 \tag{12}$$

with ε_n taken from (4) and (8), resemble the spectrum of an electron in a magnetic field, but the branches of the parabola go downward from p_y. The separation of the ε_n-levels decreases rapidly as n increases, and above the line $\varepsilon = 2g - tp_y^2$ the spectrum becomes that of free two-dimensional motion. In the neighborhood of the second saddle point the spectrum is inverted,

$$\varepsilon_{(\pi,0)}(n, p_y) = -\varepsilon_{(0,\pi)}(n, p_y). \tag{13}$$

In the absence of a wave the density of states has a logarithmic singularity on the line $|\varepsilon| = 0$:

$$\rho_0(\varepsilon) = \rho_{00}\ln\left(\frac{t}{|\varepsilon|}\right), \quad \rho_{00} = \frac{L^2}{(2\pi)^2 t}. \tag{14}$$

The wave smooths out this singularity.

If the wave is sufficiently long [Eq. (1)], electron motion is quasiclassical both in the continuous spectrum region and in the region of states localized along the direction of the wave. Hence, for an arbitrarily directed wave the density of states is given by the integral

$$\rho(\varepsilon) = \int\frac{dxdp_x}{2\pi}\int\frac{dydp_y}{2\pi} \times \delta[\varepsilon + 2t(\cos p_x + \cos p_y) - 2g\cos(\mathrm{kr})]. \tag{15}$$

Integration over momenta and along the direction perpendicular to the wave's direction yields

$$\rho(\varepsilon) = \frac{1}{\pi}\int_0^\pi dX\rho_0(\varepsilon + 2g\cos X). \tag{16}$$

Note that (16) depends explicitly neither on the size nor on the direction of vector $\mathbf{k}$. Substituting (14) into (16) yields

$$\rho(\varepsilon) = \rho_{00}\left[\ln\left(\frac{t}{|\varepsilon|}\right) - J\left(\frac{2g}{\varepsilon}\right)\right], \tag{17}$$

where

$$J\left(\frac{2g}{\varepsilon}\right) = \frac{1}{\pi}\int_0^\pi dX\ln(1 + \frac{2g}{\varepsilon}\cos X) = \begin{cases}\ln(g/|\varepsilon|), & 2g > \varepsilon\\ \ln[1 + \sqrt{1 - (2g/\varepsilon)^2}], & 2g < \varepsilon\end{cases}.$$

We see that the density of states in the layer between $-2g$ and $2g$ "freezes" at a constant level:

$$\rho(\varepsilon) = \rho_{00}\ln(t/g), \quad |\varepsilon| < 2g. \tag{18}$$

In regions adjacent to this layer the density of states is higher than the initial density of states (14) by a small quantity:

$$\rho(\varepsilon) = \rho_{00}\left[\ln\left(\frac{t}{|\varepsilon|}\right) + \frac{g^2}{\varepsilon^2}\right], \quad \varepsilon \gg 2g. \tag{19}$$

The density of states $\rho(\varepsilon)$ is depicted in Fig. 1b (the dashed curves designate the logarithmic peak in the density of states (14) of the unperturbed spectrum).

3. INSTABILITIES TO FORMATION OF A DEFORMATION WAVE

Knowing the density of states, we can easily find the thermodynamic potential of the electron system and study the stability at $T = 0$. In the one-dimensional case the problem can be solved here exactly, while in the two-dimensional only with logarithmic accuracy.

1. We begin with the one-dimensional case. If the chemical potential lies below the upper edge of the discrete spectrum (7) ($\mu < 2g$), using Eq. (9) we arrive at the following expressions for the number of particles N, the thermodynamic potential Ω, and the energy $\mathscr{E} = \Omega + \mu N$ (here μ is measured from the bottom of the initial band, and the length L is assumed equal to unity):

$$N(\mu) = \frac{k}{2\pi}n(\mu) = N_c[E(\varkappa) - (1 - \varkappa^2)K(\varkappa)],$$
$$\Omega = -4\mathscr{E}_c[(4\varkappa^2 - 2)E(\varkappa) + (3\varkappa^2 - 2)(\varkappa^2 - 1)K(\varkappa)],$$
$$\mathscr{E} = \mathscr{E}_c[(2\varkappa^2 - 1)E(\varkappa) + (6\varkappa^2 - 1)(\varkappa^2 - 1)K(\varkappa)], \tag{20}$$
$$\left(\frac{\partial\Omega}{\partial g}\right)_\mu = \frac{3\Omega/2 + \mu N}{g}, \quad \varkappa^2 = \frac{1}{2} + \frac{\mu}{4g},$$
$$\mathscr{E}_c = \frac{2g}{9}N_c, \quad N_c = \frac{4}{\pi^2}\left(\frac{g}{t}\right)^{1/2}.$$

If the chemical potential lies in the continuous spectrum region ($\mu > 2g$), we have

$$N(\mu) = N_c\varkappa E(\varkappa^{-1}), \quad \left(\frac{\partial\Omega}{\partial g}\right)_\mu = \frac{3\Omega/2 + \mu N}{g},$$
$$\mathscr{E}(\mu) = \mathscr{E}_c\varkappa^3[(2 - \varkappa^{-2})E(\varkappa^{-1}) + 4(1 - \varkappa^{-2})K(\varkappa^{-1})], \tag{21}$$
$$\Omega(\mu) = -4\mathscr{E}_c\varkappa^3[(4 - 2\varkappa^{-2})E(\varkappa^{-1}) + (\varkappa^{-2} - 1)K(\varkappa^{-1})].$$

For the sake of comparison we give the expressions for the case of unperturbed motion:

$$\rho_0(\mu) = (2\pi)^{-1}(\mu t)^{-1/2}, \quad N_0 = \pi^{-1}(\mu/t)^{1/2}, \quad \Omega_0 = -\frac{2}{3}\mu N_0, \quad \mathcal{E}_0 = \frac{1}{3}\mu N_0 . \tag{22}$$

We see that the deformation variations of all thermodynamic quantities are the greatest when $\mu \lesssim 2g$ and, with a further increase in the chemical potential, decrease in the following manner:

$$\delta N = N(\mu) - N_0(\mu) \propto \mu^{-3/2}, \quad \delta\Omega \sim \delta\mathcal{E} \propto \mu^{-1/2}. \tag{23}$$

The thermodynamic functions $\Omega(g,\mu)$ and $\mathcal{E}(g,\mu)$ and their first derivatives are continuous in g, and $|\partial^2\Omega/\partial g^2| \propto \ln(|2g-\mu|^{-1}) \to \infty$ near $g = \mu/2$. What is important is that for all g values the thermodynamic potential Ω is a decreasing function of g, that is, $(\partial\Omega/\partial g)_\mu < 0$. Hence, the system is unstable to an increase in deformation.

The equilibrium values of g are determined from the condition that the Landau functional

$$F = \Omega(g,\mu) + V(g) \tag{24}$$

assumes the minimum value. We write the expression for the deformation energy in the form of a generalized Hooke's law:

$$V(g) = \frac{1}{2}Qg^2.$$

Then the equilibrium value of g is determined from the following equation:

$$g = Q^{-1}|\partial\Omega/\partial g|. \tag{25}$$

Figure 2 depicts $|\partial\Omega/\partial g|$ as a function of g. According to (20), $|\partial\Omega/\partial g| \propto \sqrt{g/t}$ as $g \to 0$, and from (21) we find that $|\partial\Omega/\partial g| \sim g/\sqrt{\mu t}$ as $g \to 0$.

From Fig. 2 we see that for $\mu > 0$ and $Q < Q_0 = g/\pi\sqrt{\mu t} = 2\rho_0(\mu)$ the initial state with $g = 0$ is absolutely unstable to the transition to a "deformed" state ($g \neq 0$). In the interval $Q_0 < Q < Q_c$, with $Q_c \approx 1.14Q_0$, the state with $g = 0$ becomes metastable. In the interval $Q_c < Q < Q_1$, with $Q_1 \approx 1.25Q_0$, the deformed state is metastable. Finally, for $Q > Q_1$ Eq. (25) has no solutions with $g \neq 0$.

It is essential that in the deformed state (stable or metastable), the carriers on the Fermi surface are localized. This implies that if at a fixed elastic modulus the occupancy of the band is decreased, the transition to the deformed state occurs jumpwise at

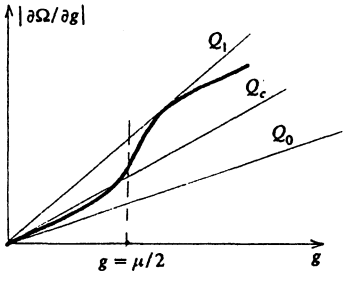

FIG. 2.

$$\mu = \mu_c \approx (Q^2 t)^{-1}. \tag{26}$$

Assuming that $Q \sim \omega_D^{-1}$, we arrive at the estimate (2) for μ_c. For $\mu < 0$ the carriers are localized on discrete levels with $-2g < \varepsilon < 0$, irrespective of the value of the elastic energy. In this sense the value $\mu = 0$ determines the maximally unstable state of the system. The electron number $N_0 = 0.2N_c$ corresponds to this state.

A remark is in order. For the band spectrum $\varepsilon_p = -2t\cos p$ the above results refer directly to a low occupancy of the initial band ($\mu \ll t$) and can easily be applied to the case of an almost completely filled state via transition to the hole representation.

2. Let us now discuss instability in a two-dimensional system. Knowing the variation $\delta\rho = \rho - \rho_0$ of the density of states (15)–(19), we can easily find the variations of thermodynamic quantities. With logarithmic accuracy,

$$\delta\Omega \approx \delta\mathcal{E}, \quad \delta N(\mu) = -\mu\delta\rho(\mu), \quad \delta\mathcal{E} \approx -\rho_{00}g^2\ln[t/(|\mu| + 2g)] \tag{27}$$

(μ is measured from the middle of the initial band). A decrease in the total electron energy in the presence of a wave may lead to spontaneous formation of a wave of deformation as in the one-dimensional case. But because $\delta\mathcal{E}$ is a smooth function of g in the two-dimensional case, the transition occurs in a way similar to a second-order phase transition. Substituting (27) into the Landau functional (25), we arrive at the instability condition in the form

$$2\rho_{00}\ln[t/(|\mu| + 2g)] > Q, \tag{28}$$

which is met only when the elastic modulus is fairly low. Since $\rho_{00}/Q \sim \omega_D/t \ll 1$, condition (26) is very stringent. For instance, when the band is half-filled, at $|\mu| = 0$, equilibrium deformation is of the scale

$$g_c \approx t\exp(-t/\omega_D). \tag{29}$$

For $|\mu| > g_c$ the homogeneous state is stable. In the inhomogeneous state local delocalization takes place. More precisely, the carriers move freely along one axis, while along the other the motion is localized.

3. When the quasiclassical conditions (1) and (3) are met, the density of states and hence the thermodynamic potentials do not explicitly depend on k. The wave vector of the inhomogeneous state can be fixed by the following mechanisms: (1) corrections to the quasiclassical solution, (2) tunneling of carriers between wells, and (3) the dependence on k of amplitude g and the elastic energy $V(g)$. For one thing, bearing in mind that g determines the magnitude of the interaction of carriers with a quasiclassical state of the boson field, its dependence on k can be expressed as follows:

$$g(k) = g_0 k^\alpha N_k^\beta,$$

where N_k is the number of bosons in the quasiclassical state. For the interaction with acoustic phonons, $\alpha = \beta = 1/2$. In this case the mechanism that fixes k is anharmonicity. Since $g \to 0$ as $k \to 0$, the equilibrium values of the wave vector clearly cannot be too small. Our paper, however, does not consider this aspect.

4. GENERAL DESCRIPTION AND QUANTIZATION OF QUASICLASSICAL MOTION

In this section we describe the quasiclassical motion of electrons in long-wave periodic potentials of a more general form than the above case of a static wave along one of the principal axes.

1. We start with the two-dimensional case. For a static wave pointing in an arbitrarily chosen direction,

$$g(x, y) = g\cos(k_1 x + k_2 y). \tag{30}$$

The motion and the shape of the spectrum change drastically in the neighborhood of the values p_{xm} and p_{ym} that satisfy the condition

$$k_1 \frac{\partial \varepsilon_0}{\partial p_x} + k_2 \frac{\partial \varepsilon_0}{\partial p_y} = 0. \tag{31}$$

This condition specifies the region of anomalous condensation of energy values. Hence, a perturbation in the form (30) leads in the neighborhood of the values specified by (31) to transformation of a large number of levels.

The quasiclassical trajectories for a system with the Hamiltonian

$$H = \varepsilon_0(p_x, p_y) - g\cos(k_1 x + k_2 y)$$

are determined by the following equations of motion:

$$\begin{aligned} &\dot{p}_x = -2k_1 g\sin X, \qquad \dot{p}_y = -2k_2 g\sin X, \\ &\dot{X} = k_1 \frac{\partial \varepsilon_0}{\partial p_x} + k_2 \frac{\partial \varepsilon_0}{\partial p_y}, \qquad X = k_1 x + k_2 y. \end{aligned} \tag{32}$$

The first two equations imply that aside from energy the system has an additional integral of motion:

$$P_0 = k_2 p_x - k_1 p_y, \qquad \dot{P}_0 = 0. \tag{33}$$

The variable conjugate to X is $p_1 = p_x/2k_1$ or $p_2 = p_y/2k_2$. We select the pair (p_1, X). Condition (31) now determines the position of the condensation points (Van Hove points) $p_{1m}(P_0)$ of the energy values $\varepsilon_0(p_1, P_0)$. For each fixed value of P_0 this condition, combined with (33), assumes the form $\partial\varepsilon_0/\partial p_1 = 0$. Near the extremal points for the electron energy we have

$$\varepsilon_{p_0} = \varepsilon - \varepsilon_0(p_{1m}, P_0) = \frac{1}{2}\varepsilon''_{0m} q_1^2 - 2g\cos X, \tag{34}$$

where

$$\varepsilon''_{0m} = 2k_1^2 \left(\frac{\partial^2 \varepsilon_0}{\partial p_x^2}\right)_{p_x = p_{xm}} = \frac{1}{2}\left(\frac{\partial^2 \varepsilon_0}{\partial p_1^2}\right)_{p_1 = p_{1m}}, \qquad q_1 = p_1 - p_{1m}.$$

Thus, the motion in the neighborhood of extremal points is described by the universal and exactly solvable model of a simple pendulum (34). Quantization of (34) produces a spectrum of the form (4) for each fixed value of P_0. The energy levels in (4) correspond to the quasiclassical trajectories of finite motion with $\varepsilon_p < 2g$ in the phase plane $\{q_1; X\}$. These trajectories describe phase oscillations satisfying the equation $\ddot{X} + \omega_m^2 \sin X = 0$, with $\omega_m^2 = 2g\varepsilon''_{0m}$. The maximum possible value of q_1 for these trajectories is $q_{1\max} = \sqrt{8g/\varepsilon''_{0m}}$. The expansion in (34) is valid for $q_{1\max} \ll p_{1m}$.

2. Next we apply the above description to the electron spectrum of a square lattice [Eq. (11)]. We introduce the angle φ that specifies the direction of the wave: $k_1 = k\cos\varphi$ and $k_2 = k\sin\varphi$. In the neighborhood of a saddle point the Hamiltonian in (11) with perturbation (30) is diagonalized in the new canonical variables:

$$\begin{aligned} q_1 &= \sqrt{2}k[p_x\sin\varphi - p_y\cos\varphi], \\ q_2 &= \sqrt{2}k[-p_x\cos\varphi + p_y\sin\varphi], \\ X &= k(x\cos\varphi + y\sin\varphi), \qquad Y = k(x\cos\varphi - y\sin\varphi). \end{aligned} \tag{35}$$

A wave along one of the principal axes, as in (11), corresponds to $k_2 = 0$ and $\varphi = 0$.

As a result of the transformation specified by (35), Eq. (34) becomes

$$\varepsilon = -4tk^2(q_1^2 - q_2^2)\cos 2\varphi - 2g\cos X. \tag{36}$$

Combining the condition $q_{1\max} = \sqrt{g/tk^2|\cos 2\varphi|} \ll p_{1m} = \pi/2k\cos(\varphi - \pi/4)$ with the requirement that

$$\omega_m = 4(gtk^2|\cos 2\varphi|)^{1/2} \ll g, \tag{37}$$

we arrive at a condition for the applicability of solutions obtained from model (34):

$$k^2|\cos 2\varphi| \ll \frac{g}{t} \ll \left|\operatorname{tg}\left(\varphi - \frac{\pi}{4}\right)\right|. \tag{38}$$

At $\varphi = 0$ this condition coincides with (1), while it becomes much more stringent as $\varphi \to \pi/4$. Quantization of (36) yields spectra of the form (12) for $\cos 2\varphi < 0$ and of the form (13) for $\cos 2\varphi > 0$ [with k replaced by $k|\cos 2\varphi|^{1/2}$ in (12) and (13)]. As condition (37) implies, as φ grows the level separation decreases but the number of levels in each well increases:

$$n_{max} = \frac{1}{\pi}\left(\frac{g}{tk^2|\cos 2\varphi|}\right)^{1/2} \tag{39}$$

At the same time the region (38) of quasilocalized states becomes narrower, that is, we see that the region with the discrete spectrum is the biggest when the wave is directed along one of the principal axes [$\varphi = 0$ in (37) and (39)]. This is the case considered by Eq. (11). Via Eqs. (37) and (39) one can easily understand why the density of states in (15) and (16) is direction-independent. The reason is that as the direction changes, an increase in the number of levels in a well corresponds to a decrease in the number of wells that "fit" into length L. As a result the dependence on direction in the density of states vanishes. Clearly, the density of states begins to depend on $\mathbf{k}$ when $k^2 \approx g/t$ and the quasiclassical conditions (1), (2), and (37) break down.

3. Let us now consider the interaction with a traveling wave (for simplicity we restrict our discussion to the one-dimensional case)

$$g(x, t) = g\cos(kx - \omega_k t), \tag{40}$$

where ω_k is the oscillation frequency. Such a perturbation leads to quantization of the electron spectrum in the neighborhood of point p_m satisfying the condition

$$k\left(\frac{\partial \varepsilon_0}{\partial p}\right)_{p=p_m} = \omega_k l \tag{41}$$

with l an integer. For the optical dispersion law, $\omega_k = \omega_0 + \alpha k^2$, point p_m is generally a common point of the electron spectrum. In the neighborhood of this point the electron energy has the form (34) with $X = kx - \omega_k t$. Correspondingly, the spectrum is determined by Eqs. (4) and (8). In the neighborhood the density of states (9) has a logarithmic peak.

However, in contrast to the problems considered above, the eigenfunctions of the Hamiltonian $H = \varepsilon_0(p) + g(x,t)$ possess certain quasienergies[16] (similar to the quasi-momentum in a lattice) that coincide with its eigenvalues. This model is apparently capable of describing, among other things, the interaction of carriers with weakly decaying critical oscillations of the order parameter above the transition point.

4. A final remark is in order. It deals with singularities in the density of states of carriers with a "long-wave" Kronig–Penney potential. Such a potential may occur if a periodic domain structure is formed in the sample, with the domains characterized by different values of some sort of a parameter (magnetization, spontaneous polarization, etc.), and interacts with the carriers. The potential corresponds to the splitting of the peak in the density of states, the root peak in the one-dimensional case or the logarithmic one in the two-dimensional, into two similar peaks separated by a distance of $2g$. Such a singularity structure in the density of states may lead to system instability to formation of a large-scale domain structure.

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