Magnetic Breakdown Induced Peierls Transition

A. M. Kadigrobov,[1,2] A. Bjeliš,[2] and D. Radić[2]

[1]*Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany*
[2]*Department of Physics, Faculty of Science, University of Zagreb, POB 162, 10001 Zagreb, Croatia*

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We predict a new type of phase transition in a quasi-one-dimensional system of interacting electrons at high magnetic fields, the stabilization of a density wave which transforms a two-dimensional open Fermi surface into a periodic chain of large pockets with small distances between them. We show that quantum tunneling of electrons between the neighboring closed orbits enveloping these pockets transforms the electron spectrum into a set of extremely narrow energy bands and gaps that decreases the total electron energy, thus leading to a magnetic breakdown induced density wave ground state analogous to the well-known instability of the Peierls type.

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Interacting electrons with quasi one-dimensional (Q1D), i.e., open and corrugated, Fermi surfaces show in many cases instabilities leading to a density wave (DW) ground state with a broken translational symmetry [1]. This type of phase transition, predicted by Peierls in 1955 [2], occurs due to divergent charge fluctuations which open the gap at the Fermi surface and so lower the energy of the new ground state. While the dominance of a repulsive Coulomb or an attractive phonon mediated electron-electron interaction are as a rule responsible for respective spin or charge modulation of DW, its stabilization depends on the degree of nesting between the left and right two-dimensional Fermi surfaces shown in Fig. 1. Nesting in real materials is always imperfect, leading to two-dimensional [3] pockets of finite size after determining the optimal wave vector of DW ordering, $\mathbf{Q} = (2k_F + \delta k_{\|}, b^*/2 + \delta k_{\perp})$, where k_F and b^* are Fermi wave number and transverse reciprocal lattice vector, respectively, while $\delta k_{\|,\perp}$ are small corrections. Unlike the nested parts of the Fermi surface, these pockets develop a weaker gap in the electron spectrum, or even remain gapless. The pockets thus act against the DW, and, if large enough, may completely eliminate it.

A qualitative change, however, takes place after applying strong enough magnetic field $\mathbf{H}$ perpendicular to the plane (p_x, p_y) in Fig. 1. Landau quantization of band states then reduces the transverse delocalization of electrons, making the system ''more one-dimensional'' [4] and therefore more susceptible to the DW ordering. DWs are then strengthened, or even newly established in systems which otherwise remain metallic down to $T = 0$. The latter case of field-induced density wave (FIDW) is particularly relevant for our further considerations. The best known examples are those realized in a series of Bechgaard salts with spin modulation [5], in which the FIDW order takes place in available magnetic fields up to ~50 T, provided the deviation form perfect nesting is not large. The pockets with discrete Landau orbits are then small and, after establishing DW gap in dominant ''nesting'' parts of Fermi surface, quite distant one from another.

The Landau quantization leads to the localization of electron motion, therefore increasing the band energy in general, or leaving it unchanged for the discrete set of values of $\mathbf{H}$ for which the Fermi energy lays exactly in the middle between two neighboring Landau levels [6]. Still, it contributes to the FIDW stabilization through an additional gain in the correlation energy part due to the improved longitudinal localization of electron states.

At this point we come to our central question, namely, is it possible to stabilize a density wave order with the help of orbital quantization in the quasi one-dimensional band, but

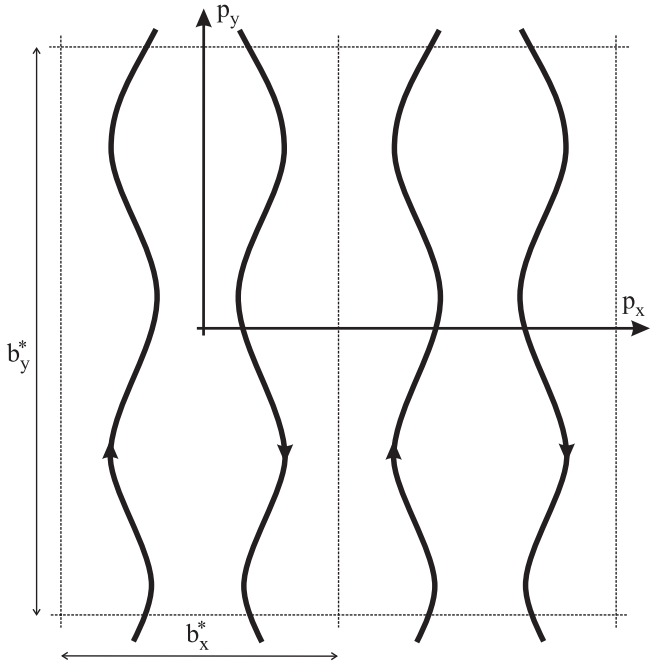

FIG. 1. Quasi one-dimensional Fermi surface, $\varepsilon(\vec{p}) = \varepsilon_F$, where $\varepsilon(\vec{p})$ is the electron dispersion law and ε_F is the Fermi energy, with arrows denoting directions of semiclassical electron motion under a magnetic field perpendicular to the plane (p_x, p_y). b_x^* and b_y^* are reciprocal lattice constants.

through a predominant decrease of the band energy due to the magnetic breakdown [7,8]? This magnetic breakdown induced density wave (MBIDW) is possible only by strengthening the tunneling between neighboring pockets, i.e., by choosing the DW wave vector which, oppositely to FIDW in Bechgaard salts, favors short and weak tunnel barriers together with large pockets between them. In the present work we examine this new possibility by using the standard mean field approach for DW instability [9] and the semiclasical treatment of MB tunneling [8], and establish the conditions under which this gain overwhelms the elastic energy loss due to the lattice deformation [10], leading so to the MBIDW stabilization.

Qualitative considerations.—Let us choose the deformation wave vector $\mathbf{Q} = (Q \approx 2k_F, 0)$ creating a static periodic lattice distortion and a charge modulation $V(x)$ with the period $2\pi\hbar/Q$ that combines open trajectories with opposite directions of the electron motion, shown by arrows in Fig. 2. We encounter a chain of closed orbits encircling large pockets and small areas between them (shown with thick dots) at which MB takes place, that is an electron moving along a semiclassical section of the chain, say 1, is scattered at the MB area to section 2 and section $2'$ with the amplitude probabilities ρ and τ respectively ($|\rho|^2 + |\tau|^2 = 1$), with the MB probability

$$|\rho|^2 = \exp(-\gamma), \tag{1}$$

where $\gamma \equiv \pi|V_0|^2/\sigma|v_x v_y|$. Here v_x and v_y are longitudinal and perpendicular projections of the electron velocity $\vec{v} = \partial\varepsilon(\vec{p})/\partial\vec{p}$ at the point of the magnetic breakdown, $\sigma = \hbar eH/c$, e and c are the electron charge and the light velocity, respectively, while V_0 is the nondiagonal matrix element of $V(x)$. For the electron-phonon system within the mean field approximation, $|V_0| = 2gb$, where g is the coupling constant and $b = \langle b_Q \rangle$ is the mean value of the phonon annihilation operator at the wave number Q (see, e.g., [9]), here directly proportional to the amplitude of the lattice displacement. Thus, due to the finite lattice distortion $V(x)$ electron scatters in a periodic set of regions of MB, latter having a role analogous to that of atomic lattice in an one-dimensional metal.

In order to understand qualitatively the structure of the energy spectrum of an electron on the orbit chain let us assume at first that $|V(x)|$ is negligibly small while the strength of the magnetic field is finite. In this case $|\rho|^2 = 1$ and the electron moves along an open trajectory 1-2-3 ... or $1'$-$2'$-$3'$ ... (trajectories I and II, respectively). It is known [11] that the electron spectrum $E_n^{I,II}(P_{x0})$ of such motion is continuous and characterized by a discrete quantum number n and a continuous momentum P_{x0}. Here superscripts refer to trajectories I and II, while P_{x0} is the generalized momentum projection conserved in the Landau gauge with the vector potential $\vec{A} = (-Hy, 0, 0)$. The electron velocities are $v^{I,II} = dE_n^{I,II}/dP_{x0}$ ($v^I > 0$ and $v^{II} < 0$). This electron spectrum is represented by the dotted straight lines in Fig. 3(a).

For a finite $V(x)$, trajectories I and II are coupled by the finite tunneling probability. The degeneracy at the crossing points in the electron spectrum is then lifted by $|\tau|^2$, producing there energy gaps analogous to those in the spectrum of a real one-dimensional electron gas created by the charge modulation $V(x)$ itself [12].

If the Fermi energy occurs in the middle of one of these gaps, the electron band energy decreases. This energy gain

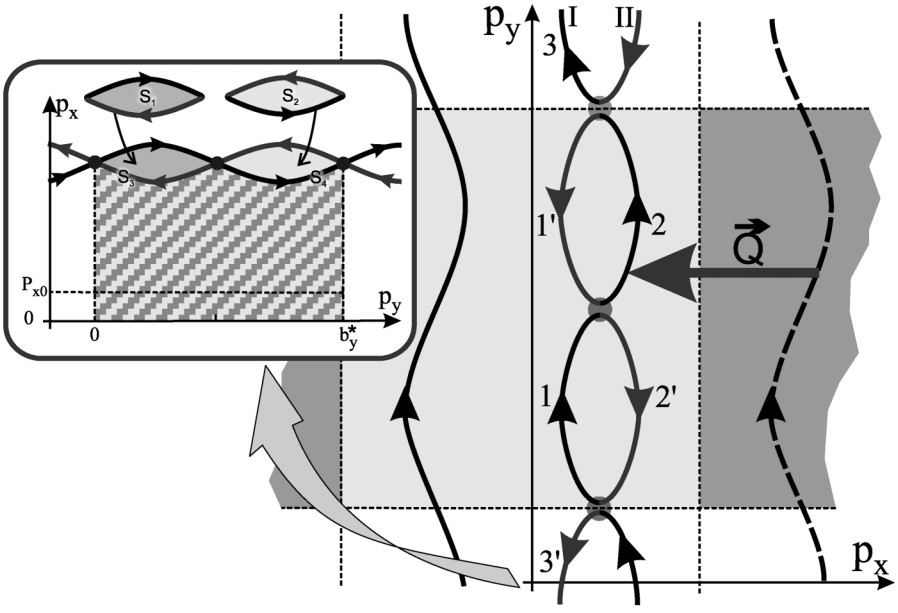

FIG. 2. (a) Periodic net of large closed orbits separated by small classically inaccessible MB arrears (thick dots). $\vec{Q} = (Q \approx 2k_F, 0)$ is lattice deformation wave vector, and the distance between closed orbits is proportional to the product of electron mass and deformation potential $V(x)$. (b) Areas of closed orbits, $S_{1,2}$, and areas under open orbits, $S_{3,4}$ for the respective left and right motion of electrons, determine the phases of semiclassical electron wave functions defined in the text.

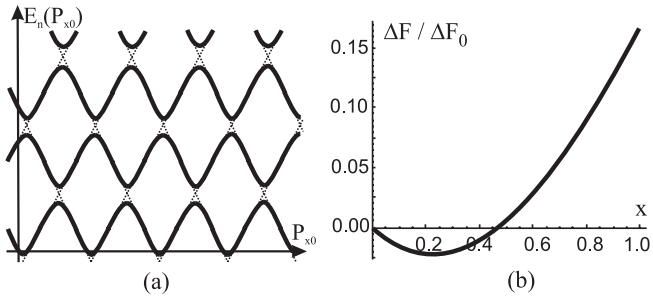

FIG. 3. (a) Energy spectrum for electrons shown in Fig. 2 in the regime of strong MB ($|\tau|^2 \ll 1$). n is the MB band number and P_{x0} is the conserved generalized electron momentum. The period of $E_n(P_{x0})$ is $2\pi\sigma/b_y^*$, while the widths of the energy bands and gaps are $\Delta E_{\text{band}} \sim |\rho|^2\hbar\omega_c$ and $\Delta E_{\text{gap}} \sim |\tau|^2\hbar\omega_c$ respectively (ω_c is the cyclotron frequency). Dotted straight lines denote the electron spectrum in the absence of MB. (b) The free energy difference $\Delta F/\Delta F_0$ vs $x \equiv (\pi g^2/\sigma|v_x v_y|)b^2$ for $\gamma \equiv (\sigma|v_x v_y|/\pi g^2)(\hbar\omega_Q/\Delta F_0) = 0.8$, showing stable minimum of DW ground state at $x_0 \approx 0.22$.

grows by increasing the gap $\propto |\tau|$. As $|\tau|^2 = 1 - |\rho|^2$ increases by increasing $|V_0|$, as is seen from Eq. (1), the energy band gain is favored by the increase of the charge modulation $V(x)$. However, by increasing $V(x)$ one increases the lattice energy and, as a result, competition of these two tendencies gives the optimal value of the charge modulation $V(x)$.

Analytical calculations.—In the $\vec{p}$-space the electron moves along classical trajectories $p_x^{(l)}(p_y)$ (marked by $l = 1, 1', \ldots$ in Fig. 2) between the points of MB. Corresponding semiclassical wave functions are

$$a^{(l)} \exp\left\{-\frac{i}{\sigma}\int^{p_y}[p_x^{(l)}(\bar{p}_y) - P_{x0}]d\bar{p}_y\right\}, \tag{2}$$

where $p_x^{(l)}(p_y)$ are solutions of the equation $\varepsilon_s(p_x, p_y) = E$ while $\varepsilon_s(\vec{p})$ is the electron dispersion law for a finite $V(x)$ and at $H = 0$, $s = 1, 2$ indexing the new electron bands. At the points of MB the incoming and outcoming functions (2) are coupled by the MB 2×2 unitary matrix [8,13,14]

$$\hat{\tau} = e^{i\Psi}\begin{pmatrix} |\tau|e^{i\eta} & |\rho|e^{i\nu} \\ -|\rho|e^{-i\nu} & |\tau|e^{-i\eta} \end{pmatrix}, \tag{3}$$

e.g., $a_2 = \exp(i\Psi)(a_1|\rho|\exp(i\nu) + a_{1'}|\tau|\exp(i\eta))$. The phases depend on the MB parameter γ from Eq. (1). In the limit $\gamma \ll 1$ (that is $|\tau|^2 \ll 1$) to which we limit our calculations of MBIDW, $\eta \approx -\pi/4 - \gamma\ln\gamma$, $\nu \approx 0$, $\Psi \approx 0$.

Matching the wave functions (2) at the MB points with use of the matrix (3) and taking into account the electron phase gains between them one finds the dispersion function

$$D(E, P_{x0}) = \cos\bar{\Phi}_- - |\tau|^2\cos\Phi_+ - |\rho|^2\cos\left(\Phi_0 - \frac{P_{x0}b_y^*}{\sigma}\right). \tag{4}$$

Here $\bar{\Phi}_- = \Phi_- + 2\Psi$, $\Phi_\pm = (1/2\sigma)(S_1(E) \pm S_2(E))$ and $\Phi_0 = (1/2\sigma)(S_3(E) - S_4(E)) + 2\nu$, while $S_{1,2,3,4}(E, Q)$ are the areas enclosed by electron trajectories which depend on the position of the crossing points of trajectories I and II determined by $\vec{Q}$ (see Fig. 2). The electron spectrum is determined by dispersion equation $D(E, P_{x0}) = 0$.

If $|\rho|^2 = 0$, this equation gives a set of discrete Landau levels, while in the case $|\rho|^2 \neq 0$ the degeneracy with respect to P_{x0} is lifted and the electron spectrum depends on a continuous quantum number, $E = E_n(P_{x0})$, where the band number n enumerates solutions of the dispersion equation. Solving this equation in the limit $|\tau|^2 \ll 1$ one finds the electron spectrum presented in Fig. 3(a).

In order to find an explicit formula for the density of states (DOS) for electrons moving along the MB chain, we express it in terms of the spectral function (4) as follows:

$$\nu_{\text{MB}}(E) = \int\sum_n \delta(E - E_n(P_{x0}))\frac{dP_{x0}}{2\pi\hbar} = \int |D'(E, P_{x0})|\,\delta(D(E, P_{x0}))\frac{dP_{x0}}{2\pi\hbar}, \tag{5}$$

where here and below $f' \equiv \partial f/\partial E$. Integrating with respect to P_{x0} we find

$$\nu_{\text{MB}}(E) = \frac{\sigma}{(2\pi)^2}\Theta(|\rho|^2 - |\cos\Phi_- - |\tau|^2\cos\Phi_+|) \times \frac{|\phi'_-\sin\Phi_- - |\tau|^2\phi'_+\sin\Phi_+|}{\sqrt{|\rho|^4 - (\cos\Phi_- - |\tau|^2\cos\Phi_+)^2}}, \tag{6}$$

where $\Theta(x)$ equals unity for $x \geq 0$ and zero otherwise. From here one easily sees that at $|\tau|^2 = 0$ (that is at $V_0 = 0$) DOS is equal to the one in the absence of MBIDW.

Equation (6) permits to find the number of electrons $N = \int[\exp(E - \mu)/T + 1]^{-1}\nu(E)dE$ and the electron free energy $F = N\mu - T\int\ln[1 + \exp(\mu - E)/T]\nu(E)dE$, μ being the chemical potential. We calculate them expanding the right-hand side of Eq. (6) in a double Fourier series in $\Phi_\pm$ and in a power series in $|\tau|^2$. Below we solve the problem in the vicinity of the critical temperature T_c in which the order parameter and the potential V_0 are small, so that $|\tau|^2 \ll 1$ and we can keep only terms of the lowest order ($\sim |\tau|^2$) in the above-mentioned power series.

After finding N and F we take into account the conservation of electron number and determine the change of the chemical potential $\delta\mu = \mu_{\text{MB}} - \mu_0$, where μ_{MB} and μ_0 are chemical potentials at $V(x) \neq 0$ and $V(x) = 0$, respectively. Inserting it in the free energy and neglecting terms of the order of $|\tau|^4\hbar\omega_c/\varepsilon_F$ and $\tau^2(\hbar\omega_c/\varepsilon_F)^2$, we find the difference of the total free energies in the presence and the absence of MBIDW at $T > \hbar\omega_c^{(+)}/\pi$, where $\omega_c^{(+)} = eH/m_+^*c$ with the effective mass given by $m_+^* = (m_1^* + m_2^*)/2$ and $m_{1,2}^* \equiv |\partial(S_{1,2})/\partial\varepsilon|$:

$$\Delta F = \Delta F_0\left[1 - \exp\left(-\frac{\pi g^2 b^2}{\sigma|v_x v_y|}\right)\right]\cos\frac{S_+}{2\sigma}\sin\frac{S_-}{2\sigma} + b^2\hbar\omega_Q; \quad (7)$$

$$\Delta F_0 \equiv kT\exp\left\{-\frac{\pi T}{\hbar\omega_c^{(+)}}\right\}.$$

Here $S_\pm = S_1(\mu_0, Q) \pm S_2(\mu_0, Q)$ is the effective electron loop area, and the last term is the lattice elastic energy given by phonon frequency ω_Q at momentum Q. Equation (7) is valid in the regime $\sigma \lesssim |S_-| \ll S_+$.

From Eq. (7) it follows that ΔF has a series of minima at the discrete set of lattice deformation wave numbers Q_n for which $S_-(\mu_0, Q)/2\sigma = (\pi/2)(2n+1)$ with integer values of n (for $\partial S_1/\partial Q \approx -\partial S_2/\partial Q$) [15]. On the other hand, the minimization of Eq. (7) with respect to b^2 shows that ΔF is negative and has an absolute minimum at

$$b^2 = \frac{\sigma|v_x v_y|}{\pi g^2}\ln\left[\lambda\frac{\mu_0|\cos(S_+/2\sigma)|\pi T}{m_+^*|v_x v_y|\hbar\omega_c^+}\exp\left(-\frac{\pi T}{\hbar\omega_c^{(+)}}\right)\right] \quad (8)$$

as shown in Fig. 3(b). Here $\lambda = g^2/(\hbar\omega_{Q_n}\mu_0)$ is the dimensionless electron-phonon coupling constant (see [9]). The corresponding critical temperature for the transition to the MBIDW state is

$$T_c \approx \frac{\hbar\omega_c^+}{\pi}\ln\left(\lambda\frac{\mu_0|\cos(S_+/2\sigma)|}{m_+^*|v_x v_y|}\right) \quad (9)$$

provided $\lambda\mu_0|\cos(S_+/2\sigma)|/m_+^*|v_x v_y| > 1$.

In conclusion, we have shown that the MBIDW instability may occur in quasi-one-dimensional conductors in a wide range of parameters and at any finite magnetic field. The topological prerequisite for such instability is the open Fermi surface of the type shown in Fig. 1, which after a periodic breaking of symmetry from Fig. 2, leads to the lattice of closed orbits connected by barriers at cross points. The magnetic field assisted tunneling through these barriers is crucial for the stabilization of MBIDW. MB introduces a qualitative change in electron dynamics, transforming the continuous spectrum of quasi-one-dimensional interacting electrons into a set of alternating narrow energy bands $\sim|\rho|^2\hbar\omega_c$ and energy gaps $\sim|\tau|^2\hbar\omega_c$. Just a mere Landau quantization of such closed electron orbits does not lead to the DW stabilization since it only rises the band energy due to the localization of electron motion. Only by delocalization of motion introduced by MB, whose negligence was probably the reason why this effect was not predicted in preceding literature, the total energy is lowered enough to grant the stability of DW ground state.

We have also shown that the free energy of MBIDWs has local minima at a set of discrete values of the deformation wave vector Q, indicating the role of resonances between neighboring orbits with generally different size (Fig. 2). We remind that this series of wave vectors belong to the "antinesting" regime, which again reflects the essential differences between MBIDWs and standard FIDWs, the latter being the consequence of logarithmic anomalies in the DW correlation function due to the almost perfect nesting between left and right Fermi surfaces in Fig. 1. The dependence of T_c on H has a periodic (in $1/H$) set of gaps for a given Q_n [Eq. (9)], in contrast to the corresponding dependence for FIDWs [16]. This, together with a qualitatively different dependence on the coupling constant and band parameters, could be a guide in the search for MBIDWs. Another one is fast magnetoresistance oscillations due to the formation of relatively large closed orbits (Fig. 2). The regime wider than that of Eq. (7) and the peculiarities of the MBIDW phase diagram will be analyzed in a more detailed presentation.

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