Peierls-type structural phase transition in a crystal induced by magnetic breakdown

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Abstract. We predict a new type of phase transition in a quasi-two dimensional system of electrons at high magnetic fields, namely 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. The 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 which decreases the total electron energy, thus leading to a magnetic breakdown induced density wave (MBIDW) ground state. We show that this DW instability has some qualitatively different properties in comparison to analogous DW instabilities of Peierls type; e.g. the critical temperature of the MBIDW phase transition arises and disappears in a peculiar way with a change of the inverse magnetic field.

1 Introduction

A specific topology of an open Fermi surface with two corrugated sheets related by the reflection symmetry is the origin of numerous examples of modulated ground states with generally incommensurate periodicities. These are well-known charge or spin density wave (DW) ground states, widely investigated during last decades. DW ground states are observed in materials with a quasi-one-dimensional crystal lattice, or materials which, due to other reasons, show strong internal anisotropy of conducting band electronic states [1].

In the absence of external magnetic field the longitudinal component $Q_x$ of the DW momentum $Q$ has a value that is equal or close to $2p_F$, with Fermi momentum $p_F = n\hbar\pi/a$ where $a$ is the longitudinal lattice constant, and $n$ is the number of electrons per site filling the band for which only the spin degeneracy is assumed. As is seen in Figure 1, $2p_F$ is the mean distance between two (“upper” and “lower”) Fermi sheets.

The DW in the absence of magnetic field may be stabilized provided one geometric and one energetic condition are obeyed. Geometrically, its transverse component $Q_y$ has to respect the nesting requirement, i.e. to allow for the largest possible phase space for the condensation of electron-hole pairs carrying the momenta $\pm Q$. Correspondingly, the great part of the new Fermi surface is gapped. Still, the nesting in real materials is imperfect, so that the Fermi surface of DW state contains mutually distant pockets in which the DW gap is degraded

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{(a) An open electron Fermi surface, with two branches “+” and “−”, shifted by deformation momentum $Q$ into $p_{F,1,2}(p_y)$. Arrows depict electron trajectories with the opposite directions of motion at corresponding branches in magnetic field. Expressions that determine the shape of trajectories $p_{\pm}(p_y)$ are given by equation (A.4) in Appendix A. $a^* \equiv 2\pi\hbar/a$ and $b^* \equiv 2\pi\hbar/b$ are the reciprocal lattice constants in $x$- and $y$-direction of momentum space, respectively, corresponding to the real space lattice constants $a$ and $b$. (b) After the degeneracy is lifted at the crossing points due to DW potential, the chain with two types of electron orbits is formed: the large ones (with area $S_+$ in $p$-space) and the small ones between them. In the finite magnetic field, the magnetic breakdown between neighboring $S_+$ trajectories takes place through the area occupied by small pockets (MB-regions).}
\end{figure}

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or even vanishes. Energetically, the electron-electron or
electron-phonon coupling responsible for the condensation
of electron-hole pairs, have to be strong enough in order
to get a sufficient correlation energy gain and stabilize the
DW order.

Even if the above conditions are not obeyed, field-
induced density wave (FIDWs) orderings may be stabilized
after applying a strong enough external magnetic field \( H \)
perpendicular to the \((x, y)\) plane. As was pointed out in
our previous work [2], two possibly competitive mech-
anisms may lead to FIDWs.

The first one may be realized if the nesting is not far
from perfect, i.e. in the regime \( t'_{y} \ll t_{y} \), where \( t_{y} \) is the
transverse band width, and \( t'_{y} \) is the imperfect nesting
parameter. It is based on the “one-dimensionalization”
of electron spectrum due to the Landau quantization of
band states within distant, presumably small, pockets re-
main ing after establishing the 2\(p_{F}\) modulation [3,4]. The
magnetic field energy relevant for this type of FIDWs is
characterized by the scale of cyclotron energy which is
in the present case given by \( \hbar \omega_{c} = ev_{F}H/b'c \) where \( v_{F} \) is
the longitudinal Fermi velocity, and \( b' \) is the
transverse reciprocal lattice constant in momentum space.
FIDWs then can be stabilized provided \( \hbar \omega_{c} \) is of the or-
der of imperfect nesting parameter \( t'_{y} \). This requirement
is accessible with magnetic fields of the order of up to
few tens tesla for various families of quasi-one-dimensional
and quasi-two dimensional materials like Bechgaard salts,
\( \alpha \)-ET compounds, etc.

While in this regime the effects of tunneling between
distant pockets are negligible, the alternative choice of
DW period, for which the pockets are large and barri-
ers between them narrow, leads to a novel mechanism of
DW stabilization. It originates from the decrease of the
total electron energy due to the creation of finite barriers
(instead of simple crossing points in the absence of DW)
between neighboring pockets. The energy decrease comes
from the magnetic breakdown between neighboring pock-
ets which opens the gaps in one-dimensional sub-bands,
the latter appearing due to the orbital quantization in
the case of an open (quasi-one-dimensional) conducting
band. Such finite barriers go together with the formation
of lattice periodic modulation, which in turn counterbal-
ances the band energy gain with the increase of the lat-
tice energy. The outcome is the ordered DW, stabilize
by the magnetic field assisted tunneling, i.e. by the one-
particle processes, and not by the electron-electron scat-
tering like in the regime of nested DWs. On the contrary,
the electron-electron correlations, illustrated here by the
electron-phonon coupling, oppose, and eventually equili-
brate, the stabilization of MBIDWs.

With magnetic breakdown having the central role in
this kind of DW ordering, it is necessary to investigate
how the details characterizing the barriers influence the
electron spectrum and the free energy of the ordered state.
More precisely, one comes to the problem of finding the
barrier configuration that is the most favorable one for
the DW stabilization, leading to the highest corresponding
critical temperature.

In the previous work [2], we have considered the case of
the DW momentum equal to \( (2p_{F}, 0) \), i.e. the succession
of same pockets separated by a simple point-like barriers
without internal structure, the distance between neighbor-
ning barriers being equal to \( b' \). In the present analysis
we concentrate to the ordering with the DW momentum
roughly equal to \( (2p_{F} - \Delta t_{y}/v_{F}, 0) \). This is the regime of
largest possible pockets, i.e. the limit of full “anti-nesting”
shown in Figure 1. The distance between neighboring bar-
riers is now equal to \( b' \). In the latter choice the “upper”
and “lower” sub-bands do not cross but touch each other,
so that the large pockets are not separated by barriers,
but by small pockets with a peculiar local band disper-
sion. As our present analysis shows, these small pockets
play the role of effective magnetic barriers with a qualita-
tively enhanced effect of field assisted tunneling between
large pockets. Consequently, we come to the central result
of this work, namely that the fully anti-nesting regime
from Figure 1 is the best candidate for the MBIDWs.

The overview of the paper is as follows: in Section 2 we
present the spectrum and the density of states of quasi-
one-dimensional electron band with periodic perturbation
introduced by the DW formation, all under magnetic field
with magnetic breakdown (MB) induced tunneling be-
 tween electron trajectories treated within the framework
of semiclassical formalism. In Section 3 we calculate the
energy balance between energy loss of delocalized elec-
tron due to the MB tunneling and gain due to the DW
formation that leads to the magnetic breakdown induced
transition of Peierls type. There we predict the magnetic
breakdown induced density wave (MBIDW) and present
its phase diagram on the domain of magnetic field and
critical temperature. Concluding remarks are given in Sec-
ction 4. An Appendix, provided in the end, contains math-
ematical details related to the calculation of results from
the main text, namely Appendix A for Section 2 and Ap-
pendix B for Section 3. In Section A.1 we present the
calculation of the resulting band structure of quasi-one-
dimensional band under the periodic perturbation. Sec-
ction A.2 contains the details of quantum-mechanical cal-
culation of novel MB tunneling process for the particular
bands relevant for the present problem. Furthermore, in
Section A.3 we present the semiclassical formalism used
to describe electrons apart from the MB region and calcu-
late the new band structure under the regime of magnetic
breakdown. Finally, in Section A.4 we show the construc-
tion of the MB tunneling matrix used to connect the semi-
classical solutions from the different regions and provide
the novel tunneling probability for the proposed model.
Appendix B contains the details of the Fourier expansion
of electron density of states under the MB regime.

2 Spectrum and density of states
of electrons under magnetic field

We consider a metal with an open Fermi surface assuming
that the dispersion law of conduction electrons \( \varepsilon(p_{x}, p_{y}) \)
depends only on two projections of the electron quasi-
momentum \( p = (p_{x}, p_{y}) \). It can be the case either of
We show below that the most favorable MBIDW deforma-
ergy spectrum $\varepsilon(p_x, p_y) = \varepsilon_F$ consists of two branches, \textquotedblleft+\textquotedblright\ (upper) and \textquotedblleft−\textquotedblright\ (lower),

\begin{equation}
\varepsilon_{\pm}(p) = \varepsilon_F \pm \nu_F(p_x \mp p_F) - 2t_y \cos \frac{b p_y}{\hbar},
\end{equation}

where $\varepsilon_F$ and $\nu_F$ are the Fermi energy and velocity, respectively (see Appendix A, Eqs. (A.1)–(A.5) for details).

We assume that a static periodic lattice distortion creates a modulation potential $V(x)$ with period $2\pi \hbar/Q_x$. The deformation momentum $Q \approx (2p_F - 4t_y/\nu_F, 0)$, with the optimal value to be determined later from the DW condensation condition, combines open trajectories $p_{x+}^{-1}(p_y)$ and $p_{x-}^{-1}(p_y)$ with opposite directions of the electron motion. These trajectories are the upper and the lower branches of the Fermi surface depicted by thick solid lines in Figure 1a. Therefore, the combined trajectories are

\begin{equation}
\begin{aligned}
p_x^{(1)}(p_y) &= p_x^{-}(p_y) + Q_x, \\
p_x^{(2)}(p_y) &= p_x^{+}(p_y).
\end{aligned}
\end{equation}

We shall show below that the most favorable MBIDW deformation vector $Q_x$ is close to the one at which the trajectories $p_x^{(1)}(p_y)$ and $p_x^{(2)}(p_y)$ touch each other. Hence, the new energy spectrum $E_{1,2}(p_x, p_y)$ of the crystal in the presence of the modulation potential $V(x)$ has peculiar points in the energy space near the Fermi energy $\varepsilon_F$ at which the equipotential surfaces $E_{1,2}(p_x, p_y) = \varepsilon_F$ change their topology with a change of the electron energy $\varepsilon$. The details of electron spectrum in the vicinity of these points are presented in Appendix A, equation (A.11), Figure A.1. Here we consider dynamics of electrons in the presence of the modulation potential $V(x)$ under a strong magnetic field $H$ at which the Larmor radius is much smaller than the electron free path length $l_0$, that is

\begin{equation}
\frac{c p_F}{e H} \ll l_0,
\end{equation}

where $c$ is the light velocity and $e$ is the electron charge. On the other hand, we assume that the magnetic field satisfies the inequalities

\begin{equation}
S_{\text{small}} < \sigma \ll S_+; \quad \sigma \equiv \frac{e H}{c},
\end{equation}

where $S_{\text{small}}$ and $S_+$ are the areas of the small and large orbits within the trajectory chain respectively (see Fig. 1b). In this case the electron dynamics may be treated semiclassically between the MB regions around the small pockets (marked area in Fig. 1b) in which the semiclassical approximation is not valid. As we show in Appendix A – Section A.4, equation (A.34), in these regions a peculiar combination of intra- and inter-band MB transitions results in the dependence of the MB probability on the magnetic field and the Fermi energy that qualitatively differs from the conventional one [5] and, as we prove in Section 3, it is the most favorable for the stabilization of the density wave.

In order to find the wave function of an electron $G(P_{x0}, P_y)$ in the momentum representation between the MB regions, one may use the Onsager-Lifshitz Hamiltonian [6,7]

\begin{equation}
E \left( P_{x0} + i \sigma \frac{d}{dP_y}, P_y \right) G(P_{x0}, P_y) = \varepsilon G(P_{x0}, P_y),
\end{equation}

where $E(p_x, p_y)$ is the electron energy band in the absence of the magnetic field, corresponding to the large pocket in Figure 1b, $P$ is the generalized momentum, and $\sigma$ is its $x$ component conserved in the Landau gauge of the vector potential $A = (-Hy, 0, 0)$. As the chain of the trajectories under consideration is periodic, Hamiltonian (5) is supplemented with a periodic boundary condition:

\begin{equation}
G(P_{x0}, P_y) = G(P_{x0}, P_y + b^*),
\end{equation}

where $b^*$ is the period of the reciprocal lattice in the $P_y$-direction. In addition, in the MB regions, the eigenfunctions are coupled by the MB condition presented below.

The semiclassical solution of equation (5) can be written in the form:

\begin{equation}
G^{(I)}_{1,2} = \frac{C_{1,2}}{\sqrt{|v_{1,2}|}} \exp \left\{ - \frac{i}{\sigma} \int_{P_y}^{P_y'} \frac{p_x^{(1,2)}(P_y') - P_{x0}}{2t_y} dP_y' \right\}
\end{equation}

in the region $-3b^*/2 < P_y < -b^*/2$ (region I), and

\begin{equation}
G^{(II)}_{1,2} = \frac{C_{1,2}}{\sqrt{|v_{1,2}|}} \exp \left\{ - \frac{i}{\sigma} \int_{P_y}^{P_y'} \frac{p_x^{(1,2)}(P_y') - P_{x0}}{2t_y} dP_y' \right\}
\end{equation}

in the region $-b^*/2 < P_y < b^*/2$ (region II), with $v_{1,2} = \partial E/\partial p_x$ at $p_x = p_x^{(1,2)}(P_y)$. Here and below we treat the MB regions as point-like objects, neglecting their length in comparison with the length of the semiclassical trajectories between them. Note that the quantum inter-band transitions between the new energy bands $E_1(p_x, p_y)$ and $E_2(p_x, p_y)$ under the magnetic field are significant for the values of $p \sim \sqrt{\sigma} \ll b^*$ [8,9]. The dependence of the kinematic momentum $p_x^{(1,2)}(P_y)$ on $P_y$ is found from the equation

\begin{equation}
E(p_x, P_y) = \varepsilon,
\end{equation}

where constants $C_{1,2}^{(I,II)}$ are matched by the $2 \times 2$ MB matrix

\begin{equation}
\begin{pmatrix}
C_{1,2}^{(I)} \\
C_{1,2}^{(II)}
\end{pmatrix}
= e^{i\Theta} \begin{pmatrix}
t & r \\
-r^* & t^*
\end{pmatrix}
\begin{pmatrix}
C_{1,2}^{(I)} \\
C_{1,2}^{(II)}
\end{pmatrix}.
\end{equation}

Due to the unitarity of MB matrix, the matrix elements satisfy $|t|^2 + |r|^2 = 1$, where $|t|^2$ and $|r|^2$ are the MB probabilities for an incident electron to pass through or to be reflected at the MB region, respectively (see Fig. 2), $\Theta$ is the phase factor specific for the particular MB configuration. For the case under our consideration, the MB
In order to find the electron density of states (DOS), we use the approach developed by Slutzkin for spectra of electrons under magnetic breakdown (see review paper [10]).

Using the identity

$$\sum_n \delta(\varepsilon - E_n) = \left| \frac{\partial D}{\partial \varepsilon} \right| \delta(D) \quad (17)$$

(see Eqs. (12), (15)), the electron DOS

$$\nu(\varepsilon) = \frac{1}{L_y} \int_0^{\Delta P_x} \frac{dP_x}{2\pi \hbar} \left| \frac{\partial D(\varepsilon, P_x)}{\partial \varepsilon} \right| \delta \left(D(\varepsilon, P_{x0}) \frac{dP_{x0}}{2\pi \hbar} \right) \quad (18)$$

can be rewritten in the form

$$\nu(\varepsilon) = \frac{1}{L_y} \int_0^{\Delta P_x} \left| \frac{\partial D(\varepsilon, P_{x0})}{\partial \varepsilon} \right| \delta \left(D(\varepsilon, P_{x0}) \frac{dP_{x0}}{2\pi \hbar} \right) \quad (19)$$

where $L_y$ is the width of the sample in $y$-direction and $\Delta P_x = (eH/\sigma)L_y$ is the maximal value of $P_{x0}$ at which the center of localization of the electron wave function remains inside the sample.

Substituting expression (12) into (19) and integrating the latter with respect to $P_{x0}$, one finds the density of states

$$\nu(\varepsilon) = \frac{2|S_+|}{(2\pi \hbar)^2} \frac{\sin \Phi(\varepsilon)}{|t|^2 - \cos^2 \Phi(\varepsilon)} \theta \left(|t|^2 - \cos^2 \Phi(\varepsilon)\right) \quad (20)$$

where $\Phi(\varepsilon) = S_+(\varepsilon)/2\sigma$ and $S_+ = dS_+/d\varepsilon$. For example, for the initial spectrum of electrons (1), one has

$$S_+(\varepsilon) = 2b^* (\varepsilon - \varepsilon_F + 2t_y)/v_F, \quad S_+ = 2b^* /v_F. \quad (21)$$

Therefore, there are energy “gaps” in the density of states determined by equation (16). The widths of the gaps are of the order of $|r|^2 /S_+ \sim |r|^2 \hbar \omega_c$, where the width of the energy bands is of the order of $|t|^2 \hbar \omega_c$, where $\omega_c = eH /m_0 c$ is the electron cyclotron frequency and $m_0^* /m_0 \equiv S_+$ plays the role of electron cyclotron effective mass for a semiclassical motion of the electron under an external magnetic field. We show below that such a dramatic transformation of the electron spectrum under magnetic breakdown can result in a peculiar instability of Peierls type.

### 3 Magnetic breakdown induced Peierls transition

We have assumed that a static distortion of the crystal combines open trajectories into a chain of closed orbits with small MB regions between them as it is shown in Figure 1. As a result, the initially continuous electron spectrum transforms into a series of alternating narrow energy gaps and bands, hence the Fermi energy of the electron system should inevitably attain a new position on the energy scale. We find a new value of the Fermi energy $\varepsilon_F$ from the condition that the number of electrons conserves under the MB induced Peierls-type phase transition, that is

$$N(\varepsilon_F) = N_0(\varepsilon_F^0). \quad (22)$$

![Graphical presentation of the magnetic breakdown scattering processes. The directions of arrows show the motion directions of electrons; $C_1^{(I)}, C_2^{(I)}$ and $C_1^{(II)}, C_2^{(II)}$ are the constant factors in the wave functions of the incoming and outgoing electrons, respectively.](image-url)
Here

\[ N = \int_0^\infty \frac{\nu(\varepsilon)}{\exp \left( \frac{\varepsilon}{k_B T} \right) + 1} d\varepsilon \]  

(23)

is the density of electrons moving under conditions of the magnetic breakdown, having the density of states \( \nu(\varepsilon) \) defined by equation (20) and \( T \) is the temperature. We define

\[ N_0(\varepsilon_F^{(0)}) = \nu_{in} \varepsilon_F^{(0)} \]  

(24)

as the density of electrons in the initial lattice (in the absence of the DW) with the initial density of states \( \nu_{in} = S'_i/(\pi \hbar)^2 \) and the initial Fermi energy \( \varepsilon_F^{(0)} \) (for the dispersion law in Eq. (1), \( \nu_{in} = 2b^*/\nu_F(\pi \hbar)^2 \), see Eq. (21)).

In order to carry out the integration in equation (23), we use the Fourier expansion of DOS (see Appendix B, Eq. (B.1)). Assuming that temperature \( T \) is sufficiently large with respect to \( \hbar \omega_c \), we keep only the first Fourier harmonics with \( A_0 = 1 \) and \( A_2 = -|r|^2 \) (see Eq. (B.7)). Inserting it in equation (23) one finds

\[ N = \nu_{in} \varepsilon_F - 2\nu_{in} \int_0^\infty |r(\varepsilon)|^2 \cos \left( \frac{\varepsilon + \varepsilon_F}{\sigma} \right) \exp(\varepsilon - \varepsilon_F)/T + 1 d\varepsilon. \]  

(25)

While writing equation (25), we took into account the dependence of the reflection probability at MB regions \(|r|^2\) on electron energy \( \varepsilon \). As it is shown in Appendix A, \( r(\varepsilon) \) is equal to zero at \( \varepsilon < \varepsilon_c^{(2)} \), where \( \varepsilon_c^{(2)} < \varepsilon_F \) is the energy at which the open electron trajectories touch each other at the fixed DW wave vector (see Fig. A.1). Taking the integral in equation (25), one finds

\[ N = \nu_{in} \varepsilon_F - 4\pi \nu_{in} |r(\varepsilon_F)|^2 T \exp \left( -\frac{\pi T}{\hbar \omega_c} \right) \sin \left( \frac{\varepsilon_F}{\sigma} \right). \]  

(26)

Using equations (22) and (24), one finds the correction to the Fermi energy \( \delta \varepsilon_F = \varepsilon_F - \varepsilon_F^{(0)} \) in the form

\[ \delta \varepsilon_F = |r|^2 4\pi T \exp \left( -\frac{\pi T}{\hbar \omega_c} \right) \sin \left( \frac{\varepsilon_F}{\sigma} \right). \]  

(27)

In the right-hand side of the above equation, all the quantities are taken at \( \varepsilon = \varepsilon_F^{(0)} \). Using equation (27) and neglecting terms of the order of \( |r|^2 \hbar \omega_c/\varepsilon_F^{(0)} \), one finds a correction to the thermodynamical potential of electrons caused by the arising of the DW in the form:

\[ (\delta \Omega)_{T,\varepsilon_F^{(0)}} = N_0(\varepsilon_F^{(0)}) |r|^2 4\pi T \exp \left( -\frac{\pi T}{\hbar \omega_c} \right) \sin \left( \frac{\varepsilon_F}{\sigma} \right). \]  

(28)

Using equation (28), and taking into account that a correction to the free energy \( \delta F \) at constant \( T \) and \( n \) is equal to \( (\delta \Omega)_{T,\varepsilon_F^{(0)}} \) at constant \( T \) and \( \varepsilon_F^{(0)} \) (see, e.g., Ref. [11]), one finds change of the free energy per one particle:

\[ \delta F = |r|^2 4\pi T \exp \left( -\frac{\pi T}{\hbar \omega_c} \right) \sin \left( \frac{\varepsilon_F}{\sigma} \right) + \hbar \omega_c \Delta^2/2g^2. \]  

(29)

where the last term is the lattice elastic energy given by phonon frequency \( \omega \) at momentum \( Q \), \( g \) is the electron-phonon coupling constant, and \( \Delta \) is the energy gap produced in the electron spectrum by the DW in the absence of the magnetic field [12] (see Appendix A – Sect. A.1 for details of gap opening in the electron spectrum and DW potential matrix elements). As one can see from equation (29), the electronic part of the free energy is positive if \( |r|^2 \hbar \omega_c/|\varepsilon_F^{(0)}| > 0 \), meaning that the considered MB induced Peierls transition may take place only at magnetic fields for which \( S_x, y/\sigma < 0 \). Also, equation (29) shows that, due to the dependence of \( |r|^2 \) on the parameter \( a_1 \) (see Eq. (A.33)) emerging from the quantum-mechanical solution of the MB problem through the band-touching region (see Appendix A – Sect. A.4 and Eq. (A.18)), the largest (negative) energy gain for electrons is proportional to the largest value of parameter \( a_1 \). On the other hand, parameter \( a_1 \) depends on the electron energy as well as on the band configuration defined by the DW momentum through parameter \( \eta \) (the parameter \( \eta \) is given by Eq. (A.16), see also Fig. A.1),

\[ a_1 = 2^{2/3} \pi \text{Ai} \left( \frac{2^{2/3} \eta}{\pi} \right) \]  

(30)

where \( \text{Ai}(x) \) is an Airy function. As it follows from equation (30), \( a_1 \sim |\eta|^{-1/4} \) for \( |\eta| \gg 1 \), while \( a_1 \sim 1 \) for \( |\eta| \leq 1 \) (see Fig. 3). Therefore, the deformation momentum that stabilizes the DW is found from the condition \( \eta(Q_x, \varepsilon_F^{(0)}) = \eta_{\text{max}} \approx -0.65 \), and hence it is equal to

\[ Q_x = 2\nu_F \left( 1 - \eta_{\text{max}} \frac{1}{\varepsilon_F^{(0)}} \beta \right) - \frac{2}{\nu_F} \left( 2t_y - V_+ \right), \]  

(31)

where \( \beta = 2 \left( \pi^2 t_y/t_x \right)^{1/3} \cos^{-1} \left( \frac{\hbar \nu_F}{|Q_x|} \right) \) is a parameter appearing due to the anisotropy of the band (see Appendix A – Sect. A.2, Eq. (A.17)), which is in the case of quater-filled Bechgaard salts of the order of 1. The size of the pocket \( S_{\text{small}} \) is also determined by \( \eta_{\text{max}} \). Taking this value of the deformation momentum \( Q_x \) and using equation (A.33), one finds that the probability of MB reflection is

\[ |r|^2 = \frac{\Delta^2}{\beta^2 (\hbar \omega_c)^{4/3} x^{2/3}} \left( 1 - \frac{\Delta^2}{\beta^2 (\hbar \omega_c)^{4/3} x^{2/3}} \right), \]  

(32)
where $\Delta$ is an order parameter related to the off-diagonal matrix element of the DW potential, i.e., gap in the one-electron spectrum perturbed by the DW potential (see Appendix A, Sect. A.1, Eq. (A.11), $\Delta \equiv |V_{12}|$). Inserting it in equation (29) one obtains the free energy of the system expanded in terms of the order parameter $\Delta$:

$$
\delta F = \left[ \frac{28\pi T \exp(-\pi T/\hbar \omega_c) \sin(S_+/\sigma)}{2\pi g^2} \right]^2 \Delta^2 - \frac{\hbar \omega_Q}{g^2} \left[ \frac{28\pi T \exp(-\pi T/\hbar \omega_c) \sin(S_+/\sigma)}{\beta^4(\hbar \omega_c)^{4/3} e^{2/3} F} \right] \Delta^4.
$$

(33)

From here one finds the equation for the critical temperature $T_c$:

$$
\exp(\pi T_c/\hbar \omega_c) = \frac{56g^2}{\hbar \omega_Q \beta^2(\hbar \omega_c)^{1/3} e^{2/3} F} \left( -\sin \frac{S_+}{\sigma} \right) \times \Theta \left[ -\sin \frac{S_+}{\sigma} \right].
$$

(34)

Using equation (34) one may write the free energy of the system in terms of the order parameter $\Delta$ and the critical temperature $T_c$ of MB induced Peierls transition in the form:

$$
\delta F = \frac{\hbar \omega_Q}{g^2} \left\{ \frac{\pi(T - T_c)}{\hbar \omega_c} \Delta^2 + \frac{\Delta^4}{\beta^2(\hbar \omega_c)^{4/3} e^{2/3} F} \right\}.
$$

(35)

Based on equation (34), the critical temperature can be approximately written with the logarithmic accuracy as

$$
T_c \approx \frac{\hbar \omega_c}{\pi} \ln \left\{ \frac{56}{\beta^2} \left( \frac{\varepsilon_F}{\hbar \omega_c} \right)^{1/4} \left( -\sin \frac{S_+}{\sigma} \right) \right\}
$$

(36)

provided the expression under the logarithm is greater than 1. Here $\lambda = g^2/(\hbar \omega_Q \varepsilon_F)$ is the dimensionless electron-phonon coupling parameter (see Ref. [12]). The phase diagram of MBIDW, the dependence of the critical temperature on the inverse magnetic field, is shown in Figure 4. Its peculiar behavior in the inverse magnetic field, exhibiting periodic appearance and disappearance of ordered phases within normal conducting phase, opens the possibility of magnetic field controlled conducting state of the sample. It changes from the metallic state ($T_c = 0$) to a nearly isolating one ($T_c \neq 0$), thus changing the sample resistance by orders of magnitude by a small variation of magnetic field.

Finally we compare the present result with our previous work [2]. Previously we have fixed the wave vector of the DW to $(2\pi F, 0)$, making electron trajectories simply to cross each other, in order to explore the possibility of MBIDW condensation in the simplest case even in a non-optimal configuration in which the MB regions have no internal structure. By letting the DW wave vector vary and finding the optimal value, we came to the new band configuration, in which the trajectories nearly touch each other, when the novel MB probability for tunneling region with particular internal structure had to be calculated. We note that the reflection probability $|r|^2 \approx (\hbar \omega_c)^{-4/3} e^{2/3} F$ in the present configuration is multiplied by additional large parameter $(\varepsilon_F/\hbar \omega_c)^{1/3}$ in comparison to the standard expression for magnetic breakdown $|r|^2 \approx (\hbar \omega_c)^{-1} e^{-F}$ used previously for the case of electron tunneling through MB regions without internal structure (see the details in Appendix A – Sect. A.4, Eqs. (A.33)–(A.35)). Therefore, one needs proportionally lower magnetic field to achieve the same effect. Indeed, the expression for the critical temperature in the present case (36) contains the same large parameter under logarithm which defines $T_c^{\text{max}}$ thus rising it proportionally.

Regarding the experimental observation of the effect, it depends a lot on the quality of the sample. The longitudinal electric fields in the sample, i.e. dislocation fields, destroy quantum coherence of semiclassical wave packages thus deteriorating the MBIDW effect. The ad hoc criterion for the MB related effects, like the one that we predict, is usually the ability of the sample to exhibit de Haas van Alphen effect since it undergoes the same restrictions.

4 Conclusion

We have shown that system with an open Fermi surface under a homogeneous magnetic field $H$ is unstable with respect to a structural phase transition of a peculiar type, under which an open Fermi surface is transformed into a chain of large pockets separated with small ones having a strong band dispersion and playing the role of effective barriers between them. Quantum tunneling between the neighboring large pockets caused by the magnetic field (magnetic breakdown) transforms the electron spectrum into a series of alternating very narrow energy gaps and bands which decreases the energy of the electronic system that in its turn stabilizes the density wave. We have found that the optimal deformation momentum of the density wave has a completely “anti-nesting” character at which the shifted branches of the Fermi surface nearly touch each other. We have also shown that the phase diagram
containing the critical temperature of this magnetic breakdown induced phase transition $T_c(H^{-1})$ is nearly periodic in the inverse magnetic field, featuring a series of alternating narrow “MBIDW-windows” ($T_c \neq 0$) and gaps ($T_c = 0$). Comparing the present result with the previous one for simple $2pF, 0$ instability [2], that generates MB tunneling between neighboring pockets without peculiar band structure inbetween, we find that now the MB tunneling probability is enhanced by large factor $(\varepsilon_F/\hbar\omega_c)^{1/3}$ consequently leading to the proportionally lower magnetic field and higher critical temperature for the same MBIDW phase transition.

Appendix A: Dynamics of electrons under magnetic field near points of the topological transition in the electron spectrum

The conventional magnetic breakdown matrix [10] describes the situation in which the electron tunnels between two large pockets of different electron energy bands (interband tunneling). In this Appendix we analytically investigate the dynamics of electrons in the vicinity of the touching points of two classical trajectories (see Fig. 1) that is near the topological phase transition of $2\delta \frac{F}{F}$ order [13]. In this case the magnetic breakdown combines both the inter-band tunneling between neighboring large and small orbits and the intra-band one between neighboring large orbits that qualitatively changes the conventional magnetic breakdown matrix.

A.1 The band structure in the absence of magnetic field

In the two-dimensional case the electron energy band within the tight binding description can be written in the form:

$$\varepsilon(p) = -2t_x \cos \frac{ap_x}{\hbar} - 2t_y \cos \frac{bp_y}{\hbar},$$

(A.1)

where $p = (p_x, p_y)$ denotes electron momentum, $t_x, t_y > 0$ are electron transfer integrals and $a$, $b$ are lattice constants in $x$- and $y$-direction respectively with an energy origin taken in the middle of the band. Fermi surface, defined by $p_F^\pm(p_y)$, follows from the condition $\varepsilon[p_F^\pm(p_y), p_y] = \varepsilon_F$, where the Fermi energy $\varepsilon_F$ is determined by the number of available electrons filling the band. This surface includes two points $\pm p_F \equiv \pm p_F^+(p_y = h\pi/2b)$, that are roots of the expression $\varepsilon_F = -2t_x \cos(\alpha p_y/\hbar)$, where points $\pm p_F$ determine positions of two (“upper” and “lower”) strict Fermi planes in the case $t_y = 0$.

Now we assume $t_x \gg t_y$. This means that $p_F^+(p_y)$ will always be near $p_F$ or $-p_F$, and that we can expand the first term in (A.1) in terms of $p_F^+(p_y) \mp p_F$. With Fermi velocity given as

$$v_F = \frac{2at_x}{\hbar} \sin \frac{p_F a}{\hbar}, \quad (A.2)$$

one gets two sheets (“+” – upper, always close to $+p_F$, “−” – lower, always close to $-p_F$, in accordance with Fig. 1) representing the open Fermi surface:

$$p_{x,\pm}^+(p_y) = \pm p_F^+ \pm \frac{2t_x}{v_F} \cos \frac{bp_y}{\hbar}. \quad (A.3)$$

The “iso-energetic” sheets for energies $\varepsilon$ around $\varepsilon_F$ are given by

$$p_{x,\pm}^\pm(p_y) = \pm p_F \pm \frac{\varepsilon - \varepsilon_F}{v_F} \pm \frac{2t_y}{v_F} \cos \frac{bp_y}{\hbar}. \quad (A.4)$$

Without periodic perturbation, the momentum $p$, i.e. each pair $(p_x, p_y)$ of its components, is a good quantum number. We denote the wave functions by $\varphi^\pm_{\varepsilon} (r)$. The corresponding eigen-energies are

$$\varepsilon_{\pm}(p) = \varepsilon_F \pm v_F(p_x \mp p_F) - 2t_y \cos \frac{bp_y}{\hbar}. \quad (A.5)$$

for $p_x$ close to $\pm p_F$.

In the presence of a density wave, the Schrödinger equation with perturbation is

$$\left( \tilde{H}_0 + V(x) \right) \psi(r) = E\psi(r), \quad (A.6)$$

where $\tilde{H}_0$ is the Hamiltonian of a conduction electron in the unperturbed crystal discussed above. As assumed in the main text, the DW modulation potential $V(x)$, periodic with momentum $Q$, shifts the branches of the Fermi
surface and forms the touching points (see Fig. 1) which are the subject of analysis in this Appendix. Since the perturbation couples states from “+" and “–" sheets of the Fermi surface, $Q_x$ should be close to $2p_F$, deviating from it on the scale $t_F/v_F$. $V(x)$ is presumably dependent on $x$ only, also it is relatively weak with respect to the bandwidth parameters $v_Fp_F$ and $t_F$, therefore it can be treated as a perturbation to the Hamiltonian $\hat{H}_0$ outside the range of these touching points. Within this range we perform the standard diagonalization procedure for two (almost) degenerate states. The corresponding wave functions for these states are $\varphi_1 \equiv \langle \varphi^\pm_{p_x} | \varphi_p \rangle (r)$ and $\varphi_2 \equiv \langle \varphi^+_p | \varphi^\mp_{p_x} \rangle (r)$, where $p_x$ is defined in the main text, equation (2). The sought-for wave functions $\Psi$ near the degeneracy points in Figure 1 can be written as linear combinations

$$\Psi = \beta_1 \varphi_1 + \beta_2 \varphi_2. \quad (A.7)$$

Inserting $\Psi$ into equation (A.6), multiplying the resulting equation by $\varphi^\dagger$ and then by $\varphi_+^\dagger$ and integrating, one obtains the following set of equations for two branches $s = 1, 2$ in the the energy spectrum, $E_s(p)$, and corresponding coefficients $\beta_s$:

$$\begin{align*}
(\varepsilon_1 + V_{11} - E)\beta_1(p) + V_{12}\beta_2(p) &= 0 \\
V_{12}\beta_1(p) + (\varepsilon_2 + V_{22} - E)\beta_2(p) &= 0.
\end{align*} \quad (A.8)$$

Here we define $\varepsilon_s \equiv \varepsilon - (p_x - Q_x, p_y)$, $\varepsilon_2 \equiv \varepsilon - (p_x, p_y)$ and $V_{ss'} \equiv \langle \varphi_s | V(x) | \varphi_{s'} \rangle$ are matrix elements of the perturbing potential. Using the spectrum $\langle A.5 \rangle$, after a convenient shift of momentum origin $p_x \to p_x + Q_x/2$, $p_y \to p_y + b^*/2$ (to the trajectory-touching point), we obtain

$$\varepsilon_{1,2}(p) = \varepsilon_0 + v_F p_x - 2t_y \left(1 - \cos \frac{b p_y}{h}\right), \quad (A.9)$$

where

$$\varepsilon_0 \equiv \varepsilon_F - v_F p_F + v_F Q_x/2 + 2t_y. \quad (A.10)$$

From equation (A.8) it follows that the eigenvalues of the total Hamiltonian $\hat{H}$ (Eq. (A.6)) in the vicinity of the degeneracy points are

$$E_{1,2}(p) = \varepsilon_0 + V_+ - \alpha p_y^2 + \sqrt{(v_F p_x + V_+)^2 + |V_{12}|^2}, \quad \alpha = \frac{t_y b^2}{h^2}, \quad V_\pm \equiv \frac{1}{2}(V_{22} \pm V_{11}), \quad (A.11)$$

with $m^*_\sigma$ has the role of a dynamic effective electron mass in the transverse direction, obtained after expanding $\varepsilon_{1,2}(p)$ near the touching point $(p_x, p_y)$ = $(p_F - 2t_y/v_F, b^*/2)$ (now shifted to the momentum space origin), i.e. $\varepsilon_{1,2} \approx \varepsilon_0 + v_F p_x - \alpha p_y^2$. The eigenvalues $E_{1,2}(p)$ are two new electron energy bands separated by an energy gap $\Delta = |V_{12}|$. An investigation of equation (A.11) shows that there are two peculiar points $\varepsilon_{1,2}^\pm = \varepsilon_0 + V_\pm + |V_{12}|$ in the new electron dispersion law at which the equipotential surfaces $E_{1,2}(p_x, p_y) = \varepsilon$ change their topology (see Fig. A.1).

### A.2 Magnetic breakdown through the band-touching region

The Hamiltonian of a conduction electron in a metal under magnetic field in the coordinate representation is

$$\hat{H}(\vec{p} - \frac{\mathbf{e}}{c} \mathbf{A}(r), \mathbf{r})$$

where $\hat{H}(\vec{p}, \mathbf{r})$ is the electron Hamiltonian in the absence of magnetic field, $\mathbf{p} = -i\hbar \partial / \partial r$ is the electron momentum operator and $\mathbf{A}$ is the vector potential.

In the momentum presentation, Lifshitz and Kosevich [6] and Onsager [7] suggested the conduction electron Hamiltonian in the form equation (5), in which the electron quasi-momentum $\mathbf{p}$ in the electron dispersion law $\varepsilon_s(\mathbf{p})$ is substituted with $\mathbf{p} - (e/c)\mathbf{A}$, where the gauge potential is chosen in the Landau gauge, i.e. $\mathbf{A} = (-\mathbf{H} \mathbf{y}, 0, 0)$. As it was proved by Zilberman [14], one gets the Onsager-Lifshitz Hamiltonian, in the case when the band number is conserved, by using the complete orthonormal set of modified Bloch functions $\chi_{s,p}(r) = e^{i\mathbf{p} \mathbf{r}} \chi_s(r) + e^{i\mathbf{H} \mathbf{y} \mathbf{r}} \chi_s(r)$, where $\chi_s(r)$ are the periodic function. Such functions are called the Zilberman functions.

As it was shown in references [8,9], in the region of magnetic breakdown, where the band number is not conserved, one gets the Hamiltonian by expanding the electron wave function $\Psi(r)$ in the form $\Psi(r) = \sum_{s=1}^{2} \int dp_g(s) \chi_{s,p}(r)$ resulting in the above-mentioned substitution in equation (A.8):

$$\begin{align*}
\left(\varepsilon_1 + i\sigma \frac{d}{dp_y}, p_y + V_{11} - E\right) g_1(p) + V_{12} g_2(p) &= 0 \\
V_{12} g_1(p) + \left(\varepsilon_2 + i\sigma \frac{d}{dp_y}, p_y + V_{22} - E\right) g_2(p) &= 0
\end{align*} \quad (A.13)$$

where $\sigma = e c H/c$, $V_{ss'} = \langle \chi_s | V(r) | \chi_{s'} \rangle$ and $\mathbf{P}_0$ is conserved longitudinal electron momentum due to the chosen Landau gauge. Introducing expression (A.9) and expansion around the touching point as in previous section, then summing and subtracting the equations in (A.13), leads us to system

$$\begin{align*}
iv_F \frac{d g_1^{(-)}(p_y)}{d p_y} + (-\alpha p_y^2 + \varepsilon^{(1)} - E) g_1^{(+)}(p_y) &= 0 \\
iv_F \frac{d g_2^{(+)}(p_y)}{d p_y} + (-\alpha p_y^2 + \varepsilon^{(2)} - E) g_2^{(-)}(p_y) &= 0
\end{align*} \quad (A.14)$$

with $V_{12} = |V_{12}| e^{i\theta}$ and $g^{(\pm)} = g_2 \pm g_1$, $g_1, g_2(p) \equiv \exp| -\frac{i}{2} (P_{0x} + \frac{V_{12}}{2}) p_y + \frac{1}{2} \mathbf{g}_1, g_2(\mathbf{p}) \equiv \exp| -i (\varepsilon^{(3)}/3 + \eta \xi) + u_2(\xi) \exp -i (\varepsilon^{(3)}/3 + \eta \xi) \equiv u_1(\xi)$. System (A.14) reduces to:

$$\begin{align*}
i \frac{d u_1(\xi)}{d \xi} &= -\gamma c^{-1}(\xi^{2} + 2\eta) u_2(\xi) \\
i \frac{d u_2(\xi)}{d \xi} &= \gamma c^{i}(\xi^{2} + 2\eta) u_1(\xi),
\end{align*} \quad (A.15)$$
where \( \omega_b \equiv \frac{dU}{m^*_b} \), \( \kappa \equiv \hbar \omega_y/\epsilon_b \), while \( \epsilon_b = m^*_b v^2_F/2 \) is of the order of Fermi energy, and two emerging parameters are defined as:

\[
\gamma = -\frac{|V_{12}|}{\beta(\hbar \omega_c)^{2/3} \xi_{1/3}^{1/3}} \\
\eta = -\frac{\epsilon_0 + V_{ss} - \epsilon}{\beta(\hbar \omega_c)^{2/3} \xi_{1/3}^{1/3}},
\]

with

\[
\beta \equiv \left( \frac{\omega_y}{\omega_c} \right)^2 \frac{\epsilon_b}{\hbar \omega_y} \left( \frac{\pi^2 t_y}{t_x} \right)^{1/2} \frac{2}{\cos(\alpha_F)}.
\]

In the case of quarter-filled Bechgaard salts parameter \( \beta \approx 0.7 \) is of the order of 1. Parameter \( \gamma \), that mixes functions \( u_1 \) and \( u_2 \), appears as a magnetic breakdown parameter, while \( \eta \) gives criterion of validity of semiclassical description, i.e. as long as \( |\eta| \lesssim 1 \) and \( |\xi| \lesssim 1 \), the full quantum treatment is required because the functions in equation (A.15) are not fast oscillating. We should note the difference between this case and conventional magnetic breakdown problem in metals when semiclassical approximation is valid as long as the area of closed electron orbit in \( p \)-space is much bigger than \( \sigma \). Here much wider area than just small closed electron orbit in Figure A.1e requires the quantum treatment. Parameter \( |\gamma| \ll 1 \) is required to be small in our approach consequently permitting us to build a perturbation theory \( u = u^{(0)} + \gamma u^{(1)} + \gamma^2 u^{(2)} + \ldots \) in order to solve the system (A.15). The asymptotic boundary conditions, i.e. the requirement of matching \( u(x) \) to semiclassical solutions in the limit \( \xi \to \pm \infty \), will be determined in the next section. Integrating the system (A.15) we get \( u(-\infty) = u^{(0)}(0) \) and \( u(\infty) = \hat{T} u^{(0)} \), where \( \hat{T} \) is unitary matrix with elements \( T_{11} = 1 + \gamma^2 a_2 \), \( T_{12} = i\gamma a_1 \), with coefficients given by:

\[
\begin{align*}
\alpha_1 &\equiv \int_{-\infty}^{\infty} e^{-i(2y^3/3 + 2\eta y)} \, dx = 2^{2/3}\pi \text{Ai} \left( 2^{2/3} \eta \right) \\
\alpha_2 &\equiv \int_{-\infty}^{\infty} e^{-i(2y^3/3 + 2\eta y)} \, dx = \int_{-\infty}^{\infty} e^{-i(2y^3/3 + 2\eta y)} \, dy,
\end{align*}
\]

where \( \text{Ai}(x) \) is an Airy function. In terms of \( u(\infty) \) we obtain

\[
\hat{g}_{1,2} (\xi) \equiv u_{1,2} (\infty) e^{\pm i \left( \frac{\xi}{2} + \eta \xi \right)}
\]

in the limit \( |\xi| \gg 1 \). From expressions (A.19), one easily gets starting coefficients

\[
\begin{align*}
g_{1,2} &\approx \frac{1}{\sqrt{2\pi}} u_{1,2} (\infty) e^{\pm i \left( \frac{1}{2} |P_{ss}| + \frac{1}{2} \right)} e^{\pm i \left( \frac{\xi}{2} + \eta \xi \right)}
\end{align*}
\]

with redefined parameters

\[
\eta_s \equiv -\frac{\epsilon_0 + V_{ss} - \epsilon}{\beta(\hbar \omega_c)^{2/3} \xi_{1/3}^{1/3}}
\]

into which we have absorbed dependency on \( V \)-matrix elements. Factor \( v^2_F \) additionally appears due to normalization of electron current density to 1. Note that \( |\xi| \gg 1 \) corresponds to \( m^*_b v^2 F_{1/3} \ll |p_y| \ll m^*_b v_F \) where it is possible to expand the transversal electron dispersion up to square contribution \( \alpha \omega_y^2 \) used in the equations above. That limit gives the quantum mechanical description of the region in which the quantum MB transitions are absent, but which still overlaps with the semiclassical description (next section). There the matching of quantum and semiclassical solution is done.

### A.3 The semiclassical solution

Since magnetic breakdown transitions are absent in the region \( |\xi| \gg 1 \), both \( u(\xi) \approx \text{const.} \), one may use Onsager-Lifshitz Hamiltonian in the form:

\[
E_s \left( P_{ss} + i\sigma \frac{d}{dp_y} p_y \right) G_s (p) = \epsilon G_s (p), \quad \text{(A.22)}
\]

where electron dispersion attain the form \( E_s (p) \approx \epsilon_s(p) + V_{ss} \) since we are far away from the band-touching point. Using the form of \( \epsilon_{1,2}(p) \) given by expression (A.9), one gets system of equations for \( G_{1,2} \):

\[
\begin{align*}
\sigma v_F \frac{dg_{1,2}}{dp_y} &\equiv \left[ -v_F P_{00} \pm \left( \epsilon_0 + V_{11,22} \right) \\
&- \epsilon - 2t_y \left( 1 - \cos \frac{b_p y}{h} \right) \right] G_{1,2}.
\end{align*}
\]

Equations in system (A.23) are not coupled and integration simply gives

\[
G_{1,2}(p) = \frac{C_{1,2}}{\sqrt{v_F}} e^{\pm i \left( \frac{P_{ss}}{v_F} + S_{1,2} (p) \right)},
\]

where \( S_{ss} (p_y) = \pm 2t_y + \frac{2m^*_b v_F^2 k^2/3}{G_{1,2} (p)} \) is semiclassical action, \( C_{1,2} \) are normalization constants and \( v_F^{-1/2} \) factor again appears due to normalization of electron current density to 1. In order to match the obtained semiclassical solutions to the quantum-mechanical solutions from previous chapter, we introduce variable \( \xi \) in the same way \( p_y = m^*_b v_F \xi \). Also, since \( m^*_b v_F \ll 1 \), we expand \( \sin \frac{b_p y}{h} \) in \( S_{ss} (p_y) \) within the semiclassical region \( 1 \ll |\xi| \ll \kappa^{-1/3} \) into Taylor series up to \( \sim \xi^3 \). This yields semiclassical solutions in the form

\[
G_{1,2}(p) = \frac{C_{1,2}}{\sqrt{v_F}} e^{\pm i \left( \frac{P_{ss}}{v_F} + S_{1,2} (p) \right)} e^{\pm i \left( \frac{\xi}{2} + \eta \xi \right)}.
\]

### A.4 Magnetic breakdown tunneling matrix

To match quantum to semiclassical solution, i.e. to match the coefficients \( g_{1,2} \) to \( G_{1,2} \), one more step is required. We should note that equation (A.22) for coefficients \( G_{1,2} \) is obtained using expansion of solution \( \psi(r) = \sum_{m,p} \int d^{3}g \mathcal{G}(m)(p) x_{m,p}(r) \) in terms of “total” Zilberman functions \( X_{m,p}(r) = e^{ipr} U_{m,p+eH_y/c_p_y}(r) \). This \( U(r) \) is
periodic, i.e. featuring the total Hamiltonian (A.6) with perturbation \( V(r) \). On the other hand, quantum solution, resulting with coefficients \( g_{1,2} \), is obtained using the expansion in terms of Zilberman functions \( \chi_{s,p}(r) \) corresponding to unperturbed Hamiltonian \( \hat{H}_0 \). In order to match two sets of coefficients, the expansion in the same set of Zilberman functions should be used, i.e. we expand \( X \) in terms of coefficients \( \epsilon^\gamma \Psi \), i.e.

\[
X \text{ in terms of set of Zilberman functions should be used, i.e. we expand}\]

\[
g_s(p) = \frac{2}{\pi} \beta_{s,m} \left( P_{x_0} + \frac{eHy}{c}, p_y \right) G_m(p). \tag{A.26}
\]

Comparison of two expansions for \( \Psi \) leads to connection between coefficients \( g_s(p) = \sum_{m=1}^{2} \beta_{s,m} \left( P_{x_0} + \frac{eHy}{c}, p_y \right) G_m(p) \). After utilizing the standard substitution as before \( \frac{eHy}{c} \rightarrow i\epsilon \frac{d}{dp_y} \) for deriving the Onsager-Lifshitz Hamiltonian, the previous expression reduces to set of differential equations for coefficients \( G_m \) in terms of given \( g_s \), i.e.

\[
g_s(p) = \frac{2}{\pi} \beta_{s,1} \left( P_{x_0} + \frac{i\epsilon \sigma d}{dp_y} \right) G_1(p) + \frac{2}{\pi} \beta_{s,2} \left( -\frac{dS}{dp_y}, p_y \right) G_2(p). \tag{A.27}
\]

Coefficients \( \beta_{s,m} \) are exactly obtained from the system (A.8) and after normalization they read: \( \beta_{11} \approx \sqrt{V_{12}/V_{12}}, \beta_{20} = \frac{1}{\sqrt{V_{12}/V_{12}}}, \beta_{20} \approx \frac{1}{\sqrt{V_{12}/V_{12}}}, \beta_{21} \approx \frac{1}{\sqrt{V_{12}/V_{12}}} \). After neglecting \( \beta_{21} \approx \frac{1}{\sqrt{V_{12}/V_{12}}} \) contributions in expression (A.27), we obtain equations for coefficients

\[
g_1(p) \approx e^{i\Phi} G_1(p), \quad g_2(p) \approx -ie^{-i\Phi} G_2(p) \tag{A.28}
\]

\((e^{i\Phi} = V_{12}/|V_{12}|) \) valid both in “left” \( (\xi \rightarrow \infty) \) and “right” \( (\xi \rightarrow \infty) \) semiclassical region. Using expression (A.28) we can match coefficients given by equations (A.20) and (A.25). Denoting the semiclassical normalization constants \( C_s \) from expression (A.25) in “left” region as \( C_4^{(I)} \) and in “right” region as \( C_4^{(II)} \), the matching conditions read

\[
C_4^{(I)} = u_1(0),
\]

\[
-ic_4^{(II)} = u_2(0),
\]

\[
C_4^{(II)} = (1 + \gamma^2 a_{12})u_1(0) + i\gamma a_{11}u_2(0),
\]

\[
-iC_2^{(II)} = (1 + \gamma^2 a_{22})u_2(0) - i\gamma a_{11}u_1(0).
\]

Finally, from system (A.29), we obtain connection between the incoming and outgoing waves through the MB region (see Fig. 2)

\[
\begin{pmatrix}
C_4^{(I)} \\
C_4^{(II)}
\end{pmatrix} = \hat{T}
\begin{pmatrix}
C_4^{(I)} \\
C_4^{(II)}
\end{pmatrix} \tag{A.30}
\]
given in terms of MB tunneling matrix

\[
\hat{T} = e^{i\theta} \begin{pmatrix}
t & r \\
-r^* & t
\end{pmatrix} \tag{A.31}
\]

where

\[
t = 1 - \frac{1}{2} \gamma^2 |a_{11}|^2, \quad r = -\gamma a_{11} \tag{A.32}
\]

define the tunneling probabilities of transmission through and reflection at the MB region, respectively. The corresponding phase is \( \theta = -\gamma^2 \text{Im}(a_{11}), \) all given up to \( \gamma^2 \) accuracy. The main result of the paper is expressed in terms of \( |r|^2 \) which we need up to \( \gamma^4 \) accuracy. After a tedious, but quite straightforward procedure analogous to the one presented above, one obtains

\[
|r|^2 \approx |a_{11}|^2 \gamma^2 (1 - \gamma^2), \tag{A.33}
\]

where \( a_{11} \) and \( \gamma \) are defined by equation (A.18) and equation (A.16), respectively. We have obtained equation (A.33) by solving the set of equations (A.13) in the region where the semiclassical approximation is not valid, using the perturbation theory in \( |\gamma| < 1 \) and then using an asymptotic form of this solution to match semiclassical wave functions on the neighboring large orbits. Following from equation (A.18), one gets \( a_{11} \sim 1 \) for \( |\eta| \sim 1 \) and

\[
|r|^2 \approx \frac{|V_{12}|^2}{\beta^2 h\omega_c e_F}. \tag{A.34}
\]

Also, one can see from equations (A.15) and (A.16), if \( |\eta| \gg 1 \) (achievable either by increasing the energy or further increase of DW vector \( Q_y \)), the small orbits in Figure A.1e become semiclassically large and magnetic breakdown occurs in the small areas \( \sim \sigma \) between them and the large neighboring orbits. However, for \( |\eta| \gg 1 \), one has \( a_{11} \propto |\eta|^{-1/4} \), consequently getting from equation (A.33) the standard expression for the MB reflection probability

\[
|r|_{\text{std}}^2 \approx \frac{\pi |V_{12}|^2}{(\sigma v_0 v_{10})^2} \sim \frac{|V_{12}|^2}{h\omega_c e_F}. \tag{A.35}
\]

where \( v_0 \) is the electron velocity in the MB region. Comparing expressions (A.34) and (A.35) shows that our configuration yields additional large parameter comparing to the standard situation, i.e. \( |r|^2 = |r|_{\text{std}}^2 (\varepsilon_F/h\omega_c)^{1/3} \), meaning that proportionally lower magnetic field is now required to achieve the same effect.

**Appendix B: Fourier series expansion of the density of states**

The right-hand side of equation (20) is a periodic function of the phase \( \Phi \) and hence it can be expanded in a Fourier series

\[
\nu(E) = \frac{2}{(2\pi\hbar)^2} \sum_{k=-\infty}^{+\infty} A_k e^{ik\Phi(E)}, \tag{B.1}
\]
where the Fourier coefficients are

\[ A_k = \int_{-\pi}^{\pi} e^{-ik\phi} \sin \phi |\Theta(|t|^2 - \cos^2 \phi)\frac{d\phi}{\sqrt{|t|^2 - \cos^2 \phi}} \frac{1}{2\pi}. \]  

(B.2)

Reducing the interval of integration to (0, \pi), one finds

\[ A_k = (1 + (-1)^k) \int_{0}^{\pi} e^{-ik\phi} \sin \phi |\Theta(|t|^2 - \cos^2 \phi)\frac{d\phi}{\sqrt{|t|^2 - \cos^2 \phi}} \frac{1}{2\pi}. \]  

(B.3)

that is only even Fourier harmonics with \( k = 2l, l = 0, \pm 1, \pm 2, \ldots \) are not equal to zero: \( A_{2l} \neq 0, A_{2l+1} = 0. \)

Using the equality

\[ \cos 2l\phi = \sum_{p=0}^{l} C_{2p}^l (-1)^{l-p} \cos^{2p} \phi \sin^{2(l-p)} \phi, \]  

(B.4)

after rather simple transformation one finds

\[ A_{2l} = A_{-2l} = 2 \frac{l}{\pi} \sum_{p=0}^{l} C_{2p}^l (-1)^{l-p} J_p^{(l)}, \quad l = 0, 1, 2, \ldots \]  

(B.5)

where

\[ J_p^{(l)} = |t|^2 p \int_{0}^{1} x^{2p} \frac{1 - |t|^2 x^2}{\sqrt{1 - x^2}} \frac{1}{x} dx. \]  

(B.6)

In particular, from here and equation (B.5) it follows that

\[ A_0 = 1, \quad A_2 = |t|^2 - 1 = -|r|^2. \]  

(B.7)

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