Non-Fermi-liquid magic angle effects in high magnetic fields

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Non-Fermi-Liquid Magic Angles Effects

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We investigate a theoretical problem of electron-electron interactions in an inclined magnetic field in a quasi-one-dimensional (Q1D) conductor. We show that they result in strong non-Fermi-liquid corrections to a specific heat, provided that direction of a magnetic field is far from the so-called Lebed's Magic Angles (LMA). If magnetic field is directed close to one of the LMA, the specific heat corrections become small and the Fermi-liquid picture restores. As a result, we predict Fermi-liquid - non-Fermi-liquid angular crossovers in the vicinities the LMA directions of the field. We suggest to perform the corresponding experiment in the Q1D conductor $(Per)_2Au(mnt)_2$ under pressure in magnetic fields of the order of $H \simeq 20\ T$.

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It is well known that closed electron orbits in a magnetic field in metals are characterized by the de Haas-van Alphen and Shubnikov-de Haas quantum oscillations [1]. For open orbits, the Landau quantization is not possible and another quantum effect - the Bragg reflection from boundaries of the Brillouin zone - play an important role [2-4]. In particular, it has been shown [5-8] that the latter effect results in the appearance of angular magnetic oscillations, such as the so-called Lebed's Magic Angles (LMA), Danner-Kang-Chaikin's (DKC) oscillations, and Lee-Naughton-Lebed's (LNL) ones. It is important that the DKC and LNL oscillations are well explained within the Fermi liquid approach to open quasi-one-dimensional (Q1D) pieces of the Fermi surface in the Q1D conductors $(TMTSF)_2X$ (X=ClO_4, PF_6, etc.), $(DMET)_2I_3$ and some others [6-8,4]. On the other hand, in many cases, the LMA phenomena are experimentally claimed [9-13] to be of the non-Fermi-liquid nature. This was claimed by Chaikin's group for the Nernst effect in the $(TMTSF)_2PF_6$ [9,10,12], by Brooks' group - for the Nernst effect in the $(TMTSF)_2ClO_4$ [11], and recently by Uji's group [13] - for the Hall effect in the $(TMTSF)_2ClO_4$. In our opinion, some non-Fermi-liquid effects were also observed in the LMA resistive experiments in the Q1D compound $(Per)_2Au(mnt)_2$ by D. Graf et al. [14].

The first non-Fermi-liquid theory of the LMA phenomenon was suggested in Ref. [15]. In particular, we showed [15] that an inverse electron-electron scattering time increased at the LMA directions of a magnetic field due to some commensurability effects in "one-dimensionalizied" electron spectrum in a Q1D conductor, resulting from the Bragg reflections. Yakovenko first studied the same "commensurability" effects in several thermodynamic properties of a Q1D conductor [16], including specific heat (see also Refs.[17,18]). Note that the physical conclusion of the work [16] was similar to that of Ref.[15] that a Q1D metal became more 1D at the LMA directions of the field. There are two main goals of the current Rapid Communication. First one is that we consider the case of high magnetic fields and make conclusion that, at directions of the magnetic field far from one of the LMA, the corrections to specific heat from electron-electron interactions are strong and, thus, we expect to have some kind of non-Fermi-liquid. The second our goal is to show that, at the LMA directions of a magnetic field, Q1D system become 2D one and, thus, the discussed above corrections become small. Therefore, Fermi-liquid restores in the near vicinity of the LMA directions. As a result, in a tilted magnetic field, we expect non-Fermi-liquid - Fermi-liquid angular crossovers. This result is opposite to the previous statements of Refs.[15-17], since below we make use of more realistic model of a Q1D spectrum. Note that very recently we have suggested non-Fermi-liquid - Fermi-liquid crossovers in a Q1D conductor [19]. There are two crucial difference between the current work and Ref.[19]. First, the LMA phenomenon has not been considered in Ref. [19]. Second, in Ref.[19], we have considered transport property - an inverse electron-electron scattering time.

Let us first consider a simplified Q1D electron spectrum, used in Refs.[15-17,19],

$$\epsilon(\mathbf{p}) = \pm v_F(p_x \mp p_F) - 2t_y \cos(p_y a_y) - 2t_z \cos(p_z a_z), \tag{1}$$

in a magnetic field, inclined in $(\mathbf{y}, \mathbf{z})$ plane:

$$\mathbf{H} = (0, \sin\alpha, \cos\alpha)H, \ \ \mathbf{A} = (0, -\cos\alpha, \sin\alpha)Hx, \tag{2}$$

where $v_F p_F \gg t_y, t_z$. Then, by using the Peierls substitution method for open electron spectrum [2], $\mathbf{p} \to \mathbf{p} - (\frac{e}{c})\mathbf{A}$, we come to the following Schrödinger-like equations:

$$\left\{\mp i v_F \frac{d}{dx} - 2t_y \cos\left[p_y a_y - \frac{\omega_y(\alpha)}{v_F}x\right] - 2t_z \cos\left[p_z a_z + \frac{\omega_z(\alpha)}{v_F}x\right]\right\}\phi_\epsilon^\pm(x; p_y, p_z) = \epsilon\ \phi_\epsilon^\pm(x; p_y, p_z), \tag{3}$$

where e and c are the electron charge and the velocity of light, correspondingly; energy ϵ is counted from the Fermi level. It is important that Eq.(3) can be exactly solved,

$$\phi_{\epsilon}^{\pm}(x;p_y,p_z)=\exp\left(\frac{\pm i\epsilon x}{v_F}\right)\exp\left\{\mp il_y(\alpha)\left(\sin\left[p_ya_y-\frac{\omega_y(\alpha)}{v_F}x\right]-\sin[p_ya_y]\right)\right\}\exp\left\{\pm il_z(\alpha)\left(\sin\left[p_za_z+\frac{\omega_z(\alpha)}{v_F}x\right]-\sin[p_za_z]\right)\right\}, \tag{4}$$

where

$$\omega_y(\alpha)=\frac{ev_Fa_yH\cos\alpha}{c},\ \omega_z(\alpha)=\frac{ev_Fa_zH\sin\alpha}{c} \tag{5}$$

and

$$l_y(\alpha)=\frac{2t_y}{\omega_y(\alpha)},\ l_z(\alpha)=\frac{2t_z}{\omega_z(\alpha)}. \tag{6}$$

It is easy to prove that at high enough magnetic fields directed far from $\mathbf{y}$ and $\mathbf{z}$ axes, where

$$H\geq H^*=\max\left\{\frac{2t_yc}{ev_Fa_y\cos\alpha}\ ,\frac{2t_zc}{ev_Fa_z\sin\alpha}\right\}\ , \tag{7}$$

wave functions (4) become almost 1D since $l_y(\alpha),l_z(\alpha)\leq 1$.

Let us consider the following more realistic Q1D electron spectrum, which takes into account additional possibilities for electron jumping in $(\mathbf{y},\mathbf{z})$ plane:

$$\begin{aligned}\epsilon(\mathbf{p})=&\pm v_F(p_x\mp p_F)-2t_y\cos(p_ya_y)-2t_z\cos(p_za_z)\\&-2t\cos(p_ya_y+p_za_z)-2t\cos(p_ya_y-p_za_z),\end{aligned} \tag{8}$$

where $t<t_y,t_z$ is overlapping of electron wave functions along the following LMA directions

$$\tan[\alpha_{(1,1)}]=\frac{a_y}{a_z} \tag{9}$$

and

$$\tan[\alpha_{(1,-1)}]=-\frac{a_y}{a_z}. \tag{10}$$

By making use of the Peierls substitution method, the corresponding Schrödinger-like equation in this case can be written as

$$\begin{aligned}&\left\{\mp iv_F\frac{d}{dx}-2t_y\cos\left[p_ya_y-\frac{\omega_y(\alpha)}{v_F}x\right]-2t_z\cos\left[p_za_z+\frac{\omega_z(\alpha)}{v_F}x\right]-2t\cos\left[p_ya_y+p_za_z-\frac{\omega_y(\alpha)-\omega_z(\alpha)}{v_F}x\right]\right.\\&\left.-2t\cos\left[p_ya_y-p_za_z-\frac{\omega_y(\alpha)+\omega_z(\alpha)}{v_F}x\right]\right\}\\&\times\psi_{\epsilon}^{\pm}(x;p_y,p_z)=\epsilon\ \psi_{\epsilon}^{\pm}(x;p_y,p_z),\end{aligned} \tag{11}$$

It is possible to prove that Eq.(11) has the following solutions:

$$\begin{aligned}\psi_{\epsilon}^{\pm}(x;p_y,p_z)=&\exp\left(\frac{\pm i\epsilon x}{v_F}\right)\exp\left\{\frac{\mp 2it}{\omega_y(\alpha)-\omega_z(\alpha)}\right.\\&\left.\times\left(\sin\left[p_ya_y+p_za_z-\frac{\omega_y(\alpha)-\omega_z(\alpha)}{v_F}x\right]-\sin[p_ya_y+p_za_z]\right)\right\}\exp\left\{\frac{\mp 2it}{\omega_y(\alpha)+\omega_z(\alpha)}\left(\sin\left[p_ya_y-p_za_z+\frac{\omega_y(\alpha)+\omega_z(\alpha)}{v_F}x\right]-\sin[p_ya_y-p_za_z]\right)\right\}\phi_{\epsilon}^{\pm}(x;p_y,p_z),\end{aligned} \tag{12}$$

where $\phi_{\epsilon}^{\pm}(x;p_y,p_z)$ are given by Eq.(4).

Let us consider the case of high magnetic field (7), inclined far from the main crystallographic axes **y** and **z**. Then, all contributions to wave functions (12) are almost 1D with the exception of

$$\Psi(x;p_y,p_z)=\exp\left(\frac{\pm i\epsilon x}{v_F}\right)\exp\left\{\frac{\mp 2it}{\omega(\alpha)}\left(\sin\left[p_y a_y +p_z a_z-\frac{\omega(\alpha)}{v_F}x\right]-\sin[p_y a_y+p_z a_z]\right)\right\}, \tag{13}$$

where $\omega(\alpha)=\omega_y(\alpha)-\omega_z(\alpha)$ and $\alpha>0$. Note that, in this Rapid Communication, we calculate specific heat in the vicinity of the LMA (9), i.e. at

$$|\delta\alpha|\ll 1,\quad \delta\alpha=\alpha-\alpha_{(1,1)}\ . \tag{14}$$

Therefore, below we will consider Eq.(13) as effective electron wave functions in a high magnetic field.

Let us qualitatively discuss the effective wave functions (13) behavior with changing direction of a magnetic field from the LMA direction (9) and how this results in Fermi-liquid - non-Fermi-liquid angular crossovers. If direction of a magnetic field exactly coincides within the LMA (9), then it is easy to show from Eq.(13) that effective electron wave functions become the following:

$$\Psi(x;p_y,p_z)=\exp\left(\frac{\pm i\epsilon x}{v_F}\right)\times\exp\left[\frac{\pm i4tx}{v_F}\cos\left(p_y a_y+p_z a_z-\frac{\omega_y-\omega_z}{2v_F}\right)\right]. \tag{15}$$

Note that in Eq.(15), we can shift electron momentum inside function cos(...) and obtain 2D wave functions, which do not depend on a magnetic field,

$$\Psi(x;p_y,p_z)=\exp\left(\frac{\pm i\epsilon x}{v_F}\right)\times\exp\left[\frac{\pm i4tx}{v_F}\cos(p_y a_y+p_z a_z)\right], \tag{16}$$

and which are characterized by a pure 2D electron spectrum:

$$\epsilon(\mathbf{p})=\pm v_F(p_x\mp p_F)-2t\cos(p_y a_y+p_z a_z). \tag{17}$$

[Note that, physically, 2D wave functions (16), independent of a magnetic field, come from the fact that electron momentum component for spectrum Eq.(8) is conserved when magnetic is applied along the LMA (9).] For 2D electrons (17), we expect Fermi-liquid behavior. As shown later it corresponds to small corrections to electron specific heat from electron-electron interactions. On the other hand, if a magnetic field is applied not close to the LMA direction (9) (i.e., $|\delta\alpha|\gg 2t/\omega\ll 1$), then effective wave functions (13) becomes pure 1D and we expect non-Fermi-liquid behavior. Below, it is shown that the latter situation corresponds to the appearance of corrections to electron specific heat due to electron-electron interactions of the order of a specific heat of free electrons.

Since the effective electron wave functions are known (13), we can define Matsubara's finite temperature Green's functions by means of the following standard formula [20]:

$$G^{\pm}(x,x_1;p_y,p_z)=\sum_{\epsilon}\frac{\Psi^{\pm}(x,;p_y,p_z)\left[\Psi^{\pm}(x_1;p_y,p_z)\right]^{*}}{i\omega_n-\epsilon}, \tag{18}$$

where $\omega_n=2\pi T(n+1/2)$ is the so called Matsubara frequencies. As a result of straightforward calculations, we obtain

$$G^{\pm}(x,x_1;p_y,p_z)=\frac{-i\ sgn(\omega_n)}{v_F}\exp\left[\pm\frac{\omega_n(x-x_1)}{v_F}\right]\exp\left\{\frac{\mp 2it}{\omega(\alpha)}\left[\sin\left(p_y a_y+p_z a_z-\frac{\omega(\alpha)x}{v_F}\right)-\sin\left(p_y a_y+p_z a_z-\frac{\omega(\alpha)x'}{v_F}\right)\right]\right\} \tag{19}$$

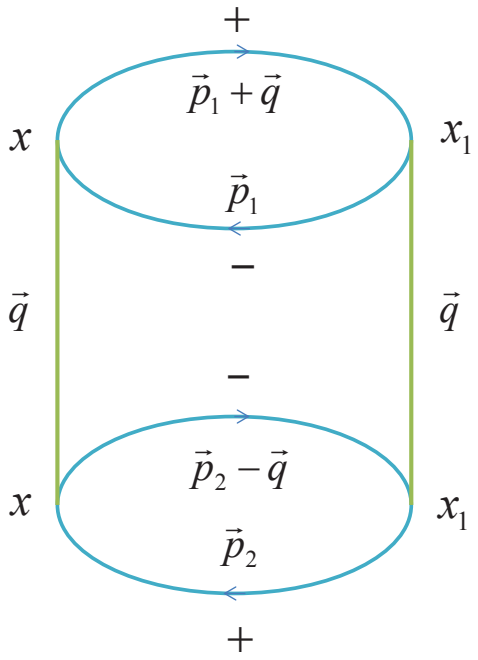

FIG. 1: One of the Feynman's diagrams, corresponding to the lowest order corrections to electron free energy from electron electron interactions. Solid lines with arrows stand for electron Green's functions, whereas solid lines without arrows represent electron electron interactions. All electrons have the same spin projection on a magnetic field.

for $\pm\omega_n(x-x_1)<0$.

Below, let us calculate the lowest order corrections to electron free energy, resulting from electron-electron interactions. Note that there are several corresponding Feynman's diagrams. One of them is shown in Fig.1, where (+) and (−) correspond to electrons from right and left pieces of the Q1D Fermi surface (8), respectively. There are two types of the diagrams: (a) without the paramagnetic Pauli term, corresponding to spin splitting in a magnetic field, and (b) with the paramagnetic term. We have proved that the diagram without the Pauli term give maximal corrections to electron specific heat. Therefore, below we calculate free energy correction, resulting from such diagrams with one of them being shown in Fig.1. If we consider δ^3-function electron-electron interactions, it is possible to demonstrate that the corresponding correction to free energy per one electron is

$$\Delta F(\alpha)=-\frac{\pi^3 g^2 T^3}{p_F v_F}\int_{1/\epsilon_0}^{\infty} dx\ \frac{\cosh(2\pi T x)}{\sinh^3(2\pi T x)}\ J(x,\alpha), \tag{20}$$

where

$$J(x,\alpha)=\int_0^{2\pi}\frac{d\phi}{2\pi}\ J_0^2\left\{\frac{8t}{\omega(\alpha)}\sin\left[\frac{\omega(\alpha)x}{2}\right]\cos(\phi)\right\} \tag{21}$$

with g and ϵ_0 being the effective electron coupling constant and cut-off energy, correspondingly; $J_0(...)$ is the Bessel function of the first order. From Eqs.(20) and (21), it is possible to derive the correction to specific per one electron:

$$\Delta C(\alpha)=-\frac{3}{4}g^2 C_0\int_0^{\infty}\left(\frac{x^2}{\sinh^2(x)}\right)'''\tilde{J}(x,\alpha)\ , \tag{22}$$

where $C_0=k_B\pi^2 T/3(p_F v_F)$ is a specific heat of non-interacting electrons per one electron, k_B is the Boltzmann constant, and

$$\tilde{J}(\alpha,x)=\int_0^{2\pi}\frac{d\phi}{2\pi}\ J_0^2\left\{\frac{8t}{\omega(\alpha)}\sin\left[\frac{\omega(\alpha)x}{4\pi T}\right]\cos(\phi)\right\}. \tag{23}$$

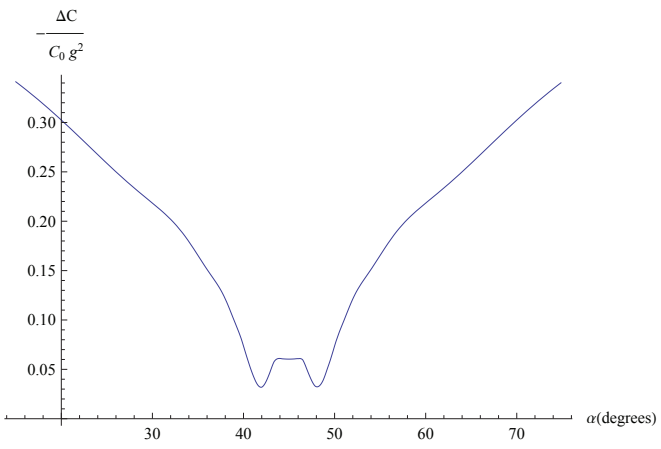

FIG. 2: Normalized correction to electron specific heat, $-\Delta C/(g^2 C_0)$, due to the Feynman's diagrams of Fig.1 is numerically calculated by means of Eqs.(22) and (23). The main minimum of the correction, corresponding to the LMA with $\alpha = 45^o$, is split into two secondary dips.

Below, we numerically calculate the integral (22) as a function of angle α. For the calculations, we use the following values of the parameters: $a_y = a_z$ [i.e., $\alpha_{(1,1)} = 45^o$ in Eq.(9)], $8t/\omega_y(0) = \sqrt{2}$, and $\omega_y(0)/(4\pi T) = 10\sqrt{2}$ (see Fig.2). It is possible to show that for large values of $|\delta\alpha| = |\alpha - 45^o|$ the correction to electron specific heat (22) in a Q1D conductor can be estimated as

$$\Delta C \simeq -\frac{g^2}{2} C_0. \tag{24}$$

Since in general $g^2 \sim 1$, the correction (24) is strong and we expect in this region of angles some kind of non-Fermi-liquid behavior in a metallic phase. As seen from Fig.2, close to the first LMA, $\alpha_{(1,1)} = 45^o$, there is a broad but strong minimum, where the corrections become at leat 10 times smaller in a magnitude. Therefore, we can expect some kind of angular non-Fermi-liquid - Fermi-liquid crossover (or phase transition) in the vicinity of $\alpha_{(1,1)}$. Note that these calculations support our previous results about 1D nature of electron wave functions (12) and 2D nature of electron wave function (16),(17) at different directions of a magnetic field in a Q1D conductor. On the other hand, such secondary effect as splitting of a minimum of the specific heat correction magnitude, shown in Fig.2, is due to oscillation of the function $\left(x^2/\sinh^2(x)\right)^{'''}$ in Eq.(22) and, thus, does not have a clear physical meaning.

Here, let us discuss a generalization of our theory on a more realistic Q1D electron spectrum, which can be represented as

$$\epsilon(\mathbf{p}) = \pm v_F(p_x \mp p_F) - 2\sum_{mn} t_{m,n} \cos(m a_y + n a_z), \tag{25}$$

where m and n are the integers. It is easy to understand that, in this case, electron wave functions become pure 2D at infinite number of the LMA,

$$\tan[\alpha_{m,n}] = \left(\frac{m}{n}\right)\left(\frac{a_y}{a_z}\right), \tag{26}$$

and, thus, we may expect the appearance of minima of a magnitude of specific heat correction due to electron-electron interactions at a series of the LMA (26) at infinite small temperature. Nevertheless, we argue that, at finite temperature T, there are only several "effective LMA" from Eq.(26), which satisfy the condition $t_{m,n} \geq T$. We expect that minima of the specific heat correction appear only for such "effective LMA". Another point is that $m = 0$ and $n = 0$ in Eq.(26), corresponding to the main crystallographic axes, $\mathbf{a}_y$ and $\mathbf{a}_z$, are also the LMA and all statements of the article are valid for them.

To summarize, we have predicted the Fermi-liquid - non-Fermi-liquid angular crossovers in a high magnetic field in Q1D conductors at the LMA directions of the field. From one side, our current results support, from a thermodynamic point of view, the pioneering statement of Ref.[19] that Fermi-liquid - non-Fermi-liquid angular crossovers have to exist, when a magnetic field is applied in the vicinities of the main crystallographic axis, $\mathbf{a}_y$ and $\mathbf{a}_z$. On the other, hand

our current results are more general than the results of Ref.[19] and predict the above-mentioned angular crossovers to exist at directions of a magnetic field close to the all "effective" LMA, given by Eq.(26). Below, we suggest to perform the described in the article experiment in the Q1D conductor $(Per)_2Au(mnt)_2$ in a metallic phase under pressure. If we take its band parameters [14], $v_F = 1.7 \times 10^7\ cm/s$, $t_y \simeq 20\ K$, $t_z < t_y$, we obtain that inequality (7) corresponds to magnetic fields, $H \geq 25\ T$. Note that, our present detailed numerical calculations (see Fig.2) correspond to very low temperature region, $T \simeq 0.1\ K$, nevertheless, our very preliminary numerical calculations show that the suggested LMA effects exist in $(Per)_2Au(mnt)_2$ also at $T \simeq 1\ K$, although, in the latter case, they are characterized by much smaller magnitudes. We stress that, at the LMA directions of a magnetic field (26), we have established "two-dimensionalization" of the Q1D electron spectrum (8), (25), in contrast to the previous statements [15,16], where increase of "one-dimensionalization" of the simplified Q1D spectrum (1) was considered. As a result, we have predicted minimums of a magnitude of the correction to specific heat (see Fig.2), instead of maximums, suggested in Ref.[16]. Since the correction due to electron-electron interactions is negative, we conclude that there have to exist maximums of specific heat in Q1D conductors at the LMA, instead of minimums [16].

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[1] See, for example, A.A. Abrikosov, *Fundamentals of the Theory of Metals* (North-Holland, Amsterdam, 1988).
[2] L.P. Gorkov and A.G. Lebed, J. Phys. (Paris) Lett. **45**, L433 (1984).
[3] M. Heritier, G. Montambaux, and P. Lederer, J. Phys. (Paris) Lett. **45**, L943 (1984).
[4] *The Physics of Organic Superconductors and Conductors*, edited by A.G. Lebed (Springer, Berlin, 2008).
[5] A.G. Lebed, JETP Lett. **44**, 114 (1986) [Pis'ma Zh. Eksp. Teor. Fiz. **44**, 89 (1986)].
[6] G.M. Danner, W. Kang, and P.M. Chaikin Phys. Rev. Lett. **72**, 3714 (1994).
[7] I.J. Lee and M,J. Naughton, Phys. Rev. B **58**, R13343 (1998).
[8] See, for example, Si Wu and A.G. Lebed, Phys. Rev. B **82**, 172504 (2010) and references therein.
[9] W. Wu, I.J. Lee, and P.M. Chaikin, Phys. Rev. Lett. **91**, 056601 (2003).
[10] W. Wu, N.P. Ong, and P.M. Chaikin, Phys. Rev. B **72**, 235116 (2005).
[11] E.S. Choi, J.S. Brooks, H. Kang, Y.J. Jo, and W. Kang, Phys. Rev. Lett. **95**, 187001 (2005).
[12] W. Wu and P.M. Chaikin, Phys. Rev. B **76**, 153102 (2007).
[13] K. Kobayashi, H. Satsukawa, J. Yamada, T. Terashima, and S. Uji Phys. Rev. Lett. **112**, 116805 (2014).
[14] D. Graf J.S. Brooks, E.S. Choi, M. Almeida, R.T. Henriques, J.C. Dias, and S. Uji, Phys. Rev. B **80**, 155104 (2009).
[15] A.G. Lebed and Per Bak, Phys. Rev. Lett. **63**, 1315 (1989).
[16] V.M. Yakovenko, Phys. Rev. Lett. **68**, 3607 (1992); Erratum **70**, 519 (1993).
[17] A.G. Lebed, J. Phys. I (France) **2**, 2005 (1992).
[18] A.G. Lebed, J. Phys. I (France) **4**, 351 (1994).
[19] A.G. Lebed, Phys. Rev. Lett. **115**, 157001 (2015).
[20] A.A. Abrikosov, L.P. Gor'kov, and I.E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1975).
[21] I.S. Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series, and Products*, 5th edition (Academic Press, New York, 1994).