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# Valuation of characteristic ratios for high- $T_c$ superconductors with anisotropic gap in the conformal transformation method

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## Abstract

The application of a method of conformal-like transformation of the two-dimensional momentum space is presented and discussed with regard to two-dimensional anisotropic superconductors. A new function, the kernel of the density of states, and some integral formulae are derived, interpreted and studied for a few specific cases. Evidences for the incompatibility between the Van Hove scenario and the conformal transformation method with respect to a couple of characteristic ratios, i.e. the transition temperature and the specific heat jump, are displayed in detail for d- and p-wave pairing. The established method allows us to obtain the gap equation in a standardized form common to the models of superconductivity with an arbitrary dispersion relation. Classification of superconductors with respect to the valuation of characteristic ratios is proposed and commented on.

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## 1. Introduction

A view dominating in most of the present approaches is that the enhancement of the transition temperature  $T_c$  in superconducting cuprates can be explained in the frame of the Van Hove scenario with conventional pairing mechanisms like electron–phonon interaction or spin-fluctuation [1–16]. In this paper we shall proceed with the assumptions that the HTSC mechanism in layered cuprate metal oxides is governed by the Cooper pairing of fermions (electrons or holes) through the exchange of virtual bosons (phonons, magnons, plasmons or

excitons), the gap equation in the momentum space can be obtained in a self-consistent manner employing the Matsubara Green function formalism and it can be written in the general form

$$\Delta_{\mathbf{p}} = \frac{1}{N} \sum_{\mathbf{p}'} V_{\mathbf{p},\mathbf{p}'} \frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}} \tanh \frac{E_{\mathbf{p}'}}{2T} \quad (1)$$

where  $V_{\mathbf{p},\mathbf{p}'}$  is the effective pairing potential,  $E_{\mathbf{p}} = \sqrt{\xi_{\mathbf{p}}^2 + \Delta_{\mathbf{p}}^2}$ ,  $\xi_{\mathbf{p}} = \epsilon_{\mathbf{p}} - \mu$ . This equation should be complete with another self-consistent equation

$$2n = \frac{1}{N} \sum_{\mathbf{p}} \left( 1 - \frac{\xi_{\mathbf{p}}}{E_{\mathbf{p}}} \tanh \frac{E_{\mathbf{p}}}{2T} \right)$$

which gives the chemical potential  $\mu$  as a function of the conduction band filling  $n$  for the normal metallic phase.

The form of the pairing potential  $V_{\mathbf{p},\mathbf{p}'}$  determines the form of the order parameter (gap)  $\Delta_{\mathbf{p}}$  which in general is not isotropic and its anisotropic structure cannot be eliminated from equation (1) even in the limit  $T = T_c$ , unlike in the pure isotropic case (s-wave pairing).

In most of the approaches where the Van Hove scenario is employed, the summation over the momentum  $\mathbf{p}$  taken from a two-dimensional space is solely replaced by the integration over the particle energy  $\xi$  according to the relation  $\frac{1}{N} \sum_{\mathbf{p}} \dots = \int d\xi v(\xi) \dots$ . The density of states  $v(\xi)$  for the normal state can be expressed as [12–14]

$$v(\xi) = \frac{a^2}{4\pi^2} \int_{\xi=\xi_{\mathbf{p}}} \frac{df}{|\nabla_{\mathbf{p}} \xi_{\mathbf{p}}|} \quad (2)$$

where  $a$  denotes the lattice constant and  $df$  is an element of the Fermi surface. The Van Hove singularities in  $v(\xi)$  correspond to the flat regions of  $\xi_{\mathbf{p}}$  where  $\nabla_{\mathbf{p}} \xi_{\mathbf{p}} = 0$ . The derived or just postulated forms of the density of states which are employed in the Van Hove scenario possess a singularity or a narrow maximum located on the Fermi surface or in its vicinity. The presence of a strong fluctuation in the density of states is a consequence of doping and implies high  $T_c$  values in layered cuprate superconductors [5, 8, 11, 12, 14, 16, 18–26]. However, in such approach the number of degrees of freedom for a particle in the momentum space ( $p_1, p_2$ ) is reduced only to 1, corresponding to the particle energy  $\xi$ . This weakness of the Van Hove scenario causes that it is not effective for systems with an anisotropic order parameter depending on the angle  $\varphi$ . Therefore in models of p-wave or d-wave superconductors one should always keep two coordinates  $\xi$  and  $\varphi$ , and it also applies to the strong coupling theory [26].

In order to overcome this problem for layered crystals of the cuprate metal oxides with d-wave pairing, Pashitskii *et al* [27] proposed to replace the density of states by a function  $v(\xi, \theta)$  being an expansion of the density of states into the Fourier series in the angle  $\theta$  between one of the main crystallographic axes in the plane of layers and the particle momentum  $\mathbf{k}$  lying on the Fermi surface. For the sake of simplicity they included only the first two terms of the expansion which satisfied the symmetry group  $C_{4v}$  of the cuprate plane  $\text{CuO}_2$ . In order to find the coefficients of the expansion they employed the density of states on quasi-1D and quasi-2D portions of the closed and roughly cylindrical Fermi surface. However, such approach and the obtained results do not seem to be correct, since the average value of  $v(\xi, \theta)$  over  $\theta$  should be reduced to the form of the density of states if their method is applied to the pure s-wave pairing.

We propose an independent formalism based on the conformal transformation of the momentum space, which can be treated as an extension of the Van Hove scenario with the actual number of degrees of freedom. This formalism allows us to standardize models of superconductivity and to clarify the role of the dispersion relation in the classification of

superconductors. It also provides evidences that models with reduced number of degrees of freedom cannot be successfully applied to p-wave or d-wave superconductors.

## 2. Transformation of the reciprocal space

We consider an effective one-band model with a one-particle dispersion relation being a differentiable function of the momentum  $\mathbf{p}$ , which can be written in the form  $\xi = \xi(p_1, p_2)$ , and the momentum vector  $\mathbf{p}$  is of the form  $\mathbf{p} = p_1\mathbf{e}_1 + p_2\mathbf{e}_2$ . We also assume that the form of the dispersion relation under consideration has been renormalized by means of the mass operator, so it includes all two-particle interactions and a finite doping, self-consistently.

The versors  $\mathbf{e}_1, \mathbf{e}_2$  form a basis of the momentum space so that they are basis vectors of the reciprocal CuO plane. The Fermi surface (line) is defined by the equation  $\xi(\mathbf{p}) - \mu = 0$ , where  $\mu$  is the Fermi energy (chemical potential).

### 2.1. Orthonormalization of the reciprocal space

For an anisotropic system with a parallelogram-like reciprocal lattice the basis  $\mathbf{e}_1, \mathbf{e}_2$  is not orthonormal. Nevertheless, performing a linear (orthonormal) transformation  $\mathbf{D}$ , described by a  $2 \times 2$  matrix, which keeps the topology of the reciprocal planar lattice, the momentum space can be transformed in such a way that in the new space with the orthonormal basis  $\mathbf{f}_1, \mathbf{f}_2$ , where  $\mathbf{f}_i = \mathbf{D}_{i1}\mathbf{e}_1 + \mathbf{D}_{i2}\mathbf{e}_2$ , the reciprocal lattice becomes a square one. In this transformed space the vector  $\mathbf{p} = p_1\mathbf{e}_1 + p_2\mathbf{e}_2$  is replaced by an equivalent vector  $\mathbf{p}' = p_1\mathbf{f}_1 + p_2\mathbf{f}_2$ . Since  $\mathbf{p}' = p'_1\mathbf{e}_1 + p'_2\mathbf{e}_2$ , the introduced components fulfil the relation  $p_i = \mathbf{D}_{1i}^{-1}p'_1 + \mathbf{D}_{2i}^{-1}p'_2$ , where  $\mathbf{D}^{-1}$  denotes the inverse matrix. Now the dispersion relation as a function of the momentum components  $p'_1, p'_2$  determined in the orthonormal system reads  $\xi = \xi(\mathbf{D}_{11}^{-1}p'_1 + \mathbf{D}_{21}^{-1}p'_2, \mathbf{D}_{12}^{-1}p'_1 + \mathbf{D}_{22}^{-1}p'_2)$ . Hereafter, we assume that in dispersion relations the particle energy is measured from the Fermi level. Taking  $\xi = \text{const}$  we can find the equi-energy lines (in particular for  $\xi = 0$  we get the Fermi line). The shape of these lines can be quite arbitrary, although it should always reflect the symmetry of the system. Moreover, it implies that we must not treat this system of fermions as the Landau Fermi liquid. On the other hand, we have to remember that after the transformation  $\mathbf{D}$ , the summation or integration in the new coordinate system requires including the Jacobian of the form

$$J(\mathbf{p}') = \left| \frac{\partial p_i}{\partial p'_j} \right|$$

which is now constant, and  $J(\mathbf{p}') = \det(\mathbf{D}^{-1})$ . Considering an anisotropic system in which the basis vectors of its reciprocal two-dimensional lattice  $\mathbf{e}_1, \mathbf{e}_2$  are not orthonormal and they are not of the same length, we may assume that  $|\mathbf{e}_1| = 1$ . Then the orthonormal transformation is represented by the matrix

$$\mathbf{D} = \begin{bmatrix} 1 & 0 \\ -\cot \alpha & \frac{1}{|\mathbf{e}_2| \sin \alpha} \end{bmatrix}$$

where  $\alpha$  is the angle between vectors  $\mathbf{e}_1$  and  $\mathbf{e}_2$ , and the Jacobian reads  $J(p'_1, p'_2) = |\mathbf{e}_2| \sin \alpha$ . After employing the above transformation we have at our disposal a system with an orthonormal basis  $\mathbf{f}_1$  and  $\mathbf{f}_2$  such that  $|\mathbf{e}_1| = |\mathbf{f}_1| = |\mathbf{f}_2|$ .

For instance, if the dispersion relation is of the parabolic form in the initial system, i.e.

$$\xi(p_1, p_2) = \frac{1}{2m^*} (p_1^2 + p_2^2) - \mu$$

where  $m^*$  denotes the effective mass and  $\mu$  is the chemical potential, then in the transformed system

$$\xi(p'_1, p'_2) = \frac{1}{2m^*} [(p'_1)^2 + 2p'_1 p'_2 |\mathbf{e}_2| \cos \alpha + (p'_2)^2 |\mathbf{e}_2|^2] - \mu.$$

After the rotation of the coordinate system by the angle  $\beta = \frac{1}{2} \arctan\left(\frac{2|\mathbf{e}_2| \cos \alpha}{1 - |\mathbf{e}_2|^2}\right)$  it reduces to a more symmetric, simplified, and equivalent form

$$\xi(p'_1, p'_2) = \frac{1}{2m_1} (p'_1)^2 + \frac{1}{2m_2} (p'_2)^2 - \mu \quad (3)$$

where  $m_1$  and  $m_2$  are some mass parameters, whose precise definitions can now be omitted. The Jacobian of the coordinate system rotation is always equal to 1. Thus, in this new Cartesian coordinate system the equi-energy lines are concentric ellipses. In such a way we display that the increase in the symmetry of the coordinate system is followed by the change of the form of the dispersion relation which can become more composed. Thus, the symmetry properties of the system which correspond to the crystal lattice symmetry can be transferred into the dispersion relation.

## 2.2. Generalized conformal transformation of the reciprocal space

Now, our intention is to construct a new orthonormal space in which  $\xi$  stands for one of the coordinate axes. Since  $\nabla \xi$  is perpendicular to the equi-energy line, the following condition for the gradient direction has to be fulfilled:

$$\frac{dp_1}{\partial \xi / \partial p_1} = \frac{dp_2}{\partial \xi / \partial p_2}. \quad (4)$$

On the other hand, by virtue of Picard's theorem, we state that the solution of the differential equation

$$\frac{dp_1}{dp_2} = \frac{\partial \xi / \partial p_1}{\partial \xi / \partial p_2}$$

always exists and is a one-parameter family of integral curves  $\phi = \phi(p_1, p_2)$ , where the curves  $\phi(p_1, p_2) = C$  are called isoclines. Note that defining the Pfaff's differential form as

$$D\Xi(p_1, p_2) = -\frac{\partial \xi}{\partial p_2} dp_1 + \frac{\partial \xi}{\partial p_1} dp_2$$

equation (4) can be read as a Pfaff's equation  $D\Xi(p_1, p_2) = 0$ . The Pfaff's equation of two independent variables always possesses an integrating factor  $\gamma = \gamma(p_1, p_2)$ , such that  $\gamma(p_1, p_2) D\Xi(p_1, p_2) = d\phi(p_1, p_2)$  is a total differential. Thus,

$$-\gamma(p_1, p_2) \frac{\partial \xi}{\partial p_2} = \frac{\partial \phi}{\partial p_1} \quad \gamma(p_1, p_2) \frac{\partial \xi}{\partial p_1} = -\frac{\partial \phi}{\partial p_2} \quad (5)$$

and hence the gradients  $\nabla \xi$  and  $\nabla \phi$ , which define the perpendicular directions to the equi-energy curves and isoclines, respectively, obey the condition

$$\nabla \xi \cdot \nabla \phi = \frac{\partial \xi}{\partial p_1} \frac{\partial \phi}{\partial p_1} + \frac{\partial \xi}{\partial p_2} \frac{\partial \phi}{\partial p_2} = 0$$

which ensures that the new two-dimensional system of curvilinear coordinates  $(\xi, \phi)$  is orthogonal. In general, the coordinate  $\xi$  which is the particle energy can vary in the conduction band, while the range of the coordinate  $\phi$  can be chosen arbitrarily and it can be infinite.

In order to simplify investigations one can formally replace  $\phi$  by the angular coordinate, e.g.,  $\varphi$  using trigonometric functions. Then the range of the new coordinate becomes finite. Note that for a function  $\varphi = \varphi(\phi)$  we have the relation

$$\nabla\varphi = \frac{d\varphi}{d\phi}\nabla\phi$$

which ensures that the coordinate system  $(\xi, \varphi)$  is also orthogonal, since  $\nabla\xi \cdot \nabla\varphi = 0$ . Moreover, employing the symmetry of the system, which is directly reflected in the form of the dispersion relation, we can restrict our consideration to the representative region of the  $(p_1, p_2)$ -plane, and the range of the angular coordinate  $\varphi$  can be settled in regard to the full rotation of the plane, i.e.  $0 \leq \varphi < 2\pi$ . Then we can assume that locally, in separated regions of the  $(p_1, p_2)$ -plane, we can derive  $p_1$  and  $p_2$  as functions of  $\xi$  and  $\varphi$ , because both functions  $\xi(p_1, p_2)$  and  $\varphi(p_1, p_2)$  are differentiable. On the other hand, we emphasize that the analytical forms of  $p_1$  and  $p_2$  as functions  $\xi$  and  $\phi$  or  $\varphi$  can be derived merely for a few specific forms of the particle energy, nevertheless they can be always found numerically. Therefore the present method allows us to transform the two-dimensional Cartesian coordinate system  $(p_1, p_2)$  into a specific curvilinear orthogonal coordinate system  $(\xi, \phi)$  employing given  $\xi = \xi(p_1, p_2)$  and found  $\phi = \phi(p_1, p_2)$  relations.

In the standard approaches a conformal mapping is given by a single-valued complex analytic function, where its real and imaginary parts define equi-energy curves and isoclines, respectively, and they satisfy the Cauchy–Riemann conditions. Since we do not require that

$$\frac{\partial\xi}{\partial p_1} = \frac{\partial\phi}{\partial p_2} \quad \frac{\partial\xi}{\partial p_2} = -\frac{\partial\phi}{\partial p_1}$$

and conditions of the Cauchy–Riemann type are fulfilled only if  $\gamma(p_1, p_2) \equiv 1$ , we maintain that the present formalism constitutes a generalization of the conformal transformation, contrary to the standard conformal transformation where these conditions must be fulfilled. Note that in this formalism the function  $\phi(p_1, p_2)$  is not given and it is derived in relation to  $\xi(p_1, p_2)$ , therefore these functions must satisfy the conditions (5). Thus  $\gamma(p_1, p_2)$ , and hence  $\phi(p_1, p_2)$ , can always be scaled by an arbitrary multiplicative constant.

The generalized conformal transformation introduces local changes of the density of states in the  $(\xi, \phi)$ -space which can be expressed by means of the Jacobian

$$J(\xi, \phi) = \begin{vmatrix} \frac{\partial p_1}{\partial \xi} & \frac{\partial p_1}{\partial \phi} \\ \frac{\partial p_2}{\partial \xi} & \frac{\partial p_2}{\partial \phi} \end{vmatrix} \quad (6)$$

which in general must be derived in the  $(\xi, \phi)$ -space locally in order to ensure it to be a single-valued function.

Therefore, replacing the summation over quantum-mechanical states by the integration over the particle energy one has to include also the integration over  $\phi$

$$\sum_{\mathbf{p}} \dots = \frac{2}{(2\pi)^2} \int d\xi \int d\phi J(\xi, \phi) \dots \quad (7)$$

where the last integral is over the whole range of  $\phi$ . In order to reduce the formula to the form applied in the Van Hove scenario we define the average density of states in the  $(\xi, \phi)$ -space for a fixed  $\xi$  as  $\nu(\xi) = \frac{2}{(2\pi)^2} \int d\phi J(\xi, \phi)$ , which is the same density of states as defined by equation (2). Then for the case when the *anonymous* integrand in equation (7) is independent of  $\phi$ , the rhs of this formula reduces to the form postulated in the Van Hove scenario, and

$$\frac{2}{(2\pi)^2} \int d\xi \int d\phi J(\xi, \phi) \dots = \int d\xi \nu(\xi) \dots$$

However, when the integrand is a function of  $\xi$  and  $\phi$ , as e.g. for p-wave or d-wave paired superconductors, one must take into account that in general

$$\int d\phi \mathcal{K}(\xi, \phi) \dots \neq \frac{1}{\int d\phi'} \int d\phi' \mathcal{K}(\xi, \phi') \int d\phi \dots \quad (8)$$

where  $\mathcal{K}(\xi, \phi) = \frac{2}{(2\pi)^2} J(\xi, \phi)$  is the kernel of the density of states and its value corresponds to the local deformation or modification of quantum-mechanical states in the  $(\xi, \phi)$ -space, which is a result of the applied transformation. Moreover, the integration on the rhs of equation (8) depends on the choice of  $\phi$ .

Therefore, in some other approaches, this variable is chosen as the angular variable  $0 \leq \varphi < 2\pi$ , the same as introduced in the standard polar coordinate system. Although such choice ensures that

$$\int_0^{2\pi} \frac{d\varphi}{2\pi} \mathcal{K}(\xi, \varphi) \dots = \int_0^{2\pi} \frac{d\varphi}{2\pi} v(\xi) \dots \quad (9)$$

when the *anonymous* integrand is independent of  $\varphi$ , and

$$v(\xi) = \int_0^{2\pi} \frac{d\varphi}{2\pi} \mathcal{K}(\xi, \varphi)$$

it proves that the Van Hove scenario cannot be applied to other than the pure s-wave pairing.

### 3. Examples of kernels of the density of states

In order to substantiate accuracy of the developed formalism we discuss in details two specific but adequately simple forms of the dispersion relation for a planar square lattice.

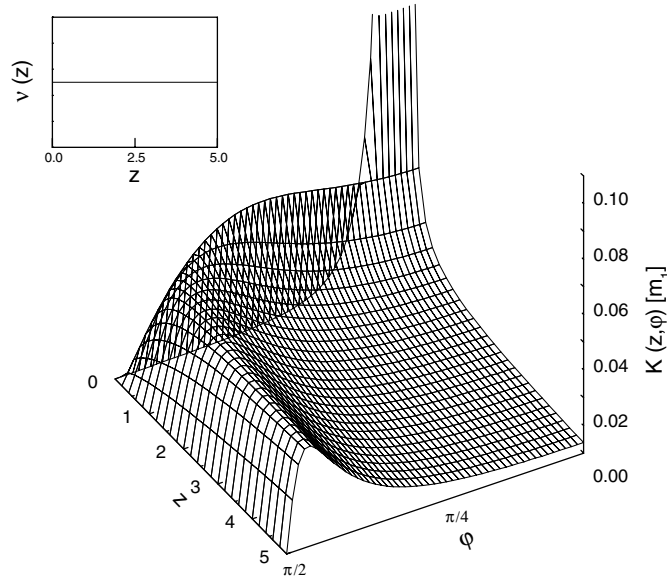
#### 3.1. Anisotropic system with a parabolic energy spectrum

The described method allows us to transform a parabolic energy spectrum from an anisotropic momentum space to a planar square lattice. Then according to equation (3) the dispersion relation reads  $\xi(k_1, k_2) + \mu = \mu^*[(k_1)^2 + \varrho(k_2)^2]$ , where  $k_i = ap_i$ ,  $\mu^* = (2m_1a^2)^{-1}$ ,  $\varrho = m_1/m_2$  and  $a$  is the lattice constant. The solution of Pfaff's equation (4) leads to the relation  $k_2k_1^{-\varrho} = \phi$ . According to the symmetry of the problem, which is of the group  $C_{2v}$ , we can restrict our investigation to the quadrant  $k_1, k_2 \geq 0$ , which implies that  $k_2k_1^{-\varrho} \geq 0$  for arbitrary  $k_1, k_2$  and  $\varrho \neq 0$ , so  $\phi$  can be taken as  $\phi = \tan \varphi$ , where  $0 \leq \varphi \leq \pi/2$ .

Since the problem cannot be solved analytically for an arbitrary  $\varrho$ , we consider the cases  $\varrho = 1$  and  $\varrho = \frac{1}{2}$ . For  $\varrho = 1$  we have  $k_1 = \sqrt{(\xi + \mu)/\mu^*} \cos \varphi$ ,  $k_2 = \sqrt{(\xi + \mu)/\mu^*} \sin \varphi$  and  $\mathcal{K}(\xi, \varphi) = m^*/2\pi^2$ ,  $v(\xi) = m^*/\pi$ , where  $m_1 = m_2 = m^*$ . Hence,  $\mathcal{K}(\xi, \varphi)$  and  $v(\xi)$  are constant and  $v(\xi)$  is the same as in the other approaches. For  $\varrho = \frac{1}{2}$  we obtain  $k_1 = \frac{1}{4}(\sqrt{\tan^4 \varphi + 16(\xi + \mu)/\mu^*} - \tan^2 \varphi)$ , and  $k_2 = \frac{1}{2} \tan \varphi (\sqrt{\tan^4 \varphi + 16(\xi + \mu)/\mu^*} - \tan^2 \varphi)^{\frac{1}{2}}$ . Hence, according to equation (6) the kernel of the density of states has the form

$$\mathcal{K}(\xi, \varphi) = \frac{m_1}{\pi^2} \frac{\left(\sqrt{\tan^4 \varphi + 16\frac{\xi+\mu}{\mu^*}} - \tan^2 \varphi\right)^{\frac{1}{2}}}{\sqrt{\tan^4 \varphi + 16\frac{\xi+\mu}{\mu^*}}} (1 + \tan^2 \varphi).$$

$\mathcal{K}(\xi, \varphi)$  is a composed function of  $\xi$  and  $\varphi$  (cf figure 1), which for a fixed  $\xi$ , when  $\varphi$  varies from 0 to  $\pi/2$ , achieves a maximum, and  $\mathcal{K}(\xi, 0) = \frac{m_1}{2\pi^2} \left(\frac{\mu^*}{\xi+\mu}\right)^{\frac{1}{4}}$ ,  $\mathcal{K}(\xi, \frac{\pi}{2}) = 0$ . The corresponding density of states (cf figure 1, inset) proves to be independent of  $\xi$ , and  $v(\xi) = \sqrt{m_1 m_2}/\pi$ .



**Figure 1.** The kernel  $\mathcal{K}$  and the density of states  $\nu$  (inset) for an anisotropic system with a parabolic energy spectrum ( $z = (\xi + \mu)/\mu^*$ ).

### 3.2. One-band Hubbard model

Since in high- $T_c$  cuprates the conduction band can be described in the frame of the rigid-band model [7, 8], the dispersion relation for a planar square lattice [9] can be taken as  $\xi(p_1, p_2) = -2t_0 [\cos(p_1 a) + \rho \cos(p_2 a)] - t_2$ , where we take into account the nearest (but not identical in both possible directions) hoppings, as it takes place in superlattices, assuming that  $\rho$  can be an arbitrary positive number. The occupation parameter  $t_2$  fixes a shift of the Fermi level in the case of the doping and a non-half-filled band, and it can be identified with the chemical potential [5, 19]. Employing the symbols  $k_i$  as above we find the solution of Pfaff's equation in the form  $(\tan \frac{k_2}{2})(\tan \frac{k_1}{2})^{-\rho} = \phi$ . Let us emphasize that analytical solutions of the problem can be found merely for a few values of  $\rho$ , e.g.  $\rho = 1$  and  $\rho = \frac{1}{2}$ . Therefore, in order to display the routine of the elaborated method we focus on the widely discussed case  $\rho = 1$ . After some algebra we obtain [11, 12]

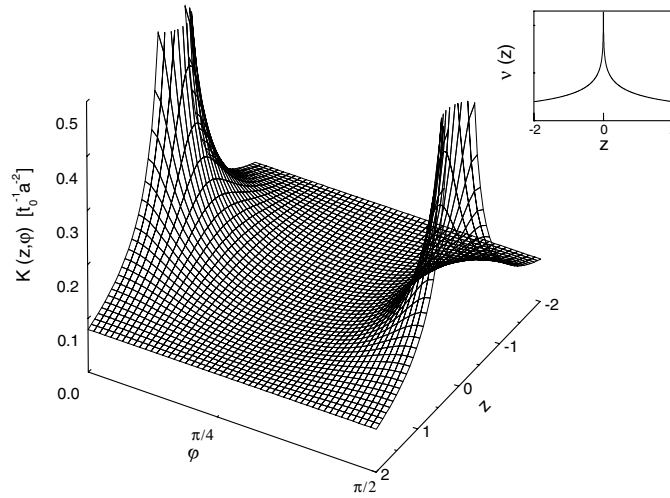
$$k_i = 2 \arctan \left[ \frac{z(1 + \phi^2) + \sqrt{(1 + \phi^2)^2 z^2 + 4\phi^2(4 - z^2)}}{2(2 - z)\phi^{2(2-i)}} \right]^{\frac{1}{2}}.$$

In order to simplify the calculations we take into account the symmetry group  $C_{4v}$ , restrict to  $k_1, k_2 \geq 0$  and introduce the following symbols  $z = (\xi + t_2)/2t_0$ ,  $\phi = \tan \varphi$ , where  $|z| \leq 2$  and  $\phi \geq 0$ , so  $0 \leq \varphi \leq \pi/2$ . The derivation of the Jacobian allows us to find the kernel of the density of states in the form

$$\mathcal{K}(\xi, \varphi) = \frac{1}{2\pi^2 t_0 a^2} \frac{1 + \tan^2 \varphi}{\sqrt{z^2(1 - \tan^2 \varphi)^2 + 16 \tan^2 \varphi}} \quad (10)$$

which also satisfies the condition  $\mathcal{K}(\xi, \frac{\pi}{2} - \varphi) = \mathcal{K}(\xi, \varphi)$ . Moreover, if  $\varphi \rightarrow \frac{\pi}{2}$ , the function  $\mathcal{K}(\xi, \varphi) \sim z^{-1}$  and it has no singularities except the case when  $z \rightarrow 0$  (cf figure 2). This particular singularity does not vanish after the averaging over  $\varphi$  and it is always revealed in





**Figure 2.** The kernel  $\mathcal{K}$  and the density of states  $\nu$  (inset) for the one-band Hubbard model.

the density of states  $\nu(\xi)$  as the Van Hove one [9, 11] (cf figure 2, inset). Integration of equation (10) over the angle  $\varphi$  yields

$$\nu(\xi) = \frac{2}{\pi^2 t_0 a^2} \frac{1}{\sqrt{8 - z^2 + 4\sqrt{4 - z^2}}} \mathbf{F} \left( \frac{\pi}{2}, \left( \frac{8\sqrt{4 - z^2}}{8 - z^2 + 4\sqrt{4 - z^2}} \right)^{\frac{1}{2}} \right) \quad (11)$$

where  $\mathbf{F}(\psi, \kappa)$  is the elliptic integral of the first kind [11, 12]. The function  $\mathbf{F}(\frac{\pi}{2}, \kappa)$  in the limit  $\kappa \rightarrow 1$  can be expanded in a specific series [11], and then we obtain the well-known [11–14] result  $\nu(\xi) = \frac{1}{\pi^2 t_0 a^2} \ln \frac{16t_0}{|\xi + t_2|}$ .

#### 4. Evidences for incompatibility between the Van Hove scenario and the conformal transformation method

In the present section we point out evident differences between the results obtained within the Van Hove scenario and within the established conformal-like transformation method for non-s-wave paired superconductors. We start from the gap equation (1) where we assume that the effective pairing potential can be separated to the form  $V_{\mathbf{p}, \mathbf{p}'} = f v(\mathbf{p}) v(\mathbf{p}')$ , where  $v(\mathbf{p})$  is an even function of  $\mathbf{p}$  for antisymmetric (singlet) spin pairing and it is an odd function for symmetric (triplet) spin pairing [28]. Moreover, as we have previously assumed, we deal with a model where many-body effects can be effectively reduced to the form of one-particle interaction, so they are included in the gap equation and other equations by means of the dispersion relation  $\xi_{\mathbf{p}}$ , or they can be gathered in the pairing channel. After performing the conformal transformation  $v(\mathbf{p})$  becomes a function of  $\xi$  and  $\varphi$ , and it can be expanded in a Fourier series in the angle  $\varphi$ ,

$$v(\mathbf{p}) = \sum_{l=0}^{\infty} v_l(\xi) \cos(l\varphi + \alpha_l)$$

and  $\alpha_0 = 0$ . Note that odd (even) coefficients of the expansion  $v_l(\xi)$  must vanish for antisymmetric (symmetric) spin pairing due to the Pauli exclusion principle. Then the order parameters for the pure s-, p-, d-, f-, g-, etc wave pairing can be taken in the form

$$\Delta(\xi, \varphi) = \Delta(T)v_l(\xi)D(\xi, \varphi) \quad (12)$$

where we assume that

$$\int_{-\omega_c}^{\omega_c} \frac{d\xi}{2\omega_c} v_l(\xi) = 1 \quad \text{and} \quad \int_0^{2\pi} \frac{d\varphi}{2\pi} |D(\xi, \varphi)|^2 = 1$$

and  $\omega_c$  is the cut-off energy. Thus

$$\begin{aligned} D(\xi, \varphi) &= 1 && \text{for s-wave pairing} \\ D(\xi, \varphi) &= \pm\sqrt{2} \cos(\varphi + \alpha_1) && \text{for p-wave pairing} \\ D(\xi, \varphi) &= \pm\sqrt{2} \cos(2\varphi + \alpha_2) && \text{for d-wave pairing} \\ D(\xi, \varphi) &= \pm\sqrt{2} \cos(l\varphi + \alpha_l) && \text{for other l-wave pairing} \end{aligned} \quad (13)$$

and  $\alpha_l$  parameters, which in general can be functions of  $\xi$ , should be determined from the stability condition. Moreover, the gap equation (1) can be rewritten in the following standardized form,

$$\begin{aligned} \Delta(\xi, \varphi) &= f v_l(\xi) \cos(l\varphi + \alpha_l) \int_0^{2\pi} \frac{d\varphi'}{2\pi} \int_{-\omega_c}^{\omega_c} d\xi' \mathcal{K}(\xi', \varphi') v_l(\xi') \cos(l\varphi' + \alpha_l) \\ &\times \frac{\Delta(\xi', \varphi')}{E(\xi', \varphi')} \tanh \frac{E(\xi', \varphi')}{2T} \end{aligned} \quad (14)$$

where  $E(\xi, \varphi) = \sqrt{\xi^2 + \Delta^2(\xi, \varphi)}$ , which is common to models of superconductivity with an arbitrary dispersion relation, realized in pure pairing states. Hence, in particular, for the BCS model,  $l = 0$ , we have  $v_0(\xi) = 1$ ,  $\Delta(\xi, \varphi) = \Delta(T)$ ,  $\mathcal{K}(\xi, \varphi) = v(0)$ , and the coupling constant  $\lambda = f v(0)$ . Besides, in most of the discussed systems one can assume that the non-vanishing coefficient  $v_l(\xi)$  varies slightly in the pairing region, so one can put  $v_l(\xi) \equiv 1$  and admit that the order parameter is independent of  $\xi$ , so  $D(\xi, \varphi) \equiv D(0, \varphi)$ , and stable states correspond to fixed values of  $\alpha_l$ . Note that within the standard approximation for the electron–electron attraction the dominant negative term of the series expansion is constant and independent of the variables  $\xi, \xi'$ , and it vanishes when  $|\xi|, |\xi'| > \xi_0$ , where  $\xi_0$  is a cut-off energy [19].

Employing algebraic methods similar to those developed in [10, 28] and substituting  $\xi = 2T_c u$  one can derive the equation

$$\ln \frac{T_c}{T_{c0}} = \int_0^{\omega_c/2T_c} \frac{du}{u} [v_l^2(2T_c u) I_2(2T_c u) - 1] \tanh u \quad (15)$$

which allows us to evaluate the normalized transition temperature with respect to the BCS approximation, when  $v_l(\xi) = 1$  and  $v(\xi) = v_0$ , where

$$v_0 = \int_{-\omega_c}^{\omega_c} \frac{d\xi}{2\omega_c} v(\xi).$$

Moreover, one finds

$$\frac{\Delta C(T_c)}{4v_0 T_c} = - \frac{\int_0^{\omega_c/2T_c} du v_l^2(2T_c u) I_2(2T_c u) \frac{d}{du} \tanh u}{\int_0^{\omega_c/2T_c} \frac{du}{u} v_l^4(2T_c u) I_4(2T_c u) \frac{d}{du} \frac{\tanh u}{u}} \quad (16)$$

which allows us to derive the reduced values of the specific heat leap. In equations (15) and (16)

$$I_{2n}(\xi) = \frac{1}{2\nu_0} \int_0^{2\pi} \frac{d\varphi}{2\pi} [\mathcal{K}(\xi, \varphi) |D(\xi, \varphi)|^{2n} + \mathcal{K}(-\xi, \varphi) |D(-\xi, \varphi)|^{2n}]. \quad (17)$$

The formulae (15) and (16), which allow us to evaluate the characteristic ratios in superconductivity, i.e.  $T_c/T_{c0}$  and  $\Delta C(T_c)/C_N(T_c)$ , have been obtained in the frame of the conformal transformation method for a non-isotropic order parameter. In the case of the Van Hove scenario these formulae keep their forms; however, the functions  $I_{2n}(\xi)$  must be rewritten as

$$I_{2n}(\xi) = \frac{1}{2\nu_0} \left[ \nu(\xi) \int_0^{2\pi} \frac{d\varphi}{2\pi} |D(\xi, \varphi)|^{2n} + \nu(-\xi) \int_0^{2\pi} \frac{d\varphi}{2\pi} |D(-\xi, \varphi)|^{2n} \right]. \quad (18)$$

Moreover, if

$$\int_0^{2\pi} \frac{d\varphi}{2\pi} |D(\xi, \varphi)|^{2n} = \int_0^{2\pi} \frac{d\varphi}{2\pi} |D(-\xi, \varphi)|^{2n}$$

they can be reduced to the form

$$I_{2n}(\xi) = I_0(\xi) \int_0^{2\pi} \frac{d\varphi}{2\pi} |D(\xi, \varphi)|^{2n}.$$

Note that for the pure l-wave pairing as defined in (13) one has

$$\int_0^{2\pi} \frac{d\varphi}{2\pi} [\pm\sqrt{2} \cos(l\varphi + \alpha_l)]^{2n} = \frac{1}{2^n} \binom{2n}{n}$$

for all  $l = 1, 2, 3, \dots$  and  $\alpha_l$ . Hence for  $n = 2$  it is equal to  $3/2$ .

Equations (15) and (16) reveal fundamental algebraic differences between the results obtained within the conformal transformation method and the Van Hove scenario. In the latter for the states (13) the expressions  $I_2(\xi)$  and  $I_4(\xi)$  are replaced as follows:  $I_2(\xi) \equiv I_0(\xi)$  and  $I_4(\xi) \equiv \frac{3}{2}I_0(\xi)$ . Such simplification of the formulae (15) and (16) causes that the ratios  $T_c/T_{c0}$  and  $\Delta C(T_c)/C_N(T_c)$  become simply identical for all non-isotropic states (13).

As has been shown before [28] stable states for the d-wave pairing are achieved for  $\alpha_2 = 0$  and  $\alpha_2 = \pi/2$ , and the suitable states after the inverse conformal transformation for the one-band Hubbard model are proportional to  $(\cos p_1a - \cos p_2a)$  and  $\sin p_1a \sin p_2a$ , respectively, which correspond to  $x^2 - y^2$  and  $xy$  symmetry. The similar procedure allows us to show that for the p-wave pairing the states with  $\alpha_1 = 0$  and  $\alpha_1 = \pi/2$  are proportional to  $\sin p_1a$  and  $\sin p_2a$ , respectively. These all functions are basis functions of the irreducible representations of the  $C_{4v}$  group and they are even or odd functions of the vector  $\mathbf{p}$ . They are chosen to be invariant under translations by reciprocal lattice vectors [29].

In order to give a detailed description of the difference between the conformal transformation method and the Van Hove scenario, we present some analytical results obtained for the one-band Hubbard model discussed in the previous section.

For the d-wave pairing, in the limit  $|z| \ll 1$ , the function  $I_2(\xi)$  defined by equation (17) can be expressed in terms of elliptic integrals

$$I_2(\xi) = \frac{1}{2\nu_0\pi^3 t_0 a^2} \sum_{s \in \{-, +\}} \frac{1}{4 - z_s^2} \left[ 4 \cos^2 \alpha_2 \mathbf{F} \left( \frac{\pi}{2}, \frac{\sqrt{4 - z_s^2}}{2} \right) + 4 \sin^2 \alpha_2 \mathbf{E} \left( \frac{\pi}{2}, \frac{\sqrt{4 - z_s^2}}{2} \right) - \sin^2 \alpha_2 z_s^2 \mathbf{F} \left( \frac{\pi}{2}, \frac{\sqrt{4 - z_s^2}}{2} \right) - 4 \cos^2 \alpha_2 \mathbf{E} \left( \frac{\pi}{2}, \frac{\sqrt{4 - z_s^2}}{2} \right) \right]$$

where  $z_{\pm} = (\pm\xi + t_2)/2t_0$ , and  $\mathbf{E}(\psi, \kappa)$  is the complete elliptic integral of the second kind. On the other hand, within the Van Hove scenario (cf equation (18)) one obtains

$$I_2(\xi) = \frac{1}{4v_0\pi^3 t_0 a^2} \sum_{s \in \{-, +\}} \mathbf{F}\left(\frac{\pi}{2}, \frac{\sqrt{4 - z_s^2}}{2}\right).$$

Although in the case of the p-wave pairing the results cannot be written in terms of elliptic integrals, one can clearly demonstrate the difference in the results obtained when employing the two discussed methods. Recall that for all states (13) the Van Hove scenario yields

$$I_2(\xi) \equiv I_0(\xi) = \frac{1}{2v_0} [\langle \mathcal{K}(-\xi, \varphi) \rangle + \langle \mathcal{K}(\xi, \varphi) \rangle] = \frac{1}{2v_0} [v(-\xi) + v(\xi)]$$

where  $\langle \dots \rangle$  denotes averaging over the angle  $\varphi$ .

For the states with  $\alpha_1 = 0$  and  $\alpha_1 = \pi/2$  the property of the kernel  $\mathcal{K}(\xi, \varphi) = \mathcal{K}(\xi, \pi/2 - \varphi)$  yields

$$\langle \mathcal{K}(\xi, \varphi) \sin^2 \varphi \rangle = \langle \mathcal{K}(\xi, \varphi) \cos^2 \varphi \rangle = \frac{1}{2} \langle \mathcal{K}(\xi, \varphi) \rangle = \frac{1}{2} v(\xi).$$

Hence, one can state that the function  $I_2(\xi)$ , defined by equation (17), evaluated in the conformal transformation method, takes the form

$$I_2(\xi) = \frac{1}{4v_0} [v(-\xi) + v(\xi)]$$

which is exactly a half of the value obtained within the former approach. Note that, in general, for an arbitrary value of the parameter  $\alpha_1$ , equation (17) is of the form

$$I_2(\xi) = \frac{1}{4v_0} \{v(-\xi) + v(\xi) + [\langle \mathcal{K}(-\xi, \varphi) \sin 2\varphi \rangle + \langle \mathcal{K}(\xi, \varphi) \sin 2\varphi \rangle] \sin 2\alpha_1\}$$

which proves that the enhancement of the transition temperature depends on orientation of the order parameter in the momentum space.

## 5. Conclusions

The established formalism based on the conformal transformation of the momentum space allows us to study crystals being both conductors, such as normal metals, or superconductors, such as A15 compounds with normal and paramagnetic impurities, 2D-like cuprates, as well as 3D-like bismuthates, Chevrel phases, heavy-fermion metals, etc [28, 30, 31]. Within this method one can precisely estimate the values of transition temperatures for new kinds of materials, e.g.,  $\text{MgB}_2$ ,  $\text{Mg}^{10}\text{B}_2$  and  $\text{Mg}^{11}\text{B}_2$  [32–34] with  $T_c$  as high as 40 K. It could also be applied to the re-investigation of novel, exotic, disordered superconductors with s-, d- [35–37] and p-wave pairing [38–41].

In the established method we assume that the dispersion relation  $\xi(p_1, p_2)$  which reflects many-particle interactions, effects of doping and other processes in real crystals in the normal phase, is an arbitrary differentiable function. Since in general  $\xi(p_1, p_2)$  is a very composed function, its form can be derived approximately or found from experiments. In real crystals the form of  $\xi(p_1, p_2)$  is modified by changes of stoichiometric relations and crystal structure deformations. The kernel of the density of states  $\mathcal{K}(\xi, \varphi)$  must be always derived individually for each fixed function  $\xi(p_1, p_2)$ . The knowledge of  $\mathcal{K}(\xi, \varphi)$  allows us to evaluate some characteristic ratios, e.g., the reduced transition temperature  $T_c/T_{c0}$ . Hence, the presented method constitutes a mapping from the stoichiometry and structure of a real crystal, through the dispersion relation and the kernel of the density of states, to the transition temperature and other thermodynamic properties. Consequently, the transition temperature is a nonlinear

functional of the dispersion relation, determined by parameters of a real crystal, therefore employing calculus of variations one can maximize the transition temperature.

On the other hand, evaluating the characteristic ratios for the s-wave paired system one can replace the kernel of the density of states  $\mathcal{K}(\xi, \varphi)$  by its average value  $\langle \mathcal{K}(\xi, \varphi) \rangle = \nu(\xi)$ . Then if  $\nu(\xi)$  is comparable for some dissimilar superconductors, i.e. systems with different dispersion relations, these superconductors reveal similar thermodynamic properties and can be classified together. Such classification can also be performed in the case of dissimilar (in the same sense as above) superconductors with anisotropic energy gap. However, in this case the criterion will be the compatibility of the expressions  $I_{2n}(\xi)$  defined by equation (17). Hence, the established formalism allows us to classify superconductors with respect to their thermodynamic properties on the basis of the integral functions  $I_{2n}(\xi)$  originating from the dispersion relation.

Within the established formalism based on the conformal-like transformation the second coordinate  $\phi$  in the mapping  $(p_1, p_2) \rightarrow (\xi, \phi)$  can be chosen as a function of another variable, arbitrarily. However, when the new variable is identified with the angular variable of the polar coordinate system and the kernel of the density of states is replaced by the standard density of states, i.e.  $\mathcal{K}(\xi, \varphi) \equiv \nu(\xi)$ , the present formalism reduces to the Van Hove scenario, which is suitable for s-wave superconductors only. Hence, the present approach can be treated as an extended Van Hove scenario.

In our previous papers [30, 31], a tight-binding model for a rectangular lattice including the nearest and the next-nearest neighbours hopping parameters has been considered. Employing a similar method we have derived complete forms of the density of states. Although the density of states has been expressed by the elliptic function of the first kind, and it reduces to the logarithmic form at the saddle point of the Van Hove singularity, the obtained formulae are not identical to some others [19, 42, 43] obtained by employing equation (2). Therefore the valuations achieved herein are evidence for the incompleteness of the Van Hove scenario.

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