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Competition mechanism between singlet and triplet superconductivity in the tight-binding model with anisotropic attractive potential

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Abstract. Based upon the tight-binding formalism a model of a high-T_c superconductor with isotropic and anisotropic attractive interactions is considered analytically. Symmetry facets of the group C_{4v} are included within a method of successive transformations of the reciprocal space. Complete sets of basis functions of C_{4v} irreducible representations are given. Plausible spin-singlet and spin-triplet superconducting states are classified with regard to the chosen basis functions. It is displayed that pairing interaction coefficients and the dispersion relation, which can be characterized by the parameter $\eta = 2t_1/t_0$, have a diverse and mutually competing influence on the value of the transition temperature. It is also shown that in the case of a nearly half-filled conduction band and an anisotropic pairing interaction the spin-singlet d-wave symmetry superconducting state is realized for small values of the parameter η, whereas in the opposite limit, for sufficiently large values, the spin-triplet p-wave symmetry superconducting state has to be formed. This result cannot be obtained within the Van Hove scenario or BCS-type approaches, where the p-wave symmetry superconducting state absolutely dominates. The specific heat jump and the isotope shift as functions of the parameter η are assessed and discussed for the d-wave symmetry singlet and the p-wave symmetry triplet states.

PACS. 74.20.Rp Pairing symmetries (other than s-wave) – 74.62.Yb Other effects

1 Introduction

In the present views on high-T_c superconductors it is accepted that due to the layered structure of copper oxides, carriers within the CuO_2 planes should be considered as a quasi-2D system of fermions. Although in some approaches, where model parameters allow one to gradually include the third dimension corrections, it is inferred that in a nearly antiferromagnetic or nearly ferromagnetic metal the electronic structure is quasi-2D and strongly anisotropic, but magnetic interactions are not exactly two-dimensional [1].

Consequently, the main applied approaches base on the 2D tight-binding band model or the 2D t–J model and the quantum Monte Carlo method. Then the one-particle (hole or electron) band-structures as well as the transformed dispersion relation of one hole in an AF background are characterized by 2D Fermi surface nesting [1–3].

On the other hand in some more composed approaches superconductivity is considered as a mixture of coexisting local pairs and itinerant fermions coupled via a charge exchange mechanism [4,5], or additional terms of energy are included, such as the formation energy of the Zhang-Rice singlet [6] or the Peierls phase factor, responsible for the diamagnetic response of the system [7]. Such approaches, which find their origin in a proposed model of the anisotropic Fermi liquid [8], allow one to display various types of superconducting behavior.

Moreover, experimental data and studies of the electron-phonon interaction in strongly correlated superconducting cuprates within the t–J model supply a direct evidence of a phonon contribution to the pairing interaction [6,9], similarly to the mixed phononic and electronic model, where the phononic pairing occurs between holes strongly dressed by AF fluctuations [2]. However, we have to emphasize that there are also some other approaches where the pairing mechanism can be of magnetic origin, as in the magnetic interaction model which is mathematically analogous to the conventional electron-phonon problem with the generalized magnetic susceptibility playing the role of the phonon propagator [1].

Therefore, in the model presented below, boson-mediated attractions providing pairing interaction channels are included. In order to estimate the transition temperature enhancement, the Van Hove scenario (VHS) employing a singular form of the density of states is

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applied [10–19]. However, the idea of VHS — where high-T_c superconductivity is achieved with the aid of a sharp peak in the density of states (DOS) in the vicinity of the Fermi level — cannot be accepted if the pairing interaction is a function of the momentum space coordinates and cannot be considered as constant. In this case the extended VHS approach must be applied [3,20].

2 Model

The effective interaction between quasiparticles in strongly correlated systems is very complex. In particular, it depends on the spin and the current carried by quasiparticles. Since for such superconducting systems, the conventional phonon-mediated pairing mechanism raises doubts, a generic, boson-mediated, strongly anisotropic pairing mechanism is assumed [1,3].

For two-dimensional models of high-T_c superconductivity, the boson-mediated pairing mechanism corresponding to on-site and nearest-neighbor interactions allows us to obtain the attractive interaction in the reciprocal space in the form (here $a_x = a_y = 1$) [3,21–23]

$$V(\mathbf{k},\mathbf{k}') = -V_0 - V_1[\cos(k_x - k_x') + \cos(k_y - k_y')], \quad (1)$$

which consists of two channels: the isotropic channel with the amplitude V_0, and the anisotropic one with the amplitude V_1. The attractive character of each channel is provided when V_0, V_1 are positive. This interaction, after some transformations, can be rewritten as

$$V(\mathbf{k},\mathbf{k}') = V^s(\mathbf{k},\mathbf{k}') + V^a(\mathbf{k},\mathbf{k}'),$$

where $V^s(\mathbf{k},\mathbf{k}') = V^s(-\mathbf{k},\mathbf{k}') = V^s(\mathbf{k},-\mathbf{k}')$ and $V^a(\mathbf{k},\mathbf{k}') = -V^a(-\mathbf{k},\mathbf{k}') = -V^a(\mathbf{k},-\mathbf{k}')$ are the spin-singlet and the spin-triplet pairing potentials, respectively, and they can be written in the following separated forms

$$\begin{aligned} V^s(\mathbf{k},\mathbf{k}') &= -V_0 - V_1(\cos k_x \cos k_x' + \cos k_y \cos k_y') \\ &= -V_0 - \frac{1}{2}V_1(\cos k_x + \cos k_y)(\cos k_x' + \cos k_y') \\ &\quad -\frac{1}{2}V_1(\cos k_x - \cos k_y)(\cos k_x' - \cos k_y'), \quad (2) \\ V^a(\mathbf{k},\mathbf{k}') &= -V_1(\sin k_x \sin k_x' + \sin k_y \sin k_y'). \quad (3) \end{aligned}$$

On the other hand the hopping mechanism coming from the 2D tight-binding model, when the nearest-neighbor and the next-nearest-neighbor integrals are taken into account, leads to the following dispersion relation

$$\xi_{\mathbf{k}} = -2t_0(\cos k_x + \cos k_y + \eta \cos k_x \cos k_y) - \mu_0, \quad (4)$$

where $\eta = 2t_1/t_0 < 1$, and t_0, t_1 represent the nearest-neighbor and the next-nearest-neighbor hopping integrals, respectively [24]. The chemical potential μ_0 fixes a shift of the Fermi level at $T = 0$ in the case of doping and a non-half-filled band, and it has been introduced in order to control the carrier concentration n ($0 < n < 1$) [7,8,14,20,25–27]. In the case of the 2D t–J model the quantum Monte Carlo method yields the one-hole dispersion relation in the AF background in the form

$$\xi_{\mathbf{k}} = -4t' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y) - \mu_0, \quad (5)$$

which corresponds to the 2D tight-binding band model where the nearest-neighbor hopping is absent ($t_0 = 0$), as in the case of a hole moving within the same sublattice to avoid distorting the antiferromagnetic background. Symbols t' and t'' denote hopping integrals between the second- and the third-nearest-neighbor Cu sites on the CuO_2 plane. The dispersion relation (5) can be transformed to the form (4) after performing changes of the momentum space variables $k_x \mapsto (k_x + k_y)/\sqrt{2}$, $k_y \mapsto (k_x - k_y)/\sqrt{2}$, replacing the lattice constant 1 by $\sqrt{2}$, and t' by t_0 as well as t'' by t_1. Since now $\eta = 2t''/t'$, the case $\eta > 1$ can be also considered [29].

Symmetry elements of the cuprate plane CuO_2 correspond to the group C_{4v}. Hence, for a two-dimensional momentum space the subsets of basis functions of irreducible representations of the group C_{4v} are usually taken in the following simplest forms (cf. Appendix A)

$$\{\cos k_x + \cos k_y\}, \quad (6)$$
$$\{\cos k_x - \cos k_y\}, \quad (7)$$
$$\{\sin k_x \sin k_y\}, \quad (8)$$
$$\{\sin k_x \sin k_y (\cos k_x - \cos k_y)\} \quad (9)$$
$$\{\sin k_x, \sin k_y\}. \quad (10)$$

Since the basic function of the first subset (6) corresponds to the trivial irreducible representation, instead of it the function equal to unity is also sometimes assumed. Then this set is replaced by $\{1\}$. All these functions are chosen to be invariant under translations by the reciprocal lattice vectors [30]. We emphasize that the above choice is one of many possible and these functions can be replaced by some more composed forms. In particular, multiplying them by $(1 - \cos k_x \cos k_y)^{-1}$ results in setting up another (more composed) set of functions being invariants of the group C_{4v} [20]. Moreover, the subset of basis functions corresponding to the irreducible representations can be taken e.g. as

$$\{\cos k_x + \cos k_y + \eta_1 \cos k_x \cos k_y\}, \quad (11)$$
$$\{(\cos k_x - \cos k_y)[1 + \eta_2(\cos k_x + \cos k_y)]\}, \quad (12)$$
$$\{\sin k_x \sin k_y [1 + \eta_3(\cos k_x + \cos k_y)]\}, \quad (13)$$
$$\{\sin k_x \sin k_y (\cos k_x - \cos k_y)[1 + \eta_4(\cos k_x + \cos k_y)]\}, \quad (14)$$
$$\{\sin k_x[1+\eta_5(\cos k_x+\cos k_y)], \sin k_y[1+\eta_5(\cos k_x+\cos k_y)]\}, \quad (15)$$

where $\eta_1, \eta_2, \ldots, \eta_5$ are real numbers.

The functions (6)–(8), which are invariants of the group C_{4v}, are usually applied to represent the pairing interaction $V(\mathbf{k},\mathbf{k}')$ in accordance with equations (2) and (3). Instead, the dispersion relation (4) can be expressed by means of the function (11) which is another invariant of the group C_{4v} fixed for the trivial irreducible representation. Although symmetry properties of the functions (6) and (11) defined by elements of the group C_{4v} are identical, these functions are not equivalent, except for the case $\eta_l = 0$. It means that if $\eta_l \neq 0$ two different sets of basis functions appear.

In some approaches to high-T_c superconductors the pairing interaction is assumed to be of a charge-coupled type mediated by bosons. Then the maximum boson energy ω_c is identified with the cut-off parameter imposed on the one-particle energy. The high-T_c superconductor is considered as a metallic system with a narrow, nearly but less than half-filled ($n \simeq 0.5$) conduction band of the width $2\omega_c$, where a non-zero pairing interaction covers the whole conduction band. The dispersion relation is taken in the form (4), thus $\mu_0 \simeq 0$ and $\mu_0 > 0$. The particle energy is localized within the conduction band, so it also satisfies the condition $-\omega_c \le \xi_{\mathbf{k}} \le \omega_c$. Moreover, the particle energy is much less than the Fermi energy E_F, i.e. $\xi_{\mathbf{k}} \ll E_F$. Therefore, in most of the discussed systems, one can assume that all regular functions of $\xi_{\mathbf{k}}$ vary slightly within the confined region of the width $2\omega_c$, and the order parameter can be considered as independent of $\xi_{\mathbf{k}}$.

In other approaches stability of various symmetry superconducting states is studied when the shape of the Fermi surface is modified as the quasiparticle concentration n and hence μ_0 are being changed. However, in this case the simplified form of the dispersion relation was taken into account. Including only the effective parameter t_0 ($\eta = 0$) Micnas et al. [26] determined the dependence of the critical temperature T_c on the concentration n, for a quasi-2D lattice, within the self-consistent RPA method, and they observed a non-monotonic dependence of T_c on n. Kuboki [27] in more precise considerations determined the phase diagram and clarified the reason for the change of the symmetry of the superconducting state due to the change of the band structure. The main results, which refer to the case $t_1 = 0$ ($\eta = 0$), show that the d-wave state is stabilized near half-filling ($\mu_0 \approx 0$), while an extended s-wave state is formed at high ($n \to 1$) and low ($n \to 0$) concentrations. In the region between d- and s-wave states spin-triplet p-wave states appear. Instead, in the case $t_1 \neq 0$ and $t_0 = 0$, p-wave states appear at and near to the half-filling, and d- or extended s-wave states are formed away from half-filling.

Recently we have shown [8,20] that after a curvilinear transformation for the dispersion relation of the form (4) with $\eta = 0$ is performed, there appears a new function — the kernel of the density of states describing the local deformation or modification of quantum-mechanical states in the (ξ, φ)-space, where the angular variable $0 \le \varphi < 2\pi$ is the same as introduced in the standard polar coordinate system. This kernel of the density of states can be written in the form

$$\mathcal{K}(\xi, \varphi) = \frac{1}{4\pi t_0} \frac{1}{\sqrt{z^2 \cos^2 2\varphi + 4 \sin^2 2\varphi}},$$

where $z = \xi / 2t_0$ and $\xi_{\mathbf{k}}$ was replaced by $\xi - \mu_0$. Note that it satisfies the conditions $\mathcal{K}(\xi, \varphi) = \mathcal{K}\left(\xi, \varphi + \frac{\pi}{2}\right)$ and $\mathcal{K}(\xi, \varphi) = \mathcal{K}\left(\xi, \frac{\pi}{2} - \varphi\right)$, which are imposed by the symmetry group C_{4v}. Moreover, if $\varphi = 0$ or $\varphi = \frac{\pi}{2}$ the function $\mathcal{K}(\xi, \varphi) \sim z^{-1}$ and it has no singularities except for the case when $z \to 0$. Since this particular divergence does not vanish after averaging over φ, and

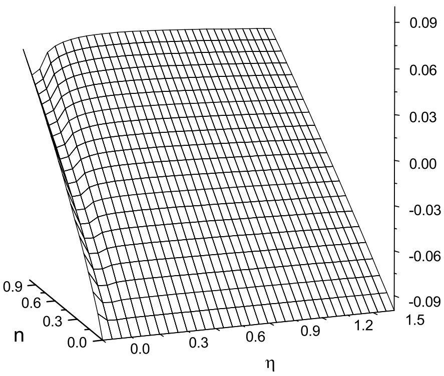

Fig. 1. The relation between μ_0 — a shift of the Fermi level, n — quasiparticle concentration and $\eta = 2t_1/t_0$. For nearly half-filled conduction band, $n \simeq 0.5$, one can assume $\mu_0 \simeq 0$ for all η.

$$\nu(\xi) = \int_0^{2\pi} \frac{d\varphi}{2\pi} \mathcal{K}(\xi, \varphi) \tag{16}$$

is the density of states (cf. Appendix B), it is always revealed in the DOS as the Van Hove singularity [8,12,14,17,31–33].

The gap equation in the momentum space, obtained in a self-consistent manner after employing the Green function formalism

$$\mathbf{\Delta_k} = \sum_{\mathbf{k}'} V(\mathbf{k}, \mathbf{k}') \frac{\mathbf{\Delta}_{\mathbf{k}'}}{E_{\mathbf{k}'}} \tanh \frac{E_{\mathbf{k}'}}{2T}, \tag{17}$$

where $E_{\mathbf{k}} = \sqrt{(\xi_{\mathbf{k}} - \mu(T))^2 + \mathbf{\Delta}_{\mathbf{k}}^2}$, along with another self-consistent equation

$$2n = \frac{1}{N} \sum_{\mathbf{k}} \left(1 - \frac{\xi_{\mathbf{k}} - \mu(T)}{E_{\mathbf{k}}} \tanh \frac{E_{\mathbf{k}}}{2T} \right), \tag{18}$$

which determines the total chemical potential i.e. μ_0 included in $\xi_{\mathbf{k}}$ and being a function of the conduction band filling n for the normal metallic phase at $T = 0$, and $\mu(T)$ expressing its temperature correction ($\mu(0) = 0$), constitute the basic equations for theoretical investigations of high-T_c superconductors. Here N denotes the total number of lattice sites.

Equation (18) in the limit $\Delta = 0$ and $T = 0$ can be employed in order to derive a relation between μ_0, n and η. The obtained relation, which can be easily derived within the present formalism, is given in Figure 1.

In the present paper we show that the basic equations studied within the tight-binding band model or a model adopted from the t–J model, after a sequence of curvilinear transformations of the coordinate system can be formulated in analytic forms depending on ξ and φ. Hence, the separated pairing interaction varies slightly in the confined region of the width $2\omega_c$, and all expressions which are functions of φ satisfy the symmetry conditions of the group C_{4v}. In such an approach, the spatial structure of the order parameter is determined by a predominant coefficient of expansion in the Fourier series in the angle φ, where odd (even) terms of the Fourier expansion must be omitted for antisymmetric (symmetric) spin pairing because of the Pauli exclusion principle.

3 Method of successive transformations

Our aim is to prove that a successive execution of some specific transformations of a two-dimensional space allows us to turn all expressions in equations (17) and (18) into functions of ξ and φ, where in the transformed integral equations an additional expression appears, namely the product of Jacobians of successive transformations (cf. Appendix B). In Appendix B we show that every change of integration variables can be formally treated as a transformation of the integration region (here in a two-dimensional space), where the deformation of the surface of the new region is taken into account by means of the Jacobian of the transformation. The product of Jacobians of the successive transformations forms the Jacobian of the complete transformation. Therefore, replacing finally the summation over quantum-mechanical states by the integration over the particle energy, the following formula can be achieved

$$\sum_{\mathbf{k}} \ldots = \int d\xi \int_0^{2\pi} \frac{d\varphi}{2\pi}\, \mathcal{K}(\xi,\varphi)\ldots,$$

where according to equation (B.8), $\mathcal{K}(\xi,\varphi) = \frac{2}{(2\pi)^2}\,\mathcal{J}(\xi,\varphi)$ is the kernel of the density of states corresponding to the local deformation or modification of quantum-mechanical states in the (ξ,φ)-space, and the density of states is given by equation (16).

The imposed symmetry of the model under consideration, which is of the group C_{4v}, allows us to limit our investigation to the quadrant $k_x,k_y \geq 0$. Then

$$\sum_{\mathbf{k}} \ldots = \frac{8}{(2\pi)^2}\int_0^{\pi} dk_x \int_0^{\pi} dk_y \ldots, \tag{19}$$

where the integration region corresponds to the appropriate part of the Brillouin zone $0 \leq k_x \leq \pi, 0 \leq k_y \leq \pi$ with the binding condition

$$-\omega_{\mathrm{c}} \leq \xi_{\mathbf{k}} + \mu_0 \leq \omega_{\mathrm{c}}. \tag{20}$$

3.1 The first transformation

We define the following transformation of the momentum space

$$k_x = \arccos(1-2x), \qquad k_y = \arccos(1-2y).$$

The corresponding Jacobian is of the form

$$J_1(x,y) = \frac{4}{\sqrt{1-(1-2x)^2}\,\sqrt{1-(1-2y)^2}}, \tag{21}$$

and the previous integration region becomes replaced by $0 \leq x \leq 1, 0 \leq y \leq 1$. Hence, the rhs of equation (19) should be replaced by

$$\frac{8}{(2\pi)^2}\int_0^1 dx \int_0^1 dy\, J_1(x,y)\ \ldots,$$

and the dispersion relation (4) obtains the form

$$z = -(1-2x) - (1-2y) - \eta(1-2x)(1-2y), \tag{22}$$

where $z = \xi/2t_0$.

3.2 The conformal-like transformation

In order to make ξ one of the integration variables we perform a conformal-like transformation [34]. Referring to the formula (22) we have the relation

$$\nabla\xi(x,y) = 4t_0\,[1+\eta(1-2y),\, 1+\eta(1-2x)],$$

which allows us to formulate the differential equation

$$\frac{dy}{dx} = \frac{1+\eta(1-2x)}{1+\eta(1-2y)}.$$

The solutions of this equation, by virtue of Picard's theorem, always exist and they form a one-parameter family of integral curves

$$\phi(x,y) = 2\,[(1+\eta)y - \eta y^2 - (1+\eta)x + \eta x^2], \tag{23}$$

which isoclines $\phi(x,y) = C$ are perpendicular to equi-energy lines $\xi(x,y) = C'$ because $\nabla\xi(x,y)\cdot\nabla\phi(x,y) = 0$.

Let us remark now, that equations (22) and (23) can be read as

$$1 - \eta\, z = XY, \qquad 2\eta\phi = X^2 - Y^2, \tag{24}$$

where $X = 1+\eta-2\eta x$, $Y = 1+\eta-2\eta y$. In order to simplify the calculation we derive the following Jacobian

$$J_2'(x,y) = \begin{vmatrix} \frac{\partial\xi}{\partial x} & \frac{\partial\xi}{\partial y} \\ \frac{\partial\phi}{\partial x} & \frac{\partial\phi}{\partial y} \end{vmatrix} = 8t_0\left(X^2+Y^2\right).$$

Hence employing the relation (B.4), we state that the Jacobian of the current transformation can be expressed as

$$J_2(\xi,\phi) = \frac{1}{8t_0}\,\frac{1}{X^2+Y^2}, \tag{25}$$

where X and Y should be found as functions of ξ and ϕ based on equations (24). Moreover, the previous integral region becomes replaced by (cf. [3])

$$\begin{aligned} -2-\eta \leq z \leq 2-\eta \qquad &\text{if} \qquad \eta \leq 1, \\ -2-\eta \leq z \leq \eta \qquad &\text{if} \qquad \eta \geq 1, \end{aligned}$$

and hence $-\phi_0(\xi) \leq \phi \leq \phi_0(\xi)$, where

$$\phi_0(\xi) = \begin{cases} \frac{1}{2(1+\eta)^2}\left(2+\eta+\frac{\xi}{2t_0}\right)\left(2+2\eta+\eta^2-\eta\frac{\xi}{2t_0}\right) & \text{if } \frac{\xi}{2t_0} \leq \eta \\ \frac{1}{2(1-\eta)^2}\left|2-\eta-\frac{\xi}{2t_0}\right|\left|2-2\eta+\eta^2-\eta\frac{\xi}{2t_0}\right| & \text{if } \frac{\xi}{2t_0} \geq \eta. \end{cases}$$

Now, the rhs of equation (19) obtains the form

$$\frac{8}{(2\pi)^2}\int_{-\omega_c}^{\omega_c} d\xi \int_{-\phi_0}^{\phi_0} d\phi\, J_1^{(1)}(\xi,\phi) J_2(\xi,\phi)\,\ldots,$$

where the variable ξ satisfies the condition (20), so $|\xi| \lll 2t_0$. We also include that after expressing x and y as functions of ξ and ϕ the Jacobian $J_1(x,y)$ obtains the form $J_1^{(1)}(\xi,\phi)$.

3.3 The third transformation

Since our aim is to transform the coordinate system in such a way that one of the coordinates is the particle energy ξ and the second one is chosen as the angular variable φ, and the symmetry of the system in the introduced coordinate system (ξ,φ) is conserved, we can define the variable φ according to the relation $y = x\tan\varphi$. Then from equations (24) we obtain the formula

$$\phi = 2(\tan\varphi - 1)\,x\left[1+\eta-\eta(1+\tan\varphi)\,x\right], \tag{26}$$

where

$$x = \frac{(1+\eta)(1+\tan\varphi)}{4\eta\tan\varphi} - \frac{\sqrt{(1+\eta)^2(1+\tan\varphi)^2 - 4\eta\left(2+\eta+\frac{\xi}{2t_0}\right)\tan\varphi}}{4\eta\tan\varphi},$$

which has the following property: if we replace φ by $\pi/2-\varphi$ then $\phi \longrightarrow -\phi$. Since in the limit $\varphi \to 0$ or $\eta \to 0$ the formula (26) is reduced to the following simple form

$$\phi = \phi_0(\xi)\,\frac{\tan\varphi - 1}{\tan\varphi + 1},$$

which retains the demanded symmetry, we define the next transformation of the plane as

$$\xi = \xi, \qquad \phi(\xi,\varphi) = \phi_0(\xi)\,f(\varphi), \tag{27}$$

where

$$f(\varphi) = \frac{\sin\varphi - \cos\varphi}{\sin\varphi + \cos\varphi}, \tag{28}$$

and $-1 \leq f(\varphi) \leq 1$ for $0 \leq \varphi \leq \pi/2$, which is taken from the integral region. The Jacobian of this transformation has the form

$$J_3(\xi,\varphi) = \frac{2}{1+\sin 2\varphi}\,\phi_0(\xi). \tag{29}$$

Finally, the rhs of equation (19) becomes

$$\frac{8}{(2\pi)^2}\int_{-\omega_c}^{\omega_c} d\xi \int_0^{\pi/2} d\varphi\, \mathcal{J}(\xi,\varphi)\,\ldots,$$

where $\mathcal{J}(\xi,\varphi) = \mathcal{J}_1^{(2)}(\xi,\varphi)\mathcal{J}_2^{(1)}(\xi,\varphi)\mathcal{J}_3(\xi,\varphi)$ is the total Jacobian of the specified transformations, and the Jacobians $\mathcal{J}_1^{(2)}(\xi,\varphi)$ and $\mathcal{J}_2^{(1)}(\xi,\varphi)$ are obtained from $\mathcal{J}_1^{(1)}(\xi,\phi)$ and $\mathcal{J}_2(\xi,\phi)$, respectively, after replacing ϕ by ξ and φ according to the relations (27).

3.4 Kernel of the density of states

In order to derive the explicit form of the Jacobian $\mathcal{J}(\xi,\varphi)$, and hence the kernel of the density of states $\mathcal{K}(\xi,\varphi)$, we have to solve equations (24). After some algebra we obtain

$$X \equiv X(\xi,\varphi) = \left[\sqrt{\left(1-\eta\frac{\xi}{2t_0}\right)^2 + \eta^2\phi_0^2(\xi)\,f^2(\varphi)} + \eta\phi_0(\xi)\,f(\varphi)\right]^{\frac{1}{2}}$$

and

$$Y \equiv Y(\xi,\varphi) = \left[\sqrt{\left(1-\eta\frac{\xi}{2t_0}\right)^2 + \eta^2\phi_0^2(\xi)\,f^2(\varphi)} - \eta\phi_0(\xi)\,f(\varphi)\right]^{\frac{1}{2}}.$$

Note that $X(\xi,\frac{\pi}{2}-\varphi) = Y(\xi,\varphi)$. Moreover, $x(\xi,\varphi) = \frac{1}{2\eta}\left[1+\eta-X(\xi,\varphi)\right]$ and $y(\xi,\varphi) = \frac{1}{2\eta}\left[1+\eta-Y(\xi,\varphi)\right]$. Hence, employing equations (21), (25) and (29) we find

$$\mathcal{K}(\xi,\varphi,\eta) = \frac{\eta^2}{4\pi t_0}\,\frac{1}{\sqrt{\eta^2-\left[X(\xi,\varphi)-1\right]^2}\sqrt{\eta^2-\left[Y(\xi,\varphi)-1\right]^2}} \times \frac{1}{\left[X(\xi,\varphi)\right]^2+\left[Y(\xi,\varphi)\right]^2}\,\frac{1}{1+\sin 2\varphi}\,\phi_0(\xi),$$

where we also include the fact that the kernel of the density of states depends on the parameter η. Consistently, we the density of states (16) takes the form

$$\nu(\xi,\eta) = \frac{2}{\pi}\int_0^{\pi/2} d\varphi\,\mathcal{K}(\xi,\varphi,\eta). \tag{30}$$

The forms of $\mathcal{K}(\xi,\varphi,\eta)$ for a few chosen values of the parameter η are given in Figure 2.

4 Pairing potential

The form of the symmetric and the antisymmetric (in the momentum space) pairing potentials, which are responsible for the formation the spin-singlet, i.e. $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$,

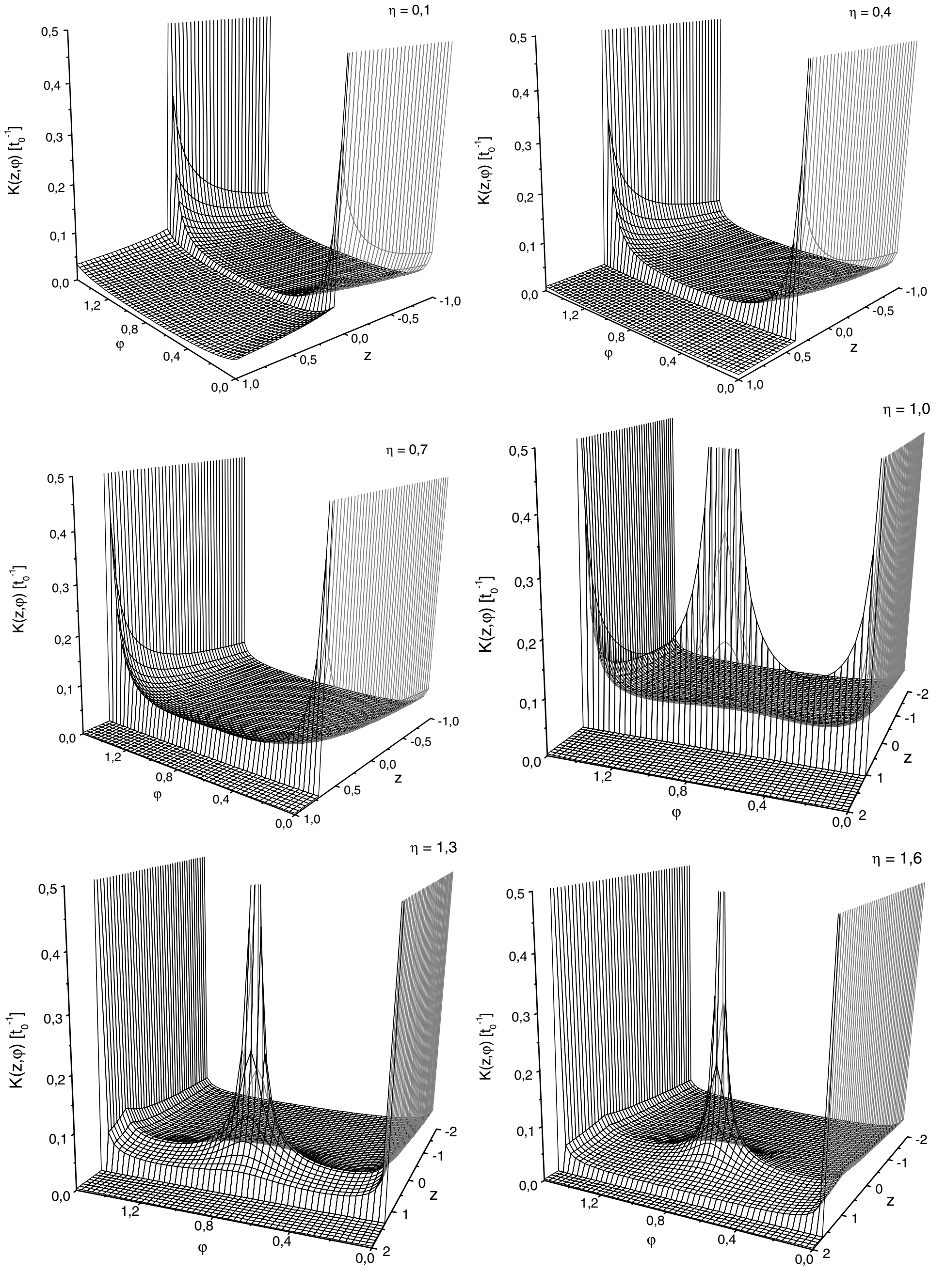

Fig. 2. The kernel of the density of states for different values of the parameter η, where $z = \xi/2t_0$.

($S = 0$, $M = 0$), s-, d-, g-wave, etc. and the spin-triplet i.e. $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$, ($S = 1$, $M = 0$), p-, f-wave, etc. Cooper pairs, respectively, are given by equations (2) and (3). Taking into account that $\cos k_x = \frac{1}{\eta}\,[X(\xi,\varphi) - 1]$, and $\cos k_y = \frac{1}{\eta}\,[Y(\xi,\varphi) - 1]$ we can rewrite the pairing potentials as

$$\begin{aligned} V^s(\xi,\varphi\,;\,\xi',\varphi') = -V_0 - \frac{1}{2\eta^2}\,V_1\,[X(\xi,\varphi) \\ +Y(\xi,\varphi) - 2]\,[X(\xi',\varphi') + Y(\xi',\varphi') - 2] \\ -\frac{1}{2\eta^2}\,V_1[Y(\xi,\varphi) - X(\xi,\varphi)]\,[Y(\xi',\varphi') - X(\xi',\varphi')] \end{aligned} \quad (31)$$

and

$$\begin{aligned} &V^a(\xi,\varphi\,;\,\xi',\varphi') = \\ &-\frac{1}{\eta^2}\,V_1\left\{(\pm)\sqrt{\eta^2 - [X(\xi,\varphi)-1]^2}\,(\pm)\sqrt{\eta^2 - [X(\xi',\varphi')-1]^2}\right. \\ &\left. +\,(\pm)\sqrt{\eta^2 - [Y(\xi,\varphi) - 1]^2}\,(\pm)\sqrt{\eta^2 - [Y(\xi',\varphi') - 1]^2}\right\}, \end{aligned} \quad (32)$$

where the sign (+) or (−) should be taken for appropriate values of φ, φ' ($0 \le \varphi, \varphi' < 2\pi$) according to the symmetry relations of the functions: $\sin k_x$, $\sin k'_x$ and $\sin k_y$, $\sin k'_y$ in the momentum space (cf. Appendix A). Hence, in the numerical analysis we can consider harmonic functions $\sin n\varphi$ and $\cos n\varphi$ of the Fourier series expansion obtained according to the relations given in Appendix C.

4.1 Permissible forms of separated potential

Working with a single Fourier component allows us to study the properties set by each harmonic function while avoiding the application of a number of free Fourier coefficients. Such approach is fully justified if the chosen Fourier component dominates the others. Then the pairing potential can be reduced to one of the following forms

1 pure s-wave pairing

$$\begin{aligned} V^s(\xi,\varphi\,;\,\xi',\varphi') &= -V_0 - V_1\,\chi_0(\xi,\eta)\,\chi_0(\xi',\eta) \\ &= -V_0 - U_0(\eta)\,v_0(\xi,\eta)\,v_0(\xi',\eta); \end{aligned}$$

2 pure p-wave pairing

$$\begin{aligned} &V^a(\xi,\varphi\,;\,\xi',\varphi') \\ &\quad= -2V_1\,\chi_1(\xi,\eta)\,\chi_1(\xi',\eta)\,[\cos\varphi\,\cos\varphi' + \sin\varphi\,\sin\varphi'] \\ &\quad= -2U_1(\eta)\,v_1(\xi,\eta)\,v_1(\xi',\eta)\,[\cos\varphi\,\cos\varphi' + \sin\varphi\,\sin\varphi']; \end{aligned}$$

3 pure d-wave pairing

$$\begin{aligned} V^s(\xi,\varphi\,;\,\xi',\varphi') &= -2V_1\,\chi_2(\xi,\eta)\,\chi_2(\xi',\eta)\,\cos 2\varphi\,\cos 2\varphi' \\ &= -2U_2(\eta)\,v_2(\xi,\eta)\,v_2(\xi',\eta)\,\cos 2\varphi\,\cos 2\varphi'; \end{aligned}$$

4 pure g-wave pairing

$$\begin{aligned} V^s(\xi,\varphi\,;\,\xi',\varphi') &= -2V_1\,\chi_4(\xi,\eta)\,\chi_4(\xi',\eta)\,\cos 4\varphi\,\cos 4\varphi' \\ &= -2U_4(\eta)\,v_4(\xi,\eta)\,v_4(\xi',\eta)\,\cos 4\varphi\,\cos 4\varphi'; \end{aligned}$$

Here $v_l(\xi,\eta) = \chi_l(\xi,\eta)/\bar{\chi}_l(\eta)$, $U_l(\eta) = V_1\,[\bar{\chi}_l(\eta)]^2$, and

$$\bar{\chi}_l(\eta) = \frac{1}{2\omega_c}\int_{-\omega_c}^{\omega_c} \chi_l(\xi,\eta)\,d\xi$$

is the η-dependent mean value of the Fourier coefficient $\chi_l(\xi,\eta)$ in the pairing region. For a fixed value of the parameter η the functions $U_l(\eta)$ modify coupling coefficients of the pairing channel diversely for different l, and hence they have a significant influence on the ultimate choice of the symmetry of the superconducting state, i.e. the angular structure of the order parameter, which coincides with the Cooper pairs wave function of a pure pairing state. In Figure 3 the forms of the Fourier coefficients corresponding to a specific symmetry of the pairing potential are presented for $0 < \eta \leq 1.62$ [24,28,29].

However, in order to analyze the competition between different symmetry types of superconducting states we have to compare the transition temperatures $T_c(l,\eta)$ derived from the gap equation.

4.2 Order parameter and basic equations

Reduction of the pairing potential (1) to one of the separable forms 1–4 causes that the order parameter must be taken as

$$\mathbf{\Delta}(\xi,\varphi,l,\eta) = \mathbf{\Delta}(T)\,v_l(\xi,\eta)\,D(\varphi,l),$$

where $v_0(\xi,\eta) \equiv 1$ if $V_0 \gg V_1$. The angular structure of the order parameter is determined by the Fourier harmonics as follows

$$\begin{aligned} &D(\varphi,0) = 1 && \text{for} \quad s\text{-wave pairing} \\ &D(\varphi,1) = \sqrt{2}\,\cos(\varphi+\beta_1) && \text{for} \quad p\text{-wave pairing} \\ &D(\varphi,2) = \sqrt{2}\,\cos 2\varphi && \text{for} \quad d\text{-wave pairing} \\ &D(\varphi,4) = \sqrt{2}\,\cos 4\varphi && \text{for} \quad g\text{-wave pairing} \end{aligned}$$

where solely $\beta_1 = 0,\ \pm\pi/4,\ \pi/2$ can be included. Then the gap equation (17) can be rewritten in the following standardized form

$$\begin{aligned} 1 = U_l(\eta)\int_0^{2\pi}\frac{d\varphi}{2\pi}\int_{-\omega_c}^{\omega_c} d\xi\;\mathcal{K}(\xi,\varphi,\eta)\,\frac{v_l^2(\xi,\eta)\,D^2(\varphi,l)}{E(\xi,\varphi)} \\ \times\tanh\frac{E(\xi,\varphi)}{2T}, \quad (33) \end{aligned}$$

which is common to models of superconductivity with an arbitrary dispersion relation realized in pure pairing states. Moreover, equation (18) reads

$$\begin{aligned} 2n = \int_0^{2\pi}\frac{d\varphi}{2\pi}\int_{-\omega_c}^{\omega_c} d\xi\;\mathcal{K}(\xi,\varphi,\eta)\,\Bigg[1 - \frac{\xi-\mu}{E(\xi,\varphi)} \\ \times\tanh\frac{E(\xi,\varphi)}{2T}\Bigg], \quad (34) \end{aligned}$$

where $E(\xi,\varphi) = \sqrt{(\xi-\mu)^2 + \mathbf{\Delta}^2(\xi,\varphi)}$, and $\mu = \mu_0 + \mu(T)$. We also define the mean value of the density of states (30) as

$$\nu_0(\eta) = \frac{1}{2\omega_c}\int_{-\omega_c}^{\omega_c} d\xi\,\nu(\xi,\eta). \quad (35)$$

4.3 The BCS-type approximation

Let us concentrate hereafter on the case of nearly half-filled system with $\mu_0 \simeq 0$ and assess the actual pairing coefficients and the transition temperatures applying the BCS-type approximation when $\mu(T) \simeq 0$. Replacing the kernel of the density of states by $\nu_0(\eta)$ and putting $v_l(\xi,\eta) \equiv 1$ we can reduce the gap equation (33) to the BCS-type form. Hence, the actual dimensionless pairing coefficients take the form $\nu_0(\eta)U_l(\eta)/2$ and the transition temperatures can be expressed as

$$T_{c0}(l,\eta) = \frac{2e^{\gamma}}{\pi}\omega_c\exp\left[-\frac{2}{\nu_0(\eta)U_l(\eta)}\right], \quad (36)$$

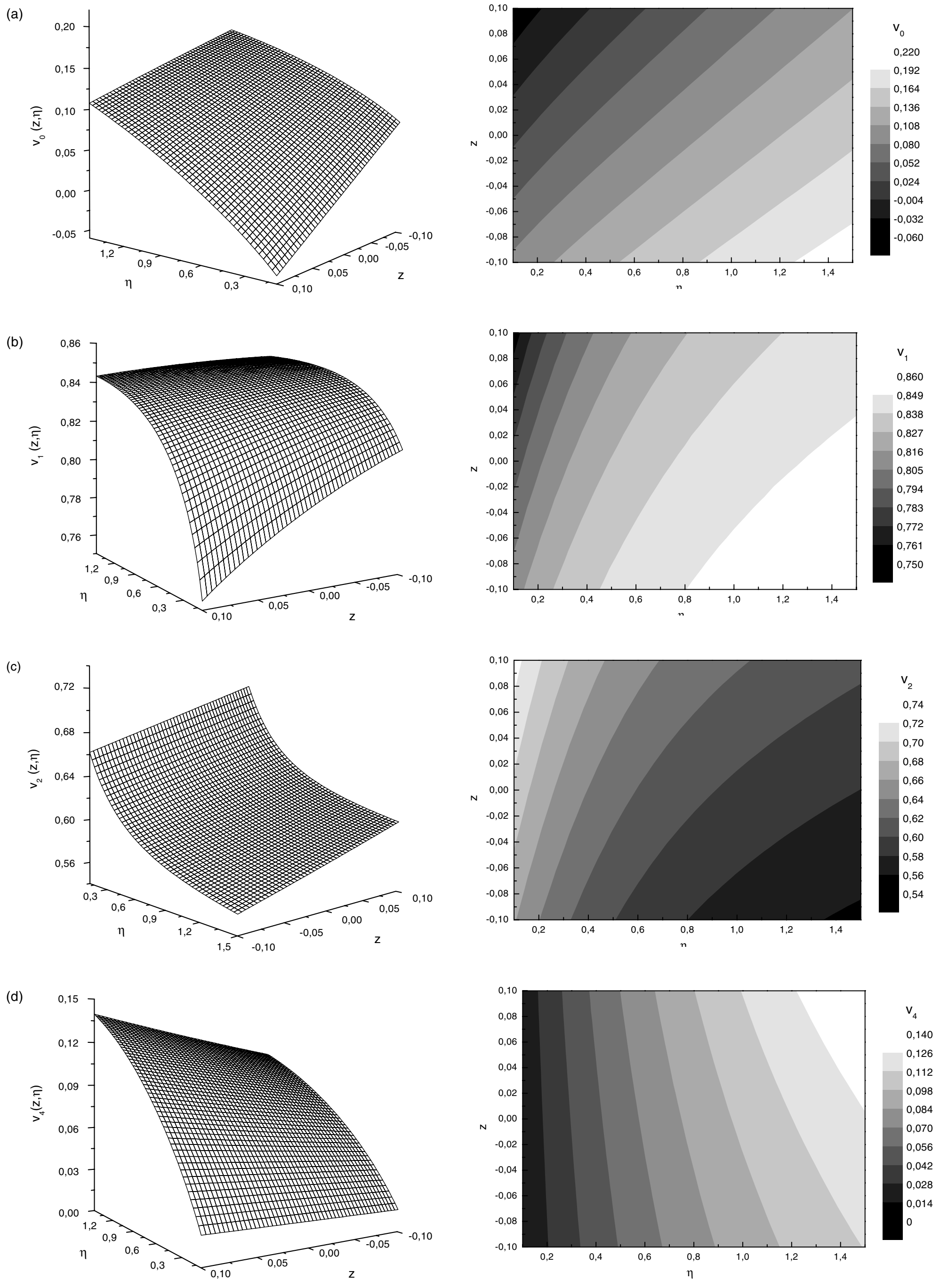

Fig. 3. The Fourier coefficients $\chi_l(\xi,\eta)$ corresponding to: (a) *s*-wave, (b) *p*-wave, (c) *d*-wave, (d) *g*-wave symmetry of the pairing potential for different values of the parameter η, where $z = \xi/2t_0$.

where $\gamma \approx 0.577$ is the Euler constant.

The comparison of forms of the actual pairing coefficients and transition temperatures in the BCS-type approximation are presented in Figures 4a and 4c, respectively. Moreover, in Figure 4b the dependence of the reduced mean value of the density of states on the parameter η is displayed. The obtained results show that within the BCS-type approximation the *d*-wave state is preferred if exclusively spin-singlet pairs can be formed. On the other hand, since $U_1(\eta) > U_2(\eta)$ for all values of η the spin-triplet ($S = 1$, $M = 0$) *p*-wave state is the preferred one, in general. The isotropic *s*-wave pairing could be realized only if the amplitude V_0 dominated over V_1. Then U_0 should be replaced by V_0 and $v_0(\xi,\eta) \equiv 1$. In the opposite case, the anisotropic pairing is preferred.

4.4 Application of the obtained equations

Equations (33) and (34) can be applied to derive the amplitude $\Delta(T)$ of the order parameter and the chemical potential $\mu(T)$ for the superconducting phase with the symmetry corresponding to $l = 0, 1, 2$ or 4. They also allow us to estimate some characteristic parameters of a

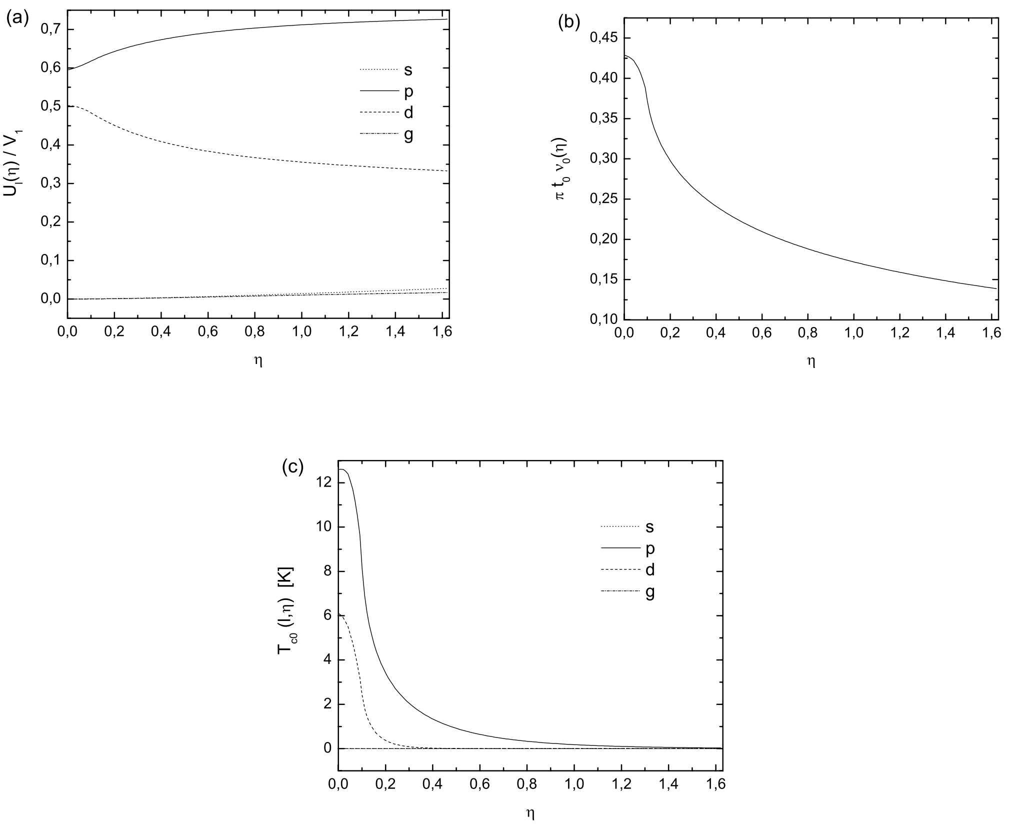

Fig. 4. The BCS-type approximation. (a) The relation between actual s-wave (dot), p-wave (solid), d-wave (dash), g-wave (dash-dot) symmetry pairing coefficients $U_l(\eta)$ and V_1 as functions of η ($0 < \eta \leq 1.62$). (b) The reduced mean value of the density of states $\pi t_0 \nu_0(\eta)$ and (c) the appropriate transition temperatures $T_{c0}(l,\eta)$ for $V_1 = 2\pi t_0$ and $\omega_c \approx 560$ K.

superconductor. Employing algebraic methods as developed in [18,34] and including $z = \xi/2t_0$, $\varsigma = \mu(T)/2t_0$, $c = \omega_c/2t_0$, and substituting $\tau = T/t_0$ we can derive the equation

$$\ln\frac{\tau_c(l,\eta)}{\tau_{c0}(l,\eta)} = \frac{1}{2}\int_{-c}^{c} dz\, \left[\frac{1}{z-\varsigma_c} v_l^2(z,\eta) I_2(z,l,\eta) \times \tanh\frac{z-\varsigma_c}{\tau_c(l,\eta)} - \frac{1}{z}\tanh\frac{z}{\tau_c(l,\eta)}\right], \quad (37)$$

which allows us to evaluate the transition temperature $T_c(l,\eta) = \tau_c(l,\eta)t_0$ with respect to $T_{c0}(l,\eta)$ defined by equation (36), where $\varsigma_c = \mu(T_c)/2t_0$ must be found from equation (34) after putting $\Delta = 0$. Moreover, the reduced value of the specific heat jump at the transition temperature are of the form

$$\frac{\Delta C\,(T_c(l,\eta))}{\nu_1(l,\eta)\,T_c(l,\eta)} = -\frac{8\int_{-c}^{c} dz\, v_l^2(z,\eta) I_2(z,l,\eta)\frac{d}{dz}\tanh((z-\varsigma_c)/\tau_c(l,\eta))}{\tau_c^2(l,\eta)\int_{-c}^{c}\frac{dz}{z-\varsigma_c} v_l^4(z,\eta) I_4(z,l,\eta)\frac{d}{dz}\frac{\tanh((z-\varsigma_c)/\tau_c(l,\eta))}{z}}, \quad (38)$$

where

$$\nu_1(l,\eta) = \frac{\nu_0(\eta)}{2\tau_c}\int_{-c}^{c} dz\, v_l^2(z,\eta)\, I_2(z,l,\eta)\cosh^{-2}\frac{z-\varsigma_c}{\tau_c},$$

$$I_{2n}(z,l,\eta) = \frac{1}{\nu_0(\eta)}\int_0^{2\pi}\frac{d\varphi}{2\pi}\,\mathcal{K}(z,\varphi,\eta)\,D^{2n}(\varphi,l),$$

and $I_0(z,l,\eta) \equiv I_0(z,\eta)$. Moreover, it can be shown that $I_2(z,1,\eta) = I_0(z,\eta)$ [34].

The formulas (37) and (38) allow us to evaluate the characteristic ratios in superconductivity, i.e. T_c/T_{c0} and $\Delta C(T_c)/C_N(T_c)$, where the normal state specific heat

$$C_N(T,\eta) = \frac{4\,\nu_0(\eta)\,T}{\tau^3}\int_{-c}^{c} dz\, I_0(z,\eta)\,(z-\varsigma)^2\cosh^{-2}\frac{z-\varsigma}{\tau}.$$

According to the definition of the isotope shift, $\alpha = -\,\partial\ln T_c/\partial\ln M$, and the relation $T_{c0}M^{1/2} = \text{const.}$, the isotope shift can be found from the formula

$$\alpha(l,\eta) = \frac{1}{2}\left(\frac{\partial\ln T_{c0}(l,\eta)}{\partial\ln T_c(l,\eta)}\right)^{-1}.$$

Hence, employing equation (37) one can find

$$\alpha(l,\eta) = \tau_c(l,\eta) \times\left[\int_{-c}^{c} dz\, v_l^2(z,\eta) I_2(z,l,\eta)\,\cosh^{-2}\frac{z-\varsigma_c}{\tau_c(l,\eta)}\right]^{-1}, \quad (39)$$

where terms of smaller orders are omitted. According to the obtained formula the isotope shift is a composed function of η.

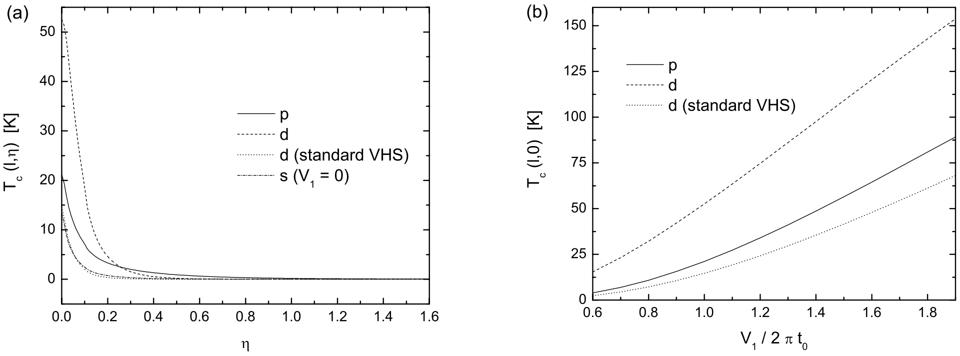

Fig. 5. (a) The transition temperatures $T_\mathrm{c}(1,\eta)$ (solid) and $T_\mathrm{c}(2,\eta)$ (dash) obtained within the extended VHS for $V_1 = 2\pi t_0$ and $V_0 = 0$ in comparison with the transition temperatures $T_\mathrm{c}^*(2,\eta)$ (dot) obtained in the frame of the standard VHS, and $T_\mathrm{c}^*(0,\eta)$ (dash-dot) obtained for $V_0 = 2\pi t_0\,[\bar{\chi}_2(0)]^2$ and $V_1 = 0$. (b) Supreme values of the transition temperatures $T_\mathrm{c}(1,0)$ (solid), $T_\mathrm{c}(2,0)$ (dash), $T_\mathrm{c}^*(2,0)$ (dot) for $0.6 \le V_1/2\pi t_0 \le 1.9$.

In the BCS-type approximation, when $v_l(z,\eta) \equiv 1$, $\nu(z,\eta) = \nu_0(\eta)$, and $I_{2n}(z,l,\eta) = 1$, we have $\nu_1(\eta) = \nu_0(\eta)$, $C_\mathrm{N}(T,\eta) = \frac{2}{3}\pi^2\nu_0(\eta)\,T$ and $\alpha(l,\eta) = 1/2$.

Note that in the Van Hove scenario method we have to replace $\mathcal{K}(z,\varphi,\eta)$ by $\nu(z,\eta)$ where $\nu(z,\eta) = I_0(z,\eta)\,\nu_0(\eta)$. In such case all expressions $I_{2n}(z,l,\eta)$ reduce to the forms

$$I_{2n}(z,l,\eta) = \left[\frac{1}{2^n}\binom{2n}{n}(1-\delta_{l0}) + \delta_{l0}\right] I_0(z,\eta),$$

so $I_2(z,l,\eta) = I_0(z,\eta)$ for $l = 0,1,2,4$. The latter relation causes that equations (37) and (39) become identical for all l after including $v_l(z,\eta) \cong 1$, what implies that the transition temperatures $T_\mathrm{c}(l,\eta)$ keep their mutual relations as for $T_{\mathrm{c}0}(l,\eta)$, the isotope shifts $\alpha(1,\eta)$ and $\alpha(2,\eta)$ coincide, and the spin-triplet p-wave symmetry superconducting state is preferred by this model.

5 Numerical results

The obtained formulas (37)–(39) allow us to estimate T_c, $\varDelta C(T_\mathrm{c})$ and α as functions of the parameter η in a simple manner. They also enable us to study them in detail and compare with the respective values evaluated in the case when solely the function of the density of states is taken into account. Employing the experimental data [12,29], where one can find $\eta = 0.375,\ 0.917,\ 1.055,\ 1.113$ or 1.53, $t_0 = 0.24$ eV (≈ 2800 K), and $\omega_\mathrm{c} = 0.026 \div 0.065$ eV, we may chose $\omega_\mathrm{c} = 0.0048$ eV (≈ 560 K), and hence $c = \omega_\mathrm{c}/2t_0 \approx 0.1$. Because the reduced transition temperature $\tau_\mathrm{c}(l,\eta) = T_\mathrm{c}(l,\eta)/t_0$ should satisfy the relation $\tau_\mathrm{c}(l,\eta) \le 0.05$ (i.e. $T_\mathrm{c}(l,\eta) \le 140$ K), then $\tau_\mathrm{c}(l,\eta) < c$ or $\tau_\mathrm{c}(l,\eta) \ll c$.

In numerical evaluations we take into consideration that $0 < \eta \le 1.62$, and we assume that the effective dimensionless pairing coefficient $\frac{1}{2}\nu_0(\eta)U_2(\eta) < 0.41$, what satisfies the weak-coupling condition, though the pairing coefficient V_1 can be large ($V_1 = 2.87\,\mathrm{eV}$) such that the standard dimensionless coefficient achieves the limit $\frac{1}{2}\nu_0(0)V_1 = 0.815$. Moreover, we also assume that $V_0 = 0$, except for the case of s-wave symmetry superconducting state when we assume that $V_0 = 2\pi t_0\,[\bar{\chi}_2(0)]^2$ and $V_1 = 0$ (cf. Fig. 5a).

In Figure 5 we present transition temperatures obtained from equation (37) after employing equation (36) for p-wave and d-wave symmetry superconducting states.

The results obtained within the developed formalism of the extended Van Hove Scenario [34] show that for $V_1 = 2\pi t_0 = 1.5\,\mathrm{eV}$, when $\frac{1}{2}\nu_0(0)U_2(0) = 0.215$, the supreme values of the transition temperatures are equal to $T_\mathrm{c}(1,0) = 21.1$ K, $T_\mathrm{c}(2,0) = 52.6$ K and $T_\mathrm{c}(2,\eta) > T_\mathrm{c}(1,\eta)$ for $0 < \eta < 0.256$. Moreover, $T_\mathrm{c}(1,0.256) = T_\mathrm{c}(2,0.256) = 2.47$ K, and $T_\mathrm{c}(1,1.62) = 0.031$ K, $T_\mathrm{c}(2,1.62) = 4.41 \times 10^{-6}$ K. Hence, in cuprates the d-wave symmetry superconducting state is realized for sufficiently small η. Instead, when η exceeds a characteristic value, the p-wave symmetry spin-triplet pairs should appear. Hence, the p-wave pairing becomes plausible by virtue of the t–J model where magnetic correlation effects in the $\mathrm{CuO_2}$ planes determine the dispersion relation, which then has a direct influence on the coefficients of the Fourier expansion of the pairing potential [1,3].

Therefore, we maintain that in the cuprate superconductors no large on-site Coulomb repulsion is necessary to destabilize the s-wave pairing, since the forms of the separated potential responsible for the formation of d-wave or p-wave pairing dominate. Moreover, any on-site interaction (attractive or repulsive) always drops out of the d-, g- and p-wave gap equation (33), cf. reference [3].

The transition temperature $T_\mathrm{c}^*(2,\eta)$ obtained according to the standard Van Hove Scenario, when $I_2(z,2,\eta)$ is replaced by $I_0(z,\eta)$, is lower that $T_\mathrm{c}(2,\eta)$ and $T_\mathrm{c}(1,\eta)$ for all η, and it coincides with $T_\mathrm{c}^*(0,\eta)$ of the s-wave symmetry superconducting state obtained for $V_0 = 2\pi t_0\,[\bar{\chi}_2(0)]^2$ and $V_1 = 0$. Thus, the application of the standard VHS leads to the conclusion that in the t–J model the p-wave pairing must be exclusively realized for all values of the parameter η.

Moreover, the derived supreme values of the transition temperatures reveal the relation $T_\mathrm{c}(2,0) > T_\mathrm{c}(1,0) > T_\mathrm{c}^*(2,0)$ for the discussed range of the parameter V_1, and only $T_\mathrm{c}(2,0)$ can exceed 100 K for the effective dimensionless pairing coefficient equal to 0.308.

In Figures 6a and 6b we present the reduced specific heat jump at the transition temperature and the isotope

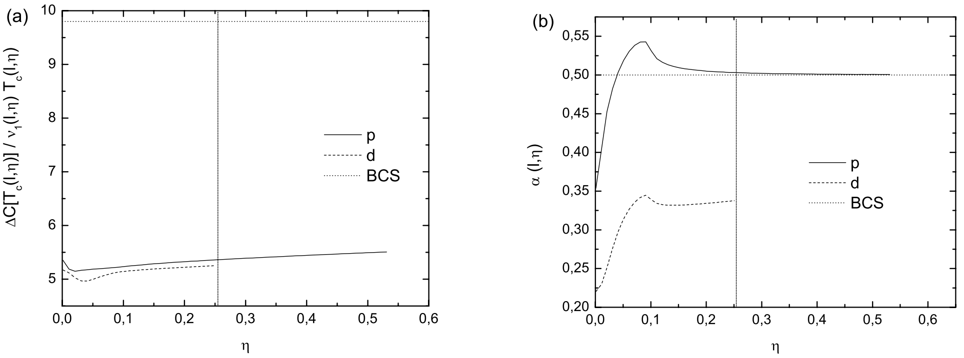

Fig. 6. (a) The reduced value of the specific heat jump at the transition temperature for p-wave (solid) and d-wave (dash) symmetry superconducting states plotted against the BCS-model value 9.38 (dot). In the limit $\eta \to 0$ they are equal to 5.35 and 5.17, respectively, though they are almost constant around 5.3 for all values of the parameter η under consideration. (b) The isotope shift $\alpha(l, \eta)$ for p-wave (solid) and d-wave (dash) symmetry superconducting states plotted against the BCS-model value 0.5 (dot). In the limit $\eta \to 0$ they are equal to 0.35 and 0.22, respectively. Note that the supreme value $\alpha(2, 0.091) = 0.345$ and for $\eta \geq 0.256$ $\alpha(1, \eta) \approx 0.5$.

shift $\alpha(l, \eta)$ for p-wave and d-wave symmetry superconducting states.

We should also mention that the reduced specific heat jump evaluated for d-wave symmetry superconducting state in the standard VHS approach is around 20 per cent greater than that presented in Figure 6a, whereas the isotope shift coincides with that obtained for the p-wave symmetry superconducting state presented in Figure 6b.

The above discussion evidences that the lack of the competition between singularities in the kernel of the density of states and pairing coefficients as in the BCS-type or standard VHS approaches causes that the p-wave symmetry superconducting state absolutely dominates, since it corresponds to the largest absolutely pairing coefficient $U_1(\eta)$. This fact implies that these approaches cannot be employed in investigations of anisotropic superconductors [8,20,34].

6 Conclusions

Within the present formalism we have demonstrated that the anisotropic model of a high-T_c superconductor with a dispersion relation established in the frame of the two-dimensional one-band tight-binding or t–J approaches and a boson-mediated strongly anisotropic pairing mechanism, whose elements of symmetry form the group C_{4v}, can be transformed into the (ξ, φ)-space, where the Fourier harmonics $\cos n\varphi$ and $\sin n\varphi$ are basis functions of irreducible representations of the group C_{4v}. As distinct from other approaches [3,21,23] the set of functions ($\cos n\varphi$, $\sin n\varphi$) we have applied is complete and orthonormal. This property allowed us to express the pairing interaction in terms of the Fourier harmonics by means of orthogonal projections. Then the structure of the order parameter is determined by the dominant Fourier component of the separable potential. Although particular terms of the separated potential contain Fourier harmonics with different n, the values of the functions $\chi_{4i}(\xi, \eta)$, $\chi_{1+4i}(\xi, \eta)$ and $\chi_{2+4i}(\xi, \eta)$ decrease with increasing i. Hence, the plausible s-, p-, d-, or g-wave symmetry superconducting states correspond merely to 1, $\cos(\varphi + \alpha_1)$, $\cos 2\varphi$, or $\cos 4\varphi$, respectively, i.e. when n is a small number. Thus, the pairing potential after expansion in a double Fourier series allows us to define and identify the order parameter with respect to harmonic functions $\sin n\varphi$ and $\cos n\varphi$.

The obtained results prove that the characteristic parameters in the t–J or two-dimensional tight-binding band models like the transition temperature, the specific heat jump, and the isotope shift can be derived in an analytic manner. The obtained form of the gap equation, which contains analytic functions of the one-particle energy ξ and the polar angle φ, coincides with the results of the extended Van Hove scenario [8,20,34], and can be employed to find the order parameter amplitude $\Delta(T)$, and other thermodynamic functions [35].

According to the developed formalism both the anisotropic attractive potential and dispersion relation have a crucial impact on the value of the transition temperature for a fixed symmetry superconducting state. The anisotropic attractive potential can be expanded in a double Fourier series (cf. Sect. 4.1), and the parameters $U_l(\eta) = V_1 \left[\bar{\chi}_l(\eta)\right]^2$ correspond to the coupling constants in the BCS-type factorizable interaction. Instead, the dispersion relation implies the form of the kernel of the density of states and its singularities, which are necessary to enhance the transition temperature. Since the effective dimensionless parameter $\frac{1}{2}\nu_0(\eta)\, U_l(\eta)$ is a decreasing function of η for all l, one should apply the weak-coupling formalism also for a strong attractive anisotropic potential until $V_1 = 2.87$ eV, or for a very strong attractive anisotropic potential, if η is sufficiently large. Detailed numerical calculations show that the spin-singlet d-wave symmetry superconducting state is preferred for small values of η, when singularities of $\mathcal{K}(\xi, \varphi)$ are near to the Fermi surface, what is expected for the phonon-mediated pairing, as in the 2D one-band tight-binding model. On the other hand for sufficiently large η, as in the t–J model, which is relevant to the magnon-mediated pairing, the spin-triplet p-wave symmetry superconducting state has to be formed. So, if strong magnetic correlations determine the pairing potential (of a magnetic origin) and form the dispersion relation, the spin-triplet p-wave superconducting state is preferred [1,3].

We have considered the problem of stability of spin-singlet and spin-triplet superconducting states in dependence on the ratio of the next-nearest-neighbor and nearest-neighbor transfer integrals $\eta = 2t_1/t_0$ for near half-filling when $n \simeq 0.5$ and $\mu_0 \simeq 0$. This is distinct from the problems where stability of spin-singlet and spin-triplet superconducting states was investigated in dependence on the carrier concentration n (the reduced electron density) with $\eta = 0$ [26,27], or $t_0 = 0$ and $t_1 \neq 0$ which corresponds to $\eta \to \infty$ [27].

The presented results agree with some obtained by Kuboki [27] in two specific cases when the used parameters coincide, i.e. for $\eta = 0$ and $\mu_0 = 0$ ($n = 0.5$) the $d_{x^2-y^2}$-wave superconducting state is stabilized, and for $\eta \gg 1$ and $\mu_0 = 0$ the p-wave superconducting state dominates. Moreover, one can note that the enhancement of n (if $\eta = 0$), or η (if $n = 0.5$) results in the replacement of the stable d-wave superconducting state by the p-wave one, what suggests the equivalent impact of the both parameters η and n.

The estimated values of the reduced specific heat jump for p-wave and d-wave symmetry superconducting states show that they are comparable and almost constant for all η under discussion, whereas the values of the isotope shift for the d-wave symmetry superconducting state are about 1.5 times smaller than the respective values of the isotope shift in the p-wave symmetry superconducting state.

Moreover, we have also demonstrated that the transition temperatures evaluated for d-wave symmetry superconducting state within the standard Van Hove scenario approach and p-wave symmetry superconducting state, which are identical both in the extended and standard Van Hove scenario, prefer the p-wave symmetry superconducting state for all values of η, just as does the BCS-type approximation. This crucial result proves that while considering a model of a superconductor with anisotropic pairing potential one has to include the kernel of the density of states $\mathcal{K}(\xi,\varphi)$, which corresponds to the product of Jacobians of subsequently performed transformations, instead of the density of states $\nu(\xi)$ as e.g. in the standard Van Hove scenario.

Although the parameter η is fixed and constant for each superconductor, one can modify the application range of the model by placing the system in an uniform perpendicular magnetic field. Since we take into account spin-triplet paired states with the spin projection $S_z = 0$ and spin-singlet paired states, which are affected by the magnetic field due to the Zeeman coupling, ineffectively, the Zeeman coupling leads solely to a renormalization of the chemical potential $\mu \to \bar{\mu} = \mu \pm \frac{1}{2} g \mu_B H$. Thus, the magnetic field H moves singularities in $\mathcal{K}(\xi,\varphi)$ away from the Fermi surface, and reduces the enhancement of the transition temperature. Therefore, eventually for sufficiently large H the field-induced transition from spin-singlet to spin-triplet superconductivity should be observed, as it has been reported recently [7].

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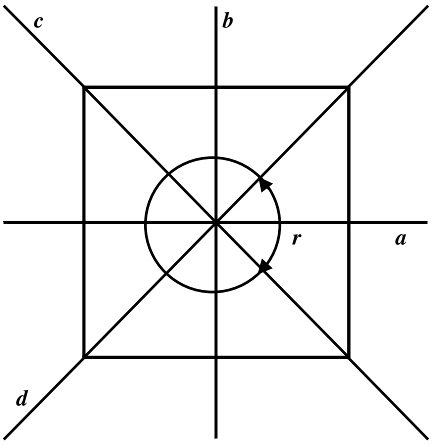

Fig. A.1. Elements of tetragonal planar symmetry corresponding to the group C_{4v}.

Appendix A: Basis functions of C_{4v} irreducible representations

The symmetry group of a square (in a two-dimensional space), denoted as C_{4v}, possesses one four-fold axis of symmetry, where r defines the rotation by the angle $\pi/2$, and four planes of symmetry a, b, c, d, which intersect at this axis. Hence, the group $C_{4v} = \{e, r, r^2, r^3, a, b, c, d\}$, where e is the identity element, possesses eight elements of symmetry as shown in Figure A.1, and it is a non-abelian group. This elements can be separated into five equivalence classes, namely two single-element: $\{e\}$, $\{r^2\}$, and three two-element: $\{r, r^3\}$, $\{a, b\}$, $\{c, d\}$. It implies that the group C_{4v} possesses five irreducible representations, i.e. four different one-dimensional and one two-dimensional. Hence, there must always exist six basis functions gathered in four subsets containing one function: $\{f_1\}$, $\{f_2\}$, $\{f_3\}$, $\{f_4\}$ and one subset containing two functions: $\{f_5\ f_6\}$. These subsets are invariants of the group C_{4v}. Hence, the symmetry elements $\{e, r, r^2, r^3, a, b, c, d\}$ acting on the functions f_1, f_2, f_3, f_4 leave them unchanged (up to the sign), whereas acting on the functions f_5, f_6 they can form a linear combination of them. The properties of the invariant functions $\{f_i\}$, $i = 1, 2, 3, 4$ can be classified with the reference to particular elements g of the group C_{4v} as follows:

A. The single-element subset $\{f_1\}$ of basis functions, corresponding to the trivial representation, such that $g f_1 = f_1$ for all $g \in \{e, r, r^2, r^3, a, b, c, d\}$.
B. The single-element subset $\{f_2\}$ of basis functions, corresponding to the representation with the trivial representation of the subgroup C_{2v}, such that $g f_2 = f_2$ if $g \in \{e, r^2, a, b\}$ and $g f_2 = -f_2$ if $g \in \{r, r^3, c, d\}$.
C. The single-element subset $\{f_3\}$ of basis functions, corresponding to the representation with the trivial representation of another tetra-subgroup, such that $g f_3 = f_3$ if $g \in \{e, r^2, c, d\}$ and $g f_3 = -f_3$ if $g \in \{r, r^3, a, b\}$.

D. The single-element subset $\{f_4\}$ of basis functions, corresponding to the representation with the trivial representation of the cyclic subgroup, such that $g\,f_4 = f_4$ if $g \in \{e, r, r^2, r^3\}$ and $g\,f_4 = -f_4$ if $g \in \{a, b, c, d\}$.

The properties of the invariant subset of basis functions $\{f_5,\, f_6\}$ corresponding to the two-dimensional irreducible representation can be classified with the reference to particular elements g of the group C_{4v} in one of the following two manners

E$_s$. The two-element subset of the functions $\{f_5,\, f_6\}$ for the two-dimensional representation representation:

$$\begin{aligned} &g\,f_5 = f_5 \mathrm{if} g \in \{e,a\}, \quad g\,f_5 = -f_5 if g \in \{r^2,b\},\\ &g\,f_5 = -(-1)^s f_6 \mathrm{if} g \in \{r,d\}, \; g\,f_5 = (-1)^s f_6 \mathrm{if} g \in \{r^3,c\}, \end{aligned}$$

and

$$\begin{aligned} &g\,f_6 = f_6 \mathrm{if} g \in \{e,b\}, \quad g\,f_6 = -f_6 \mathrm{if} g \in \{r^2,a\},\\ &g\,f_6 = -(-1)^s f_5 \mathrm{if} g \in \{r^3,d\}, \; g\,f_6 = (-1)^s f_5 \mathrm{if} g \in \{r,c\}, \end{aligned}$$

where $s = 1$ or 2. Acting with the elements of the group C_{4v} on a two-dimensional momentum space with Cartesian coordinate system, the components of the vector $\mathbf{k} = [k_x,\, k_y]$ are being transformed as follows:

$$\begin{aligned} &g\,k_x = k_x \mathrm{if} g \in \{e,a\}, \qquad g\,k_x = -k_x \mathrm{if} g \in \{r^2,b\},\\ &g\,k_x = k_y \mathrm{if} g \in \{r,d\}, \qquad g\,k_x = -k_y \mathrm{if} g \in \{r^3,c\}, \end{aligned}$$

and

$$\begin{aligned} &g\,k_y = k_y \mathrm{if} g \in \{e,b\}, \; g\,k_y = -k_y \mathrm{if} g \in \{r^2,a\},\\ &g\,k_y = k_x \mathrm{if} g \in \{r^3,d\}, \quad g\,k_y = -k_x \mathrm{if} g \in \{r,c\}. \end{aligned}$$

The above relations after including the formula $g\,f_i(k_\alpha) = f_i(g\,k_\alpha)$, where $i = 1, 2, \ldots, 6$ and $\alpha = x$ or y, allow us to choose invariant subsets of basis functions in accordance with the introduced classification in the form given by (6)–(10). Since $g \cos k_x \cos k_y = \cos k_x \cos k_y$ for all $g \in C_{4v}$, one has the right to define invariant subsets of basis functions as (11)–(15).

In the case of the polar coordinate system the elements of the group C_{4v} acting on the angular coordinate φ transform it in the following manner

$$\begin{aligned} &e\,\varphi = \varphi, r\,\varphi = \varphi - \frac{\pi}{2}, r^2\,\varphi = \varphi - \pi, r^3\,\varphi = \varphi - \frac{3\pi}{2},\\ &a\,\varphi = -\varphi, b\,\varphi = \pi - \varphi,\; c\,\varphi = \frac{3\pi}{2} - \varphi, d\,\varphi = \frac{\pi}{2} - \varphi. \end{aligned}$$

Hence, applying the formula $g\,f(\varphi) = f(g\,\varphi)$ to the Fourier harmonics: $1, \cos n\varphi, \sin n\varphi$, where $n = 1, 2, 3, \ldots$, we state that $g\,1 = 1$ for all $g \in C_{4v}$, and moreover

$$e\,\cos n\varphi = \cos n\varphi, \qquad e\,\sin n\varphi = \sin n\varphi$$

$$r\,\cos n\varphi = \begin{cases} (-1)^i \cos n\varphi \text{ if } n = 2i \\ (-1)^i \sin n\varphi \text{ if } n = 1+2i \end{cases}$$

$$r\,\sin n\varphi = \begin{cases} (-1)^i \sin n\varphi \text{ if } n = 2i \\ -(-1)^i \cos n\varphi \text{ if } n = 1+2i \end{cases}$$

$$r^2\,\cos n\varphi = (-1)^n \cos n\varphi, \qquad r^2\,\sin n\varphi = (-1)^n \sin n\varphi$$

$$r^3\,\cos n\varphi = \begin{cases} (-1)^i \cos n\varphi \text{ if } n = 2i \\ -(-1)^i \sin n\varphi \text{ if } n = 1+2i \end{cases}$$

$$r^3\,\sin n\varphi = \begin{cases} (-1)^i \sin n\varphi \text{ if } n = 2i \\ (-1)^i \cos n\varphi \text{ if } n = 1+2i \end{cases}$$

$$a\,\cos n\varphi = \cos n\varphi, \qquad a\,\sin n\varphi = -\sin n\varphi$$

$$b\,\cos n\varphi = (-1)^n \cos n\varphi, \qquad b\,\sin n\varphi = -(-1)^n \sin n\varphi$$

$$c\,\cos n\varphi = \begin{cases} (-1)^i \cos n\varphi \text{ if } n = 2i \\ -(-1)^i \sin n\varphi \text{ if } n = 1+2i \end{cases}$$

$$c\,\sin n\varphi = \begin{cases} -(-1)^i \sin n\varphi \text{ if } n = 2i \\ -(-1)^i \cos n\varphi \text{ if } n = 1+2i \end{cases}$$

$$d\,\cos n\varphi = \begin{cases} (-1)^i \cos n\varphi \text{ if } n = 2i \\ (-1)^i \sin n\varphi \text{ if } n = 1+2i \end{cases}$$

$$d\,\sin n\varphi = \begin{cases} -(-1)^i \sin n\varphi \text{ if } n = 2i \\ (-1)^i \cos n\varphi \text{ if } n = 1+2i \end{cases}$$

where $i = 0, 1, 2, \ldots$ The obtained relations allow us to perform the following classification for the functions 1, $\cos n\varphi$ and $\sin n\varphi$.

1. The functions 1 and $\cos 4i\varphi$, $i = 1, 2, 3, \ldots$, are invariants and each of them has the same properties as function f_1 of the subset A.
2. The functions $\sin 4i\varphi$, $i = 1, 2, 3, \ldots$, are invariants and each of them has the same properties as function f_4 of the subset D.
3. The functions $\cos(1+4i)\varphi$ and $\sin(1+4i)\varphi$ for a fixed $i = 0, 1, 2, \ldots$, have the same properties as functions f_5 and f_6, respectively, of the invariable subset E$_1$.
4. The functions $\cos(2+4i)\varphi$, $i = 0, 1, 2, \ldots$, are invariants and each of them has the same properties as function f_2 of the subset B.
5. The functions $\sin(2+4i)\varphi$, $i = 0, 1, 2, \ldots$, are invariants and each of them has the same properties as function f_3 of the subset C.
6. The functions $\cos(3+4i)\varphi$ and $\sin(3+4i)\varphi$ for a fixed $i = 0, 1, 2, \ldots$, have the same properties as functions f_5 and f_6, respectively, of the invariable subset E$_2$.

Thus, all Fourier harmonics: $1, \cos n\varphi, \sin n\varphi$ can be collected in only five possible types of invariant subsets.

Appendix B: Curvilinear transformations

General properties of curvilinear transformations and their relation to the density of states and its kernel can be considered as follows: for two arbitrary, orthogonal, curvilinear coordinate systems in a d-dimensional space, $x_1, \ldots, x_d$ and $y_1, \ldots, y_d$, where $d = 2$ or 3, the coordinates of a vector in the former system can be always expressed as functions of coordinates in the latter one, i.e. $x_i = x_i(y_1, \ldots, y_d)$ and $y_j = y_j(x_1, \ldots, x_d)$, where $i, j = 1, \ldots, d$, and $\hat{\mathbf{x}}_1, \ldots, \hat{\mathbf{x}}_d$ is a basis of orthogonal unit vectors associated with the point $[x_1, \ldots, x_d]$ of this space. Since we consider curvilinear systems, their basis vectors defined for particular points of the space can be oriented accidentally. The infinitesimal translation vector fixed at the point $[x_1, \ldots, x_d]$ has the form $d\mathbf{x} = \sum_{i=1}^{d} \hat{\mathbf{x}}_i dx_i$, whereas the same vector $d\mathbf{x}$ in the other coordinate system can be expressed as $d\mathbf{x} = \sum_{i=1}^{d} \frac{\partial \mathbf{x}}{\partial y_i} dy_i$, where the vectors $\hat{\mathbf{y}}_i = \frac{\partial \mathbf{x}/\partial y_i}{|\partial \mathbf{x}/\partial y_i|}$ form an orthonormal basis of the other coordinate system, and they are tangent to the lines y_i, so for particular points of the space they are oriented accidentally as well. The following relation

$$dy_i = \nabla_{\mathbf{x}} y_i \cdot d\mathbf{x} = \sum_{j=1}^{d} \nabla_{\mathbf{x}} y_i \cdot \frac{\partial \mathbf{x}}{\partial y_j} \, dy_j,$$

fulfilled for each coordinate y_i implies that

$$\nabla_{\mathbf{x}} y_i \cdot \frac{\partial \mathbf{x}}{\partial y_j} = \delta_{ij}. \tag{B.1}$$

The area of an infinitesimal rectangle defined in a two-dimensional space or the volume of an infinitesimal cuboid defined in a three-dimensional space, where the vector $d\mathbf{x}$ is its diagonal originating from the vertex $[x_1, \ldots, x_d]$, can be expressed as $d\tau = [\hat{\mathbf{x}}_1 dx_1, \ldots, \hat{\mathbf{x}}_d dx_d] = \prod_{i=1}^{d} dx_i$. Here, for $d = 3$ the symbol $[\cdot, \cdot, \cdot]$ denotes the triple product of three vectors, instead for $d = 2$ the symbol $[\cdot, \cdot]$ is the exterior product of two vectors. Note that in the other coordinate system the corresponding infinitesimal element of the space has the form

$$d\tau' = \prod_{i=1}^{d} dx_i = \left[\frac{\partial \mathbf{x}}{\partial y_1} dy_1, \ldots, \frac{\partial \mathbf{x}}{\partial y_d} dy_d\right] = \mathcal{J}(y_1, \ldots, y_d) \prod_{i=1}^{d} dy_i, \tag{B.2}$$

where

$$\mathcal{J}(y_1, \ldots, y_d) = \left[\frac{\partial \mathbf{x}}{\partial y_1}, \ldots, \frac{\partial \mathbf{x}}{\partial y_d}\right] = \left|\frac{\partial x_i}{\partial y_j}\right| \tag{B.3}$$

is the Jacobian of the transformation from the former to the latter coordinate system. Performing a rotation of the former coordinate system one can make the versors $\hat{\mathbf{x}}_i$ overlap versors $\hat{\mathbf{y}}_i$, and hence $d\tau' = d\tau = \prod_{i=1}^{d} dx_i$. Since the Jacobian of the coordinate system rotation is always equal to 1, then according to the theorem about the multiplication of determinants we state that the Jacobian (B.3) keeps its form. Moreover, the total symmetry of the problem under consideration ensures that for the inverse transformation (from the latter to the former coordinate system) equation (B.2) must be of the form

$$\prod_{i=1}^{d} dy_i = \mathcal{J}'(x_1, \ldots, x_d) \prod_{i=1}^{d} dx_i,$$

where $\mathcal{J}'(x_1, \ldots, x_d) = \left|\frac{\partial y_i}{\partial x_j}\right|$, which allows us to conclude that the introduced Jacobians satisfy the relation

$$\mathcal{J}(y_1, \ldots, y_d)\, \mathcal{J}'(x_1, \ldots, x_d) = 1. \tag{B.4}$$

On the other hand, taking into account that the new coordinate system is orthonormal then including equation (B.1) the Jacobian (B.3) reads

$$\mathcal{J}(y_1, \ldots, y_d) = \left|\frac{\partial \mathbf{x}}{\partial y_1}\right| \cdot \ldots \cdot \left|\frac{\partial \mathbf{x}}{\partial y_d}\right| = \frac{1}{|\nabla_{\mathbf{x}} y_1| \cdot \ldots \cdot |\nabla_{\mathbf{x}} y_d|}. \tag{B.5}$$

Let us emphasize that the Jacobian of any transformation as well as the gradient of a function, in particular $|\nabla_{\mathbf{x}} y_i|$, are invariants of an orthogonal transformation. The infinitesimal translation vector originating from the vertex $[x_1, \ldots, x_d]$, which is the diagonal of the element $d\tau$ can be written in the form $d\mathbf{x} = \sum_{i=1}^{d} \hat{\mathbf{y}}_i dx_i$. Then $dy_i = \nabla_{\mathbf{x}} y_i \cdot d\mathbf{x} = |\nabla_{\mathbf{x}} y_i|\, dx_i$, and hence

$$dx_i = \frac{dy_i}{|\nabla_{\mathbf{x}} dy_i|}. \tag{B.6}$$

Employing jointly equations (B.2), (B.5) and (B.6) we obtain the following formula

$$\mathcal{J}(y_1, \ldots, y_d) \prod_{i=1}^{d} dy_i = dy_1 \frac{\prod_{i=2}^{d} dx_i}{|\nabla_{\mathbf{x}} y_1|}, \tag{B.7}$$

where the differential elements dx_2, or $dx_2\, dx_3 = dS$ belong to a curve or a surface perpendicular to the vector $\nabla_{\mathbf{x}} y_1$.

Referring the present consideration to the orthogonal momentum $\mathbf{k}$-space, for which the curvilinear, orthogonal transformation of the coordinate system is given, and where the first coordinate represents the one-particle energy spectrum ξ, employing equation (B.7) one can state that the following definitions of the density of states, for $d = 2$ or 3

$$\nu(\xi) = \frac{2}{(2\pi\hbar)^d} \int \frac{\prod_{i=2}^{d} dk_i}{|\nabla_{\mathbf{k}} \xi|},$$

$$\nu(\xi) = \frac{2}{(2\pi\hbar)^d} \int \mathcal{J}(\xi, \ldots, \xi_d) \prod_{i=2}^{d} d\xi_i$$

are quite equivalent. Here ξ_2, or ξ_2 and ξ_3 are the remaining coordinates of the used curvilinear system. Note that the integration in the former expression is taken over one- or two-dimensional surface for the fixed energy ξ, whereas the integration in the latter expression is taken over finite or infinite intervals of well-defined coordinates ξ_2, or ξ_2 and ξ_3, respectively, which can be chosen in any manner. To simplify the notation we define the kernel of the density of states as

$$\mathcal{K}(\xi,\ldots,\xi_d)=\frac{2}{(2\pi\hbar)^d}\,\mathcal{J}(\xi,\ldots,\xi_d). \tag{B.8}$$

Then

$$\nu(\xi)=\int\mathcal{K}(\xi,\ldots,\xi_d)\prod_{i=2}^{d}d\xi_i.$$

Appendix C: Symmetry properties of separable parts of pairing interactions

The separated parts of pairing interactions (2) and (3) have the following symmetry properties with regard to elements of the group C_{4v}:

1. the functions 1 and $\cos k_x+\cos k_y$ are invariants and they have the same properties as the function f_1 of the subset A;
2. the function $\cos k_x-\cos k_y$ is an invariant and it has the same properties as function f_2 of the subset B;
3. the functions $\sin k_x$ and $\sin k_y$, have the same properties as functions f_5 and f_6, respectively, of the invariant subset E_1.

the corresponding functions of φ given in equations (31) and (32) must possess the same symmetry properties. Let us note that the function $f(\varphi)$ defined by equation (28), which is of the form

$$f(\varphi)=\frac{|\sin\varphi|-|\cos\varphi|}{|\sin\varphi|+|\cos\varphi|},$$

when $0\le\varphi<2\pi$, has the same properties as function f_2 of the subset B. Hence, $g\,X(\xi,\varphi)=X(\xi,\varphi)$ if $g\in\{e,r^2,a,b\}$ and $g\,X(\xi,\varphi)=Y(\xi,\varphi)$ if $g\in\{r,r^3,c,d\}$ as well as $g\,Y(\xi,\varphi)=Y(\xi,\varphi)$ if $g\in\{e,r^2,a,b\}$ and $g\,Y(\xi,\varphi)=X(\xi,\varphi)$ if $g\in\{r,r^3,c,d\}$. This implies that

1′. the function $[X(\xi,\varphi)+Y(\xi,\varphi)-2]/2\eta$ is an invariant and it has the same properties as function f_1 of the subset A,
2′. and the function $[Y(\xi,\varphi)-X(\xi,\varphi)]/2\eta$ is an invariant and it has the same properties as function f_2 of the subset B.
3′. Moreover, the functions $(\pm)\frac{1}{2\eta}\sqrt{\eta^2-[X(\xi,\varphi)-1]^2}$ and $(\pm)\frac{1}{2\eta}\sqrt{\eta^2-[Y(\xi,\varphi)-1]^2}$ have the same properties as functions f_5 and f_6 of the invariant subset E_1, respectively.

The obtained relations and the classification of the Fourier harmonics performed in 6 evidence that the Fourier expansions of the specified functions must have the following forms

$$\frac{1}{2\eta}[X(\xi,\varphi)+Y(\xi,\varphi)-2]=\frac{\chi_0(\xi,\eta)}{\sqrt{2}}+\sum_{l=1}^{\infty}\chi_{4l}(\xi,\eta)\cos 4l\varphi,$$

where

$$\chi_0(\xi,\eta)=\frac{\sqrt{2}}{\eta\pi}\int_0^{\pi/2}[X(\xi,\varphi)+Y(\xi,\varphi)-2]\;d\varphi$$

and

$$\chi_{4l}(\xi,\eta)=\frac{2}{\eta\pi}\int_0^{\pi/2}[X(\xi,\varphi)+Y(\xi,\varphi)-2]\;\cos 4l\varphi\,d\varphi$$

for $l=1,\,2,\ldots$, and

$$\frac{1}{2\eta}\;[Y(\xi,\varphi)-X(\xi,\varphi)]=\sum_{l=0}^{\infty}\chi_{2+4l}(\xi,\eta)\cos(2+4l)\varphi,$$

where

$$\chi_{2+4l}(\xi,\eta)=\frac{2}{\eta\pi}\int_0^{\pi/2}[Y(\xi,\varphi)-X(\xi,\varphi)]\;\cos(2{+}4l)\varphi\,d\varphi,$$

and

$$(\pm)\frac{\sqrt{2}}{2\eta}\sqrt{\eta^2-[X(\xi,\varphi)-1]^2}=\sum_{l=0}^{\infty}\chi_{1+4l}(\xi,\eta)\cos(1{+}4l)\varphi,$$

and

$$(\pm)\frac{\sqrt{2}}{2\eta}\sqrt{\eta^2-[Y(\xi,\varphi)-1]^2}=\sum_{l=0}^{\infty}\chi_{1+4l}(\xi,\eta)\sin(1{+}4l)\varphi$$

where

$$\chi_{1+4l}(\xi,\eta)=\frac{2\sqrt{2}}{\eta\pi}\int_0^{\pi/2}\sqrt{\eta^2-[X(\xi,\varphi)-1]^2}\cos(1{+}4l)\varphi\,d\varphi$$

$$=\frac{2\sqrt{2}}{\eta\pi}\int_0^{\pi/2}\sqrt{\eta^2-[Y(\xi,\varphi)-1]^2}\;\sin(1+4l)\varphi\,d\varphi$$

for $l=0,\,1,\,2,\ldots$.

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