Tight-Binding non-magnetic disorder DOS and residual DOS revisited for Unconventional Superconductors

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Abstract

In this paper, we present the calculation of the density of states (DOS) and the residual density of states (RDOS) for two unconventional superconductors – strontium-doped lanthanum cuprate La2-xSrxCuO4, which is a high-temperature superconductor (HTSC) with singlet pairing, and strontium ruthenate Sr2RuO4, with a triplet pairing in the Fermi surface’s γ-sheet. The calculations were carried out in the framework of the tight-binding (TB) approach with first neighbors’ interaction in the presence of nonmagnetic pair breaking disorder, using the experimental values for Δ0 and other TB parameters taken from ARPES data. For the case of the singlet HTSC such as La2-xSrxCuO4, DOS and RDOS in Born’s and Unitary limits can be treated numerically with a dimensionless disorder parameter ζtriplet, which happens to be one order of magnitude smaller as to compare with ζsinglet in the case of quasi-nodal paring in the FS γ-sheet for the triplet Sr2RuO4. We demonstrate that the unitary limit persists in the calculation of both DOS and RDOS for the γ-sheet of triplet Sr2RuO4, showing the formalism for the calculation of RDOS in the TB case for both symmetry groups of the order parameter (OP) and compare our theoretical results with several experimental data and theoretical reports found in the scientific literature. Finally, we show that for the highest values of dimensionless disorder parameter ζsinglet and the majority values of ζtriplet both compounds are mostly dwelling in the unitary limit.

Keywords: densities of states; residual density of states, dirty non-magnetic unconventional superconductors, singlet nodal line superconductors, triplet quasi-point nodes superconductors, D1h point group crystal symmetry, irreducible representation B1g, irreducible representation E2g, impurity non-magnetic quantum levels, tight-binding, Fermi averages, advanced solid-state teaching, quasiparticles decay.

1. Introduction

The density of states (DOS) is a quantum concept extensively used in Statistical Mechanics and Solid State Physics. The DOS represents the number of the energy states available of a physical system per unit of energy [1,2,3]. Since in solid-state physics, energy levels in crystals can be represented as a continuum, the DOS can be plotted as a two-dimensional function of the energy curve. In general, DOS tells us the information about the number of quantum levels distributed over an energy interval. Therefore, it is a measure of how many quantum states are in a small range of energy avoiding the use of concept of the phase space, which is more related to the classical variables (q, p) where q is the generalized position, and p is the generalized linear momentum, that are used in statistical mechanics and kinetics physics widely.

In solid-state physics, the most general DOS is expressed in terms of the system’s energy. As some authors point out [2], each element of volume/area in the phase space of linear position q and momenta p is replaced by a weighting factor in an energy integral, which is easier to work with at the quantum level. The DOS can be written as a sum of infinite Dirac delta functions with energies corresponding to the set of eigenvalues ϵi of the
Hamiltonian. In this work, we use the reduced Planck system of units \((\hbar = k_B = c = 1)\) to have a single experimental unit of measurement (meV), which is used in ARPES technique, and it is considered very instructive. DOS equation for equal number of spin up and down quasiparticles states is therefore

\[
D(\omega) = \frac{2}{V} \sum_l \delta(\omega - \omega_l) = \frac{d \Theta}{d \omega}. \quad (1)
\]

The intermediate equation in (1) represents the sum of the number of different energy states at a particular quantum level that quasiparticles are allowed to occupy, i.e., is the sum of the number of quasiparticles levels per unit volume and energy. They are generally called quasiparticle levels with two terms: a real term, and also an imaginary decaying energy term due to scattering processes [4] as we will see for the case of superconductors with non-magnetic impurities. However, from a macroscopic point of view, the DOS is defined as the final expression in equation (1), i.e., as the proportionality coefficient between the number of macroscopically allowed quantum states \((\Theta)\) and an infinitesimal energy interval between \(\omega\) and \(\omega + d\omega\) in a two-dimensional space with variables \((\omega, \Theta)\) \([1, 2]\).

In superconductors, however, the expression for the DOS looks different, normal quasiparticles energy levels do not exist below \(T_c\) for the BCS superconductors with a gap \([5]\), or it changes its behavior as a function of energy for unconventional superconductors with or without impurities \([6]\), so the most generally accepted equations are the following.

For a single sheet/band superconductor using non-magnetic impurity scattering formalism \([6]\), we use equation

\[
N(\bar{\omega}) = N_F \mathcal{R}[g(\bar{\omega})], \quad (2)
\]

where \(\mathcal{R}\) means the real part of the function \(g(\bar{\omega})\) and at the Fermi level, the number of states \(\Theta\) is huge and at the Fermi level \(N_F \sim 10^{15} eV^{-1}\). The function \(g(\bar{\omega}) = \left(-\frac{\bar{\omega}}{\sqrt{\bar{\omega}^2 - \Delta_0^2(k_x, k_y)}}\right)_{FS}\) has real and imaginary terms. In this expression the self-consistent frequency \(\bar{\omega}\) has replaced the energy \(\epsilon\), since we use Planck reduced units and the accent mark symbol on the frequency, i.e. \(\sim\), means self-consistently. If \(\bar{\omega}\) has \(\mathcal{R}(real)\) and \(\mathcal{I}(imaginary)\) terms, then equation 2 is valid. If \(\bar{\omega}\) has only a \(\mathcal{R}(real)\) part, then the symbol \(\mathcal{R}\) is omitted \([3, 5]\).

For those reasons, a few points to notice here from a pedagogical point of view are: First, we use the TB approach for ARPES parameters \([7]\) and a TB average \("<...>_{FS}\"\) over a single Fermi surface sheet for both materials which will be explained in section 3. Second, we use the 2D dimensional space \((k_x, k_y)\) adequate for the first Brillouin zone and an anisotropic treatment. Third, the use of \(\bar{\omega}\) requires a numerical calculation that implies uncommon numerical routines. For pedagogical purposes we use a smaller subset of \(\bar{\omega}\) values from the ones obtained from the imaginary part of the elastic scattering cross-section according to \([8]\) taken from the following works \([9, 10, 11, 12]\).

In reference \([8]\), \(\bar{\omega}\) was calculated for isotropic FS high \(T_c\) superconductors, in \([9]\) the work was done for High \(T_c\) cuprates using anisotropic TB, and in \([10, 11, 12]\), the calculation of \(\bar{\omega}\) was used to study the FS two dimensional \(\gamma\) - TB sheet of \(Sr_2RuO_4\), allowing us at that moment, to infer some macroscopic classical properties using a Wigner distribution probabilities approach as is advice in \([13, 14]\).

Instead, we address in this work, a pedagogical introduction to the DOS and residual DOS calculation for two unconventional superconductors widely mentioned in the scientific literature in the case that the pair breaking
occurs due to a non-magnetic field or due to additional impurity levels of an in-situ element (estequiometric).

Second, if we are dealing with more than one sheet, the DOS is calculated according to equation (3) (which is shown here for the case of the 3 FS sheets of Sr₂RuO₄):

\[
\frac{N(\omega)}{N_F} = p^\gamma N^\gamma (\frac{\omega}{\Delta_0}) + p^{\alpha\beta} N^{\alpha/\beta} (\frac{\omega}{\Delta_0^{\alpha/\beta}}) \tag{3}
\]

Equation (3) is very suitable to calculate theoretically and to fit 3D experimental low-temperature data for unconventional superconductors with several sheets on the FS (such as the triplet superconductor strontium ruthenate, which has three sheets α, β (1D) and γ (2D)), in a non-self-consistent way using a TB parametrization. TB, allows to calculate and fit experimental low-temperature data such as ultrasound attenuation in the normal and superconducting states α(T) [15,16,17], electronic thermal conductivity κ(T) [18,19] and electronic specific heat C(T) [20,21].

In equation (3), \(p^{\alpha\beta}\) is defined to be the fraction of the density of states in the normal metal associated with the α/β sheets. The quantity \(p^\gamma\) is the fraction of the normal-state density of states associated with the γ sheet. The relation between these two quantities is \(p^\gamma + 2p^{\alpha\beta} = 1\) and it can be found experimentally from viscosity (ultrasound) measurements and fitted to a TB model in the normal state of a bulk crystal [16]. The frequency \(\omega\) in equation (3) is also given in (meV), and it is no self-consistently calculated, which is valid when the quasiparticles lifetime (\(\tau_s\)) in the superconducting phase is almost the same constant normal state lifetime, i.e. \(\tau_s \approx \tau_n\), in the majority of the energy interval [11,22]. The curves obtained with the DOS’s calculations, can be used to interpret quantum mechanical effects such as tunneling in dirty d-wave unconventional superconductors. Additionally, they can be used to fit several experimental properties in bulk or thin-film metallic alloys using TB parameters in meV, taken from ARPES or other experimental techniques.

In solid-state physics, if the most general DOS equation is expressed in terms of the momenta of the system [1,2,3], the sums \(\sum_{kx,ky,kz} f\), where \(f\) is a function that approximate the \(\delta(\omega - \omega_k)\) expression over the linear 3D momentum anisotropic space \((k_x, k_y, k_z)\) or the 2D analog space \((k_x, k_y)\), are adequate for QM calculations on the first Brillouin zone, with first (2D) and second neighbors (3D). We replace in some cases the sums by a weighting factor into an energy integral, which is easier to deal with at the QM level [2].

The structure of this work is as follows: In section 2 some details of the computational approach were outlined referring to previous work for the details of the TB model and equations. In section 3, a detailed DOS calculation for both model was numerically performed for several cases of experimental interest but pointing out the differences among them instructively. Finally, in section 4, the behavior of the residual density of states DOS was addressed for both models using TB.

2. TB Computational details for the DOS and the residual DOS with Fermi averages

For the calculation of the DOS and the residual DOS of singlet and triplet superconductors, we use a TB model with ARPES parameters, that have been extensively explained in references for the case of the imaginary part of the elastic scattering cross-section [9,10,11] detailing the equations and analysis for the quasiparticles elastic scattering lifetime \(\tau_i\) in the reduced phase space.

The equation, we have used in the case, taking into account dirty superconductors for numerical purposes, (which usually is not showcase in textbooks, where the Green function formalism is emphasized), is pointed out
here as a pedagogical contribution to this paper, and it can be used by advanced student in solid-state physics, it is the following:

\[
\frac{N(\tilde{\omega})}{N_F} = \frac{3(\tilde{\omega})}{\sqrt{2} \rho_k} \sqrt{1 + \frac{a_k}{\rho_k}} + \frac{3(\tilde{\omega})}{\sqrt{2} \rho_k} \sqrt{1 - \frac{a_k}{\rho_k}}.
\]

where \(\Re(\tilde{\omega})\), and \(\Im(\tilde{\omega})\) are the real and imaginary part of the scattering self-consistent cross-section, and the other symbols in equation (3) are three expressions: \(a_k = \Re(\tilde{\omega})^2 - \Im(\tilde{\omega})^2 - \Delta_k^2\), \(b = 2 \Re(\tilde{\omega}) \Im(\tilde{\omega})\), and \(\rho_k = \sqrt{a_k^2 + b^2}\).

The tight-binding Fermi averages in the 2D sum "\(\Sigma_{kx,ky}(\ldots)\)" can be performed by a very useful identity given by

\[
\Sigma_k^\infty (\ldots) = \frac{1}{4 \pi^2} \int \frac{dS_F}{|\vec{v}_k|} \int d\mathcal{E} (\ldots) \tag{5}
\]

In expression (5), \(\mathcal{E}\) is the energy of the normal state quasiparticles, the Fermi velocity is given by the gradient of the \(\epsilon\), \(\vec{v}_k = \text{grad} \mathcal{E}\), the surface \(k\)-space element is expressed as \(dS_F = \sqrt{d k_x^2 + d k_y^2}\) and the normal state density of states at the “Fermi level” \(N_F\) used in equations (3) and (4) is given by the equation [6] for which we perform the integral (5) in the first Brillouin zone as

\[
N_F = \frac{1}{4 \pi^2} \int \frac{dS_F}{|\vec{v}_k|} \tag{6}
\]

We have used the standard C language program to calculate the DOS from equations (2-6). The optimization of the self-consistent DOS was carried out using a home-developed algorithm to find the numerical solution of equation (2) and which have explained in equations 4, 5, and 6, using a minimization routine based on the non-linear Levenberg-Marquardt method for the self-consistency \(\tilde{\omega}\), and an integration routine [24]. A different treatment on how to deal with the DOS calculation in unconventional high Tc cuprates is found in the mongraphy [25].

Returning to the old problem of nodal behavior in unconventional superconductors, among recent developments, we have selected two examples for the pedagogical analysis of DOS and residual DOS, where some exciting theories and experiments still continue to appear in the current literature [25,26,27,28,29].

First, a 2D TB Scalapino line nodes model [30,31,32] in strontium doped 214 lanthanum copper oxide superconductor \(\text{La}_{2-x}\text{Sr}_x\text{CuO}_4\) (\(T_c \approx 44.35\) K for a polycrystalline sample [41]) with TB ARPES values (\(\epsilon = 0.4, \epsilon_F = 0.4, \Delta_0 = 33.9\) meV, and with an OP with even parity \(\epsilon\) to the irreducible representation \(B_{1g}\) of the \(D_{4h}\) point symmetry group. Second, a 2D TB \(\gamma\) sheet Miyake Narikiyo quasi-point nodes model [36] ternary compound \(\text{Sr}_2\text{RuO}_4\) (\(T_c \approx 1.5\) K for a bulk clean sample) with the TB ARPES values (\(\epsilon = 0.4, \epsilon_F = -0.4, \Delta_0 = 1.0\) meV, and with a OP with odd parity \(\epsilon\) to the irreducible representation \(E_{2u}\) of the \(D_{4h}\) point symmetry group [33,34,35,36]. We would like to point out the intriguing 2D electronic nature of this material discovered in [37].

To take into account the non-magnetic disorder effects into the DOS and the residual DOS with an adequate parametrization, we use the Born limit given by \(\epsilon \kappa F \gg 1\) or \(\epsilon \kappa F \ll 1\), where \(\epsilon\) -is the mean dressed quasiparticles free path, \(\kappa\) -is the lattice parameter, \(\kappa F\) -is the Fermi momentum, and the unitary metallic limit with: \(\epsilon \kappa F \sim \epsilon \kappa F \sim 1\). We use the parameter \(c\) which is inverse to the scattering strength \(U_0\) to describe the dispersion limit, being \(c = 0\) the strong unitary limit and \(c = 0.4\) the weak Born limit for cuprates [9] and \(c = 0.4\) the intermediate limit for strontium ruthenate [10].
During the 70s to the 80s, the formalism and some phenomenology of the physics for non-magnetic impurity scattering treatment in normal metals and alloys were pedagogically described in the textbook [38]. In monography [39] it was noticed that in studying the DOS behavior in alloys, we unquote their phrase: “...a feature of one-site approximations (referring to first neighbors)... and also that the density of states (DOS) in the vicinity of the resulting band edges behaves like $\sqrt{\mathcal{E} - \mathcal{E}_c}$”, pointing out that singularities in DOS behavior in disordered systems such as those involving non-magnetic impurities, or stoichiometric non-magnetic atomic potential $U_0$. Pedagogically, we think that this effect is of extreme importance in order to study and understand disorder effects in metallic solids.

A few tuitional words for the use of the ARPES measurements are the following. ARPES in an experimental technique mainly developed in the 90s. It has served well its purpose by giving theorists with experimental parameters that allow the study of unconventional superconductors as the two mentioned in this pedagogical work for several reasons. First, it serves for both approximations, the free-electron approximation developed in the 50s and 60s [4], or the tight-binding approach developed in the 80s [7]. It also is used for physical phenomena with different dispersion mechanisms, i.e., the elastic and inelastic scattering cases (we refer here for the case were linear momentum - $p$ is not conserved and energy - $\varepsilon$ is conserved).

It helps to infer physical parameters such as the zero gap magnitude $\Delta_0$, a key parameter in the superconducting DOS. We consider instructive to remember that ARPES technique is related to a fundamental equation which plays a role quasiparticles interaction phenomena, “the Fermi Golden Rule (FGR)”. A robust introduction to ARPES and FGR can be found in [40]. We ought to point out the most of the physics involved in non-equilibrium transport properties can be related to the mean free path, the lifetime, the scattering cross-section, and the DOS levels of some of those quasiparticles, and henceforth, the FGR, informers us about the Fermi energy level, giving us as instructors of advanced solid-state courses a great scholastic method, i.e., relevant physical quantities obtained by ARPES technique such as the Fermi energy, the zero gap magnitude, and the hopping TB parameters can be used to perform numerical modeling.

3. TB numerical and visualization results for the self-consistent DOS with non-magnetic disorder

Figure 1 shows the density of states DOS, calculated numerically using equation (2), normalized by the density of states at the Fermi level $N(\tilde{\omega})/N_F$ as a function of normalized frequency $\omega/\Delta_0$, in the clean limit (without non-magnetic impurities) and the parameter for the “concentration of disorder $\sim \Gamma^+$” is the dimensionless new parameter $\zeta = \Gamma^+ / \Delta_0 = 0$. It is observed that, at zero energy, there are no dressed QM quasiparticle states if $\zeta = 0$. Then, the number of occupied states starts to grow linearly, as should be for the 1D irreducible representation $B_{1g}$ of the $D_{4h}$ point group, since it represents nodal lines in the reduced scattering space until an energy value exactly equal to that of the Gap $\Delta_0$ is reached.

At $\omega = \Delta_0$, there is a drastic change in slope, as observed in figure 1. In BCS clean superconductors, the DOS presents a singularity for $\omega = \Delta_0$, and for $\omega/\Delta_0 = 1$ values below $\Delta_0$, it is a forbidden region only for dressed non-magnetic quasiparticles [5].
Figure 1. Superconducting density of states (DOS) for a 2D tight binding Scalapino line nodes in strontium doped 214 lanthanum copper oxide with $\zeta = 0$. Line nodes are expected for the irreducible representation $B_{1g}$ of the $D_{4h}$ point symmetry group. $N(0) = 0$ as it should be, with no residual density of states at zero energies.

Figure 2 shows five curves calculated for different values of the normalized non-magnetic disorder parameter $\zeta = 0.001, 0.005, 0.010, 0.015, 0.020$ in the unitary limit when the inverse strength parameter $c = 0$. At zero frequency, it is observed that there are residual states for all 5 values of $\zeta = \zeta_{\text{singlet}}$, which is a consequence of the presence of non-magnetic impurities in the reduced phase scattering space for the line nodes model. It is noticed that a higher concentration of impurities given by $\zeta$ increases the amount of occupied dressed quasiparticle states at the frequency value $\omega = 0.0$ meV. $N(0)/N_F$ is bigger for the thinner line ($\zeta = 0.020$) compared to other curves, the thicker line ($\zeta = 0.001$) has a considerable amount of residual DOS. That is a particular characteristic of the unitary scattering limit in the DOS, as was previously explained in [6] and references therein.

Figure 2. Superconducting density of states (DOS) for a 2D tight-binding Scalapino line nodes in strontium $La_{2-x}Sr_xCuO_4$ with $\zeta = 0.001, 0.005, 0.010, 0.015, 0.020$ for the irreducible representation $B_{1g}$ of the $D_{4h}$ point symmetry group. Residual $N(0) \neq 0$, as it should be, since there are dressed normal quasiparticles levels at zero energy due to the strong scattering potential (unitary limit).
Figure 3, shows the superconducting DOS behavior for a weaker scattering potential with \(c = 0.4\) and the dimensionless parameter \(\zeta = 0.001, 0.005, 0.010, 0.015, 0.020\). The strength is \(c = 0.4\), this value was established as the Born limit for the case of nodal line superconductors in the TB limit, analyzing the imaginary scattering cross-section [9].

However, the number of residual DOS states \(\frac{N(0)}{N_F}\) weakly increases as \(\zeta\) increases and it is noticeably smaller compared to \(\frac{N(0)}{N_F}\) values in Figure 2 with a strong elastic scattering, suggesting that a strong non-magnetic dispersion potential produces more occupied states DOS states, than weaker scattering potentials at zero energy. This can be defined as the signature for the unitary state in residual DOS analysis compare with the maximum observed in the analysis of the imaginary function \(\Im \left[ \tilde{\omega} \right] \left( \omega + i 0^+ \right)\) [9].

Figure 3. Superconducting density of states (DOS) for a 2D TB Scalapino nodal line model in strontium \(La_{2-x}Sr_xCuO_4\) with \(\zeta = 0.001, 0.005, 0.010, 0.015, 0.020\) for the irreducible representation \(B_{1g}\) of the \(D_{4h}\) point symmetry group. Residual \(N(0) \neq 0\), but is very small compared to Figure 2, as it should be, since there are very few dressed DOS states at zero energy due to the weak Born scattering limit \(c = 0.4\).

The next step in our program is to do the same calculation for the FS \(\gamma\)-sheet of the ternary triplet superconductor strontium ruthenate \([31, 32, 33, 34, 35]\) for the 2D irreducible representation \(E_{2u}\) of the \(D_{4h}\) point symmetry group. Figure 4 shows six curves calculated for different values of the normalized non-magnetic disorder parameter \(\zeta = \Gamma^\ast/\Delta_0\); now we have six values \(\zeta_{\text{triplet}} = \zeta = 0.00, 0.01, 0.02, 0.03, 0.10, 0.20\) in the unitary limit when the inverse elastic scattering parameter \(c = 0\). The first contrast concerning the nodal lines DOS drawn in Figures 1 - 3, is that the dimensionless parameter for the triplet case \(\zeta = \Gamma^\ast/\Delta_0\) is one order of magnitude bigger. Consequently, we use the following notation for pedagogical purposes \((\zeta_{\text{triplet}}/10 \sim \zeta_{\text{singlet}})\). This is partially explained because the FS \(\gamma\)-sheet TB model uses an experimental \(\Delta_0 = 1.0\) meV value, that is an order of magnitude smaller than for the nodal line TB model with \(\Delta_0 = 33.9\) meV, and therefore the triplet case has a much smaller reduced scattering space.

Generally speaking, in the triplet pairing \(Sr_2RuO_4\), \(Sr\) atoms belong to the lattice with an additional non-magnetic impurity DOS level in the energy zone. Thus \(Sr\) atoms are part of the \(D_{4h}\) tetragonal structure and also are the centers on which non-magnetic elastic scattering occurs, giving rise to a strong pair breaking mechanism and an additional impurity level, with a disorder dimensionless parameter \(\zeta = \zeta_{\text{triplet}}\) an order of magnitude bigger than
for the nodal lines cuprates, as is clearly seen when we numerically calculate the DOS using TB. That means we have a much smaller reduced phase scattering space in terms of the imaginary scattering cross-section [10,11].

Figure 4 shows that in the absence of non-magnetic impurity levels (black line with $\zeta = 0.00$), we do not observe non-zero values for the DOS $N(\tilde{\omega})/N_F$ as for BCS superconductors (there is no pair breaking conducting to dressed level states). It occurs below 0.83 meV in this calculation. Generally speaking, this value depends on the choice of all TB parameters, i.e., how close will be the FS $\gamma$-sheet to the zero-gap $\Delta_0$ value in the MN model (see figure 1 in [11] and figures 1-2 in [12]).

It means that in the absence of non-magnetic impurity levels in the FS $\gamma$-sheet in Sr$_2$RuO$_4$, the material behaves like BCS superconductors [5,11,36], with only Cooper pair quasiparticles. For a parameter value of $\zeta = 0.01$, we observe still an intermedia well-formed BCS gap (from $\omega \in (0.4,0.83)$ meV, and with a small quantity of dressed DOS states at low frequencies due to strong scattering unitary regime in the reduced phase scattering space, when the mean free path $\ell$ is comparable to the inverse of the Fermi length $|k_F|^{-1}$, but for $\zeta = 0.05$ it agrees with an inhomogeneous phase mentioned in [11] where there are not dressed electron and hole levels forming the MN tiny gap [10, 11, 12, 36].

It also agrees with [10] in the sense that only the unitary limit persists for the numerical superconducting DOS calculation in the FS $\gamma$-sheet in Sr$_2$RuO$_4$. It is noticed that a higher concentration of impurity levels given by the values $\zeta = 0.01, 0.05, 0.10, 0.15, 0.20$, the number of occupied quasiparticles states at low and higher frequencies increases, that is a consequence of having an increasing reduced phase scattering space [11], but is still very small compare with the High $T_c$ case [9].

The tiny Miyake-Narikiyo FS $\gamma$-sheet gap predicted in [36] is observed in Figure 4 for a value of $\zeta = 0.05$ as was previously observed in [10,11,12] using the imaginary part analysis of the scattering cross-section $\Im [\tilde{\omega}] \left( \omega + i \ 0^+ \right)$. The linear behavior numerically observed in Figure 4 for the DOS in the clean limit ($\zeta = 0.00$)
in the frequency interval \( \omega \in (0.82, 1.20) \text{ meV} \) is a numerical error in our DOS calculation (due to the lack of fast computer facilities to perform the \( \omega \) integration with more \( \omega \) points).

For the values of the disorder parameter \( \zeta = 0.10, \ 0.15, \ 0.20 \), there are normal state DOS levels available, and the peak at \( \omega = 1.4 \) considerable reduces with a tendency where \( N(\omega) \sim N_F \) above \( T_c \). Therefore, in the superconducting \( \text{Sr}_2\text{RuO}_4 \) “DOS”, we observe both phases, one without electronic levels (BCS type) and another with normal-state dressed quantum levels, contrasting with the High \( T_c \text{ La}_2\text{xSr}_x\text{CuO}_4 \) case where always dressed electronic levels are present.

4. **TB numerical results for the residual DOS with non-magnetic disorder \( \eta_c \) pair breaking**

The residual \( (\omega = 0) \) DOS equation (7) is theoretically obtained by setting up \( \omega = i \alpha \) in equation 2, that is if \( \tilde{\omega} = \omega + i \alpha \), with \( \alpha \) a new phenomenological disorder numerical parameter \( (0 \leq \alpha \leq 1) \). If we use this approach, this is not a self-consistent, but a fixed point numerical calculation. In such a case, we get the following general equation for \( \frac{N(0)}{N_F} \), obtaining a dimensionless and non-self-consistent disorder parameter \( C_0 = \frac{\alpha}{\Delta_0} \), obtaining

\[
N(0) = N_F \left( \frac{C_0}{\sqrt{C_0^2 + \Delta_0^2(k_x,k_y)}} \right)_{FS} (7)
\]

Equation (7) depends on the symmetry of the order parameter (OP) and the elastic scattering limits of the imaginary part of the elastic scattering cross-section, i.e., unitary, intermedia and Born cases [41] (see the isotropic expression in [41] and the TB expressions of Table 1 in order to compare the formalism).

The plot of the residual functional dependence \( \frac{T_c}{T_{c0}} = f \left( \frac{N(0)}{N_F} \right) \) strongly depends on the Larkin equation (8) for suppression of dressed DOS states in the case of non-magnetic disorder in unconventional superconductors, when the critical temperature \( T_c \) is decreased as a function of the pair breaking parameter \( \eta_c \) [42],

\[
\ln \frac{T_c}{T_{c0}} = \psi \left( \frac{1}{2} \right) - \psi \left( \frac{1}{2} + \eta_c \right) = \psi' \left( \frac{1}{2} \right) \frac{\Gamma^+}{2\pi T_c} (8)
\]

In equation (8), the Cooper pair breaking parameter is represented by a dimensionless \( \eta_c = -\frac{4\pi}{1.764} \ln \frac{T_c}{T_{c0}} \), the other quantities in equation (8) are the following: \( T_{c0} \) is the transition temperature for a clean superconductor \( (\alpha = 0) \), \( T_c \) represents the transition temperature for dirty superconductors, i.e., \( \alpha \neq 0 \), \( \psi(x) \) is the digamma function, and \( \psi'(x) \) - its derivative.

Table 1 summarizes in the TB case, the expressions needed for the calculation of the functional shape in the relationship \( \frac{T_c}{T_{c0}} = f \left( \frac{N(0)}{N_F} \right) \), for the cases that we numerically plot in this section; these equations can be obtained after some long algebraic manipulations using equations (7) and (8).

The difference with previous works [36,41], is in the FS average \( \langle ... \rangle_{FS} \), the basis function \( \phi_k \) in the case of a singlet nodal line OP, and the complex triplet vector OP \( d_k \) are the ones stated in section 2, with first neighbors hopping TB parameters, a discussion with second and third neighbors for the MN triplet \( \gamma \) sheet model is given in their original work [36].
Theoretically it is known that the concentration of impurities suppresses the critical temperature $T_{c0}$ and the Gap equation temperature dependence [6,39,40]. The residual DOS also changes as a function of $T_c$, as it is shown accordingly to table 1. Noticeable in this work that the parameter $C_0$ depends on the Fermi TB averages. In order to numerically evaluate the polynomial expressions involved, it is more convenient to simplify the analysis to the weak dispersion (Born), and the strong dispersion (unitary) limits (see Table 1 for a summary).

Table 1: $C_0$ parameter, and residual density of states equations; summarized for both irreducible representations, $B_{1g}$ and $E_{2u}$ of the symmetry point group $D_{4h}$ for Born, intermedia and unitary scattering limits.

| Residual Density of states RDOS TB formalism | Expressions for $C_0$ in the Born and intermedia limits | Expressions for $C_0$ in the unitary limit | Residual DOS equations for Born and intermedia scattering limits | Residual DOS equations for the Unitary scattering limit |
|---------------------------------------------|--------------------------------------------------------|------------------------------------------|---------------------------------------------------------------|---------------------------------------------------------------|
| **Singlet line nodes case for the scalar OP** | $C_0 = \pi \eta_c \left(\frac{C_0}{\sqrt{C_0^2 + \phi_0^2}}\right)_{FS}$ | $C_0 = \pi \eta_c \left(\frac{\sqrt{C_0^2 + \phi_0^2}}{C_0}\right)_{FS}$ | $\frac{N(0)}{N_F} = \frac{C_0}{\pi \eta_c}$ | $\frac{N(0)}{N_F} = \left(\frac{C_0}{\pi \eta_c}\right)^{-1}$ |
| **Triplet quasi-point nodes case for the triplet vector OP** | $C_0 = \pi \eta_c \left(\frac{C_0}{\sqrt{C_0^2 + |d^K|^2}}\right)_{FS}$ | $C_0 = \pi \eta_c \left(\frac{\sqrt{C_0^2 + |d^K|^2}}{C_0}\right)_{FS}$ | $\frac{N(0)}{N_F} = \frac{C_0}{\pi \eta_c}$ | $\frac{N(0)}{N_F} = \left(\frac{C_0}{\pi \eta_c}\right)^{-1}$ |

The results of the numerical calculation using equations taken from Table 1 are shown in Figure 5 for the case of La$_{2-x}$Sr$_x$CuO$_4$. At zero $T_c/T_{c0}$ the largest residual DOS value for both cases is obtained (for unitary and Born limits). On the other hand, as $\frac{N(0)}{N_F}$ increases, $T_c/T_{c0}$ ratio falls to zero, faster for a weak scattering Born non-magnetic potential limit than for the unitary limit. In addition, from Figure 5, we see that the unitary limit presents a curve that always has the same sign in slope; meanwhile the Born limit changes it signs and even has a linear behavior dependence for $N(0) \sim \frac{1}{2} N_F$.

Figure 6 compares the unitary limit for the compound strontium doped 214 lanthanum copper oxide for different experimental values of Sr doping obtained experimentally and denoted by the letter x [45]. Sr doping has been extensively studied in the cuprate La$_{2-x}$Sr$_x$CuO$_4$ for smaller orders of strontium concentration recently [43,44]. The color points with Sr impurity atoms are from values of specific electronic heat capacity $C(T)$ in the superconducting state, where in Figure 6 the gray color corresponds to $x = 0.10$, green color corresponds to $x = 0.18$, blue color corresponds to $x = 0.20$, and red color corresponds to $x = 0.22$ [45].

We see a clear tendency for the experimental red points with $x = 0.22$ corresponding to the value $\zeta_{\text{singlet}} = 0.020$ (in the DOS calculation) in correspondence with both the unitary theoretical residual DOS limit and the self-consistent DOS unitary case. Phenomenologically, this can be explained by comparison with the case of strontium ruthenate, where, upon scattering by stoichiometric Sr atoms, for all values of the non-magnetic $U_0$ potential, the $\gamma$-sheet is in the limit of unitary elastic scattering (see Fig. 2 in reference [10]).
Figure 5. Numerical calculation of the residual DOS in the case of the singlet La\textsubscript{2-x}Sr\textsubscript{x}CuO\textsubscript{4} line nodes in the Born and the unitary limits following equations in Table 1.

Figure 6. Fits of the previous curve for the unitary (U\textsubscript{0} >> 1, c = 0) limit in La\textsubscript{2-x}Sr\textsubscript{x}CuO\textsubscript{4} to experimental values from reference [45]. Different colors correspond to different values of the hopping parameter x.

Figure 7 shows the results for the reduced DOS in the case of the triplet Sr\textsubscript{2}RuO\textsubscript{4} with quasi-point. At zero \( \frac{T_c}{T_{c0}} \) we see the largest residual normalized DOS value \( \frac{N(0)}{N_F} \) for both cases (unitary and intermediate scattering as in [10] for the function \( \Im [\tilde{\omega}] (\omega + i 0^+) \), and as \( T_c \) increases \( \frac{N(0)}{N_F} \) falls to zero, faster for an intermediate scattering. We ought to remember from [10] that the Born limit does not play a significant role in the case of the FS \( \gamma \)-sheet for the case of stoichiometric non-magnetic strontium DOS impurity levels.

In figure 7, \( \frac{T_c}{T_{c0}} \) falls to zero slowly if the fixed point calculation is done for the unitary limit. As in the case of line nodes, the unitary triplet limit presents a curve that always has the same decreasing behavior in slope; the intermediate limit changes its slope weaker, slightly contrasting with the OP nodal line situation in Figure 5, where there is a clear intermediate linear behavior.
Figure 7 also compares the unitary limit for the compound strontium ruthenate, for four different experimental values originally calculated in [36]. In this case we recall that non-magnetic Sr atoms add an additional impurity level in the energy zone, since, Sr atoms are part of the structure. The experimental blue color points were taken from reference [46] accordingly to [36], confirming for the TB illustrative case, the MN original results.

Therefore, the experimental evidences that the FS $\gamma$-sheet of Sr$_2$RuO$_4$, is in the unitary elastic scattering limit makes it an instructive example to study in advanced superconductivity and solid-state courses, since three approaches can be used: The $\Im [\tilde{\omega}] (\omega + i 0^+)$, the $N(\omega)/N_F$ and the $N(0)/N_F$ analyses. Comparing them with the same ARPES experimental parameters and first neighbor hopping parameters is very instructive.

Finally, for an experimental detailed verification of the Larkin equation (8) using the superconducting electronic thermal conductivity $\kappa(T)$, see the experimental work [47]. The work [49] accomplish an extended recent analysis with several important remarks concerning these two compounds.

![Figure 7. Numerical calculation of the residual DOS in the case of the triplet Sr$_2$RuO$_4$ quasi-point nodes model for the intermedia and the unitary limits following equations in Table 1. The blue color shows the previous curve fits corresponding to the unitary limit in Sr$_2$CuO$_4$ with experimental values obtained in [46] and confirmed in [36].](image)

5. Conclusions

This work was aimed at pedagogically revisiting the calculation of the density of states (DOS) and the residual DOS with energy values taken from a self-consistent calculation of the imaginary part of the elastic scattering cross-section for two important realistic models, that can be used for instructional purposes. The strontium-substituted lanthanum cuprate, and strontium ruthenate compounds, where the dressed DOS levels, in the reduced phase scattering space come from non-magnetic pair breaking disorder, or in situ additional strontium atoms impurity levels.

The models used were the first TB neighbors 2D nodal line (Scalapino [28]), and the 2D tiny quasi-point FS $\gamma$-sheet nodes (Miyake and Narikiyo [36]), with an anisotropic TB [9,10,11] parametrization. We focused our study of the DOS and residual DOS, on the three types of non-magnetic scattering (the Born, intermedia and unitary limits). Revisiting the DOS and the residual DOS numerical modeling with non-magnetic disorder phenomena in a self-consistent 2D TB model, is a subject of interest in the field of superconductivity and its instructional practice. Finally, it helps us to confirm our numerical results using the imaginary part of the scattering cross-
section presented recently, where long time consuming computer calculations were made for a whole set of impurity concentration values and wide computing consuming energy ranges.

For the high $T_c$ compound strontium doped 214 lanthanum copper oxide the DOS was numerically calculated for the clean ($U_0 = 0$), Born ($U_0 << 1$), and unitary limits ($U_0 >> 1$), for six values non-magnetic disorder, starting with clean, then very diluted to most optimal normalized (dimensionless) non-magnetic Sr doping values ($\zeta_{\text{singlet}} = 0.000, 0.001, 0.005, 0.010, 0.015, 0.020$), noticing that the self-consistent DOS behavior previously results in the literature were reproduced. However, our dimensionless doping parameter, realistically, starts from an order of magnitude of $10^{-3}$, as recent experiments suggest [43,44], with the doping parameter $x \sim \zeta_{\text{singlet}}$.

For the unconventional $\text{Sr}_2\text{RuO}_4$, the DOS was numerically calculated for the unitary limit for six values of local non-magnetic disorder potential ($U_0 > 1$, $c = 0$), starting with clean to optimal dimensionless non-magnetic impurity levels of disorder with the values ($\zeta_{\text{triplet}} = 0.00, 0.01, 0.05, 0.10, 0.15, 0.20$), noticing that the results from the original DOS of the MN model were reproduced [36]. In this case, we find the tiny gap for the value $\zeta = 0.05$ as it was recently found using the imaginary part of the scattering elastic cross-section [10,11,12].

Subsequently, we calculated the residual DOS using a TB approach for both models. We also reproduced the results previously found in the literature but taking into account the dimensionless parametrization and anisotropic effects of the FS, for the residual DOS, we find that it is natural to find the unitary limit in the triplet FS $\gamma$ - sheet. In this case, the dimensionless non-magnetic disorder is a the pair breaking parameter $\eta_c$.

Finally, we would like to emphasize the tutoring structure of this paper where the analysis of the density of states (DOS) and its residual part (both being quantum observables) can be used in a tight-binding (TB) approach. Contrasting the 2D modelling of these superconductors is didactic. The DOS and residual (RDOS) procedure using a quantum observable as the density of states, can be compared with the imaginary elastic scattering cross-section $\Im \{\omega\} (\omega + i 0^+)$, calculations (where thousands of $\omega$ points are needed to obtain whole sets of Wigner distribution probability curves) granting researchers with a classical window to superconductors [13,14,50], and which are more computing demanding and more complex to analyze [48,50]. TB ads an instructive aspect as well, since those dressed quantum levels can be treated with hopping QM parameters from ARPES data. Additionally, an interesting work will be to calculate the DOS and the residual RDOS for the case of a flat band limit with point nodes and in the metallic ground state, as it has been recently calculated the imaginary part of the scattering cross-section for $\text{Sr}_2\text{RuO}_4$ [12].

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