



A NONLINEAR MINIMIZATION CALCULATION OF THE RENORMALIZED FREQUENCY $\tilde{\omega}$ IN DIRTY d -WAVE SUPERCONDUCTORS

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ABSTRACT

This work performs a comparative numerical study of the impurity average self-frequency $\tilde{\omega}$ in an unconventional superconducting alloy with non-magnetic impurities. Two methods are used: the Levenberg-Marquardt algorithm as a nonlinear minimization problem, and a fixed-point iteration procedure. The unconventional superconducting renormalized by impurities $\tilde{\omega}$ is a self-consistent complex nonlinear equation with two varying parameters: the impurity concentration Γ^+ and the strength of the impurities c , for which its numerical solution is a computational challenge. This study uses an order parameter that corresponds to the high-temperature superconducting ceramics (HTS) with a well-established gap symmetry. The results reveal the computational efficiency of the non-linear minimization technique by improving the calculations of the $\tilde{\omega}$ computation when using a two-dimensional parameter space (Γ^+ , c), particularly in the unitary regime, where the imaginary part of $\tilde{\omega}$ is a complicated expression of those parameters; this allows to enhance the study of the universal behavior of this particular quantum mechanical state.

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Keywords:Nonlinear minimization algorithm, fixed-point routine, HTS dirty d -wave superconductors, self-consistent frequency, quasi-particle lifetime, superconducting density of states.

INTRODUCTION

The effect caused by nonmagnetic impurities in unconventional superconductors play a fundamental role in the understanding of their physical properties when these materials are doped. We use an order parameter well established for the high-temperature superconductors (HTS) (Maeno *et al.*, 1994). Superconducting ceramics have a transition temperature T_c close to the boiling point of liquid Nitrogen: $T_{Ni} = -195.79$ degrees Celsius (Bergemann *et al.*, 2003). Although these materials are fragile in their elastic properties, they aim to revolutionize the technology of electrical conduction without energy loss (Kamerlingh Onnes, 1911a, 1911b, 1911c). In particular, these materials lose their superconducting properties as soon as nonmagnetic impurities are added. For example, for *YBCO* ceramics doped with Zn impurities, the transition temperature T_c begins to decrease rapidly (Maeno *et al.*, 1994).

We know that for the HTS, the energy gap corresponds to a paired singlet quantum state with a $d_{x^2-y^2}$ symmetry, for example, in hole-doped cuprate superconductors such as $YBa_2Cu_3O_7$ and $Tl_2Ba_2CuO_6$ (Tsuei and Kirtley, 2000; Annett, 1995). The superconducting gap for this

symmetry has lines nodes on the Fermi surface, and the energy gap corresponds to the one-dimensional irreducible representation B_{1g} of the tetragonal point symmetry group D_{4h} . They are called d -wave superconductors and they have elastic impurity scattering preserving the total kinetic energy. The d -wave gap changes sign as a function of the azimuthal angle θ with line nodes in the energy spectra as it is illustrated in Figure 1.

The task of this work is to obtain the solution of the equation for $\tilde{\omega}$ for a wide range of (Γ^+ , c) parameters. This complex nonlinear two-dimensional equation is very difficult to solve by conventional iterative algorithms. Instead of that, in this work we solve $\tilde{\omega}$ using two numerical routines; throughout this study $\tilde{\omega}$ is the renormalized frequency, γ represents the inverse of the residual average lifetime τ at zero frequency, and N/N_0 is the normalized superconducting density of states (DOS). We calculate and studied the DOS at low energies. The DOS gives insight information about the temperature behavior of some relevant thermodynamic and kinetic quantities in unconventional superconductors that are experimentally measured such as the specific electronic heat $C(T)$, the thermal conductivity $\kappa_{ij}(T)$ and the sound attenuation $\alpha_{ij}(T)$ (Contreras *et al.*, 2004; Contreras, 2011;

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Contreras *et al.*, 2014). These measurements help to clear up the structure of the gap symmetry.

This work consists of five sections. The first section introduces the subject of the dirty d -wave (HTS) and limits our study to a spherical (isotropic) Fermi surface with a line-nodes order-parameter of the one-dimensional representation B_{1g} of the tetragonal group D_{4h} . The second section explains shortly the $\tilde{\omega}$ formalism given by Mineev and Samokhin (1999), and also follows the approach by Schachinger and Carbotte (2003) that does some of these numerical calculations in a different physical context (the residual absorption at zero temperature of the optical spectral weight). Briefly, we derive and explain equations (2) and (4) and refer the readers to these two references for further details. The third section briefly introduces and explains the way the two algorithms work and their main differences (the implementation advantages and/or disadvantages). The fourth section presents the numerical solutions of equations (2) and (4) by comparing the fixed-point iteration procedure and the nonlinear minimization algorithm. The fifth section performs a numerical evaluation of the normalized DOS in the unitary and Born regimes. The calculation of the low energy DOS is crucial for the impurity case, because it shows the limit which belongs to the HTS d -wave superconductors. We conclude with a summary of the main results and some final thoughts are provided for some further research.

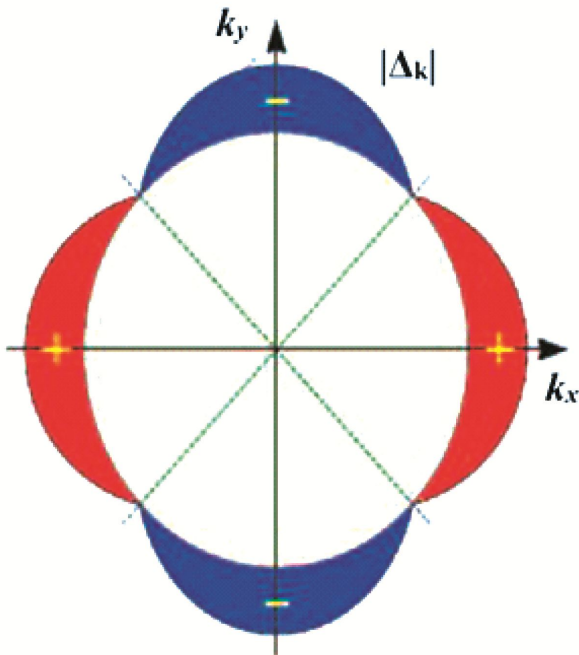


Fig. 1. The $d_{x^2-y^2}$ gap for the one-dimensional irreducible representation B_{1g} of the tetragonal point symmetry group D_{4h} for a spherical Fermi surface.

THE $\tilde{\omega}$ FORMALISM FOR NONMAGNETIC IMPURITIES

In the case of unconventional superconductors with a singlet pairing state such as the HTS, when nonmagnetic impurities effects are added, the interaction Hamiltonian between impurities and Cooper pairs is given by the following expression:

$$H = U_0 \sum_{i,j} \hat{c}_f^+ \hat{c}_i(1)$$

where U_0 is the interaction potential, \hat{c}_i and \hat{c}_f^+ are the annihilation and creation operators of the Cooper pairs. When multiple elastic scattering of a Cooper pair occurs (Mineev and Samokhin, 1999; Smith and Walker, 2000; Landau and Lifshitz, 1965); the $\tilde{\omega}$ is not only given in the Born limit (weak potential with $U_0 \ll 1$ and a Cooper pair scattered by one impurity). Instead, a Cooper pair scatters many impurities (strong Coulomb interaction with $U_0 \gg 1$) and the calculation of the equation for the $\tilde{\omega}$ that has to be done in the unitary regime. However, the fixed-point method has problems in finding a proper $\tilde{\omega}$.

We consider the important case of weak disorder (restricting our calculation more). It means that at sufficiently low concentration of impurities, the condition $k_f l \gg 1$ (l is the mean free path) prevails and the crossed Feynman diagrams are ignored. Physically, this means that there is no interference between scattered waves having different probability amplitudes (Mineev and Samokhin, 1999; Edwards, 1961; Lussier *et al.*, 1996; Landau and Lifshitz, 1965; Puchkaryov and Maki, 1998).

We further consider the dimensionless Planck units ($\hbar = c = k_B = 1$) for the whole calculation. Nevertheless, the renormalized frequency $\tilde{\omega}$ does not depend on the angle because of the elastic impurity scattering changes. The elastic scattering is the only scattering process taken into account in our work. The dimensionless self-consistent frequency equation for $\tilde{\omega}$ in a t -matrix approximation is (Mineev and Samokhin, 1999; Schachinger and Carbotte, 2003):

$$\tilde{\omega}(\omega) = \omega + i\pi\Gamma^+ \frac{\langle g(\theta, \tilde{\omega}) \rangle_{FS}}{c^2 + \langle g(\theta, \tilde{\omega}) \rangle_{FS}^2} \quad (2)$$

In equation (2), the imaginary term is the self-energy renormalized for nonmagnetic doped impurities $\Sigma_{imp}(\tilde{\omega})$ and the Fermi averaged expression for $g(\tilde{\omega})$ is

$$g(\tilde{\omega}) = \langle \frac{\tilde{\omega}}{\tilde{\omega}^2 + |\Delta|^2} \rangle_{FS} \quad (3)$$

In equation (2), the parameter $c = 1/(\pi N_F U_0)$ and the parameter $\Gamma^+ = n_{imp}/(\pi N_F)$. For very low frequencies ($\omega \rightarrow 0$), $\tilde{\omega} = i\gamma$ and γ becomes equal to

$$\gamma(\Gamma^+, c) = \pi\Gamma^+ \frac{g(i\gamma)}{c^2 + g^2(i\gamma)} \quad (4)$$

where

$$g(i\gamma) = \langle \frac{\gamma}{\gamma^2 + |\Delta|^2} \rangle_{FS} \quad (5)$$

We call equation (4) the transcendental equation of the residual average lifetime at zero frequency with $\gamma = 1/\tau(0)$. According to equation (2), we know that γ depends on both Γ^+ and c . So, first we solve and analyze this dependency numerically for equation (4).

We write the imaginary part of equation (2) as $\text{Im}[\tilde{\omega}(\omega)] = 1/\tau(\omega)$, where $\tau(\omega)$ represents the average lifetime for the bounded quasi-stationary state and $\text{Im}[\tilde{\omega}(\omega)]$ is the disintegration probability W per unit time (Landau and Lifshitz, 1965). In other words, the calculation of the imaginary term empowers a direct evaluation of the average lifetime in a particular quasi-stationary state for a weak-elastic scattered and doped d -wave HTC superconductor.

THE ALGORITHMS

We used two different algorithms to find the numerical solution of equation (2): An iterative fixed-point method with error differences to find the sought solution for $\tilde{\omega}$ (GCC, the GNU Compiler Collection), and a minimization routine based on the nonlinear Levenberg-Marquardt method (Levenberg, 1944; Marquardt, 1963). Both were developed in a C language (Standard C11, ISO/IEC 9899:1999 - Programming languages - C), which supports complex numbers in a native way, in the GCC compiler (GNU Compiler Collection) and the open-source integrated development environment NetBeans IDE.

(A) The fixed-point method

The fixed-point algorithm (GNU Compiler Collection) iterates a maximum number of times `max_iter` equation (2). It evaluates whether the real and complex parts of equation (2) are smaller than a specified tolerance TOL between two continuous evaluations of the equation. When the smaller values are found, it converges and the solution is reached. Its performance and solution is strongly associated with the “quality” of the initial conditions and the dimensions of the parameter space involved (c, Γ^+) as we conclude in this work.

(B) The Levenberg-Marquardt algorithm

The Levenberg-Marquardt algorithm (Levenberg, 1944; Marquardt, 1963) is an iterative method that solves nonlinear quadratic systems through the combination of the descending gradient and the Gauss-Newton methods by following the behavior of the quadratic error. The

method provides a solution for the minimization of linear complex quadratic systems of equations. This implies that the minimization function must have the following special form:

$$f(x) = \frac{1}{2} \sum_{j=1}^m r_j^2(x) \quad (6)$$

where $x = (x_1, \dots, x_m)$ is a vector, and each r_j is a function $r_j: R_n \rightarrow R_n$. r_j is known as a residual (it is assumed that $m \geq n$). In this methodology, $f(x)$ is represented as a residual vector \mathbf{r} such that $\mathbf{r}: R_n \rightarrow R_n$, where $r(x) = (r_1(x), \dots, r_m(x))$. The derivatives of $f(x)$ are written using a Jacobian matrix \mathbf{J} . The methodology considers the case where every function r_j is linear, the Jacobian is constant, and \mathbf{r} is represented as a hyperplane (a 2D space parameter in our case). $\nabla^2 f(x) = \mathbf{J}\mathbf{J}^T$ is given by its quadrature, and it is obtained by solving the minimum when $\nabla f(x) = 0$, in such a case it is found that $x_{min} = -(\mathbf{J}^T\mathbf{J})^{-1}\mathbf{J}^T\mathbf{r}$ which is the solution for normalized equation (2).

Returning to the nonlinear case, we have that the distinctive feature of the least-squares problem is that given the Jacobian matrix \mathbf{J} , the Hessian $\nabla^2 f(x)$ can be found. If this is possible, r_j are approximated by linear functions, where the $r_j(x)$ and the $r_j^2(x)$ are small and the Hessian becomes $\nabla^2 f(x) = \mathbf{J}^T\mathbf{J}$ that is the same equation obtained for the linear case. This common approach applies to systems where the residuals r_j are small (in our case, a 2D (Γ^+, c) space parameter).

THE NUMERICAL RESULTS

We begin testing the two algorithms to find a solution for equation (2). Immediately it was discovered that although the fixed point algorithm has a faster runtime (Table 1), it does not manage to differentiate the parameter Γ^+ , obtaining, that no matter the value of Γ^+ is, always the imaginary part of $\tilde{\omega}$ is very similar for different values of Γ^+ as shown in Figure 4(a). This result is explained below, it means that the curve in Figure 4(b) cannot be reproduced with the fixed-point procedure.

On the other hand, the Levenberg-Marquardt nonlinear algorithm performs a minimization for equation (2) and accurately differentiates small and large values of both the parameters: Γ^+ and c . Thanks to this algorithm, we are able to find the results showed in Figure 4(b). In this analysis, Γ^+ and c were evaluated for small relative numbers that outline two physical regimes: (*) the misbehaved ill quasi-particle unitary state (Mineev and Samokhin, 1999; Schachinger and Carbotte, 2003; Bad metals and the unitary limit); (**) the Born limit where the elastic scattering, the free mean path, and the quasiparticles states physically are well defined.

Subsequently, we analyze transcendental equation (4) that represents the dispersion of quasiparticles at $\omega = 0$ and for zero temperatures. It is observed in Figure 2 that when $c = 0$ and U_0 rapidly increases, γ also increases. Moreover, $\Gamma^+ = 0.3$ meV gives the maximum γ value in figure 2, with an observed tendency for decreasing Γ^+ values. This means that for higher impurity concentration, the Cooper pair lifetime $\tau(\omega) \rightarrow 0$ decreases faster when $c \rightarrow 0$, giving that for values $c \leq 0.1$ the probability of destroying the superconducting state by the impurity is calculated correctly. Nonetheless, for γ values with relatively small U_0 given when $c \geq 0.1$, bound states still remain in the sample with a small $\tau(\omega)$. Consequently, the imaginary part of the zero-frequency dispersion decays faster, implying that the average lifetime increases faster if the potential strength is not so small. Figure 2 should be compared with the reference figure 4 bottom frame in (Schachinger and Carbotte, 2003). Also, the results shown in Figure 2 should be compared with some of the results obtained in (Puchkaryov and Maki, 1998).

Table 1. The runtime for the complex fixed-point and minimization algorithms to calculate $\tilde{\omega}(\omega)$. The table summarizes the data processing of both algorithms for a computer architecture with a 64-bit Intel I5 processor and an 8 GB RAM in a Slackware 14.2 OS (Slackware Linux Project).

Method	Running performance
Self-consistent method	24 seconds
Minimization method	15 minutes and 24 seconds

As a next step, we display the 3D figure of transcendental equation (4), $\gamma(\Gamma^+, c)$ in figure 3. We limit our discussion to places near the location of the minimum gap nodes at zero temperatures. So, in this neighborhood there are still ill-defined quasiparticles. We want to pursue the discussion by Landau and Lifshitz concerning the resonance spectrum of quasiparticles at quasi-discrete levels by quoting their own words (Landau and Lifshitz, 1965): It may happen, however, that the disintegration probability W of the system is very small. The simplest example of this kind is given by a particle surrounded by a fairly high and wide potential barrier. For such systems with a small disintegration probability, we can introduce the concept of quasi-stationary states, in which the particles move “inside the system” for a considerable period of time, leaving it only when a fairly long time interval τ has elapsed; τ may be called the lifetime of the almost stationary state concerned ($\tau \sim 1/W$, where W is the disintegration probability per unit time). The energy spectrum of these states will be quasi-discrete; it consists of a series of broadened levels, whose “width” is related to the lifetime by $\tau \sim \hbar/\Gamma$. The widths of the quasi-discrete levels are small compared with the distances between them.

It can be also seen in Figure 3 that for a zero value of Γ^+ , no matter what the value of the strength $c \sim 1/U_0$ is, a straight zero horizontal axis line $\gamma(\Gamma^+ = 0, 0 \leq c \leq 1)$ can exist even when the imaginary part disappears and the scattering phenomenon loses any physical meaning. According to our interpretation, it doesn't imply that the quasiparticles lifetime $\tau(0)$ is infinite, just its physically nonentity.

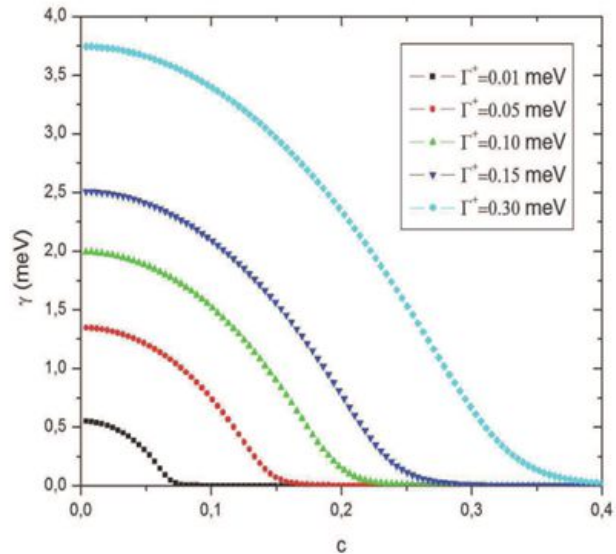


Fig. 2. The transcend equation $\gamma(c)$ as a function of the strength related parameter c for five different values of the concentration related parameter Γ^+ .

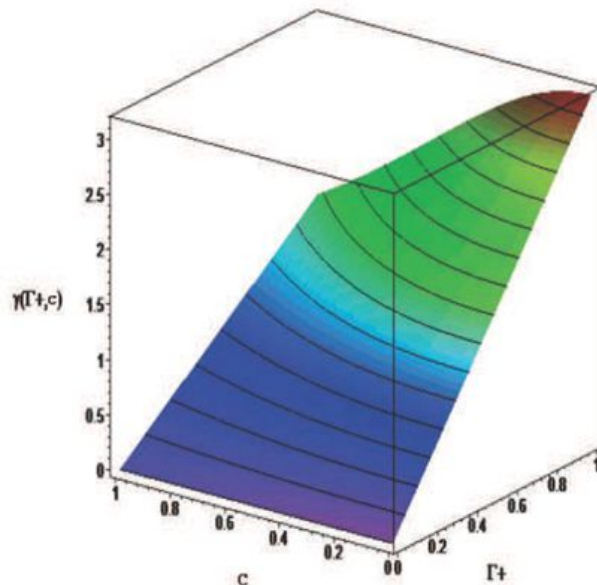


Fig. 3. The sketch of the imaginary part $\gamma(\Gamma^+, c)$ as a continuous 3D function of c and Γ^+ . The green and red neighborhoods show the smallest lifetimes $\tau(0)$, and the dark blue part shows the region with the biggest $\tau(0)$

value. This picture was obtained for gap values that are closed to the nodes of Figure 1.

As soon as small finite values of the impurities concentration appears ($\Gamma^+ \sim n_{imp}$), the 3D manifold emerges (Fig. 3) with the maximum value for the $\gamma(\Gamma^+, c)$ surface in the neighborhood of the point with $\gamma(\Gamma^+ = 1, c = 0)$ and a gap value of $\Delta_0 = 0$, $\gamma_i = 1$, and $\gamma(\Gamma^+ = 1, c = 0) = \pi$. At this point, we find the smallest lifetime $\tau(0)$ in the unitary regime and $\omega = 0$ (the red color neighborhood on the right side in figure 3). However, for the values around the point $\gamma(\Gamma^+ = 1, c = 1) = 1.57$, smaller γ means that a bigger lifetime $\tau(0)$ exist with $\omega = 0$, corresponding to a Born scattering with some remaining ill-quasiparticles states (the green color neighborhood on the left side in Figure 3). Another case of interest is when $\tilde{\omega} \neq 0$ has a constant value and the 3D manifold $\gamma(0 \leq \Gamma^+ \leq 1, c = 0)$ converts into a 2D straight line $\tilde{\omega} = \omega - i\gamma(\Gamma^+, c = 0)$. In this case, $\omega \neq 0$ has a very large potential (and a greater slope), with Γ^+ equivalent to the Landau-Lifshitz parameter Γ mentioned in their book on Quantum Mechanics (Landau and Lifshitz, 1965), Chapter XVII, section 132, equation 132.1 that resembles the unitary limit. Finally, in Figure 3 there is another case at $\tilde{\omega} = \omega - i\gamma(\Gamma^+, c = 1)$, with a straight line of smaller slope, corresponding to a Born limit with $\omega \neq 0$ and a very small potential (Landau and Lifshitz, 1965). The case when $\Delta \neq 0$ we will analyze in the future because here our discussion follows a zero-temperature approach.

Following the analysis, we calculate equation (2) corresponding to the self-frequency consistent $\tilde{\omega}$ using the minimization algorithm. This equation contains the inverse of the average lifetime states for the quasiparticles bound to the impurity (Mineev and Samokhin, 1999; Schachinger and Carbotte, 2003; Hirschfeld *et al.*, 1988). The top and bottom frames in Figures 4(a) and 4(b) respectively show that two physical limits are well established from the imaginary part of $\tilde{\omega}$: the Born and the unitary regimes.

In both cases, the figures display the unitary regime with the strength parameter interaction at $c = 0$ in black color. In such a case, the imaginary part of the frequency (the disintegration probability per unit time) $\text{Im}[\tilde{\omega}(\omega)]$ has a maximum at zero frequency $\omega = 0$. This physically shows that the magnitude of the scatter potential U_0 is strong enough to immediately break the bound state of the Cooper pair because $c = 1/(\pi N_F U_0)$. Moreover, as the interaction parameter c moves away from the unitary limit (with $\tau(0) \rightarrow 0$), the maximum of the disintegration probability $\text{Im}[\tilde{\omega}(\omega)]$ decreases as the parameter c increases (the interaction potential U_0 decreases) as a function of the frequency ω .

With the values of $c \geq 0.2$, its observed that the behavior is close to the Born limit, for which the value of the interaction potential U_0 is small in comparison with the electronic energy. Therefore, $\tau(\omega)$ increases. The top frame of figure 4 shown in this paper should be compared with the figure 1 bottom frame in (Schachinger and Carbotte, 2003). It is stated that the bottom frame in Figure 4 is showed and discussed here for the first time. The bottom part in figure 4 shows that with a very small value of $\Gamma^+ = 0.001$ meV, the disintegration probability $\text{Im}[\tilde{\omega}(\omega)]$ is very small for most of the whole frequency range and the maximum $\text{Im}[\tilde{\omega}(\omega)]$ shifts with a pronounced peak to the right values of the frequency ω .

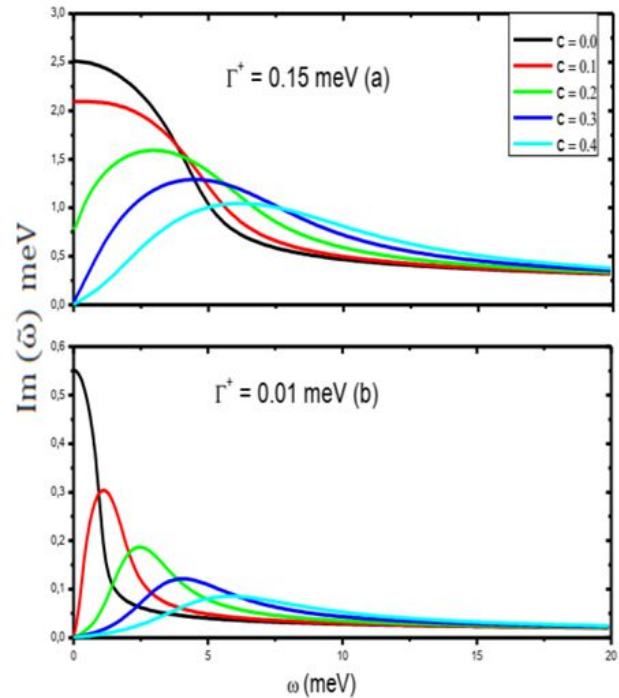


Fig. 4. $\text{Im}[\tilde{\omega}(\omega)]$ vs. ω for small concentrations of impurity (bottom-frame b, $\Gamma^+ = 0.01$ meV) and higher concentrations (top-frame a, $\Gamma^+ = 0.15$ meV) for the unitary ($c = 0.0$), intermediate ($c = 0.2$), and Born ($c = 0.4$) limits.

THE SUPERCONDUCTING DENSITY OF STATES

In this section, the DOS results are presented. In unconventional superconductors, the order parameter goes to zero at some parts of the Fermi surface. Due to this fact, the density of states at very low energy arises from the vicinity where the nodes of the order parameters are located. Well known examples of this are the HTS (Annett, 1995). In general, line nodes and point nodes give a density of states that varies at the low energy limit as ω and ω^2 , respectively (Mineev and Samokhin, 1999; Contreras, 2011).

Besides the nodes in the order parameter, scattering from non-magnetic impurities also influences the calculation of the low energy DOS (Mineev and Samokhin, 1999; Puchkaryov and Maki, 1998; Hirschfeld *et al.*, 1988). This elastic scattering mechanism leads to the lowering of T_c ; and therefore, to the suppression of the superconducting state. In general, for temperatures much smaller than T_c , the effect of having very low nonmagnetic impurities concentration can be neglected. It is found that only for very low temperatures, the effect of impurities becomes important for the unitary limit. However, for clean samples, this effect can be neglected (Contreras *et al.*, 2014; Hirschfeld *et al.*, 1988).

Therefore, in dirty d -wave (HTS) becomes interesting to reconstruct the appearance of normal states at zero temperature. Hence, we study the evolution of the gap as a function of Γ^+ . We used the minimization routine (Levenberg, 1944; Marquardt, 1963). The DOS for low frequencies ($\omega \rightarrow 0$) is calculated by the following expression (Mineev and Samokhin, 1999):

$$N(\omega) = N_{FS} \text{Re}[g(\tilde{\omega}(\omega))] \quad (7)$$

where $g(\tilde{\omega}(\omega))$ is given by expression (3), the Fermi average $\langle \dots \rangle_{FS}$ in equation (3) is performed over a spherical Fermi surface with a polar representation of the d -wave gap $\Delta = \Delta_0 \cos(2\theta)$, see in figure 1. Experimentally, the value for $\Delta_0 = 24 \times (2)^{1/2}$ meV corresponds to the maximum value obtained by the ARPES technique (Schachinger and Carbotte, 2003; Palczewski, 2010).

As the fourth result, the figure 5(a) top frame shows the unitary limit case with an a $c = 0$ strength parameter (where a single Cooper pair scatters many impurities, and n_{imp} is larger ($\gamma = 0.15$ meV); it remarkably shows that there is a large density of residual states $N(0)$ for higher concentrations of impurities $\Gamma^+ \sim n_{imp}$ (red line) mapping the zero frequency $\omega = 0$ DOS unitary behavior. However as this concentration decreases an order of magnitude, the amount of residual states $N(0)$ also decreases, the black line in Figure 5(a). Regardless of this, the same behavior persists for both curves, represented by the black and red colors corresponding to the unitary regime. The residual $N(0)$ existence changes the behavior in the universal limit of certain kinetic coefficients such as the thermal conductivity $\kappa_{ij}(T)$ and the sound attenuation $a_{ij}(T)$ (Mineev and Samokhin, 1999; Contreras *et al.*, 2004; Contreras *et al.*, 2014).

Bottom frame of Figure 5(b) corresponds to the case with an intermediate scatter parameter $c = 0.2$ which represents in practice the dispersion due to a single impurity, and the bound of the U_0 potential with the Cooper pair is relatively small (Born limit). We see in Figure 5(b) that

there is no residual density of states $N(0)$ at zero frequency as it was shown in (Schachinger and Carbotte, 2003) for the HTS d -wave superconductors, and in (Hirschfeld *et al.*, 1988) for the heavy fermion superconductors. For the calculation of the DOS in this work, we use two Γ^+ values to test the nonlinear minimization technique.

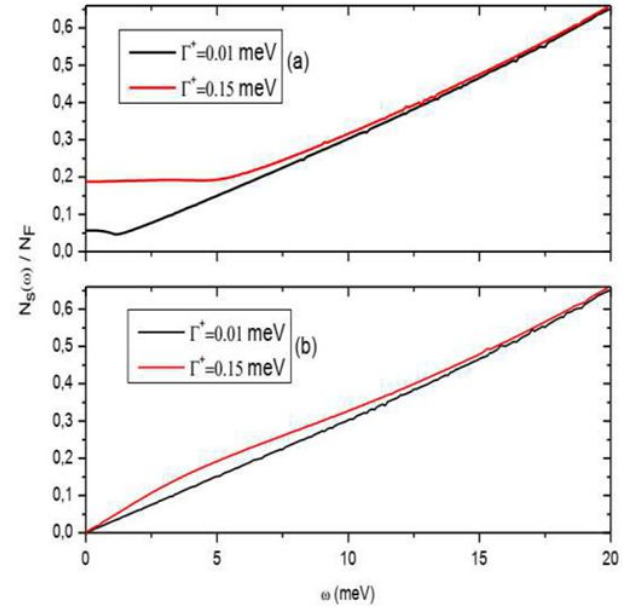


Fig. 5. The DOS normalized $N(\omega)/N_F$ for top bottom-(a) unitary regime and low bottom-(b) Born case.

CONCLUSION

This study compares and implements two algorithms to solve the imaginary nonlinear self-consistent equation for $\tilde{\omega}$ in nonmagnetic unconventional superconductors. As a main conclusion, this work states that the minimization algorithm (Levenberg, 1944; Marquardt, 1963) is the appropriated numerical procedure to solve $\tilde{\omega}$ in the complex field, when the number of varying parameters is two, that is to say, the impurity concentration Γ^+ and the strength parameter c . The cost in time showed in Table 1 correctly approaches the space parameter minimization search accounting for different Γ^+ values. On the other hand, the self-consistent fixed-point algorithm (GCC, the GNU Compiler Collection) only manages to properly solve equation (2) for the parameter c (faster according to Table 1, however, as Γ^+ changes it does not converge). That means that the fixed-point method is not suitable for a parameter space of dimension $d \geq 2$. This result is based on the exact reproduction of the imaginary part of $\tilde{\omega}$, as well as, the density of superconducting states (DOS) previously calculated in (Schachinger and Carbotte, 2003) for different values of Γ^+ .

Additionally, it was possible to obtain the inverse of the average lifetime $\tau(\omega)$ and the imaginary part (disintegration probability) $\text{Im}[\tilde{\omega}(\omega)]$ in Figure 4(b) for very small impurity concentration values of Γ^+ such as $\Gamma^+ = 0.01$ meV. This result offers a relevant approach to numerically study the unitary limit regime. To a certain extent there are strong experimental evidences that the heavy fermions superconductors UPt_3 (Lussier *et al.*, 1996; Hirschfeld *et al.*, 1988) and UPd_2Al_3 (Scheffler *et al.*, 2005) are in the unitary regime. This calculation is not reported by Schachinger and Carbotte (2003) (the authors did not mention their numerical approach to solve equation (2)). Furthermore, this report points out the importance of the use of appropriate numerical methods such as the minimization procedure (Levenberg, 1944; Marquardt, 1963) when studying elastic scattering quantum mechanical phenomena (Landau and Lifshitz, 1965; Bad metals and the unitary limit) with parameter space of dimension $d \geq 2$.

Finally, this study emphasizes that the physics of the unitary regime in superconducting metals needs further clarification (bad metals and the unitary limit; Coleman, 2015) as we stated in the fourth section, where Figure 3 is analyzed from a more general quantum mechanical approach (the footnote is added in the bibliography) (Landau and Lifshitz, 1965; Scheffler *et al.*, 2005; Bad metals and the unitary limit).

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REFERENCES

Annett, JF. 1995. Unconventional superconductivity. *Contemporary Physics*. 36(6):423-437.

Bergemann, C., Mackenzie, AP., Julian, SR., Forsythe, D. and Omichi, E. 2003. Quasi-two-dimensional Fermi liquid properties of the unconventional superconductor Sr_2RuO_4 . *Advances in Physics*. 52(7):639-725. DOI: <https://doi.org/10.1080/00018730310001621737>.

Contreras, PL. 2011. Electronic heat transport for a multiband superconducting gap in Sr_2RuO_4 . *Revista Mexicana de Física*. 57(5):395-399.

Contreras, PL., Walker, MB. and Samokhin, KV. 2004. Determining the superconducting gap structure in

Sr_2RuO_4 from sound attenuation studies below T_c . *Physical Review B*. 70(18):184528. DOI: <https://doi.org/10.1103/PhysRevB.70.184528>.

Contreras, PL., Burgos, J., Ochoa, E., Uzcategui, D. and Almeida, R. 2014. A numerical calculation of the electronic specific heat for the compound Sr_2RuO_4 below its superconducting transition temperature. *Revista Mexicana de Física*. 60(3):184-189.

Edwards, SF. 1961. The electronic structure of disordered systems. *The Philosophical Magazine: A Journal of Theoretical, Experimental, and Applied Physics (Series 8)*. 6(65):617-638. DOI: <https://doi.org/10.1080/14786436108244414>.

Hirschfeld, PJ., Wölfle, P. and Einzel, D. 1988. Consequences of resonant impurity scattering in anisotropic superconductors: Thermal and spin relaxation properties. *Physical Review B*. 37(1):83-97.

Kamerlingh Onnes, H. 1911^a. Further experiments with liquid helium. C. On the change of electric resistance of pure metals at very low temperatures, etc. IV. The resistance of pure mercury at helium temperatures. *Communications of the Physical Laboratory of the University of Leiden*. Number 120b.

Kamerlingh Onnes, H. 1911^b. Further experiments with liquid helium. D. On the change of electric resistance of pure metals at very low temperatures, etc. V. The disappearance of the resistance of mercury. *Communications of the Physical Laboratory of the University of Leiden*. Number 122b.

Kamerlingh Onnes, H. 1911^c. Further experiments with liquid helium. G. On the electrical resistance of pure metals, etc. VI. On the sudden change in the rate at which the resistance of mercury disappears. *Communications of the Physical Laboratory of the University of Leiden*. Number 124c.

Landau, LD. and Lifshitz, EM. 1965. *Quantum Mechanics*. Pergamon Press, London, UK.

Levenberg, K. 1944. A method for the solution of certain nonlinear problems in least square. *The Quarterly of Applied Mathematics*. 2(2):164-168.

Lussier, B., Taillefer, L., Buyers, WJL., Mason, TE. and Petersen, T. 1996. Influence of a magnetic field on the antiferromagnetic order in UPt_3 . *Physical Review B*. 54(10):R6873-R6876. DOI: <https://doi.org/10.1103/PhysRevB.54.R6873>.

Maeno, Y., Hashimoto, H., Yoshida, K., Nishizaki, S., Fujita, T., Bednorz, JG. and Lichtenberg, F. 1994. Superconductivity in a layered perovskite without copper. *Nature (London)*. 372:532-534.

Marquardt, DW. 1963. An algorithm for least-squares estimation of nonlinear parameters, SIAM Journal on Applied Mathematics. 11(2):431-441.

Mineev, VP. and Samokhin, KV. 1999. Introduction to Unconventional Superconductivity. Gordon and Breach, Amsterdam, The Netherlands.

Palczewski, A. 2010. Angle-resolved photoemission spectroscopy (ARPES) studies of cuprate superconductors. Ph.D. thesis. Iowa State University, USA.

Puchkaryov, E. and Maki, K. 1998. Impurity scattering in *d*-wave superconductivity. Unitarity limit versus Born limit. The European Physical Journal B. 4(2):191-194. DOI: <https://doi.org/10.1007/s100510050369>.

Schachinger, E. and Carbotte, JP. 2003. Residual absorption at zero temperature in *d*-wave superconductors. Physical Review B. 67(13):134509-1.

Scheffler, M., Dressel, M., Jourdan, M. and Adrian, H. 2005. Extremely slow Drude relaxation of correlated electrons. Nature. 438(7071):1135-1137.

Smith, MF. and Walker, MB. 2000. Quasiparticle-quasiparticle scattering in high T_c superconductors. Physica C: Superconductivity and its Applications. 341-348(Part 3):1893-1894.

Tsuei, CC. and Kirtley, JR. 2000. Pairing symmetry in cuprate superconductors. Reviews of Modern Physics. 72(4):969-1016.

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