Analysis of the approximations used in the van Hove-BCS theory.

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Abstract

An analysis of the different approaches used within the van Hove BCS model for the high temperature superconductors has been done. How far the employment of an asymptotic expression for the density of states underestimates the thermodynamic parameters, as for example, the critical temperature, the gap at zero temperature, and the known universal ratios of the BCS model, is discussed. Analytical expressions obtained for some thermodynamic functions are compared with the numerical results for which the exact 2D density of states has been considered. Approximate analytical expressions for the temperature dependence of the reduced gap, the superconducting electronic specific heat, and the critical magnetic field have been obtained and compared with the corresponding numerical results. The validity of the different approximations and of the equations obtained for the thermodynamic functions in the framework of the van Hove model are also analyzed.

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I. INTRODUCTION

For electron-phonon (e-ph) superconductors, the Eliashberg equations (EE) allow the exact calculation of the temperature dependence of the thermodynamic functions. To solve EE one needs to know the e-ph spectral distribution function, $\alpha^2 F(\omega)$, and the coulomb repulsion pseudopotential parameter, $\mu^*$. The function $\alpha^2 F(\omega)$ has been obtained from the inversion of tunneling data and calculated theoretically for several e-ph superconductors. As a rule, a very good agreement has been obtained between experimental and theoretical calculations. The parameter $\mu^*$ is more difficult to deal with in a precise way. The common practice is to fit it to the experimental critical temperature, $T_c$, through the linearized EE, valid at $T_c$. These data are then used to solve the non-linearized EE from which the free-energy difference as a function of the temperature, $T$, follows.

BCS theory is the first solution found that gave the clue to the explanation of the e-ph superconductivity. It is a weak coupling limit that, as it is to be expected, deviates sometimes strongly, from the experimental results even for some medium e-ph coupling superconductors. An important role, as reference values, has been played by the universal ratios (UR), $R_1 = 2\Delta(0)/k_B T_c$, $R_2 = \Delta C(T_c)/C_{en}(T_c)$, and $R_3 = H_c(0)/\sqrt{N(0)\Delta(0)}$, where $\Delta(T)$ is the gap function, $\Delta C(T_c) = C_{es}(T_c) - C_{en}(T_c)$ is the jump of the electronic specific heat at $T_c$, given by the difference between its value in the superconducting state $C_{es}(T_c)$ and in the normal state $C_{en}(T_c)$, $H_c$ is the thermodynamic critical magnetic field, and $N(0)$ is the density of states (DOS) at the Fermi energy. For e-ph conventional superconductors, the BCS UR do not depend on any parameter: $R_1 = 3.52$, $R_2 = 1.43$, and $R_3 = 2\sqrt{\pi}$. The BCS theory was mainly used as a reference, as a limit that helped characterize the relative strength of the e-ph coupling for conventional superconductors (CS).

In the new high-Tc superconductors (HTS), the situation is quiet different since the mechanism driving the superconducting phase transition is still unknown. Actually, it is amazing how much it has been established about HTS without knowing the mechanism. Two main attitudes have been adopted: to assume a mechanism and to calculate the ther-
modynamics that follows, or to incorporate some known facts into BCS theory which makes no assumption on the specific mechanism. Several known facts have been discussed within the BCS framework as, for example, the symmetry of the gap and the influence of the dimensionality on the phenomenon of superconductivity. In this sense, the van Hove BCS (v-BCS) scenario has been formulated by different authors. Both, analytical and numerical treatments have been carried out leading to results that present noticeable differences in the thermodynamic functions. Tunneling experiments and the dependence of the specific heat on temperature, have been analyzed following the BCS formalism. For example, the contributions that come from the CuO₂ planes, CuO chains, and c-axis, have been decoupled. The one coming from the CuO₂ plane seems to be the most important one. Most of the work has been devoted to it. In this sense, it is necessary to understand very well superconductivity on the CuO₂ plane and to analyze in detail how the different approximations used describe the phenomenon. In other words, it is important to be aware whether certain deviations from the experimental results come from physics or from mathematics.

In this paper we want to analyze three types of solutions to the van Hove scenario, i.e., the analytic ones and their approximations, the numerical “asymptotic” solution that makes use of the asymptotic behavior of the two-dimensional density of states, and what we will call the “exact” solution where the full elliptic integral of the first kind, taking place in the 2D DOS, is considered and treated numerically. The calculations presented here assume an s-wave symmetry for the gap in the CuO₂ plane since it is the most widely studied case, although it is known not to be the experimental verified result. Nevertheless, this is not important for the sake of our purpose and the analysis obtained does not change in any essential way whether we introduced or not a d-wave or a mixing of s and d gap symmetries.

The rest of the paper is organized as follows. In sec. 2, we compare the analytic, the asymptotic and the exact solution within the van Hove scenario for the gap, the critical temperature, the temperature dependence of the gap, the electronic specific heat, and the thermodynamic critical field. Discussions and conclusions are considered in sec. 3.
II. BCS MODEL WITH A VAN HOVE SINGULARITY IN THE DOS

The layered structure of the new superconducting materials leads to almost dispersionless electronic spectrum on the c-axis and therefore, as a first approximation, it can be modeled as a stack of decoupled CuO$_2$ planes. This constitutes the so called van Hove scenario. For the CuO$_2$ planes, we take the following electronic dispersion relation:

$$\varepsilon_{\vec{k}} = -2t(\cos k_x a + \cos k_y a) + 4t' \cos(k_x a) \cos(k_y a)$$, (1)

where $t$ and $t'$ are the coupling parameters between the Cu-O atoms and O-O atoms respectively, $k_x$, $k_y$ are wave vector components, and $a$ is the lattice constant. The origin of the energy is at the Fermi level, $\varepsilon_F$. The resulting topology of the electronic band structure in the first Brillouin zone for $t' = 0$ (a) and $t' = 0.4t$ (b) are shown in Fig. 1. The saddle points at $\vec{k} = (\pi/a, 0)$ and $(0, \pi/a)$ are clearly seen yielding to the van Hove singularity (vHs) which enhances the DOS. The parameter $t'$ ranges between 0 and 0.5 and it is responsible for the observed changes in the shape of the Fermi surface (compare Fig. 1(a) to Fig. 1(b)). It is worth noticing that for a fixed carrier concentration, the parameter $t'$ drives the relative position of the singularity with respect to $\varepsilon_F$. Later on, we will show how almost all superconducting properties depend on this relative position.

The single spin DOS for a stack of layers is equal to

$$N(\varepsilon) = \frac{S n_p}{a^2} \frac{N_0}{\pi} K \left[ \sqrt{\frac{16t^2 - (\varepsilon - 4t')^2}{16t^2(1 + \frac{\varepsilon}{4t})}} \right]$$, (2)

where $K(m)$ is the elliptic integral of the first kind. S is the area of the sample, $n_p$ is the number of layers, and $N_0 = 1/2\pi^2t$. The asymptotic form for $K(m)$ in the neighborhood of the singularity with $t' = 0$ is

$$N(\varepsilon) \approx \frac{S n_p}{a^2} \frac{N_0}{2} \ln \left( \frac{16}{|\varepsilon/4t|} \right)$$. (3)

The equation above allows us to obtain analytical expressions for some of the thermodynamic functions. The BCS theory equation for the gap is
\[ \Delta_{k}(T) = \frac{1}{2} \sum_{k'} V_{\bar{k},\bar{k}'} \frac{\Delta_{\bar{k}'} E_{\bar{k}'} \tanh \left( \frac{E_{\bar{k}'} }{2k_B T} \right) }{E_{\bar{k}'}^2 + \Delta_{\bar{k}'}^2 (T)^2}, \]

where \( E_{\bar{k}'} = \sqrt{\varepsilon^2_{\bar{k}'} + |\Delta_{\bar{k}'}(T)|^2} \), and \( V_{\bar{k},\bar{k}'} \) is the effective electron-electron interaction matrix element. In agreement with the BCS formulation we use the following parametrization for \( V_{\bar{k},\bar{k}'} \):

\[
V_{\bar{k},\bar{k}'} = \begin{cases} 
V_1 ; & \text{if } |\varepsilon_{\bar{k}}|, |\varepsilon_{\bar{k}'}| < \varepsilon_c \\
0 ; & \text{otherwise}
\end{cases},
\]

and \( \varepsilon_c \) is an energy cut-off. Following the standard BCS procedure, we get

\[
\frac{2}{V_1} = \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon \ N(\varepsilon) \tan \left( \sqrt{\frac{\varepsilon^2 + \Delta^2(T)}{2k_B T}} \right) \frac{\tanh \left( \frac{\sqrt{\varepsilon^2 + \Delta^2(T)}}{2k_B T} \right) }{\sqrt{\varepsilon^2 + \Delta^2(T)}}. \tag{4}
\]

### A. The gap and the critical temperature

The numerical solutions of eq. (4) with a DOS given by eq. (3) will be referred to as the “exact” solution. When eq. (3) is used instead, we will talk about “asymptotic solution”.

We, first, compare the exact to the asymptotic DOS in the calculation of \( T_c \) and \( \Delta(0) \), in particular, their dependence on the dimensionless interaction parameter \( \lambda \equiv N_0 V \), with \( V = V_1 n_p S/a^2 \). We present these results in Fig. 2. Here, \( \alpha \equiv 2t'/t \), twice the O-O second nearest neighbors hopping parameter in units of the Cu-O first nearest neighbors one. In Fig. 2(a), we present the dependence on \( \lambda \) of the critical temperature \( T_c \) and in Fig. 2(b), the one of the gap \( \Delta(0) \), normalized to the cut-off energy \( \varepsilon_c \). The curves correspond to \( \alpha = 0.01, 0.04, \) and 0.07. Both parameters, \( T_c \) and \( \Delta(0) \), increase with \( \lambda \) almost in the same way. For lower values of \( \alpha \) (Cu-O interaction stronger than the O-O one), \( T_c \) and \( \Delta(0) \) both are a very steep function of \( \lambda \). Hence, for a single plane, the dependence of the critical temperature and the gap on \( \lambda \) is strong. It is worth noticing that \( T_c \) of order 100K can be reached with \( \lambda = 0.15 \) and \( \alpha = 0.01 \). On the other hand, for higher values of \( \alpha \) (a big relative hopping energy to the O-O atoms), \( i.e \alpha = 0.07, \lambda \) would have to increase as high
as 0.25 to obtain $T_c \approx 100K$. It is worth noticing that for $\alpha = 0.07$, $\lambda$ needs to be of the order of 0.30 to get $\Delta(0)/\varepsilon_c \approx 1$.

In Fig. 3, we show the exact solution for the universal ratio, $R_1 \equiv 2\Delta(0)/k_BT_c$ as a function of $\lambda$, for the same values of $\alpha$ considered above. At $\lambda=0.15$ and $\alpha=0.01$, $R_1=3.82$; while for higher values of $\lambda$, $R_1$ tends to 4 irrespective of the parameter $\alpha$. Notice that, according to these results, the asymptotic value is reached for $\lambda$’s that might be very high compared to the expected ones in the cooper oxide superconductors. On the other hand, at low $\lambda$ values, we get the usual BCS value, i.e., $R_1 = 3.52$. On the overall, these results show that for any value of $\lambda$ and any chosen parameter $\alpha$, $3.5 \leq R_1 \leq 4$. Therefore, in any case, the 2D character of superconductivity in the cooper oxides rises $R_1$ by at most 0.5 within the BCS formulation.

Approximate analytic solutions are obtained by inserting eq. (3) into eq. (4):

$$\Delta(0) = 64t \exp \left(1 - \sqrt{\frac{4}{N_0V} + \ln^2 \left(\frac{\varepsilon_c}{64t}\right) - 1}\right),$$

$$k_BT_c = 32t \exp \left(1 - \sqrt{\frac{4}{N_0V} + \ln^2 \left(\frac{\varepsilon_c}{64t}\right) - 1}\right),$$

from which a parameter-independent universal ratio follows:

$$R_1 = \frac{2\Delta(0)}{k_BT_c} = 4.\quad (7)$$

The numerical calculations using the exact DOS converge to $R_1 = 4$ for high values of $\lambda$, so the analytic solution (7), represents an upper bound for this ratio (see Fig. 3). The $R_1$ value is smaller than those reported experimentally, where $R_1$ ranging between 4 and 8 are found. This disagreement is well outside the experimental error.

In Fig. 4, the dependence of $T_c$ on the dimensionless interaction parameter, $\lambda$, is studied. The solid lines are numerical solutions obtained from eq. (4) with the DOS given by eq. (2) and $t' = 0$. The dot–dashed lines correspond to solutions using the asymptotic behavior of the DOS (eq. (3)). Three set of curves are presented in each case: $\varepsilon_c = 20$ meV (1), 35 meV (2), and 50 meV (3). As it can be seen, the cut-off energy has a strong influence on $T_c$. At $\lambda =$
0.20, for example, the solid lines range between 100 K and 300 K for 20 meV $\leq \varepsilon_c \leq 50 \text{meV}$. It is difficult to decide for a precise value of $\varepsilon_c$ which actually acts as a free parameter and quantitative results are subject to a physical justification. In Fig. 4, we also show the results using the *exact* DOS (solid lines). Compare them to the asymptotic expression (dot–dashed lines). The *exact* DOS gives, for the same value of $\varepsilon_c$, always higher values for $T_c$. At $\lambda=0.15$, for example, the *exact* $T_c$ is about twice the one obtained from the asymptotic DOS given by eq. (3). Furthermore, the analytic solution given by eq. (6) using $\varepsilon_c = 50 \text{meV}$ (dashed line) gives values for $T_c$ that are just (10%) above the numerical results using the asymptotic DOS but quite lower than the exact solution. So, the effect of the vHs is quite underestimated by using in either way the asymptotic form for $K(m)$. Any analysis of HTS based on BCS theory should take into account these very strong dependences on several parameters before reaching any even qualitative conclusion. This is a main result of this paper. We will illustrate it further.

**B. Temperature dependence of $\Delta(T)/\Delta(0)$**

The temperature dependence of the reduced gap, $\Delta(T)/\Delta(0)$, on the reduced temperature $T/T_c$ is presented in Fig. 5. For the sake of comparison the Mühlschlegel model\cite{2} is also shown (in circles). It is found that the temperature dependence of $\Delta(T)/\Delta(0)$ in the framework of the models considered here present the known universal character irrespective of the value of the parameters $\alpha$, $\varepsilon_c$ and $\lambda$.

In the following, approximate analytic expressions for the gap at low temperatures and close to $T_c$ are derived. In the low temperature regime and taking $t' = 0$, eq. (4) can be cast in the form $I_1 - I_2 = -2I_{3}$, with

$$I_1 = \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon N(\varepsilon) \frac{1}{\sqrt{\varepsilon^2 + \Delta^2(0)}}; \quad I_j = \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon N(\varepsilon) \frac{[f(E)]^{j-2}}{\sqrt{\varepsilon^2 + \Delta^2(T)}} \quad (j = 2, 3) ,$$

where $f(E)$ is the Fermi-Dirac distribution function. Using eq. (3), the difference $I_1 - I_2$ is calculated in a similar way to that used in ref.\cite{11}.
\[ I_1 - I_2 \propto (1 + \ln 16) \ln \left( \frac{\Delta(T)}{\Delta(0)} \right) + \frac{1}{2} \ln^2 \left( \frac{\Delta(0)}{4t} \right) - \frac{1}{2} \ln^2 \left( \frac{\Delta(T)}{4t} \right), \]

\[ I_3 \propto \left[ \ln(16) \sqrt{\frac{\pi k_B T}{2}} - \ln \left( \frac{\Delta(0)}{4t} \right) + 1 \right] \exp \left( -\frac{\Delta(0)}{k_B T} \right). \quad (8) \]

Collecting the results for \( I_1 - I_2 \) and \( I_3 \) and taking into account that \( R_1 = 4 \), the following analytical expression for the gap, \( \Delta(T) \), is obtained

\[ \frac{\Delta(T)}{\Delta(0)} = 1 - \frac{3}{4} \left( \frac{\pi T}{T_c} + \frac{10}{3} \right) \exp \left( -\frac{2T_c}{T} \right). \quad (9) \]

Let us look now at the behavior of the gap near \( T_c \). For this purpose eq. (4) is rewritten as \( K_1 - K_2 = K_3 \) with

\[ K_1 = \int_0^\omega dx \ln \left( \frac{16}{x} \right) \frac{\tanh(\beta_c x/2)}{x}, \]

\[ K_2 = \int_0^\omega dx \ln \left( \frac{16}{x} \right) \frac{\tanh(\beta x/2)}{x}, \]

\[ K_3 = -4\beta^3 y^2 \sum_{n=1}^\infty \int_0^\omega dx \ln \left( \frac{16}{x} \right) \frac{1}{[(2n-1)^2\pi^2 + \beta^2 x^2]^2}, \quad (10) \]

where \( \beta_c = 4t/k_B T_c \), \( x = \varepsilon/4t \), \( y = \Delta(T)/4t \), \( \omega = \varepsilon_c/4t \), \( \beta = 4t/k_B T_c \), and the following identity has been used

\[ \tanh \left( \frac{b}{2} \right) = 4b \sum_{n=1}^\infty \frac{1}{(2n-1)^2\pi^2 + b^2}. \]

Since \( K_3 \) decreases strongly for large values of \( \beta x \), the upper limit can be extended to infinity and

\[ K_3 = \left( \frac{\Delta(T)}{\pi k_B T} \right)^2 \sum_{n=1}^\infty \left[ \ln(2n-1) - \frac{\ln(16\beta/\pi) + 1}{(2n-1)^3} \right]. \quad (11) \]

The difference \( K_1 - K_2 \) can be obtained using the same approach of ref[1] and results in

\[ K_1 - K_2 = (1 + \ln 16) \ln \left( \frac{T}{T_c} \right) - \frac{1}{2} \left[ \ln^2 \left( \frac{k_B T}{2t} \right) - \ln^2 \left( \frac{k_B T_c}{2t} \right) \right]. \quad (12) \]
The above equations are the starting point to develop an explicit equation for the gap close to \( T_c \). Differentiating \( K_1 - K_2 \) in eq. (12) and \( K_3 \) from eq. (11) with respect to \( T \) results in

\[
\frac{d\Delta^2(T)}{dT} \bigg|_{T_c} = -\frac{8\pi^2}{7\zeta(3)} k_B^2 T_c = -9.38k_B^2 T_c
\]

which is the same as c-BCS result. To derive the above equation the following identities have been employed:\(^{21}\)

\[
\sum_{n=1}^{\infty} \frac{1}{(2n-1)^k} = (1 - 2^{-k})\zeta(k).
\]

\[
\sum_{n=1}^{\infty} \ln(2n-1) \frac{1}{(2n-1)^k} = -(2^{-k} - 1)\zeta'(k).
\]

where \( \zeta(k) \) is the Riemann Zeta function, and \( \zeta'(k) \) its derivative. From eqs. (11) and (12) follow the functional dependence \( \Delta^2(T) = F(T) \). Irrespective to the form that the function \( F(T) \) has, for \( T \) near \( T_c \) and due to the smallness of \( \Delta^2(T) \), this can be expand in powers of \( (T - T_c) \), thus

\[
\Delta^2(T) = \left( \frac{dF}{dT} \right) \bigg|_{T_c} (T - T_c) = \left( \frac{d\Delta^2(T)}{dT} \right) \bigg|_{T_c} (T - T_c).
\]

From eq. (13), \( \Delta^2(T) \) can be cast into

\[
\Delta^2(T) = 9.38k_B^2 T_c^2 \left( 1 - \frac{T}{T_c} \right)
\]

and taking into account eq. (7) it is obtained that

\[
\frac{\Delta(T)}{\Delta(0)} = 1.53 \sqrt{1 - \frac{T}{T_c}}.
\]

The expressions for \( \Delta(T) \) given by eqs. (13) and (15), are plotted in Fig. 5 in dashed and dot-dashed lines, respectively. It can be seen that eq. (13) is valid in the range \( 0 \leq T/T_c \leq 0.4 \), whereas eq. (15) in the range \( 0.95 \leq T/T_c \leq 1 \).

C. Electronic specific heat

The fermion specific heat, \( C_{en} \), in the normal state is given by
\[ C_{en}(T) = \frac{2}{k_B T^2} \int_{-4t}^{4t} d\varepsilon N(\varepsilon) \varepsilon^2 f(\varepsilon) [1 - f(\varepsilon)] . \]  

(16)

In Fig. 6(a) the \( C_{en}(T)/T \) dependence on \( T \) is presented for different values of the parameter \( \alpha \) and \( \varepsilon_F = 0 \). For \( \alpha = 0 \), \( C_{en}/T \) has a singular behavior as the temperature decreases. On the other hand, for \( \alpha > 0.03 \) and very low temperatures, the electronic specific heat presents a linear behavior with \( T \). These features are consistent with those reported in ref. \(^2\), where the usual constant coefficient in the linear term of the specific heat becomes a function of temperature.

An approximate analytic expression for \( C_{en} \) will be now derived. After inserting eq. (3) in eq. (16) we get

\[ C_{en}(T) = \frac{\pi^2}{3} R N_0 k_B T \left[ 1.73 - \ln \left( \frac{k_B T}{4t} \right) \right] , \]

(17)

where \( R \) is the universal gas constant, \( n_p s/a^2 \) is assumed to be equal to the Avogadro’s number, and the specific heat is calculated per mole. The first term in eq. (17) is the usual contribution from constant DOS. The second one, \( T \ln T \), is due to the vHs. A similar dependence has been reported in ref. \(^1\).

The superconducting-state electronic specific heat can be written as

\[ C_{es}(T) = \frac{2}{k_B T^2} \int_{-\varepsilon_c}^{\varepsilon_c} d\varepsilon N(\varepsilon) f(E)[1 - f(E)]\left[ E^2 - \frac{1}{2} T \frac{d\Delta^2(T)}{dT} \right] . \]

(18)

For the derivative of the square of the gap as a function of \( T \) we use eq. (13). We have calculated the dependence of \( C_{es}(T)/C_{en}(T_c) \) on \( T/T_c \), for three different values of \( \alpha \) (\( \varepsilon_c = 20 \) meV, \( \lambda = 0.1 \)). We get a universal behavior consistent with the one obtained for \( \Delta(T)/\Delta(0) \).

Inserting the eq. (3) into eq. (18) results in

\[ C_{es}(T) = 4RN_0 k_B T_c \sqrt{\frac{2 T_c}{T}} \frac{\left( \frac{2T_c}{T} \right)^3}{2} \exp \left( -\frac{2T_c}{T} \right) \left[ 3.46 + \frac{1}{4} \ln \left( \frac{2T_c}{T} \right) \right] , \]

where a value of \( k_B T_c/4t = 0.015 \) has been assumed. This approximated analytical equation is valid at low temperatures (\( 0 < T/T_c < 0.4 \)) where the gap is almost independent of temperature (see Fig. 5). Finally, for the ratio \( C_{es}(T)/C_{en}(T_c) \) follows:
\[
\frac{C_{es}(T)}{C_{en}(T_c)} = 7.15 \left( \frac{2T_c}{\pi T} \right)^3 \exp \left( -2 \frac{T_c}{T} \right) \left[ 1.4 + \frac{1}{10} \ln \left( \frac{2T_c}{T} \right) \right]
\]

Notice that the expected exponential behavior has been obtained.

The specific heat jump at \( T_c \) is given by

\[
\Delta C(T_c) = -\frac{1}{k_B T_c} \left. \frac{d^2 \Delta(T)}{dT^2} \right|_{T_c} \int_{T_c-4t'}^{4t-4t'} d\varepsilon \ N(\varepsilon) f(\varepsilon) [1 - f(\varepsilon)]
\]

(19)

In Fig. 6(b) we show the dependence of \( R_2 = \Delta C(T_c)/C_{en}(T_c) \) on \( \alpha \). For low values of \( \alpha \), \( R_2 \) approaches the asymptotic behavior of 1.95 as the cut-off energy increases. At intermediate values of \( \alpha \), \( R_1 \) crosses the c-BCS value towards lower values. At \( \alpha = \frac{\varepsilon_c}{2t} \) we get a discontinuity (in disagreement with ref.\[10\]). \( \alpha = \varepsilon_c/2t \) corresponds to the vHs energy shift from the Fermi level (\( \varepsilon_F = 0 \)). The jump observed in the figure is due to the vHs (see eq. (3)). Finally the curve approaches asymptotically the c-BCS value for higher value of \( \alpha \). At higher values of \( \alpha \) a crossover to the c-BCS value of 1.43 is reached.

In order to estimate the maximal value that \( R_2 \) can reach, we take \( \alpha = 0 \). Then, from eqs. (3), (13), (17), and (19) we get

\[
\frac{\Delta C(T_c)}{T_c} = 9.38 \ R N_0 k_B \left[ 1.96 - \frac{1}{2} \ln \left( \frac{k_B T_c}{4t} \right) \right]
\]

and

\[
\frac{\Delta C(T_c)}{C_{en}(T_c)} = 2.85 \left[ \frac{1.96 - \frac{1}{2} \ln(k_B T_c/4t)}{1.73 - \ln(k_B T_c/4t)} \right].
\]

Assuming \( k_B T_c/4t = 0.015 \), we get an upper limit for \( R_2 \):

\[
R_2 = \frac{\Delta C(T_c)}{C_{en}(T_c)} = 1.95.
\]

This result is slightly higher than the conventional BCS model value. The difference represents the influence of the vHs. Even thought the value of 1.95 follows the trend to higher values in the UR, this is not high enough to be in agreement with those reported from experimental estimations (2 < \( R_2 < 4.6 \)).
D. Critical Magnetic Field

Finally, the thermodynamic critical magnetic field, $H_c(T)$, can be evaluated from the thermodynamic relationship

$$\frac{H_c^2(T)}{8\pi} = F_n(T) - F_s(T) ,$$

(20)

where the $F_n(T)(F_s(T))$ is the free energy in the normal (superconducting) state. We use eq. (2) in eq. (20) and get the reduced temperature dependence of the reduced thermodynamic critical magnetic field $H_c(T)/H_c(0)$ that appears in Fig. 7 for two different values of $\varepsilon_c$ and $\lambda$ at $\alpha = 0$ (see figure caption for details). Curve 4 is the parabolic behavior known for conventional superconductors. Notice the strong departure from the parabolic behavior.

After some straightforward but slightly lengthy algebra, we arrive at the following expression

$$\frac{H_c^2(0)}{N_0/\Omega \Delta^2(0)} = 2\pi \left[ \frac{4}{3} - \ln \left( \frac{\Delta(0)}{64t} \right) \right] ,$$

where $\Omega = a^2d$ and $d$ is the interplanar distance. From the above equation it follows that $H_c(0)$ has a similar behavior as $\Delta(0)$ as a function of $\varepsilon_c$, $\lambda$ and $\alpha$. Further, using the inequality $-\ln x > 1 - x$, for $x < 1$ and $\Delta(0)/64t \ll 1$, a lower limit for the UR $R_3 = H_c(0)/\sqrt{N_0/\Omega \Delta(0)}$ is obtained

$$R_3 = \frac{H_c(0)}{\sqrt{N_0/\Omega \Delta(0)}} > 2.16\sqrt{\pi} .$$

This result represents another UR, whose value is higher than the 3D BCS model ($2\sqrt{\pi}$), fixing a minimum for this ratio.

The temperature dependence of $H_c(T)$ near $T_c$, can be obtained in the following way. Near $T_c$, $\Delta(T)$ is a small and $F_s(T)$ can be expanded in powers of $\Delta^2(T)$. To second order, we get:

$$F_s(T) - F_n(T) = -a_1(T_c)\Delta^4(T) ,$$

(21)
\[ a_1(T_c) = \frac{1}{2} \beta^2 \sum_{n, k} \frac{1}{(2n-1)^2\pi^2 + \beta^2 c^2 k^2}. \] (22)

The sum over \( \vec{k} \) in eq. (22), can be transformed into an integral over the energy, and using eq. (11), we get

\[ H^2_c(T) = \frac{0.29}{8\pi} \left( \frac{N_0 \Delta^2(0)}{a^2 d} \right) \left[ 2.84 - \ln \left( \frac{k_B T_c}{4t} \right) \right] \left( 1 - \frac{T}{T_c} \right)^2. \]

From this expression it follows:

\[ \frac{H_c(T)}{H_c(0)} = 0.83 \left( 1 - \frac{T}{T_c} \right). \] (23)

Equation (23) has a slope of 0.83 which is smaller than the one in c-BCS (1.74). The approximate \( H_c(T) \) expression for \( T \) near \( T_c \), of eq. (23) is valid in the range \( 0.75 \leq T/T_c \leq 1 \).

III. DISCUSSION AND CONCLUSIONS

In the present paper the thermodynamics of the BCS model within the vHs scenario is carried out using both the exact DOS and its asymptotic behavior (analytically and numerically). We were interested in the intrinsic error that derives from the use of the asymptotic approximation to the van Hove DOS as compared to the exact one. For that purpose we assumed an s-wave symmetry for the gap in spite of the experimentally shown d or (d+s)-wave symmetry. For our purpose this does not make any difference. Our study helps point to specific differences with experiment that come from the mathematical approximations used rather than from physics. A first conclusion is that the widely spread use of the logarithmic asymptotic behavior near the singularity of the elliptic integral of the first kind that is obtained for the DOS in the van Hove scenario is a very disputable approximation. It can lead to results that differ substantially from the ones obtained when the exact DOS is used. So most of the analytical expressions (obtained in this way) are to be used with great care, in general, even to draw from them qualitative conclusions.

Furthermore, even using the exact DOS of the van Hove scenario, we still get (within v-BCS) a picture that does not always agree with experiment.
Numerical computations of the gap at zero temperature $\Delta(0)$ and $T_c$ as a function of the dimensionless interaction parameter, $\lambda$, were carried out for different values of $\alpha \equiv 2t'/t$, with $\varepsilon_c$, the cut-off energy, fixed (see Fig. 2). $T_c$ and $\Delta(0)$ increase with $\lambda$, but as $\alpha$ is increased, with $\lambda$ fixed, a strong decrease in both $T_c$ and $\Delta(0)$ is observed. As $\alpha$ increases, the range of possible values of $\lambda$ that are consistent with the experimental results, increase towards those often found in CS. An analysis of Fig. 2 shows that for $\lambda > 0.15$ the ratios $k_B T_c/\varepsilon_c$ and $\Delta(0)/\varepsilon_c$ are higher than one. In CS, this fact is understood as a signature of lifetime effects. Thus, for small values of $\alpha$ and $\lambda > 0.15$, many body effects should play an important role. This is consistent with the explanation given for CS to account for some high values found for $R_1$. The universal ratio, $R_1 = 2\Delta(0)/k_B T_c$, ranges between 3.5 and 4 for any values of $\alpha$ and $\lambda$, well below the experimental reported value. The highest values of $\Delta(0)$ and $T_c$ are obtained at $\alpha = 0$. We have derived analytic expressions in this limit to examine further this point. The asymptotic approximation underestimate $\Delta(0)$ and $T_c$ as compared to the exact result. It is interesting to notice further that there is but a small difference using Eq. 3 whether the problem is solved analytically or numerically (only by 10\% , see Fig. 4).

The temperature dependence of the reduced gap $\Delta(T)/\Delta(0)$ on the reduced temperature $T/T_c$ presents the known universal behavior irrespective of the value of $\alpha$, $\varepsilon_c$ and $\lambda$. Analytic expressions can be obtained for the gap at $0 \leq T \leq 0.4$ (eq. (9)) as well as at $0.95 \leq T/T_c \leq 1$ (eq. (15)). The presence of the vHs leads to higher values of $\Delta(0)$ and $T_c$ than those reported for the CS even for low values of the dimensionless interaction constant $\lambda$. Furthermore, the magnitudes $\Delta(0)$, $T_c$ and $R_1$ are strongly affected by the departure of the vHs from the $\varepsilon_F$. This is an obvious result since the number of states around $\varepsilon_F$ (that contribute to the superconductor state) decreases as the singularity moves far away from the Fermi level.

We have further calculated the specific heat. Our results appear in Figs. 6(a) and 6(b). We get for $C_{es}(T)/T$ an exponential decay at low temperature (for $a > 0$) in contrast with that reported in\cite{22,25,26}. It is possible to show, that the corresponding width in the transition region ($T$ close to $T_c$) decreases as $\alpha$ increases in agreement with experimental evidences\cite{2}.
On the other hand, in the range of temperatures close to $T_c$, and due to thermally-created quasiparticle excitations, with roughly the same weight for all directions of $\vec{k}$, qualitative differences with respect to c-BCS behavior are not found and the specific heat jump has a sharp maximum at $T_c$. We get a linear dependence of $\Delta C$ on $\Delta(0)$ instead of the quadratic dependence reported in \cite{27}. In this region a broadened step-like discontinuity, as it has been found in some CS, is presented. For $UR = \Delta C(T_c)/C_{en}(T_c)$ we found that even though the value that we have obtained is higher than that of the c-BCS it is not enough to be in agreement with experimental reported that ranges between 2 and 4.

The reduced thermodynamic critical magnetic field $H_c(T)/H_c(0)$ as a function of $T/T_c$ shows a marked departure from the characteristic parabolic dependence observed in CS. Another important feature of the curve $H_c(T)/H_c(0)$ is the change of curvature that takes place close to $0.3T_c$. The origin of this departure from the parabolic law is associated with the temperature dependence of the specific heat in the superconducting state. In ref.\cite{28} a dependence like $\sqrt{1-(T/T_c)^2}$ is proposed instead of the parabolic law. Finally, a minimum value for the ratio $R_3 = H_c(0)/\sqrt{N_0/\Omega\Delta(0)}$ is obtained (3.83) which is higher than that reports in the c-BCS theory.

Our two main conclusions are: First, the widely used logarithmic form of the DOS in the van Hove scenario is a very disputable approximation. Second, the van Hove scenario, even using the “exact” DOS although it enlightens quite a lot, might need more elements to account properly for the thermodynamics of HTS. It seems that other contributions neglected by the van Hove scenario play an important role.\cite{15}

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FIGURES

FIG. 1. Topology electronic band structure in the first Brillouin zone following eq. (1) for $t' = 0$ (a), and $t' = 0.4t$ (b). The energy is given in eV and the calculations correspond to $t = 0.25$ eV.

FIG. 2. Dependence of the critical temperature, $T_c$ (a) and the reduced gap at zero temperature, $\Delta(0)$ (b) on the dimensionless interaction constant $\lambda = N_0V$, at $\varepsilon_c = 20$ meV and $\alpha = 0.01$ (solid line), 0.04 (dashed line) and 0.07 (dot-dashed line).

FIG. 3. Dependence of the ratio $R_1 = 2\Delta(0)/k_BT_c$ on the dimensionless interaction constant $\lambda = N_0V$, for the same values of $\alpha$ and $\varepsilon_c$ of fig. 2. The c-BCS and v-BCS universal ratios are presented by thin lines.

FIG. 4. Critical temperature $T_c$ as a function on the dimensionless interaction constant $\lambda = N_0V$, for $\varepsilon_c : 20$ meV (curves 1), 35 meV (curves 2), and 50 meV (curves 3). The calculations with the exact DOS, eq. (2) and its asymptotic behavior, eq. (3) are plotted by solid and dot-dashed lines, respectively. The approximate expression given by eq. (6) is represented in dashed line for $\varepsilon_c = 50$ meV. The value of $\alpha = 0$ has been chosen for all calculated curves.

FIG. 5. Dependence of the ratio $\Delta(T)/\Delta(0)$ on the reduced temperature $T/T_c$. The $T \to 0$ (curve 1 by dashed lines) and $T \to T_c$ (curve 2 by dot-dashed lines) approaches according to eqs. (9) and (15), respectively are presented (for details see text). For comparison the c-BCS result is depicted in solid circles. The calculation correspond to $\alpha = 0$.

FIG. 6. Electronic specific heat in the normal state $C_{en}$ in units of $T$ as a function of $T$ for different values of $\alpha$ (a); The jump ratio $\Delta C(\alpha)/C_{en}(T_c)$ as a function of $\alpha$ for different values of $\varepsilon_c$ at $\lambda = 0.1$ (b). For comparison the c-BCS and the v-BCS universal ratios are presented by thin lines.
FIG. 7. Temperature dependence of $H_c(T)/H_c(0)$ on $T/T_c$ obtained from eq. (21) with the DOS given by eq. (2) for $\varepsilon_c = 35$ meV, $\lambda = 0.1$ (curve 1); $\varepsilon_c = 20$ meV, $\lambda = 0.1$ (curve 2); $\varepsilon_c = 35$ meV, $\lambda = 0.02$ (curve 3). For comparison the empirical parabolic law (curve 4) of the c-BCS (see ref. 23) is shown.
\[ 2 \Delta(0) / k_B T_c \]

- v-BCS
  - $\alpha = 0.01$
  - $\alpha = 0.04$
  - $\alpha = 0.07$

- c-BCS

$\varepsilon_c = 20$ meV
\[ \Delta(T) / \Delta(0) \]

\[ \alpha = 0 \]

\[ T / T_c \]
\[ \frac{C_{en}}{T} \text{ (mJ/mol/K^2)} \] vs. \( T \text{ (K)} \)

- \( \alpha = 0.00 \)
- \( \alpha = 0.01 \)
- \( \alpha = 0.02 \)
- \( \alpha = 0.03 \)
- \( \alpha = 0.04 \)
\[ \frac{\Delta C(\alpha)}{C_{en}(T_c)} \]

\( \alpha \)

\( \Delta C(\alpha) / C_{en}(T_c) \)

\( \varepsilon_c = 20 \text{ meV} \)
\( \varepsilon_c = 35 \text{ meV} \)
\( \varepsilon_c = 50 \text{ meV} \)
\( \varepsilon_c = 65 \text{ meV} \)

\( \varepsilon_c \) values are 20, 35, 50, and 65 meV.
\[ \alpha = 0 \]