Physica C: Superconductivity and its applications 548 (2018) 132–137

Contents lists available at ScienceDirect

Physica C: Superconductivity and its applications

journal homepage: www.elsevier.com/locate/physc

Superconducting critical temperature under pressure

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ARTICLE INFO

Article history:
Received 24 November 2017
Revised 15 January 2018
Accepted 16 January 2018

Keywords:
Superconductivity
Critical temperature
Functional derivative
Pressure

ABSTRACT

The present record on the critical temperature of a superconductor is held by sulfur hydride (approx. 200 K) under very high pressure (approx. 56 GPa.). As a consequence, the dependence of the superconducting critical temperature on pressure became a subject of great interest and a high number of papers on of different aspects of this subject have been published in the scientific literature since. In this paper, we calculate the superconducting critical temperature as a function of pressure, $T_c(P)$, by a simple method. Our method is based on the functional derivative of the critical temperature with the Eliashberg function, $\delta T_c(P)/\delta\alpha^2F(\omega)$. We obtain the needed coulomb electron-electron repulsion parameter, $\mu^*(P)$ at each pressure in a consistent way by fitting it to the corresponding T_c using the linearized Migdal–Eliashberg equation. This method requires as input the knowledge of T_c at the starting pressure only. It applies to superconductors for which the Migdal–Eliashberg equations hold. We study Al and $\beta-$Sn two weak-coupling low-T_c superconductors and Nb, the strong coupling element with the highest critical temperature. For Al, our results for $T_c(P)$ show an excellent agreement with the calculations of Profeta et al. which are known to agree well with experiment. For $\beta-$Sn and Nb, we found a good agreement with the experimental measurements reported in several works. This method has also been applied successfully to PdH elsewhere. Our method is simple, computationally light and gives very accurate results.

1. Introduction

One of the goals of the research in superconductivity nowadays is to find a system with a room critical temperature. Due to the success with the sulfur hydride under pressure [1] the detailed understanding of the different properties of a material that contribute to enhance its critical temperature, became of central interest. For this reason, one of the present lines of research is the dependence of the critical temperature on pressure, $T_c(P)$. In electron-phonon superconductors, pressure affects the vibration spectrum by shifting it to higher frequencies which can enhance or lower the critical temperature depending on details of the system under study. Also the electron-phonon interaction is affected by pressure. This is put in evidence by several experimental works [2–10].

In order to contribute to the understanding of the details that determine whether or not pressure will enhance T_c, we have developed a simple but still quite accurate method to calculate the superconducting critical temperature as a function of pressure , $T_c(P)$, . We use the density functional theory (DFT) and the density functional perturbation theory [11–13] (DFPT) to get the electron and phonon band structures and the Eliashberg function, $\alpha^2F(\omega)$, from first principles. We use the Quantum Espresso suite codes [14,15] for most of the calculations made in this work. This method applies to superconductors for which the Migdal–Eliashberg equations (MEE) [16,17] are valid to describe their superconducting properties as it is the case of the electron-phonon superconductors. The parameters that enter the linearized MEE (LMEE) are the critical temperature T_c, which can be obtained from resistivity experiments, for example, the frequency at which the sum over the Matsubara frequencies on the frequency imaginary axis is stopped, the so-called, cut-off frequency, ω_c, which can actually be fixed numerically, and the electron-electron repulsion parameter, μ^*. The electron-phonon interaction parameter, λ, is known once the Eliashberg function, $\alpha^2F(\omega)$, is known and it can also be obtained from specific heat experiments, for example. The electron-electron repulsion parameter, μ^*, requires some attention. Actually, it has not been yet neither calculated nor measured with enough precision to be useful as the parameter needed to solve the LMEE to obtain an accurate value for T_c. If T_c is known, then by solving the LMEE we can fix μ^*. When T_c is not known, several ways have been proposed to estimate μ^* so that it can be calculated from the LMEE. P.Morel and Anderson [18] suggest the following analytic formula

$$\mu^* = \frac{\mu}{1+\mu ln(\frac{E_{el}}{\omega_{ph}})} \tag{1}$$

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https://doi.org/10.1016/j.physc.2018.01.015
0921-4534/

where the dimensionless parameter $\mu = < V > N(E_F)$ is the product of the averaged screened coulomb interaction, V, and the density of states at the Fermi energy, $N(E_F)$. E_{el} and ω_{ph} are the electron and phonon energy scales, respectively. Further, Bennemann and Garland [19], Smith [4] and Neve et al. [20] give semi-empirical formulas to estimate the behavior of the coulomb pseudo-potential as a function of pressure. Liu et al. [21] and Freericks et al. [22] calculated μ^* scaled to the maximum phonon frequency, meaning to replace ω_{ph} in Eq. (1) by $\omega_{\max}$, the maximum phonon frequency. Daams and Carbotte [23] fit μ^* solving the LMEE using the experimental value of T_c. In a more recent work Bauer et al. [24] calculated corrections to μ^* based on the Hubbard–Holstein model. There is no consensus concerning the proper way to calculate μ^* under pressure or even at ambient pressure. For example, for Nb at ambient pressure, a set of different values for μ^* are reported, 0.117 [25], 0.13 [20], 0.14 [26], 0.183 [27], 0.21 [28] and 0.249 [29] which differ considerably from each other.

The rest of the paper is organized as follows. In Section 2, we present the theoretical foundations that supports our method. The method is described in Section 3. In the next Section 4, we describe some technical details of the calculation. In Section 5, we present our results and compare them with other work and to experiment. For Al, with the known successful calculations of Profeta *et al.* [9] and with experiment [2,3,8]; for Sn, with the experimental measurements of Smith and Chu [30], Berman et al. [5] and Jennings and Swenson [6]. We get a good agreement with them. For Nb, we compare our results to the experimental ones of Struzhkin et al. [7]. Finally, we summarize our work in a final Section 6.

2. Theoretical foundations

2.1. The functional derivative

The functional derivative, $\frac{\delta T_c}{\delta \alpha^2 F(\omega)}$, can be thought as a measure of the strength of the influence of a particular frequency on T_c. In this sense, a calculation of the functional derivative tells us how favorable a certain frequency range is for an increase in the transition temperature. The maximum of the functional derivative, ω_{opt}, is therefore the most important region in determining the critical temperature. Actually very useful relation between this optimum frequency and Tc does exist, namely $\hbar\omega_{opt} = CK_BT_c$ where C is a constant between 7–8 and K_B is the Boltzman constant.

From the solution of the LMEE and using the algorithm of Leavens [31] the functional derivative can be obtained. Changes in T_c, calculated using this method have been considered previously by several authors to study the influence on T_c due to changes in concentration [32] and changes in composition [33]. Also for a two-band superconductor as MgB_2 [34] or, as in our case, to study the influence of pressure [23,35].

2.2. Linearized Migdal–Eliashberg equations

Central to our calculations is the functional derivative of T_c with de Eliashberg function, $\alpha^2F(\omega)$, $\delta Tc(P_i)/\delta\alpha^2F(\omega)$, which we obtain from the solution of the Linearized Migdal–Eliashberg equations (LMEE) [16,17]. As stated before, we solve LMEE to fit μ^* to the corresponding value of T_c. On the imaginary axis, the LMEE is:

$$\rho\tilde{\Delta}_n = \pi T\sum_m\left[(\lambda_{mn} - \mu^*) - \delta_{nm}\frac{|\tilde{\omega}_n|}{\pi T}\right]\tilde{\Delta}_m, \tag{2}$$

$$\tilde{\omega}_n = \omega_n + \pi T\sum_m \lambda_{mn}sgn(\omega_n), \tag{3}$$

$$\omega_n = (2n-1)\pi T, \tag{4}$$

$$\bar{\Delta}_n = \frac{\tilde{\Delta}_n}{\rho + |\tilde{\omega}_n|}, \tag{5}$$

$$\lambda_{mn} = 2\int_0^\infty \frac{d\omega\omega\alpha^2F(\omega)}{\omega^2 + (\omega_n - \omega_m)^2}. \tag{6}$$

where T is the temperature, $\tilde{\Delta}_n$ is the gap function, ω_n is the Matsubara frequency, ρ is the pair breaking parameter and $n = 0, \pm1, \pm2, \ldots$. In particular, $\lambda_{nn} \equiv \lambda$ is the electron-phonon coupling constant. We take ω_c to be 10 times the maximum phonon frequency, $\omega_{\max}$, as suggested by Bergmann and Rainer [56]. The Eliashberg function is defined as

$$\alpha^2F(\omega) = \frac{1}{N(\epsilon_F)}\sum_{mn}\sum_{q\nu}\delta(\omega - \omega_{\vec{q},\nu}) \times \sum_{\vec{k}}|g^{\vec{q}\nu,mn}_{\vec{k}+\vec{q},\vec{k}}|^2\delta(\epsilon_{\vec{k}+\vec{q},m} - \epsilon_F)\delta(\epsilon_{\vec{k},n} - \epsilon_F) \tag{7}$$

where $g^{\vec{q}\nu,mn}_{\vec{k}+\vec{q},\vec{k}}$ is the electron-phonon coupling matrix element, $\epsilon_{\vec{k}+\vec{q}}$ and $\epsilon_{\vec{k},n}$ are the energy of the quasi-particles in bands m and n with wave vectors $\vec{k}+\vec{q}$ and $\vec{k}$, respectively. $\omega_{\vec{q},\nu}$ is the phonon energy with momentum $\vec{q}$ and branch ν. $N(\epsilon_F)$ is the electronic density of states at the Fermi energy, ϵ_F.

3. The method

To calculate the critical temperature as a function of pressure, we need only as the starting data, the critical temperature at the starting pressure, Tc_{P_i}. We make use of the Espresso codes [13] to optimize the lattice constants first and then to calculate the Eliashberg function, $\alpha^2F(\omega, P_i)$, from first principles at the starting pressure. To get the electron-electron repulsion parameter, $\mu^*_{P_i}$, we solve the Linearized Migdal Eliashberg Equation (LMEE) to fit it to the known Tc_{P_i}. We use the Mc Master programs for that purpose [23,25,36,37,55]. With these data, we calculate the functional derivative of Tc with the Eliashberg function, $\alpha^2F(\omega)$ at P_i, $\delta Tc(P_i)/\delta\alpha^2F(\omega)$ [19]. Now, we define the next pressure, say P_{i+1}, obtain the new lattice parameters, optimize them and get the new Eliashberg function, $\alpha^2F(\omega, P_{i+1})$. This new Eliashberg function differs from the previous one by

$$\Delta\alpha^2F(\omega)_{P_{i+1},P_i} = \alpha^2F(\omega, P_{i+1}) - \alpha^2F(\omega, P_i) \tag{8}$$

The change in the critical temperature is now obtained from (Rainer and Bergman [38], and Baquero and López-Olazagasti [39])

$$\Delta Tc_{P_{i+1},P_i} = \int_0^\infty \frac{\delta Tc(P_i)}{\delta\alpha^2F(\omega)}\Delta\alpha^2F(\omega)_{P_{i+1},P_i}d\omega \tag{9}$$

and then, the $Tc_{P_{i+1}}$ at the new pressure is calculated as

$$Tc_{P_{i+1}} = Tc_{P_i} + \Delta Tc_{P_{i+1},P_i}. \tag{10}$$

4. Technical details

We, first, relax the internal degrees of freedom and the lattice vectors of the corresponding structure (Al, β-Sn and Nb) using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) quasi-Newton algorithm at each pressure to get the corresponding lattice constants. From these relaxed structure configurations, we calculated the electronic and phonon band structures, electron (DOS) and phonon (PHDOS) densities of states, and the Eliashberg function $\alpha^2F(\omega)$. We used a kinetic energy cut-off of 60 Ry for the expansion of the wave function into plane waves and 240 Ry for the density. To integrate over the Brillouin zone (BZ), we used for the electronic integration a k-grid of $32\times32\times32$ and for the phononic integration a q-grid of $8\times8\times8$ according to the Monkhorst–Pack