

Functional derivatives of T_c for a two-band superconductor: application to MgB_2

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Abstract. We address the question of how phonons of various frequencies contribute to the superconducting transition temperature T_c of a multi-band superconductor by considering the functional derivatives of T_c with respect to various intraband and interband electron-phonon coupling functions. A general scheme for computing such functional derivatives is developed. The proofs are given that the functional derivatives which are diagonal in band indices are linear in phonon energy Ω at small Ω , while the functional derivatives which are off-diagonal in band indices diverge at $\Omega = 0$ as $1/\Omega$. The case of a two-band model for MgB_2 is treated numerically.

PACS. 74.20.-z Theories and models of superconducting state – 74.70.Ad Metals; alloys and binary compounds (including A15, MgB_2 , etc.) – 74.62.-c Transition temperature variations

1 Introduction

Bergmann and Rainer [1] introduced an important diagnostic tool into the Eliashberg theory of superconductivity (for a pedagogical review of Eliashberg theory see [2]). They considered the functional derivative of the superconducting transition temperature T_c with respect to the electron phonon coupling function $\alpha^2 F(\Omega)$ of an isotropic (dirty) superconductor

$$\frac{\delta T_c}{\delta \alpha^2 F(\Omega)} = \lim_{\eta \rightarrow 0} (T_c [\alpha^2 F(\Omega') + \eta \delta(\Omega' - \Omega)] - T_c [\alpha^2 F(\Omega')]) / \eta. \quad (1)$$

The functional $T_c[\alpha^2 F(\Omega)]$ is defined by the Eliashberg equations at T_c [2]. The function $\delta T_c / \delta \alpha^2 F(\Omega)$ provides answer to the question – How are the phonons of frequency Ω effective in contributing to T_c ? From the practical point of view the functional derivative $\delta T_c / \delta \alpha^2 F(\Omega)$ gives the change ΔT_c in transition temperature when $\alpha^2 F(\Omega)$ is changed by a *small* amount $\Delta \alpha^2 F(\Omega)$ (say, by applying pressure [3], by alloying [4,5], or by implanting small concentrations of hydrogen into a metal [6])

$$\Delta T_c = \int_0^{+\infty} d\Omega \frac{\delta T_c}{\delta \alpha^2 F(\Omega)} \Delta \alpha^2 F(\Omega). \quad (2)$$

The concept of functional derivative $\delta / \delta \alpha^2 F(\Omega)$ was extended by Rainer and Bergmann [4] and others to several

thermodynamic properties of isotropic superconductors (for a review and an extensive list of references see [7]).

The main conclusions of Bergmann and Rainer [1] were that $\delta T_c / \delta \alpha^2 F(\Omega)$ is always positive (they were able to prove this mathematically for the case when the Coulomb repulsion parameter μ^* [2] is zero), proportional to Ω at $\Omega \ll 2\pi T_c$ (we choose units such that $\hbar = 1$ and $k_B = 1$) and with a maximum at Ω just above $2\pi T_c$. Hence, the electron coupling to a phonon of any frequency has a positive contribution to T_c , but the small values of $\delta T_c / \delta \alpha^2 F(\Omega)$ in the low frequency region imply that the changes of $\alpha^2 F(\Omega)$ in this frequency range have no appreciable effect on T_c , in contrast to the influence of the low frequency part of $\alpha^2 F(\Omega)$ on the electron-phonon coupling parameter λ

$$\lambda = 2 \int_0^{+\infty} d\Omega \alpha^2 F(\Omega) / \Omega, \quad (3)$$

which is used in McMillan-type interpolation formulae for T_c [2].

Daams and Carbotte [8] considered the functional derivative of T_c with respect to the Fermi surface averaged electron-phonon coupling function of an anisotropic superconductor and found that $\delta T_c / \delta \alpha^2 F(\Omega)$ *diverges* at $\Omega = 0$ as $1/\Omega$. Their explicit calculations for a separable model of anisotropy $\alpha^2 F_{\mathbf{k},\mathbf{k}'}(\Omega) = (1+a_{\mathbf{k}})\alpha^2 F(\Omega)(1+a_{\mathbf{k}'})$, with the Fermi surface averages $\langle a_{\mathbf{k}} \rangle = 0$ and $\langle a_{\mathbf{k}}^2 \rangle \ll 1$, showed that at small Ω $\delta T_c / \delta \alpha^2 F(\Omega)$ goes *negative* and diverges as $-1/\Omega$. Thus in high purity anisotropic superconductors the electron coupling to low frequency phonons *decreases* T_c , which is analogous to the effect of elastic impurity scattering on transition temperature of anisotropic

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superconductors. However, Daams and Carbotte pointed out that for their choice of anisotropy parameter for Pb ($\langle a_{\mathbf{k}}^2 \rangle = 0.04$) $\delta T_c / \delta \alpha^2 F(\Omega)$ becomes negative only below $0.6T_c$ where $\alpha^2 F(\Omega)$ has very little weight and varies as Ω^2 , rendering $1/\Omega$ -divergence in functional derivative harmless. The net effect of anisotropy in the pairing interaction is to increase the T_c as the virtual scattering ($\mathbf{k} \uparrow, -\mathbf{k} \downarrow$) \rightarrow ($\mathbf{k}' \uparrow, -\mathbf{k}' \downarrow$) $\rightarrow \dots$ over the Fermi surface takes advantage of the regions where the pairing interaction is large.

A consensus has emerged (for a review see [9]) that in order to describe the superconducting properties of a 40 K superconductor MgB₂ the Eliashberg theory has to be applied to a multi-band case with [10] or without [11] gap anisotropy on different sheets of the Fermi surface. In [11] the Eliashberg equations for an effective two-band model of electronic structure and electron-phonon coupling in MgB₂ were solved and the calculated specific heat difference between the superconducting and the normal state was in good agreement with experiments over a wide temperature range below T_c . As a model for gap anisotropy the two-band model is the opposite extreme to the separable anisotropy considered in [8] – there are four Eliashberg functions $\alpha^2 F_{\sigma\sigma}(\Omega)$, $\alpha^2 F_{\pi\pi}(\Omega)$, $\alpha^2 F_{\sigma\pi}(\Omega)$ and $\alpha^2 F_{\pi\sigma}(\Omega)$, and, correspondingly, there are four functional derivatives of T_c with respect to each one of them (the band off-diagonal functions $\alpha^2 F_{\sigma\pi}$ and $\alpha^2 F_{\pi\sigma}$ are related, but are different as they are proportional to the partial electronic densities of states in π - and σ -bands, respectively). In this work we calculate the functional derivatives of T_c for the two-band model and electron-phonon coupling functions presented in [11].

The rest of the paper is organized as follows. In Section 2 we present the formalism necessary for computation of the functional derivatives of T_c with respect to various electron-phonon coupling functions in a multi-band case. We also prove that the band-diagonal functional derivatives $\delta T_c / \delta \alpha^2 F_{ii}(\Omega)$, where i is the band index, are proportional to Ω at small Ω , while the functional derivatives which are off-diagonal in the band indices, $\delta T_c / \delta \alpha^2 F_{ij}(\Omega)$ with $i \neq j$, diverge at small Ω as $1/\Omega$. In Section 3 we present and discuss our numerical results, and in Section 4 we give a summary.

2 The functional derivatives $\delta T_c / \delta \alpha^2 F_{ij}(\Omega)$

In the case of several bands $i = 1, 2, \dots$ with different partial densities of states N_i the Eliashberg equations for T_c do not have the form of a Hermitian eigenvalue problem [11]. That is because the interband electron-phonon coupling functions $\alpha^2 F_{ij}(\Omega)$ and the corresponding Coulomb repulsion parameters μ_{ij} are proportional to N_j and are not symmetric under the exchange of the band indices i and j , $i \neq j$. As a calculation of the functional derivative of T_c relies on the Hellman-Feynman theorem [1], [12] which is valid only for Hermitian matrices, it is necessary to cast the Eliashberg equations at T_c into a Hermitian eigenvalue problem. To this end one first takes the cutoff ω_c in the Matsubara frequency sums to be large

enough so that $\mu_{ij}^*(\omega_c) = \mu_{ij} \equiv V_{ij}^c N_j$, where V_{ij}^c is the Fermi surface averaged screened Coulomb matrix element between the states in the bands i and j ; clearly $V_{ji}^c = V_{ij}^c$. The electron-phonon coupling functions can be written as $\alpha^2 F_{ij}(\Omega) = \alpha^2 f_{ij}(\Omega) N_j$ with $\alpha^2 f_{ij}(\Omega) = \alpha^2 f_{ji}(\Omega)$. Then the Eliashberg equations at T_c take the form

$$\phi_i(n) = \pi T_c \sum_{jm} [\bar{\lambda}_{ij}(n-m) N_j - V_{ij}^c N_j] \frac{\phi_j(m)}{|\omega_m| Z_j(m)}, \quad (4)$$

$$\omega_n Z_i(n) = \omega_n + \pi T_c \sum_{jm} \bar{\lambda}_{ij}(n-m) N_j \frac{\omega_m}{|\omega_m|}, \quad (5)$$

$$\bar{\lambda}_{ij}(n-m) = \int_0^{+\infty} d\Omega \alpha^2 f_{ij}(\Omega) \frac{2\Omega}{\Omega^2 + (\omega_n - \omega_m)^2}, \quad (6)$$

where $\phi_i(n)$ and $Z_i(n)$ are the pairing self-energy and the renormalization function, respectively, at Matsubara frequency $\omega_n = \pi T_c (2n - 1)$ in band i . By defining

$$\bar{\phi}_i(n) = \phi_i(n) \sqrt{N_i} / \sqrt{|\omega_n| Z_i(n)}. \quad (7)$$

Equation (4) takes the form of a Hermitian eigenvalue problem

$$\bar{\phi}_i(n) = \varepsilon(T) \sum_{jm} \pi T \frac{\lambda_{ij}^s(n-m) - \mu_{ij}^s}{\sqrt{|\omega_n| Z_i(n)} \sqrt{|\omega_m| Z_j(m)}} \bar{\phi}_j(m), \quad (8)$$

where the symmetrized λ 's and Coulomb repulsion parameters are given by

$$\lambda_{ij}^s(n-m) = \sqrt{\frac{N_i}{N_j}} \int_0^{+\infty} d\Omega \alpha^2 F_{ij}(\Omega) \frac{2\Omega}{\Omega^2 + (\omega_n - \omega_m)^2}, \quad (9)$$

$$\mu_{ij}^s = \sqrt{\frac{N_i}{N_j}} \mu_{ij}, \quad (10)$$

and the eigenvalue $\varepsilon(T)$ is 1 when $T = T_c$. In terms of $\lambda_{ij}^s(n-m)$ the renormalization function $Z_i(n)$ is given by (see Eq. (5))

$$\omega_n Z_i(n) = \omega_n + \pi T_c \sum_{jm} \lambda_{ij}^s(n-m) \sqrt{\frac{N_j}{N_i}} \frac{\omega_m}{|\omega_m|}. \quad (11)$$

Next, in order not to deal with a matrix of unnecessarily large size one cuts off the Matsubara sums in (8) at a smaller energy ω_c , which is large enough so that $Z_i(n) \approx 1$ for $|\omega_n| > \omega_c$, and at the same time rescales μ_{ij}^s to the new cutoff ω_c by integrating out the high energy part of $\bar{\phi}_j(m)$ as described in [2]. The result is that μ_{ij}^s in equation (8) is replaced by $\mu_{ij}^*(\omega_c)$ where the matrix (in band indices) $\hat{\mu}^*(\omega_c)$ is related to matrix $\hat{\mu}^s$ by

$$\hat{\mu}^*(\omega_c) = \left(\hat{1} + \hat{\mu}^s \ln \frac{E_F}{\omega_c} \right)^{-1} \hat{\mu}^s, \quad (12)$$

with E_F on the order of the total bandwidth. In the case of a two-band model, which we will examine numerically

in the next section, the explicit relations between $\mu_{ij}^*(\omega_c)$ and μ_{ij}^s are ($\mu_{\pi\sigma}^s = \mu_{\sigma\pi}^s$)

$$\mu_{\sigma\sigma}^*(\omega_c) = \left[\mu_{\sigma\sigma}^s + (\mu_{\sigma\sigma}^s \mu_{\pi\pi}^s - \mu_{\sigma\pi}^s{}^2) \ln \frac{E_F}{\omega_c} \right] / D, \quad (13)$$

$$\mu_{\sigma\pi}^*(\omega_c) = \mu_{\sigma\pi}^s / D, \quad (14)$$

$$\mu_{\pi\pi}^*(\omega_c) = \left[\mu_{\pi\pi}^s + (\mu_{\sigma\sigma}^s \mu_{\pi\pi}^s - \mu_{\sigma\pi}^s{}^2) \ln \frac{E_F}{\omega_c} \right] / D, \quad (15)$$

where D is the determinant of $\hat{1} + \hat{\mu}^s \ln(E_F/\omega_c)$

$$D = 1 + (\mu_{\sigma\sigma}^s + \mu_{\pi\pi}^s) \ln \frac{E_F}{\omega_c} \\ \times (\mu_{\sigma\sigma}^s \mu_{\pi\pi}^s - \mu_{\sigma\pi}^s{}^2) \left(\ln \frac{E_F}{\omega_c} \right)^2. \quad (16)$$

Now it is easy to generalize the procedure for calculating the functional derivative of T_c given in [12] for a single-band isotropic superconductor to the case of several isotropic bands. One finds

$$\frac{\delta T_c}{\delta \alpha^2 F_{ij}(\Omega)} = - \left(\frac{d\varepsilon(T_c)}{dT} \right)^{-1} \frac{\delta \varepsilon(T_c)}{\delta \alpha^2 F_{ij}(\Omega)} \quad (17)$$

with

$$\frac{\delta \varepsilon(T_c)}{\delta \alpha^2 F_{ij}(\Omega)} = \left[\pi T_c \sum_j \sum_{n,m=1}^{N_c} \frac{\bar{\phi}_i(n)}{\sqrt{\omega_n Z_i(n)}} \frac{\bar{\phi}_j(m)}{\sqrt{\omega_m Z_j(m)}} \right. \\ \times \sqrt{\frac{N_i}{N_j}} \left(\frac{2\Omega}{\Omega^2 + (2\pi T(n-m))^2} \right. \\ \left. \left. + \frac{2\Omega}{\Omega^2 + (2\pi T(n+m-1))^2} \right) - \pi T \right. \\ \left. \times \sum_{n=1}^{N_c} \frac{\bar{\phi}_i^2(n)}{\omega_n Z_i(n)} \left(2 \sum_{l=0}^{n-1} \frac{2\Omega}{\Omega^2 + (2\pi Tl)^2} \right. \right. \\ \left. \left. - \frac{2}{\Omega} \right) \right] / \sum_k \sum_{n=1}^{N_c} \bar{\phi}_k^2(n). \quad (18)$$

The derivative $d\varepsilon(T_c)/dT (< 0)$ is conveniently calculated in the process of finding the highest T for which the largest $\varepsilon(T)$ in equation (8) is equal to 1 and $\bar{\phi}_i(n)$ are the components of the corresponding eigenvector of length dN_c , where d is the number of bands and $N_c = [\omega_c/(2\pi T_c) + 0.5]$, where $[\dots]$ denotes the integer part. Note that $\bar{\phi}_i(n)/\sqrt{\omega_n Z_i(n)} = \sqrt{N_i} \phi_i(n)/\omega_n Z_i(n) = \sqrt{N_i} \Delta_i(n)/\omega_n$, where $\Delta_i(n)$ is the gap function in band i at Matsubara frequency $i\omega_n$.

For $\Omega \ll 2\pi T_c$ one finds from equation (18) that the band-diagonal functional derivatives are given by

$$\frac{\delta \varepsilon(T_c)}{\delta \alpha^2 F_{ii}(\Omega)} = 2\pi T_c \Omega \left[\sum_i \sum_{n,m=1}^{N_c} \frac{\bar{\phi}_i(n)}{\sqrt{\omega_n Z_i(n)}} \frac{\bar{\phi}_i(m)}{\sqrt{\omega_m Z_i(m)}} \right. \\ \times \left(\frac{1}{(2\pi T_c(n-m))^2} \right. \\ \left. \left. + \frac{1}{(2\pi T_c(n+m-1))^2} \right) \right. \\ \left. - \sum_{n=2}^{N_c} \frac{\bar{\phi}_i^2(n)}{\omega_n Z_i(n)} \sum_{l=1}^{n-1} \frac{1}{(2\pi T_c l)^2} \right] \\ / \sum_k \sum_{n=1}^{N_c} \bar{\phi}_k^2(n), \quad (19)$$

and are *linear* in Ω just like in the one-band isotropic case [1]. The band-off-diagonal functional derivatives ($i \neq j$) in the small Ω limit are given by

$$\frac{\delta \varepsilon(T_c)}{\delta \alpha^2 F_{ij}(\Omega)} = \frac{2\pi T_c}{\Omega} \sum_{n=1}^{N_c} \frac{\bar{\phi}_i(n)}{\sqrt{\omega_n Z_i(n)}} \\ \times \left(\sqrt{\frac{N_i}{N_j}} \frac{\bar{\phi}_j(n)}{\sqrt{\omega_n Z_j(n)}} - \frac{\bar{\phi}_i(n)}{\sqrt{\omega_n Z_i(n)}} \right) / \sum_k \sum_{n=1}^{N_c} \bar{\phi}_k^2(n), \quad (20)$$

and diverge at $\Omega = 0$ as $1/\Omega$ just like the functional derivative of T_c with respect to the Fermi surface averaged electron-phonon coupling function of an anisotropic superconductor [8]. Note that the sum in the numerator of equation (20) can be written as $N_i \sum_{n=1}^{N_c} \Delta_i(n) (\Delta_j(n) - \Delta_i(n))/\omega_n^2$ and the sign of $\delta T_c/\delta \alpha^2 F_{ij}(\Omega)$ is determined by the relative size of the gaps $\Delta_i(n)$ and $\Delta_j(n)$ near T_c in the two bands and by the sign of $\Delta_i(n)$ near T_c for low n since the low- n terms give the largest contribution to the sum because of ω_n^2 in the denominator.

The results presented so far apply to a superconductor with *any* number of bands with isotropic intra-band and interband interactions (both electron-phonon and Coulomb). In the next section we present numerical results for an effective two-band model of MgB₂ described in [11].

3 Numerical results for a two-band model

Following the work of Liu et al. [13], Golubov et al. [11] reduced the four-band electronic structure and electron-phonon coupling in MgB₂ to an effective two-band model by exploiting the similarity of the two cylindrical (σ -bands) and the two three-dimensional (π -bands) sheets of the Fermi surface. We used the $\alpha^2 F$'s given in [11] with the coupling parameters (see Eq. (3)) $\lambda_{\sigma\sigma} = 1.017$, $\lambda_{\pi\pi} = 0.446$, $\lambda_{\sigma\pi} = 0.212$ and $\lambda_{\pi\sigma} = 0.155$. The Coulomb repulsion parameters were determined using the ratios of the *screened* Coulomb interaction parameters for MgB₂

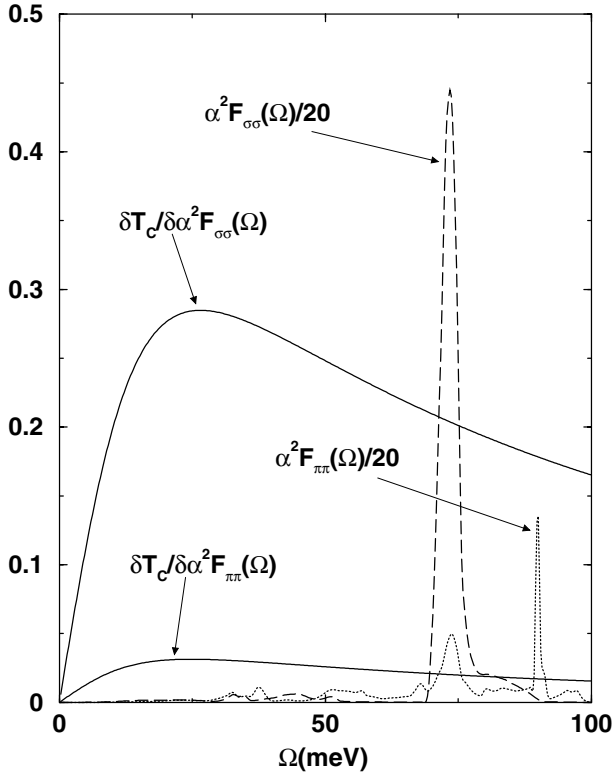


Fig. 1. The band-diagonal functional derivatives and rescaled electron-phonon coupling functions over the entire phonon energy range in MgB₂.

calculated in [14], $\mu_{\sigma\sigma} : \mu_{\pi\pi} : \mu_{\sigma\pi} : \mu_{\pi\sigma} = 1.75 : 2.04 : 1.61 : 1.00$, the density of states ratio N_{π}/N_{σ} consistent with the ratio $\lambda_{\sigma\pi}/\lambda_{\pi\sigma}$ for the spectra that we used, and using equations (10) and (13–16) with E_F set equal to the π -bandwidth of 15 eV [15] and $\omega_c = 0.5$ eV. These constraints leave the single fitting parameter $\mu_{\sigma\sigma}$ which was fitted to the experimental transition temperature of 39.4 K. The results of the fit were: $\mu_{\sigma\sigma}^*(\omega_c) = 0.19627$, $\mu_{\pi\pi}^*(\omega_c) = 0.19561$ and $\mu_{\sigma\pi}^*(\omega_c) = \mu_{\pi\sigma}^*(\omega_c) = 0.04948$.

The calculated functional derivatives are shown in Figures 1–3. In Figure 1 we present the band-diagonal functional derivatives $\delta T_c/\delta\alpha^2 F_{\sigma\sigma}(\Omega)$, $\delta T_c/\delta\alpha^2 F_{\pi\pi}(\Omega)$ and rescaled $\alpha^2 F_{\sigma\sigma}(\Omega)$ and $\alpha^2 F_{\pi\pi}(\Omega)$ over the entire phonon energy range in MgB₂. The spectra $\alpha^2 F_{\sigma\sigma}(\Omega)$ and $\alpha^2 F_{\pi\pi}(\Omega)$ are scaled down by a factor of 20 so that their shapes over the entire range of phonon energies are seen on the scale set by the size of the corresponding functional derivatives. This leaves parts of $\alpha^2 F_{\sigma\sigma}(\Omega)$ and $\alpha^2 F_{\pi\pi}(\Omega)$ that are near the maxima in corresponding functional derivatives invisible, and in Figure 2 we redraw a part of Figure 1 over a smaller energy range with the electron-phonon coupling functions shown to scale. As we proved in Section 2, $\delta T_c/\delta\alpha^2 F_{\sigma\sigma}(\Omega)$ and $\delta T_c/\delta\alpha^2 F_{\pi\pi}(\Omega)$ are linear in Ω at small energies and vanish at $\Omega = 0$. Moreover, both functional derivatives are positive with broad maxima at 9–10 times $k_B T_c$, similar to what one finds in the isotropic single-band case [1, 12]. The difference in sizes of the two functional derivatives in Figures 1 and 2 is due to the difference in sizes of the gap-functions $\Delta_{\sigma}(n)$ and

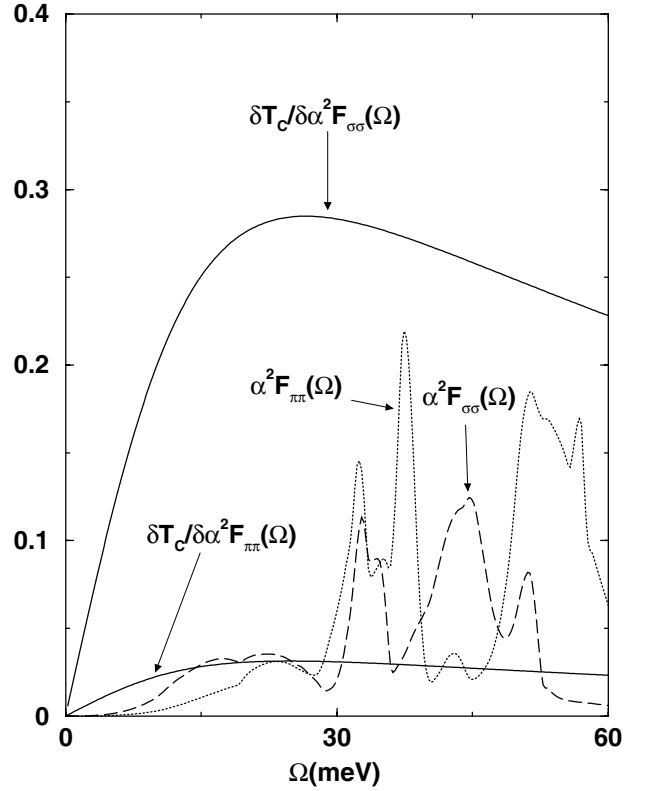


Fig. 2. The same as Fig. 1 but over a smaller energy range so that the parts of $\alpha^2 F_{\sigma\sigma}(\Omega)$ and $\alpha^2 F_{\pi\pi}(\Omega)$ that are near the maxima in the corresponding functional derivatives are drawn to scale.

$\Delta_{\pi}(n)$ near T_c in the two bands as can be deduced from equation (18) (or Eq. (19)) by noting that the normalization factor $\sum_n (\bar{\phi}_{\sigma}^2(n) + \bar{\phi}_{\pi}^2(n))$ is the same for both functional derivatives and its size is largely determined by $\bar{\phi}_{\sigma}(n)$, which is larger than $\bar{\phi}_{\pi}(n)$ ($\bar{\phi}_{\sigma}(1)/\bar{\phi}_{\pi}(1) = 3.4$). Note that in the isotropic one-band case the scale of the functional derivative of T_c varies roughly as $1/(1+\lambda)$ [16] and from Figure 1 it is clear that such a “rule” cannot be applied in determining the relative size of the band-diagonal functional derivatives of T_c in a multi-band case.

In Figure 3 we present the band-off-diagonal functional derivatives $\delta T_c/\delta\alpha^2 F_{\sigma\pi}(\Omega)$ and $\delta T_c/\delta\alpha^2 F_{\pi\sigma}(\Omega)$ together with the corresponding electron-phonon coupling functions. As we proved in Section 2, both of these functional derivatives diverge at $\Omega = 0$ as $1/\Omega$, but they also have opposite signs. Both $\alpha^2 F_{\sigma\pi}(\Omega)$ and $\alpha^2 F_{\pi\sigma}(\Omega)$ vary as Ω^2 in the limit $\Omega \rightarrow 0$ so that $1/\Omega$ -divergences in the corresponding functional derivatives are integrable, as can be deduced from equation (2).

The difference in signs between $\delta T_c/\delta\alpha^2 F_{\sigma\pi}(\Omega)$ and $\delta T_c/\delta\alpha^2 F_{\pi\sigma}(\Omega)$ is related to the fact that near T_c $\Delta_{\sigma}(n) > \Delta_{\pi}(n)$ with both gap functions *positive* at low n (see Eq. (20) and the subsequent discussion in Section 2). In order to illustrate the importance of the sign of the smaller gap $\Delta_{\pi}(n)$ at low n close to T_c , we have computed the functional derivatives for the case when $\alpha^2 F_{\pi\pi}(\Omega)$, $\alpha^2 F_{\sigma\pi}(\Omega)$ and $\alpha^2 F_{\pi\sigma}(\Omega)$ were scaled down by a factor

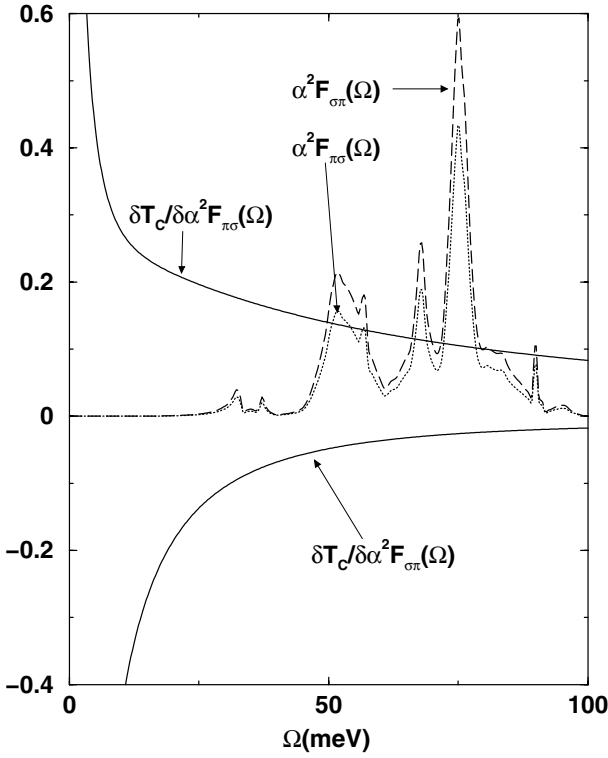


Fig. 3. The band-off-diagonal functional derivatives and electron-phonon coupling functions for MgB₂.

of 10, with $\alpha^2 F_{\sigma\sigma}(\Omega)$ and $\mu_{\sigma\sigma}^*(\omega_c)$, $\mu_{\pi\pi}^*(\omega_c)$, $\mu_{\sigma\pi}^*(\omega_c)$, $\mu_{\pi\sigma}^*(\omega_c)$ left unchanged. This produced negative $\lambda_{\pi\pi} - \mu_{\pi\pi}^*$, $\lambda_{\pi\sigma} - \mu_{\pi\sigma}^*$ and $\lambda_{\sigma\pi} - \mu_{\sigma\pi}^*$ which resulted in a solution where $\Delta_\sigma(n)$ and $\Delta_\pi(n)$ near T_c have opposite signs at low n . The corresponding functional derivatives are shown in Figure 4. Now, both band-off-diagonal functional derivatives are negative. Note that the scale of $\delta T_c / \delta \alpha^2 F_{\pi\pi}$ is roughly two orders of magnitude smaller than the other three functional derivatives.

It is important to point out that the calculated T_c for the parameters in Figure 4 was 43.7 K – substantially higher (by 10%) than the T_c of 39.4 K obtained for the parameters used to produce the results given in Figures 1–3. In fact, even higher T_c of 45.1 K was obtained by setting $\alpha^2 F_{\pi\pi}$, $\alpha^2 F_{\sigma\pi}$ and $\alpha^2 F_{\pi\sigma}$ identically equal to 0 with $\alpha^2 F_{\sigma\sigma}$ and all the Coulomb repulsion parameters left the same – i.e. no attractive interaction in π - π and σ - π channels! The corresponding functional derivatives were similar to those shown in Figure 4 and they explain why T_c is reduced as the couplings $\alpha^2 F_{\pi\pi}$, $\alpha^2 F_{\sigma\pi}$ and $\alpha^2 F_{\pi\sigma}$ are turned on from 0: $\delta T_c / \delta \alpha^2 F_{\sigma\pi}$ and $\delta T_c / \delta \alpha^2 F_{\pi\sigma}$ are both negative and much bigger in absolute value than the positive $\delta T_c / \delta \alpha^2 F_{\pi\pi}$. We finally note that if all interactions, both electron-phonon and Coulomb, in π - π and σ - π channels are set equal to zero, which effectively reduces the two-band model to one-band model, the calculated T_c was 44.6 K. This is a half degree lower than what was obtained by turning off only electron-phonon interaction in π - π and σ - π channels.

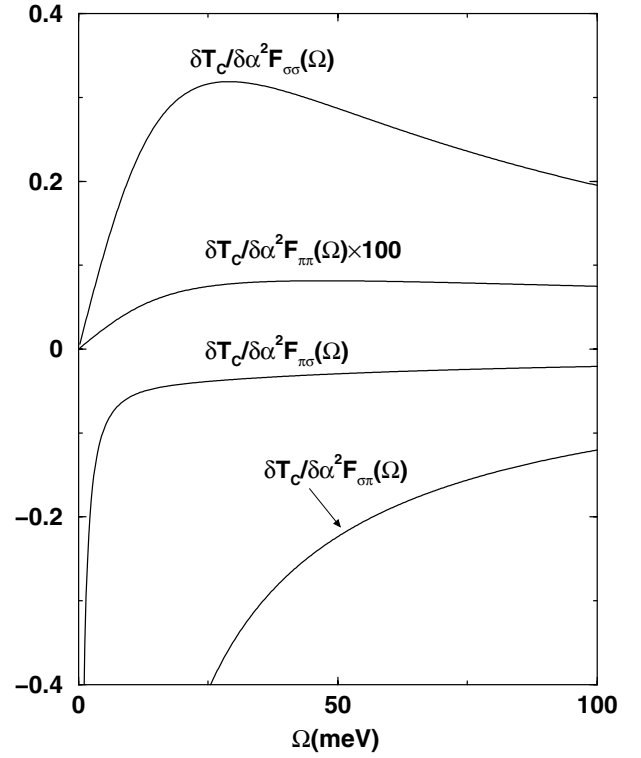


Fig. 4. The functional derivatives for the case when the strengths of $\alpha^2 F_{\pi\pi}$, $\alpha^2 F_{\sigma\pi}$ and $\alpha^2 F_{\pi\sigma}$ were scaled down by a factor of 10 with $\alpha^2 F_{\sigma\sigma}$ and $\mu^*(\omega_c)$'s left unchanged compared to those used in Figures 1–3.

4 Summary

We have developed the general formalism for calculating the functional derivatives of T_c with respect to electron-phonon coupling functions for a superconductor with several bands with isotropic intraband and interband interactions (electron-phonon and Coulomb). We proved rigorously that the band-diagonal functional derivatives $\delta T_c / \delta \alpha^2 F_{ii}(\Omega)$ are linear in Ω at small Ω , as in the isotropic single band case [1]. At the same time we proved that the functional derivatives which are off-diagonal in the band indices, $\delta T_c / \delta \alpha^2 F_{ij}(\Omega)$ with $i \neq j$, diverge at small Ω as $1/\Omega$. The calculation was carried out for a two-band model of MgB₂ using the electron-phonon coupling spectra given in [11] and the ratios of the screened Coulomb interaction parameters given in [14]. We found that the band-diagonal functional derivatives are both positive with broad maxima in the range of 9–10 times $k_B T_c$, similar to the single band isotropic case. However, the functional derivative with respect to intraband electron-phonon coupling function for the band with the smaller gap (π -band) was found to be much smaller than the corresponding functional derivative for the band with the larger gap (σ -band). The functional derivatives with respect to the interband electron-phonon coupling functions were found to diverge as $1/\Omega$ at $\Omega = 0$, but had opposite signs over the entire range of phonon energies for the parameters given in [11]. We found that the signs of these off-diagonal functional derivatives are determined by

the relative signs of the gap functions near T_c at low Matsubara frequencies in the two bands and that, in general, it is possible to have both band-off-diagonal functional derivatives negative.

The results found here give a better insight into the questions – What is the effect of phonons of frequency Ω on T_c through their couplings to electrons via various band channels? Are all coupling always contributing positively to T_c , or are some of them pair-breaking? The answers to these questions are provided in Figures 1–3.

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