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The Sensitivity of the Transition Temperature to Changes in $\alpha^2 F(\omega)$

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The transition temperature of a superconductor depends on $\alpha^2 F(\omega)$, the spectral function of the effective interaction due to phonon exchange. We discuss how strongly the transition temperature is influenced by different frequency parts of $\alpha^2 F(\omega)$. For this purpose the functional derivative $\delta T_c/\delta \alpha^2 F(\omega)$ is calculated. It is shown that all frequency regions of $\alpha^2 F(\omega)$ yield a positive contribution to T_c and that the most effective range covers frequencies, slightly above $2\pi T_c$. The functional derivative is calculated numerically for several superconductors from their measured $\alpha^2 F(\omega)$-spectra. Finally, we discuss the change in transition temperature due to the softening of $\alpha^2 F(\omega)$ which has been observed in amorphous superconductors.

1. Introduction

In superconducting tunneling experiments the Eliashberg function $\alpha^2 F(\omega)$ and the Coulomb pseudopotential μ^* can be determined. The transition temperature of a superconductor can be calculated in terms of these quantities using the linearized Eliashberg equations [1]. Such calculations reflect an integral property of the total spectrum $\alpha^2 F(\omega)$ and do not answer the question of how much different frequency parts of $\alpha^2 F(\omega)$ contribute to the calculated transition temperature T_c.

To investigate this problem one can calculate ΔT_c, the change of the transition temperature which would result if $\alpha^2 F(\omega)$ is set equal to zero in a frequency interval between ω_0 and $\omega_0 + \Delta\omega$. For small $\Delta\omega$ the change ΔT_c is proportional to $\alpha^2 F(\omega_0)$ multiplied by a weighting factor. This weighting factor is simply the appropriate functional derivative, i.e.

$$\Delta T_c = -\frac{\delta T_c}{\delta \alpha^2 F(\omega)}(\omega_0)\,\alpha^2 F(\omega_0)\,\Delta\omega. \tag{1}$$

The functional derivative, considered as a function of frequency, can therefore be thought of 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 one how favourable a certain frequency range is for an increase of the transition temperature. By means of the functional

derivative we can also investigate whether sufficiently low lying phonons are "pair-breaking" as has been suggested recently [2]. If such an effect exists the functional derivative would be negative in that frequency range. In all examples considered here the functional derivative is always positive. Furthermore we can prove this property rigorously for $\mu^*=0$ (see Appendix A). Therefore we are convinced that in thermal equilibrium phonons never have a pair-breaking effect on the transition temperature. In §2 we express the functional derivative $\delta T_c/\delta\alpha^2F(\omega)$ in terms of $\Delta(\omega_n)$, the solution of the linearized Eliashberg-equations. In §3 we present numerical results for several superconductors both crystalline (Sn, Tl, In, Hg, Pb) and amorphous (Ga, Bi, $Pb_{0.75}Bi_{0.25}$, $Sn_{0.9}Cu_{0.1}$, $Pb_{0.9}Cu_{0.1}$).

2. Theoretical Background

The transition temperature of an isotropic strong-coupling superconductor is determined by the linearized Eliashberg equations. For our purposes we found it advantageous to use the Eliashberg equations involving Green-functions defined at the imaginary frequency points

$$\begin{aligned} i\omega_j &= \pi i(2j+1)\,T, \quad j=0, \pm1, \pm2, \ldots \\ \Delta(\omega_i) &= T\sum_j \{\lambda(\omega_i-\omega_j)-\mu^*\}\frac{\pi}{|\tilde{\omega}_j|+\rho}\Delta(\omega_j), \end{aligned} \tag{2}$$

$$\tilde{\omega}_j=\omega_j+\pi T\sum_l \operatorname{sign}\omega_l\,\lambda(\omega_j-\omega_l). \tag{3}$$

In such a Matsubara-type formulation of the Eliashberg equations effects related to the thermal excitations of electrons and phonons are automatically included. Thermal phonons must be included if one wants to study the influence of low lying phonons on the transition temperature [3]. In Eqs. (2) and (3) $\lambda(\omega_i-\omega_j)$ describes the effective electron-electron attraction via exchange of phonons, and can be expressed in terms of a spectral function conventionally denoted as $\alpha^2F(\omega)$.

$$\lambda(\omega_i-\omega_j)=2\int_0^\infty d\omega\,\frac{\omega\alpha^2F(\omega)}{\omega^2+(\omega_i-\omega_j)^2}.$$

The frequency summation in the gap equation (2) should be done up to a frequency of the order of the band width. For technical reasons one only does the summation up to a cut-off frequency somewhat larger than the maximum phonon frequency. The error caused by this restricted summation can be compensated by replacing the true Coulomb repulsion parameter μ by a "pseudo-repulsion" μ^* [1]. Generally μ^*

depends on the chosen cut-off frequency. Since μ^* is determined from tunneling experiments using a cut-off at ten times the maximal phonon frequency [1, 4] we also chose this conventional cut-off frequency in our calculations. For convenience we introduced in Eq. (2) a pair-breaking parameter ρ. For a fixed temperature T the corresponding parameter $\rho(T)$ is the largest ρ such that the linear gap equation has a non-vanishing solution $\Delta(\omega_n)$. From a calculation of $\rho(T)$ one can obtain the transition temperature by solving the equation

$$\rho(T_c)=0. \tag{4}$$

ρ and T_c are functionals of the spectral function $\alpha^2 F(\omega)$. To study the relative strength of the influence of different frequency parts of $\alpha^2 F(\omega)$ on the transition temperature we calculate the functional derivative $\delta T_c/\delta\alpha^2 F(\omega)$.

This functional derivative has the following physical meaning. If $\alpha^2 F(\omega)$ is changed by a small amount $\Delta\alpha^2 F(\omega)$, the resulting change ΔT_c of the transition temperature is given by

$$\Delta T_c = \int_0^\infty d\omega \frac{\delta T_c}{\delta\alpha^2 F(\omega)} \Delta\alpha^2 F(\omega). \tag{5}$$

Within our numerical algorithm it is preferable to calculate first the functional derivative of the pair-breaking parameter ρ at fixed temperature. The functional derivative of T_c is connected with that of ρ by the relation

$$\frac{\delta T_c}{\delta\alpha^2 F(\omega)} = -\left.\frac{\delta\rho}{\delta\alpha^2 F(\omega)}\right|_{T=T_c} \Big/ \left.\frac{d\rho}{dT}\right|_{T_c}. \tag{6}$$

The simplest way of obtaining $\delta\rho/\delta\alpha^2 F(\omega)$ is to transform the gap equation via the transformation

$$\bar{\Delta}(\omega_j)=\frac{\pi}{|\tilde{\omega}_j|+\rho}\Delta(\omega_j)$$

into a hermitian eigenvalue problem for ρ,

$$\rho\bar{\Delta}(\omega_i)=T\sum_j\left\{\lambda(\omega_i-\omega_j)-\mu^*-\frac{|\tilde{\omega}_j|}{\pi T}\delta_{ij}\right\}\bar{\Delta}(\omega_j). \tag{7}$$

The Feynman-Hellman theorem yields the functional derivative of ρ as the expectation value of the functional derivative of the kernel in Eq. (7)

with the eigenvector $\bar{\Delta}(\omega_n)$. Expressing finally $\bar{\Delta}(\omega_n)$ by $\Delta(\omega_n)$ one obtains

$$\frac{\delta\rho}{\delta\alpha^2 F(\omega)} = \pi T \sum_{i,j} \left[\frac{\Delta(\omega_i)\Delta(\omega_j)}{(|\tilde{\omega}_i|+\rho)(|\tilde{\omega}_j|+\rho)} - \frac{\Delta^2(\omega_i)}{(|\tilde{\omega}_i|+\rho)^2} \operatorname{sign}\omega_i \operatorname{sign}\omega_j \right] \cdot \frac{2\omega}{\omega^2+(\omega_i-\omega_j)^2} \left\{ \sum_i \frac{\Delta^2(\omega_i)}{(|\tilde{\omega}_i|+\rho)^2} \right\}^{-1}. \tag{8}$$

For $\omega \ll 2\pi T_c$ this leads to the following behaviour of $\delta T_c/\delta\alpha^2 F(\omega)$ at low frequencies:

$$\frac{\delta T_c}{\delta\alpha^2 F(\omega)} \sim \omega \cdot \pi T_c \sum_{i \neq j} \left\{ \frac{\Delta(\omega_i)\Delta(\omega_j)}{|\tilde{\omega}_i||\tilde{\omega}_j|} - \frac{\Delta^2(\omega_i)}{|\tilde{\omega}_i|^2} \operatorname{sign}\omega_i \operatorname{sign}\omega_j \right\} \cdot \frac{2}{(\omega_i-\omega_j)^2} \left\{ -\left.\frac{d\rho}{dT}\right|_{T_c} \cdot \sum_i \frac{\Delta^2(\omega_i)}{|\tilde{\omega}_i|^2} \right\}^{-1}. \tag{9}$$

Thus the functional derivative goes to zero linearly at sufficiently low frequencies. This reduced influence of low frequency modes on T_c can be heuristically understood in the following way. At T_c the superconductor cannot feel the dynamics of lattice oscillations with frequencies small compared to T_c. Such lattice modes act more like static lattice deformations which have no influence on T_c according to Andersons theorem.

In Appendix A we prove rigorously (for $\mu^*=0$) that the functional derivative of ρ has always a positive sign. This implies that the functional derivative of T_c which differs only by the positive factor $(-d\rho/dT)^{-1}$, is also a positive function.

In order to calculate the functional derivative of T_c one needs $\Delta(\omega_j)$, the solution of the linearized gap equation and the slope of the pair-breaking parameter at T_c. The algorithm for our numerical calculation of these quantities is described in appendix B.

3. Results and Discussion

We have calculated the functional derivative of the transition temperature for several realistic superconductors whose Eliashberg function $\alpha^2 F(\omega)$ and μ^* have been determined experimentally [5–10]*. $\delta T_c/\delta\alpha^2 F(\omega)$ is shown in Fig. 1 for crystalline Sn, Tl, In, Hg, Pb and for amorphous $Sn_{0.9}Cu_{0.1}$, $Pb_{0.9}Cu_{0.1}$, Ga, Bi, $Pb_{0.75}Bi_{0.25}$. This collection of data demonstrates that the general shape of the functional derivatives is very insensitive to the different shapes of the corresponding $\alpha^2 F(\omega)$-

* Most of these data are tabulated by Rowell, McMillan and Dynes [11].

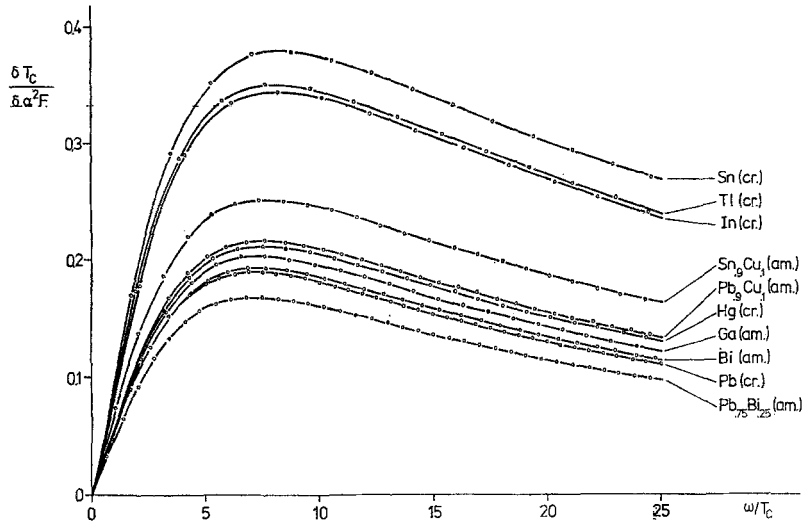

Fig. 1. Frequency dependence of the functional derivative $\delta T_c/\delta\alpha^2 F(\omega)$

Table 1. Characteristic data of the investigated superconductors. The three tabulated transition temperatures are experimentally measured ($T_{c\,\mathrm{exp}}$), calculated from Eq. (2–4) ($T_{c\,\mathrm{sc}}$) and calculated from McMillan's formula [12] for the transition temperature ($T_{c\,\mathrm{MM}}$)

Alloy	State	λ	μ^*	$\langle\omega\rangle$ |°K|	$\int\alpha^2 F(\omega)d\omega$ |°K|	$T_{c\,\mathrm{exp}}$ |°K|	$T_{c\,\mathrm{sc}}$ |°K|	$T_{c\,\mathrm{MM}}$ |°K|	$-\frac{d\rho}{dT}$
Sn	crystalline	0.716	0.111	111	40.0	3.7	3.9	3.7	0.98
Tl	crystalline	0.795	0.135	58	23.2	2.4	2.4	2.1	1.03
In	crystalline	0.805	0.121	80	32.0	3.4	3.4	3.3	1.05
$Sn_{0.9}Cu_{0.1}$	amorphous	1.9	0.04	44	41.6	6.8	6.6	6.9	1.37
$Pb_{0.9}Cu_{0.1}$	amorphous	2.08	0.04	35	35.5	6.5	6.1	5.8	1.51
Hg	crystalline	1.63	0.11	38	30.8	4.2	4.4	4.5	1.58
Ga	amorphous	2.29	0.17	62	71.5	8.5	8.8	8.4	1.63
Bi	amorphous	2.49	0.11	33	40.8	6.2	5.9	5.3	1.66
Pb	crystalline	1.55	0.13	63	48.6	7.2	7.4	6.8	1.70
$Pb_{0.75}Bi_{0.25}$	amorphous	2.76	0.14	34	46.8	6.9	6.9	5.5	1.89

spectra. Concerning the functional derivative the most important parameter for a particular superconductor is its transition temperature since it determines the scale factor for the frequency dependence of the functional derivative. The different amplitudes of the functional derivatives are mainly due to differences in $d\rho/dT$ (see Eq. 6). $d\rho/dT$ at T_c is tabulated in Table 1 together with other characteristic properties of the superconductors investigated.

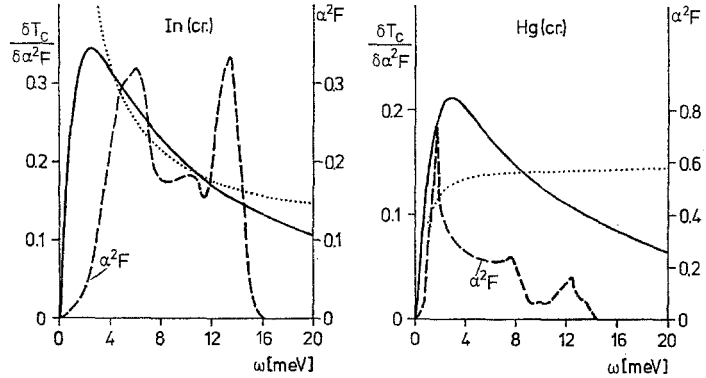

Fig. 2a and b. $\alpha^2 F(\omega)$ (dashed line) and $\delta T_c/\delta \alpha^2 F(\omega)$ (full line) for In and Hg. The dotted line shows the functional derivative of McMillan's formula*

Generally $\delta T_c/\delta \alpha^2 F(\omega)$ starts linearly at the origin and has a maximum slightly above $\omega/T_c = 2\pi$. The frequency where the functional derivative is largest can be thought of as the "optimal frequency" for a high transition temperature, since any shift of $\alpha^2 F$- weight into this region causes an increase of the transition temperature. The small functional derivative in the very low frequency region below T_c means that changes of $\alpha^2 F(\omega)$ in this range have no essential influence on the transition temperature. This is in contrast to the influence of the low frequency part of $\alpha^2 F(\omega)$ on the electron-phonon coupling parameter λ,

$$\lambda = 2 \int_0^\infty \frac{\alpha^2 F(\omega)\, d\omega}{\omega}.$$

λ depends sensitively on the low frequency behaviour of $\alpha^2 F(\omega)$.

* From McMillans interpolation formula for the transition temperature,

$$T_c = \frac{\langle \omega \rangle}{1.2} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right],$$

$$\langle \omega \rangle = \frac{\int \alpha^2 F(\omega)\, d\omega}{\int \alpha^2 F(\omega)\, d\omega/\omega},$$

one obtains the functional derivative

$$\frac{\delta T_c}{\delta \alpha^2 F(\omega)} = T_c \cdot \left[\frac{2}{\lambda \langle \omega \rangle} + \left(1.04 \frac{1+0.38\mu^*}{(\lambda - \mu^*(1+0.62\lambda))^2} - \frac{2}{\lambda}\right)\frac{1}{\omega}\right].$$

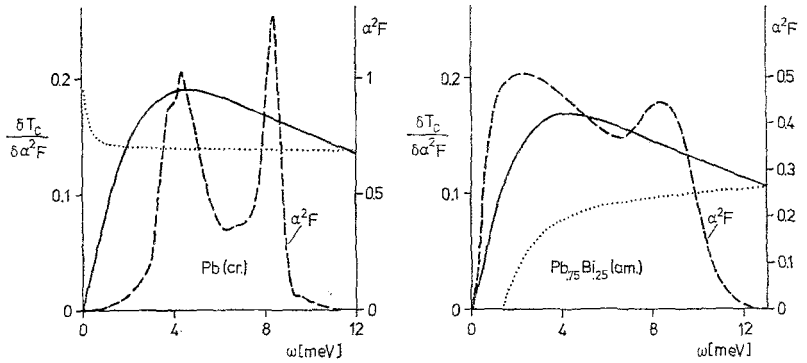

Fig. 3a and b. $\alpha^2F(\omega)$ and $\delta T_c/\delta\alpha^2F(\omega)$ for crystalline Pb and amorphous $Pb_{0.75}Bi_{0.25}$

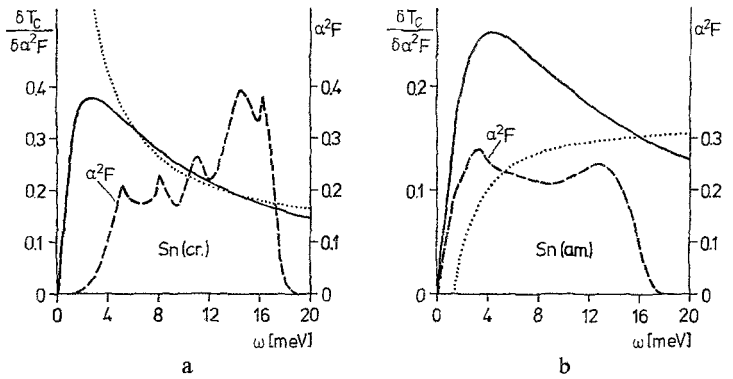

Fig. 4a and b. $\alpha^2F(\omega)$ and $\delta T_c/\delta\alpha^2F(\omega)$ for crystalline Sn and amorphous $Sn_{0.9}Cu_{0.1}$

The functional derivative of T_c is shown in Figs. 2–4 together with the corresponding Eliashberg function $\alpha^2F(\omega)$ for several characteristic superconductors. We want to demonstrate for these examples the relative location of the "optimal frequency" and the transverse and longitudinal phonon peaks in $\alpha^2F(\omega)$. For In, an example of a weak coupling superconductor, both the transverse and longitudinal phonon peaks lie above the "optimal frequency", whereas for the strong coupling superconductor Hg the transverse phonon peak lies slightly below the optimal frequency. In Fig. 3, crystalline Pb is compared with amorphous $Pb_{0.75}Bi_{0.25}$. For crystalline Pb the transverse phonon peak coincides with the optimal frequency. In amorphous $Pb_{0.75}Bi_{0.25}$ this peak is shifted towards lower frequencies. The total weight of $\alpha^2F(\omega)$ is nearly unchanged (see Table 1). This shift of $\alpha^2F(\omega)$ into a less favourable frequency range is the reason

for the decrease of the transition temperature in the amorphous state of Pb. For the weak coupling superconductor Sn the situation is quite different. Fig. 4a shows that for crystalline Sn the main weight of $\alpha^2 F(\omega)$ lies above the optimal frequency. The "softening" of $\alpha^2 F(\omega)$, which is observed in the amorphous phase (Fig. 4b) then shifts the weight of $\alpha^2 F(\omega)$ into a more favourable frequency range. This results in an increased transition temperature. Again $\int \alpha^2 F(\omega) d\omega$ remains nearly unchanged (see Table 1).

These examples demonstrate that a "softening" of $\alpha^2 F(\omega)$ can result in either a positive or a negative change in the transition temperature and that this effect can be explained by means of the characteristic shape of the functional derivative of T_c.

We would like to thank A. Baratoff for helpful discussions during the course of this study.

Appendix A

To prove that $\delta\rho/\delta\alpha^2 F(\omega)$ is positive we first notice that the denominator in Eq. (8) is positive. To investigate the sign of the numerator we rewrite the latter in the form

$$\pi T \sum_{\omega_m=0}^{\infty} \left\{ \sum_{\substack{\omega_i,\,\omega_j>0 \\ \omega_i+\omega_j=\omega_m}} \left(\varphi(\omega_i)+\varphi(\omega_j)\right)^2 - 2\cdot \sum_{\omega_i>0} \left(\varphi(\omega_i)-\varphi(\omega_i+\omega_m)\right)^2 \right\} \frac{2\omega}{\omega^2+\omega_m^2}. \tag{A.1}$$

Here

$$\omega_m = 2m\pi T, \qquad m=0,1,2,\ldots$$

and

$$\varphi(\omega_i) = \frac{\Delta(\omega_i)}{|\tilde{\omega}_i|+\rho}.$$

We now use the fact that for $\mu^*=0$ the physically relevant solution $\Delta(\omega_i)$ of the linearized gap equation (Eq. 2) does not change sign and decreases for increasing $|\omega_n|$. This follows from the positive sign of all elements of the kernel in the gap equation and from the monotonic behaviour of $\lambda(\omega_m)$. The above-mentioned properties of $\Delta(\omega_i)$ also hold for $\varphi(\omega_i)$ and lead to the inequalities

$$\sum_{\substack{\omega_i,\,\omega_j>0 \\ \omega_i+\omega_j=\omega_m}} \left(\varphi(\omega_i)+\varphi(\omega_j)\right)^2 \geqq 2 \sum_{0<\omega_i<\omega_m} \varphi^2(\omega_i) \tag{A.2}$$

and

$$2\sum_{\omega_i>0}\left(\varphi(\omega_i)-\varphi(\omega_i+\omega_m)\right)^2 \leqq 2\sum_{0<\omega_i<\omega_m}\varphi^2(\omega_i). \tag{A.3}$$

One can therefore conclude immediately that the prefactors in front of the terms $\omega/(\omega^2+\omega_m^2)$ in the expression $A1$ and therefore the total sum are never negative.

Appendix B

For the numerical calculation of the order parameter $\Delta(\omega_i)$ and the pair-breaking parameter ρ at fixed temperature T we use the following iteration procedure:

$$\Delta_{n+1}(\omega_i)=\bar{\Delta}_n(\omega_i)/\bar{\Delta}_n(\pi T),$$
$$\rho_{n+1}=\rho_n+(1-f_n)/f_n'.$$

Here

$$\bar{\Delta}_n(\omega_i)=T\sum_j\left(\lambda(\omega_i-\omega_j)-\mu^*\right)\frac{\pi}{|\tilde{\omega}_j|+\rho_n}\Delta_n(\omega_j),$$

$$f_n=\sum_i\frac{\bar{\Delta}_n(\omega_i)\Delta_n(\omega_i)}{|\tilde{\omega}_i|+\rho_n}\Big/\sum_i\frac{\Delta_n^2(\omega_i)}{|\tilde{\omega}_i|+\rho_n},$$

$$f_n'=\left\{\left(\sum_i\frac{\Delta_n^2(\omega_i)}{(|\tilde{\omega}_i|+\rho_n)^2}\right)\left(\sum_i\frac{\bar{\Delta}_n(\omega_i)\Delta_n(\omega_i)}{|\tilde{\omega}_i|+\rho_n}\right)\right.$$
$$\left.-2\left(\sum_i\frac{\bar{\Delta}_n(\omega_i)\Delta_n(\omega_i)}{(|\tilde{\omega}_i|+\rho_n)^2}\right)\left(\sum_i\frac{\Delta_n^2(\omega_i)}{|\tilde{\omega}_i|+\rho_n}\right)\right\}\left\{\sum_i\frac{\Delta_n^2(\omega_i)}{|\tilde{\omega}_i|+\rho_n}\right\}^{-2}.$$

Fewer than ten iterations were necessary, in all cases considered, to obtain $\rho(T)$ with relative accuracy of 10^{-5}. In order to avoid small fluctuations arising from the discontinuous dependence of the matrix dimension on the temperature we used a temperature mesh such that the cut-off frequency is an odd multiple of πT. T_c and $d\rho/dT$ are calculated by quadratic interpolation of $\rho(T)$ using the three temperature points nearest T_c.

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