SOLUTION OF THE SUPERCONDUCTIVITY PHYSICS INVERSE TASK: RECONSTRUCTION OF BOSON MODE SPECTRUM FROM THE TUNNEL DATA

A. I. D'yachenko, A. A. Kvachev

Donetsk Physico-Technical Institute, str. R. Luxemburg, 72, Donetsk, 340114, the Ukraine

It is well known that the tunnel density of states $N(\omega)$ of high-temperature superconductors is characterized by essential smoothing of the root peculiarity in the region of the energy gap. It can be taken into account by the Dynes approximation:

$$N(\omega) \approx N_D(\omega) \equiv \mathrm{Re}\left\{\frac{\omega + i\gamma}{\sqrt{(\omega + i\gamma)^2 - \Delta(\omega)^2}}\right\},$$

where imaginary addition $i\gamma$ effectively allows for the washing out of the quasiparticle levels, direct not linked with the electron-phonon interaction (EPI). We propose the regularization algorithm allowing one to eliminate the influence of Dynes parameter γ on the reconstructing from tunnel data spectral function $\alpha^2F(\omega)$.

Significant feature of high temperature superconductors is an unusual wide spectrum of phonon excitation and high electron-phonon interaction of a high-frequency mode. Therefore, independently of a real microscopic mechanism of HTSC, which most likely realized at "semi-chemical" level, contribution of phonon mechanism may be very important. Virtual exchange by the phonon mode renormalized the density of states of quasiparticles excitation $N(\omega)$ for superconductor S, that reflected in conductivity $\sigma(V)$ of S–I–S and N–I–S type tunnel contacts. Function $N(\omega)$ and spectral function of electron-phonon interaction $\alpha^2F(\omega)$ are connected by the nonlinear Eliashberg equations [1]

$$N = \hat{E}(\alpha^2F). \tag{1}$$

$$N(\omega) = \mathrm{Re}\left\{\frac{\omega}{\sqrt{\omega^2 - \Delta(\omega)^2}}\right\}. \tag{2}$$

The proposed program allows one to solve both the direct and the inverse problem, i.e. to calculate the tunnel conductivity $\sigma(V)$ for a given boson spectrum $\alpha^2F(\omega)$, and, vice versa, reconstruct the $\alpha^2F(\omega)$ function from an experimental curve $\sigma(V)$. It must be borne in mind, that when solving inverse task the most difficult moment is the problem to eliminate high sensitivity of the results of calculations to data error in an experimental function $\sigma(V)$. Reason of that sensitivity has a deep character and is linked with a formal absence of the inverse operator $\hat{E}^{-1}$ for the Eliashberg equations (1), i.e. far and by

$$\alpha^2F \neq \hat{E}^{-1}\{N(\Delta)\}. \tag{3}$$

To solve that problem we elaborated the regularization algorithm, which allows to suppress both the high-frequency and the low-frequency noises in the experimental data on $\sigma(V)$. In that case, the spectral function $\alpha^2F(\omega)$ was found with a minimal distortion. The program used the linearized Eliashberg equation [2],

$$g(\omega) = E_{\text{lin}}\{N_{\text{exp}}\}, \tag{4}$$

which allows one to obtain the complex energy gap $\Delta(\omega)$ from the experimental function $N(\omega)$ directly, with the use of a dispersion relationship

$$\text{Im}\left\{\frac{\omega}{\sqrt{\omega^2 - \Delta(\omega)^2}}\right\} = \frac{2\omega}{\pi}\int_{\Delta_0}^{\infty} \frac{N(\omega') - N_{\text{BCS}}(\omega')}{\omega^2 - \omega'^2}\, d\omega' \tag{5}$$

$N_{\text{BCS}}(\omega) = \text{Re}\left(\omega/\sqrt{\omega^2 - \Delta_0^2}\right)$, Δ_0 is the gap BCS in the energy spectrum of the superconductor.

The linearized equation (4) is solved by virtue of direct iteration algorithm with secured the steadiness of calculations. The calculated function $g^{(i)}(\omega)$ contains errors and by and large does not belong to the family G of EPI functions $\alpha^2(\omega)F(\omega)$, which is characterized by total conditions: $g(\omega) \in G$ if

$$g(\omega) \equiv 0 \text{ for } \omega > \omega_D;\ g(\omega) \approx \omega^{\nu},\ \omega < \omega_{\text{min}};\ g(\omega) \geq 0 \text{ for } 0 < \omega < \omega_D \tag{6}$$

Therefore the program has block corrected $g^{(i)}(\omega)$ according to conditions (6) (Fig. 1). Here (i) is the number of iteration in which the experimental function $N_{\text{exp}}(\omega)$ is corrected, ω_D is the end of phonon spectrum, ω_{min} is the energy to which $\alpha^2(\omega)F(\omega)$ can be taken as proportional to ω^{ν}, exponent $\nu > 0$ (usually $\nu = 2$). The full nonlinear Eliashberg equations $\Delta = \hat{E}(\alpha^2 F)$ (1) is used for direct calculation of complex parameter $\Delta(\omega)$ and function $N(\omega)$.

The calculated function $N(\omega) \equiv N_{\text{calc}}(\omega) \in N$, where N is a multitude of solutions of the Eliashberg equation (1), (2). The experimental function $N_{\text{exp}}(\omega)$ does not belong to multitude N therefore the inverse task (2) strictly speaking is not resolved, $N_{\text{exp}}(\omega) \notin N$.

In order to decrease the influence of uncertainty in the experimental data, we used the known character of usual experimental errors and this allows us to correct the starting function N_{exp} and compare it with the N_{calc}. In this correction some parameters $C_n \in C$ for given correction function $\delta N(C)$ are determined. Then the program eliminate an influence of the Dynes parameter γ with the help of the equations

$$N_{\text{Dynes}}(\omega) = \text{Re}\left\{\frac{\omega}{\sqrt{\omega^2 - \beta^2(\omega)\Delta^2(\omega)}}\right\},\quad \beta(\omega) = \omega/(\omega - i\gamma),$$

$$N_D(\omega) = \text{Re}\left\{\frac{\omega}{\sqrt{\omega^2 - \beta^2(\omega)\Delta_0^2}}\right\},\quad \beta(\omega) = \omega/(\omega - i\gamma),$$

$$f(\omega) = \left(\frac{\omega^2 - \beta^2(\omega)\Delta^2(\omega)}{\omega^2 - \Delta^2(\omega)}\right)^{1/2} \tag{7}$$

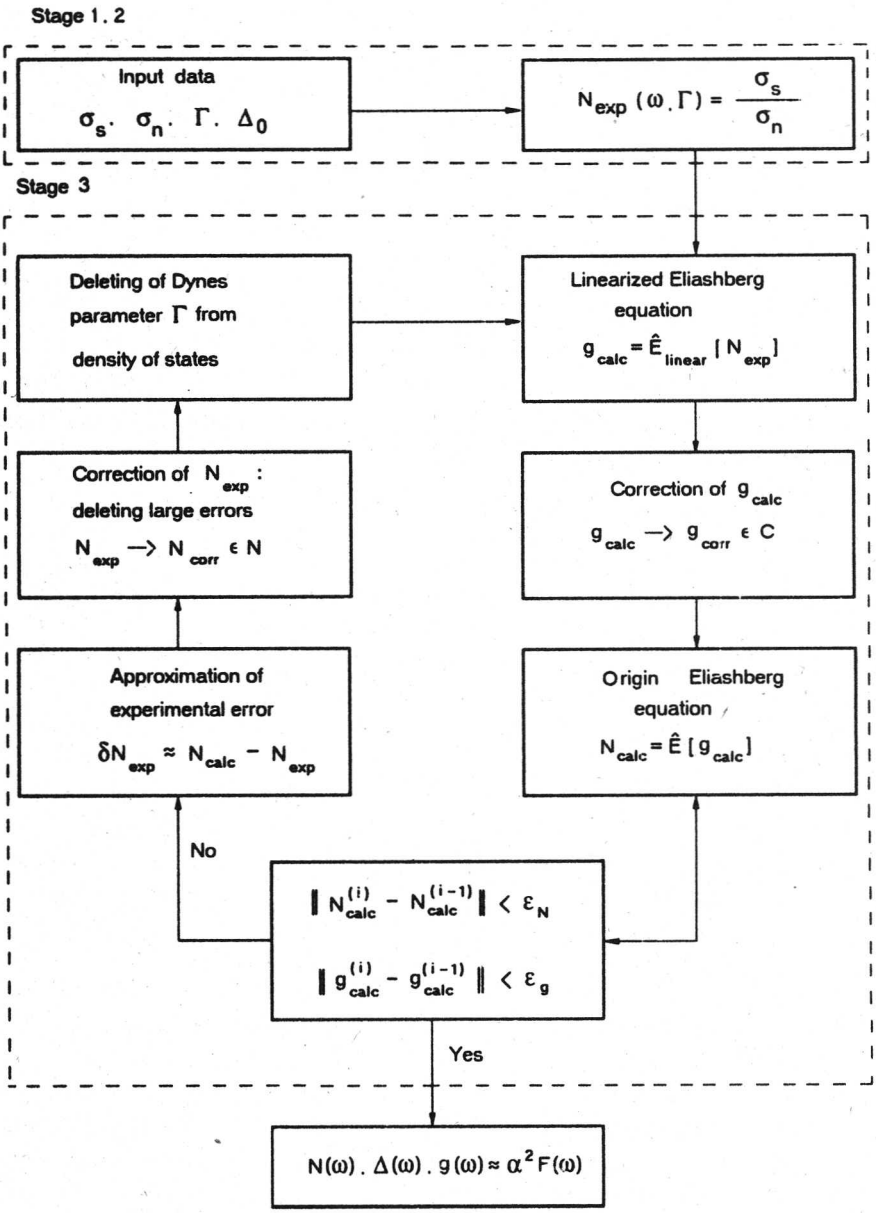

Fig. 1. Block-diagram of PHONON program

$$N_{corr}(\omega) \approx N_{exp}(\omega)\,\mathrm{Re}\,f(\omega) - \mathrm{Im}\,f(\omega)\cdot \mathrm{Im}\,S(\omega)\,,$$

$$S(\omega) = \omega/\sqrt{\omega^2 - \beta^2(\omega)\,\Delta^2(\omega)}\,.$$

The function $N_{corr}(\omega)$ is further used as "experimental" tunnel density of states. The iteration for making the correction $N_{corr}(\omega) \approx N(\omega)$ more preciseis carried out until the conditions

$$||N^{(i)} - N^{(i-1)}|| > \varepsilon_N\,, \quad ||g^{(i)} - g^{(i-1)}|| > \varepsilon_g$$

are fulfilled.

Efficiency of the program algorithm was tested on the ordinary superconductors [3], and in numerical experiments, for which the modeling function $\alpha^2F(\omega)$ was used. For model calculations of HTSC-superconductors we used the effective spectral function $\alpha^2F(\omega)$, where $F(\omega)$ was the known data on the BSCO phonon density of states [4], the parameter of electron-phonon coupling α^2 was relapsed by the constant, which was chosen so that the calculated value $T_c = 110$ K (the electron-phonon coupling constant $\lambda = 2\int \alpha^2F(\omega)/\omega d\omega \approx 3.4$ [5]).

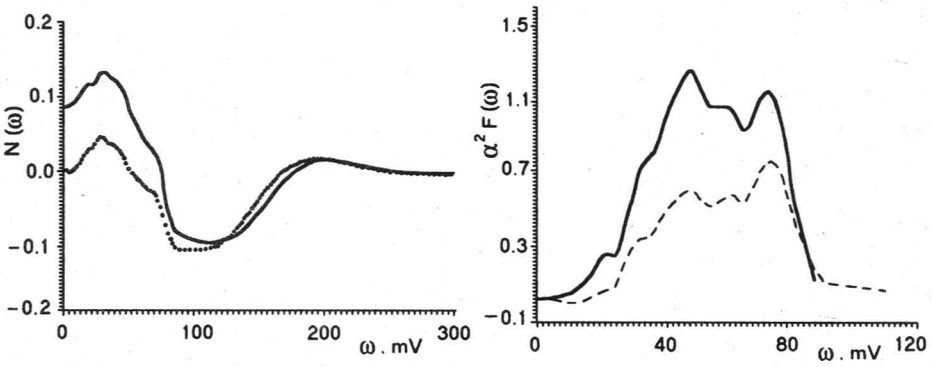

Fig. 2. The experimental (●) and calculated (–) density of states

Fig. 3. The spectral function of EPI for Bi 2223 ceramic: (solid) — influence of Dynes parameter Γ is eliminate; (dashed) — the Dynes density of states with Γ = 15 meV

As is seen from Figs. 2,3 the washing out of the $N(\omega)$ peculiarity in the region of energy gap leads to strong distortion of calculated function $\alpha^2F(\omega)$, if the corresponding correction in the program is not used. An error in the λ value may reach more than 100%.

1. *Wolf E. L.*, Principles of electron tunneling spectroscopy, Oxford University Press, New York (1985), 576 p.
2. *Galkin A. A., D'yachenko A. I., Svistunov V. M.*, Zh. Eksp.Theor. Fiz. **66**, 2262 (1974); Sov. Phys. JETP **39**, 1115 (1974).
3. *Svistunov V. M., Belogolovskii M. A., Chernyak O. I.*, Uspekhi Fiz. Nauk (Sov. Phys. Uspekhi) **151**, 31 (1987).
4. *Vedeneev S. I., Stepanov V. A.*, Physica **C162&164**, 1131 (1989).
5. *D'yachenko A. I., Kvachev A. A., Kochergin I. V. and Svistunov V. M.*, Phys. Lett. **A150**, 121 (1990).