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A STUDY OF THE THERMODYNAMIC SUPERCONDUCTING STATE PARAMETERS IN SELENIUM UNDER HIGH PRESSURE

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The thermodynamic properties of the superconducting state that induces in selenium at the pressure of 100 GPa have been described in the paper. In the framework of the Eliashberg theory values of the energy gap at the temperature of close to zero Kelvin and electron effective mass have been determined. Our study shows that the ratio of the electron effective mass to electron band mass (m_e^*/m_e) in the entire range of the superconducting state existence takes a high value and its maximum equals 1.505 for $T = T_{\rm C}$. Furthermore, it has been shown that the dimensionless ratio: $2\Delta(0)/k_{\rm B}T_{\rm C}$ deviates from the predictions of the conventional BCS theory.

Key words: superconductors, thermodynamic properties, high-pressure effects.

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I. INTRODUCTION

At ambient pressure selenium (Se) is a semiconductor. However, under high pressure exhibits electrical resistance disappearance. Crystalline Se, similar to other chalcogens like sulfur and tellurium, undergoes a sequence of phase transformations in the following way: monoclinic → bco → β-Po → bcc, at 27.8 GPa → 60 GPa → 140 GPa pressure respectively [1]. The metallic bco phases of Se is observed to be superconducting with the transition temperatures of approximately 5–4.5 K at 42–57 GPa [2].

The experimental [2] and theoretical [3] results suggest that from the physical point of view, the superconducting state in Se may have interesting properties at the range of high pressures. It prompted us to estimate the basic thermodynamic parameters of the superconducting selenium for $p = 100$ GPa. Our theoretical analysis based on numerical solutions of the Eliashberg equations. A review of anomalous thermodynamic properties of the superconducting state of simple metals like lithium, calcium and hydrogen, determined in the framework of Eliashberg formalism, can be found by the readers in the following papers [4–9] whereas for the compounds $CaLi_2$, MgB_2 and YNi_2B_2C can be found in [10–12].

II. THE ELIASHBERG FORMALISM

The strong-coupling Eliashberg formalism constitutes an extension of the original Bardeen–Cooper–Schrieffer (BCS) theory, which based on the pairing mechanism that involves an attractive interaction between electrons mediated by the lattice vibrations [13].

The Eliashberg equations on the imaginary axis formulation can be written in the following form [14]:

$$\phi_n = \frac{\pi}{\beta}\sum_{m=-M}^{M}\frac{\lambda(i\omega_n - i\omega_m) - \mu^*\theta(\omega_c - |\omega_m|)}{\sqrt{\omega_m^2 Z_m^2 + \phi_m^2}}\phi_m, \tag{1}$$

$$Z_n = 1 + \frac{1}{\omega_n}\frac{\pi}{\beta}\sum_{m=-M}^{M}\frac{\lambda(i\omega_n - i\omega_m)}{\sqrt{\omega_m^2 Z_m^2 + \phi_m^2}}\omega_m Z_m, \tag{2}$$

where $\phi_n \equiv \phi(i\omega_n)$ and $Z_n \equiv Z(i\omega_n)$ denote the order parameter function and the wave function renormalization factor, respectively; the n-th Matsubara frequency is given by the expression: $\omega_n \equiv (\pi/\beta)(2n-1)$, where $\beta \equiv (k_{\rm B}T)^{-1}$ and $k_{\rm B}$ is the Boltzmann constant. θ denotes Heaviside unit function and ω_c is the cut-off energy ($\omega_c = 3\Omega_{\max}$). The pairing kernel for the electron-phonon interaction is given by:

$$\lambda(z) \equiv 2\int_0^{\Omega_{\max}} d\Omega \frac{\Omega}{\Omega^2 - z^2}\alpha^2 F(\Omega), \tag{3}$$

where the electron-phonon interaction spectral function ($\alpha^2 F(\Omega)$) with the maximum phonon frequency ($\Omega_{\max} = 48.24$ meV) for selenium has been determined in paper [3].

Due to the absence of the experimental value for the critical temperature ($T_{\rm C}$) we are unable to determine the critical value of the Coulomb pseudopotential. In what follows in our considerations we assume the conventional value of $\mu_{\rm C}^\star = 0.1$.

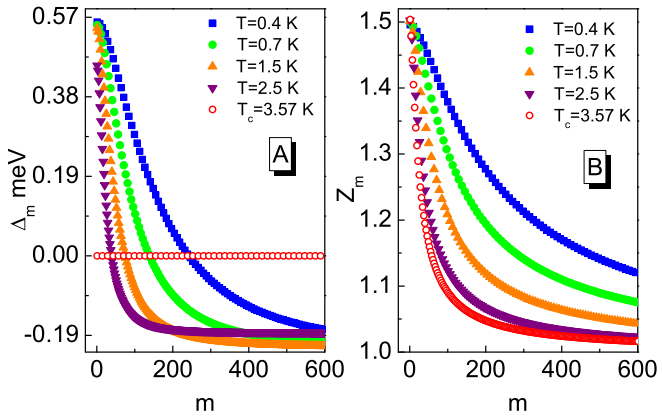

Fig. 1. (Color online.) (A) The order parameter and (B) the wave function renormalization factor on the imaginary axis for the selected temperatures; the first 600 values, respectively of Δ_m and Z_m, are presented.

The solutions of the Eliashberg equations on the imaginary axis for the temperature range from 0.4 K to T_{C} was presented in Fig. 1. In particular, in Fig. 1(A) the dependence of the order parameter's values on the successive Matsubara frequencies has been plotted. We note that with the growth of temperature the maximum of the order parameter's function ($\Delta_{m=1}$) is decreasing. Moreover, the half-width of the function becomes successively smaller. The latter property suggests that together with the growth of temperature less of the Matsubara frequencies give relevant contribution to the Eliashberg equations. In Fig. 1(B) the second solution of the Eliashberg equations has been shown. Also in this case, for the increasing values of the Matsubara frequencies the values of Z_m decrease. However, in comparison with the order parameter, this decrease is much slower.

In order to exactly calculate the value of the energy gap at the temperature close to zero Kelvin and the value of the electron effective mass we perform calculations for the Eliashberg equations on the real axis. The analytic continuation to the real frequency is then performed using the mixed representation technique. The imaginary axis Z_m and Δ_m solutions are then substituted into the Eliashberg equations of the mixed representation and then continued into the Eliashberg equations on the real axis. Such technique is more efficient than the use of the direct real frequency equations [16]. More specifically, the Eliashberg equations in the mixed representation have the following form [17]:

$$\begin{aligned}\phi(\omega+i\delta) &= \frac{\pi}{\beta}\sum_{m=-M}^{M}\left[\lambda(\omega-i\omega_m)-\mu^{*}\theta(\omega_c-|\omega_m|)\right]\frac{\phi_m}{\sqrt{\omega_m^2 Z_m^2+\phi_m^2}} \\ &+ i\pi\int_0^{+\infty}d\omega'\alpha^2F(\omega')\left[\left[N(\omega')+f(\omega'-\omega)\right]\frac{\phi(\omega-\omega'+i\delta)}{\sqrt{(\omega-\omega')^2 Z^2(\omega-\omega'+i\delta)-\phi^2(\omega-\omega'+i\delta)}}\right] \\ &+ i\pi\int_0^{+\infty}d\omega'\alpha^2F(\omega')\left[\left[N(\omega')+f(\omega'+\omega)\right]\frac{\phi(\omega+\omega'+i\delta)}{\sqrt{(\omega+\omega')^2 Z^2(\omega+\omega'+i\delta)-\phi^2(\omega+\omega'+i\delta)}}\right]\end{aligned} \tag{4}$$

and

$$\begin{aligned}Z(\omega+i\delta) &= 1+\frac{i}{\omega}\frac{\pi}{\beta}\sum_{m=-M}^{M}\lambda(\omega-i\omega_m)\frac{\omega_m Z_m}{\sqrt{\omega_m^2 Z_m^2+\phi_m^2}} \\ &+ \frac{i\pi}{\omega}\int_0^{+\infty}d\omega'\alpha^2F(\omega')\left[\left[N(\omega')+f(\omega'-\omega)\right]\frac{(\omega-\omega')Z(\omega-\omega'+i\delta)}{\sqrt{(\omega-\omega')^2 Z^2(\omega-\omega'+i\delta)-\phi^2(\omega-\omega'+i\delta)}}\right] \\ &+ \frac{i\pi}{\omega}\int_0^{+\infty}d\omega'\alpha^2F(\omega')\left[\left[N(\omega')+f(\omega'+\omega)\right]\frac{(\omega+\omega')Z(\omega+\omega'+i\delta)}{\sqrt{(\omega+\omega')^2 Z^2(\omega+\omega'+i\delta)-\phi^2(\omega+\omega'+i\delta)}}\right].\end{aligned} \tag{5}$$

In Eqs. (4) and (5), the symbols $N(\omega)$ and $f(\omega)$ denote the statistical functions of bosons and fermions, respectively.

The Eliashberg equations have been solved for 2201 Matsubara frequencies ($M = 1100$) and for the conventional value of Coulomb pseudopotental ($\mu^{\star}_{\mathrm{C}} = 0.1$) with the use of the iteration method, described in papers [18] and [19]. In the considered case the solutions of the Eliashberg equations are stable for $T \geq T_0$ ($T_0 = 0.4$ K).

III. RESULTS AND DISCUSSION

In Fig. 2, we have presented the form of the order parameter on the real axis for the selected values of temperature for the range of the frequencies from 0 to Ω_{max}. It can be observed, that for the low frequencies, the nonzero value is taken only by the real part of $\Delta(\omega)$. The obtained result proves the fact that in the considered range of the frequencies the damping effects do not exist [20]. Further, we note that the functions $\mathrm{Re}[\Delta(\omega)]$ and $\mathrm{Im}[\Delta(\omega)]$ are correlated with the Eliashberg function. The dependence of the order parameter on temperature can be seen after plotting the function of $\Delta(0)$ (see Fig. 3). Note that $\Delta(0)$ decreases with the temperature growth and takes the zero value at the critical temperature $T_C = 3.57$ K.

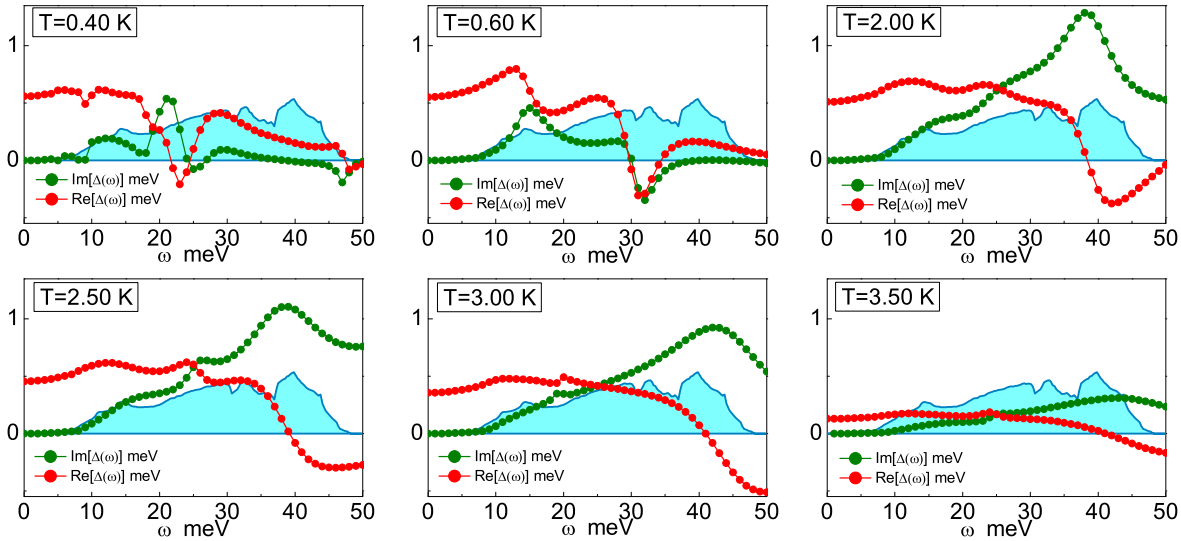

Fig. 2. (Color online.) Frequency dependence of the real and the imaginary part of the order parameter on the real axis for selected values of temperature. The rescaled Eliashberg function ($2\alpha^2 F(\omega)$) has been also plotted.

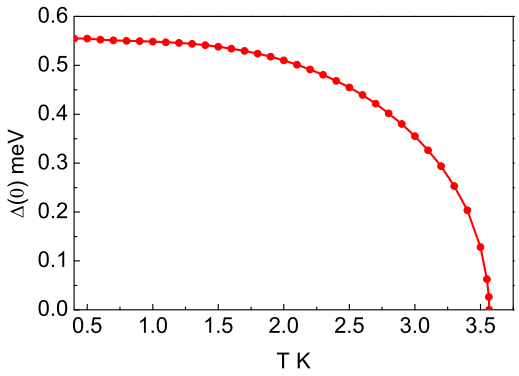

Fig. 3. Temperature dependence of the order parameter on the real axis. The function can be parameterized with the use of the expression: $\Delta(0)(T) = \Delta(0)_{T=T_0}\sqrt{1-\left(\frac{T}{T_C}\right)^{\beta}}$, where $\Delta(0)_{T=T_0} = 0.56$ meV and $\beta = 3.15$.

The knowledge of the order parameter on the real axis allows us to calculate the total normalized density of states using the following formula [21]:

$$\frac{N_S(\omega)}{N_N(\omega)} = \mathrm{Re}\left[\frac{|\omega - i\Gamma|}{\sqrt{(\omega - i\Gamma)^2 - \Delta^2(\omega)}}\right], \qquad (6)$$

where the symbols N_S and N_N denote the energy dependent density of states in the superconducting and the normal state. For the pair breaking parameter Γ we have assumed the typical value for the simple metals: 0.05 meV. The plot of the total normalized density for the selenium has been shown in Fig. 4. According to the presented data we note that with the increasing temperature, the maxima of the density function draw aside. This behavior is connected with the fact that these maxima exist near the points $\omega \pm \Delta(0)$.

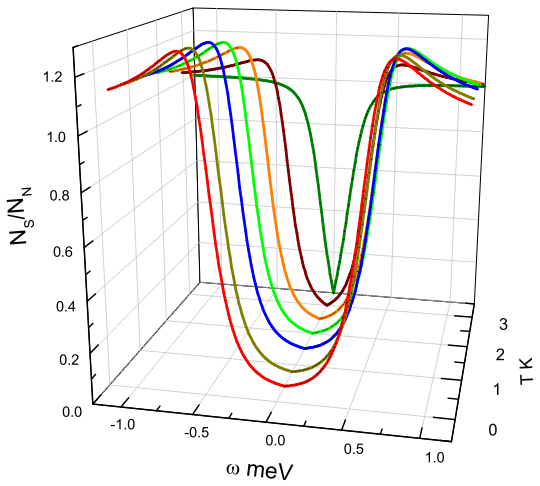

Fig. 4. (Color online.) The dependence of the total normalized density of states on the frequency for selected temperatures.

Due to a weak influence of the temperature on the wave function renormalization factor, in Fig. 5 the functions $\mathrm{Re}[Z(\omega)]$ and $\mathrm{Im}[Z(\omega)]$ have been presented only for $T = T_C$ and $\omega \in \langle 0, \Omega_{\max}\rangle$.

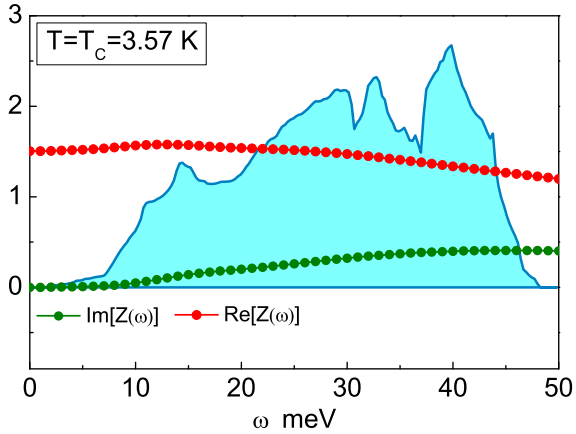

Fig. 5. (Color online.) The dependence of the real and the imaginary part of the wave function renormalization factor on the frequency for T_C. The rescaled Eliashberg function $(10\alpha^2F(\omega))$ has been also plotted.

On the basis of the plotted shape it can be noticed that for the low values of ω only the real part of the wave function renormalization factor is non-zero. This result is directly correlated with the behavior of the order parameter. For higher frequencies the shape of the real and imaginary part of $Z(\omega)$ and $\Delta(\omega)$ are slightly correlated with the Eliashberg function form.

In the framework of the Eliashberg formalism the real part of the wave function renormalization factor enables the determination of the electron effective mass (m_e^*). In particular, the ratio of m_e^* to the electron band mass (m_e) is given by: $m_e^*/m_e = \mathrm{Re}[Z(0)]$. We can observe that $\mathrm{Re}[Z(0)]$ takes the highest value for $T = T_C$ (see Fig. 6).

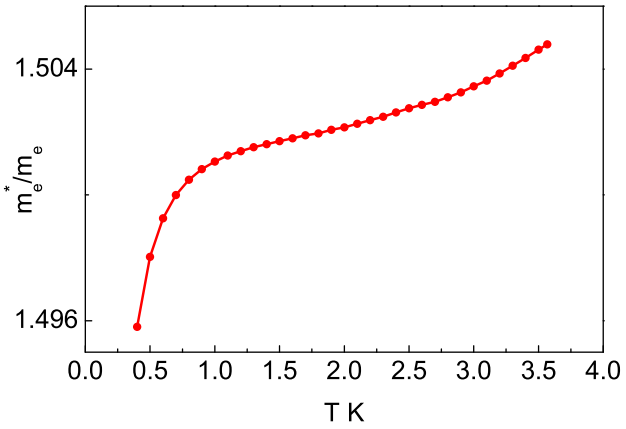

Fig. 6. The temperature dependence of the ratio m_e^*/m_e.

Thus, $[m_e^*]_{\max}$ equals $1.505m_e$. Let us notice that in the case of $T = T_C$ the electron band effective mass in the presence of the electron-phonon interactions can be calculated with a good approximation using a simple formula: $m_e^* = (\lambda + 1)\, m_e$, where the electron-phonon coupling constant λ is the integral involving the Eliashberg function: $\lambda \equiv 2\int_0^{\Omega_{\max}} d\Omega \frac{\alpha^2F(\Omega)}{\Omega}$. For selenium under the pressure at 100 GPa it has been obtained that $\lambda = 0.504$.

On the basis of the Eliashberg equations on the real axis it is possible to calculate the characteristic dimensionless ratio: $R_1 \equiv 2\Delta(0)/k_BT_C$. Let us notice that in the framework of the BCS theory the parameter R_1 takes the universal value equalling to 3.53 [22]. However, this value stands only for the weak coupling limit assumed in the original BCS theory where the critical temperature is small compared with to a logarithmic phonon frequency $(k_BT_C/\omega_{\ln} \to 0)$. In the Eliashberg theory where the electron-phonon interaction can be strong enough to make retardation effects important, the ratio $2\Delta(0)/k_BT_C$ will deviates from the BCS predictions [23]. For selenium under pressure at 100 GPa, where $k_BT_C/\omega_{\ln} = 0.014$, the value of the superconducting gap at the temperature close to zero Kelvin $\Delta(0)$ equals 0.56 meV and $T_C = 3.57$ K. As a result, we obtain $R_1 = 3.64$. This ratio takes a similar value as in the case of sulphur under pressure at 160 GPa ($R_1 = 3.7$) [24]. In the next step we have derived the analytical expression for R_1:

$$R_1 = [R_1]_{\mathrm{BCS}}\left(1 + 7.78\left(\frac{2k_BT_C}{\omega_{\ln}}\right)^2 \ln\left(\frac{2\omega_{\ln}}{k_BT_C}\right)\right), \quad (7)$$

where the logarithmic phonon frequency $\omega_{\ln} = 21.62$ meV. The presented Eq. (7) is a simple modification of the Mitrović–Zarate–Carbotte formula [25] and in the case of selenium it gives a result consistent with the data obtained using the numerical analysis of the Eliashberg equations.

IV. SUMMARY

We have used the Eliashberg formalism to precisely calculate the basic superconducting properties of selenium at 100 GPa. The Eliashberg equations have been solved on the imaginary axis and then using the analytical continuation transformed to the mixed representation and real axis. As a result of these computations the electron effective mass $[m_e^*]_{\max} = 1.505m_e$ and the superconducting energy gap at the temperature close to zero Kelvin $\Delta(0) = 0.56$ meV have been calculated. The knowledge of the value of the energy gap allows to determine the characteristic dimensionless ratio $R_1 = 2\Delta(0)/k_BT_C$. For simple metal selenium it we obtained non-BCS value: $R_1 = 3.64$.

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ВИВЧЕННЯ ТЕРМОДИНАМІЧНИХ ПАРАМЕТРІВ НАДПРОВІДНОГО СТАНУ В СЕЛЕНІ ПІД ВИСОКИМ ТИСКОМ

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У статті описано термодинамічні властивості надпровідного стану, що виникає в селені при тиску 100 ГПа. У межах теорії Еліашберґа встановлено значення енерґетичної щілини за температури, близької до абсолютного нуля, й ефективної маси електрона. Наше дослідження показує, що відношення ефективної маси електрона до маси електрона в зоні провідності (m_e^*/m_e) у всьому діапазоні існування надпровідного стану набуває високих значень і досягає максимуму 1.505 при $T = T_C$. Крім того, показано, що безрозмірне відношення $2\Delta(0)/k_B T_C$ відхиляється від оцінки традиційної теорії БКШ.