THE VAN HOVE SINGULARITY AND TWO-DIMENSIONAL CHARGE DENSITY WAWES. EXACT ANALYTICAL RESULTS

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Received 16 June 2003 in final form 29 September 2003, accepted 13 October 2003

The problem of two-dimensional charge density waves is discussed in the context of the van Hove singularity located at the Fermi level. Exact analytical expressions for the transition temperature T_{CDW}, the isotope coefficient α_{CDW}, order parameter at zero temperature $G(0)$ and discontinuity in the specific heat at critical temperature ΔC_{CDW} was derived. Our results show that in the presence of the van Hove singularity the isotope coefficient can have small values despite the fact that charge density waves originates from phonon-induced pairing. The ratio $2G(0)/k_BT_{CDW}$ varies very little, whereas the temperature dependence of ΔC_{CDW} can be different from standard result.

PACS: 74.20.-z, 74.25.Kc

1 Introduction

The pseudogap in the normal state of high-temperature superconductors is observed in the following: tuneling spectroscopy [1], the angle-resolved photoemission spectroscopy (ARPES) [2], transport properties [3] and nuclear magnetic resonance (NMR) [4].

The experimental data show that the pseudogap Δ^* evolves into the superconducting (SC) gap Δ_{SC} [5]. The pseudogap and superconducting gap have the same symmetry, d-wave type of symmetry [6]. However, the pairing fluctuations may include both s- and d- wave components [7]. Secondly, the crossover temperature T^* merges with the superconducting transition temperature T_{SC} in the overdoped region of the phase diagram. For underdoped high-temperature superconductors the normal-state pseudogap enhances the superconducting isotope effect [8]. Probably the gaps have the same microscopic origin. Therefore we assume that pseudogap is a precursor of superconducting gap formation. However, existing models of pseudogap involve several mechanisms e.g. spin gap due to antiferromagnetic correlations [9].

The existence of charge density wave (CDW) can be considered a possible scenario, which explains the anomalous property of the high-temperature superconductors [8]. We assume the phonon-induced CDW pseudogap. The CDW state stems from electron-hole coupling and charge redistribution. CDW and superconductivity can also represent different phenomena, which coexist below the superconducting transition temperature [10]. The CDW formation has strong influence on the superconductivity [8] . The ratio $2\Delta_{SC}(0)/k_BT_{SC}$, where $\Delta_{SC}(0)$ is the

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zero-temperature superconducting energy gap, in the case of CDW superconductors (weak-coupling limit) is always smaller than the classical BCS value 3.52. However, the strong electron-phonon coupling increases the ratio [11] so these effects may compensate each other in the high-temperature superconductors. In the CDW superconductors is observed also the reduction of the specific heat ΔC_{SC} at $T = T_{SC}$. The experiments demonstrated that the ratio $\Delta C_{SC}/\gamma_S T_{SC}$, γ_S is the Sommerfeld constant, is smaller than the BCS value 1.43 [8].

A competition between the CDW and superconductivity is a highly nontrivial problem. In the framework of the weak-coupling theory one can show that the many-body effects can effectively contribute to the stabilization of the superconducting phase [12]. However, the stability of CDW and superconductivity can strongly depend also on the electronic spectrum, temperature and the electron-phonon interaction-strength. The problem of the competition between the CDW and superconductivity have been in detail discussed by C. A. Balseiro and L. M. Falicov in Ref. [10]. On the other hand, the strong-coupling limit (Eliashberg's equations) is rather difficult to analyse.

It is well known that the quasi-two-dimensionality of the CuO_2 plane in high-temperature superconductors gives rise to logarithmic van Hove singularities in the electronic density of states [13] - [15]. The van Hove singularity, in the electron-phonon weak-coupling limit (s-wave channel), can enhance the T_{SC}, reduce the isotope effect. The ratio $2\Delta_{SC}(0)/k_B T_{SC}$ does not differ much from the BCS limit, whereas the dependence between ΔC_{SC} and T_{SC} is not linear. In the Eliashberg approach the transition temperature T_{SC} and the isotope coefficient α_{SC} is also strongly dependent on the structure of the density of states, the transition temperature T_{SC} is enhanced from the standard value while the isotope coefficient is small [16].

In this paper we study weak-coupling CDW state in the van Hove scenario (s-wave channel), although we should start from the Eliashberg's theory. We suggest that the weak-coupling approach is probably the first good step.

2 Results and discussion

The Hamiltonian is of the following form

$$\begin{aligned} H_{CDW} &= \sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}} - \mu)\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \\ &+ \sum_{\mathbf{k}\sigma} \Lambda_W G_0(\mathbf{k}) c^{\dagger}_{\mathbf{k}+\mathbf{Q}\sigma} c_{\mathbf{k}\sigma} \\ &+ \sum_{\mathbf{k}\sigma} \Lambda_{\omega_D} G_1(\mathbf{k})\, c^{\dagger}_{\mathbf{k}+\mathbf{Q}\sigma} c_{\mathbf{k}\sigma}, \end{aligned} \tag{1}$$

where $c^{(\dagger)}_{\mathbf{k}\sigma}$ denotes annihilation (creation) operator for an electron with momentum $\mathbf{k}$ and spin σ. The chemical potential is $\mu = 0$ so that we refer to the half-filled situation. The band energy is $\varepsilon_{\mathbf{k}} = -2t\left[\cos(k_x) + \cos(k_y)\right]$ for the nearest-neighbour hopping t. The modulation vector is $\mathbf{Q}$. We consider only the simplest form of the modulation vector, $\mathbf{Q}$=(π, π), which results in the opening of the gap in the middle of the band irrespective of the position of the chemical potential. We introduce cutoff operators Λ_W, Λ_{ω_D}, where W, ω_D are the bandwidth and the Debye phonon frequencies, respectively. The cutoff operator Λ_x is defined by

$$\sum_{\mathbf{k}} \Lambda_x f(\varepsilon_{\mathbf{k}}) \simeq \int_{-x}^{x} d\varepsilon \rho(\varepsilon) f(\varepsilon). \tag{2}$$

where x is W or ω_D, $f(\varepsilon_{\mathbf{k}})$ is the appropriate energy dependent function and $\rho(\varepsilon)$ is the density of states. For a two-dimensional square lattice and nearest-neighbour hopping integral t we can accurately reproduce the density of states by

$$\rho(\varepsilon) = b_1 \ln \left| \frac{\varepsilon}{b_2} \right|, \tag{3}$$

with $b_1 = -0.04687t^{-1}$ and $b_2 = 21.17796t$ [16]. In the numerical calculations we take t as an energy unit. The CDW order parameters are denoted by $G_0(\mathbf{k})$, $G_1(\mathbf{k})$, as follows

$$G_0(\mathbf{k}) \equiv \sum_{\mathbf{l}} \Lambda_{\omega_D} V_{\mathbf{kl}} \left\langle c^{\dagger}_{\mathbf{l}+\mathbf{Q}\uparrow} c_{\mathbf{l}\uparrow} \right\rangle, \tag{4}$$

$$G_1(\mathbf{k}) \equiv \sum_{\mathbf{l}} \Lambda_W V_{\mathbf{kl}} \left\langle c^{\dagger}_{\mathbf{l}+\mathbf{Q}\uparrow} c_{\mathbf{l}\uparrow} \right\rangle, \tag{5}$$

where $V_{\mathbf{kl}}$ is the pairing potential. We notice that the mean-field Hamiltonian in Eq.(1) can be derived directly from Fröhlich Hamiltonian (canonical transformation) [10]. The potential $V_{\mathbf{kl}}$ describes thus effective interaction between the electrons.

The pairing potential $V_{\mathbf{kl}}$ will be assumed as a model parameter throughout this paper, $V_{\mathbf{kl}} \simeq -V$, so the phonon properties are used to calculate only the isotope coefficient.

With the help of equations of motion we calculate the Green functions $\left\langle\left\langle c_{\mathbf{k}\uparrow} | c^{\dagger}_{\mathbf{k}\uparrow} \right\rangle\right\rangle$, $\left\langle\left\langle c_{\mathbf{k}\uparrow} | c^{\dagger}_{\mathbf{k}+\mathbf{Q}\uparrow} \right\rangle\right\rangle$ which determinate normal-state and CDW properties [17]. Finally, we conclude with the system of equations

$$1 = (1 + \frac{G_1}{G_0}) V \sum_{\mathbf{k}} \Lambda_{\omega_D} \chi(E_{\mathbf{k}}), \tag{6}$$

and

$$\frac{G_1}{G_0} = 1 + V \sum_{\mathbf{k}} (\Lambda_W - \Lambda_{\omega_D}) \chi(E_{\mathbf{k}}). \tag{7}$$

The temperature-dependent susceptibility function $\chi(E_{\mathbf{k}})$ is defined by

$$\chi(E_{\mathbf{k}}) \equiv \frac{1}{2E_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right), \tag{8}$$

where $E_{\mathbf{k}} \equiv (\varepsilon_{\mathbf{k}}^2 + G^2)^{\frac{1}{2}}$, $G \equiv G_0\Lambda_W + G_1\Lambda_{\omega_D}$ and $\beta \equiv 1/k_BT$, k_B is the Boltzmann constant. Equations (6), (7) originally were derived by Balseiro and Falicov (BF model) [10]. The autors calculated only the CDW-transition temperature T_{CDW} and used the constant density of states at the Fermi level. We present explicit analytical expressions for the most important CDW-parameters in the van Hove scenario. There is a difference between results derived in Ref. [10] and the ones presented here. Then, when combining equations (6), (7) and (3), one gets the equation which determines CDW-parameters.

$$\begin{aligned} 1 &= [2 + V(\int_{-W}^{-\omega_D} + \int_{\omega_D}^{W}) d\varepsilon \rho(\varepsilon) \chi(E)] \\ &\times V \int_{-\omega_D}^{\omega_D} d\varepsilon \rho(\varepsilon) \chi(E). \end{aligned} \tag{9}$$

We now calculate the CDW transition temperature T_{CDW}. We assume the weak-coupling limit, $\omega_D/(2k_BT_{CDW}) \gg 1$. Calculations similar to those presented previously [16] allow us to find the following equation for the CDW transition temperature.

$$1 = b_1 V (2 + b_1 V \phi_0) \phi, \tag{10}$$

where

$$\begin{aligned} \phi &\equiv ln\left(\frac{2k_BT_{CDW}}{b_2}\right) ln\left(\frac{a\omega_D}{k_BT_{CDW}}\right) \\ &+ \frac{1}{2} ln^2\left(\frac{\omega_D}{2k_BT_{CDW}}\right) \\ &- \left[\frac{\partial^2}{\partial n^2} 2^{1-n}\left(1 - 2^{2-n}\right)\Gamma(n)\zeta(n-1)\right]_{n=1} \end{aligned} \tag{11}$$

and

$$\left[\frac{\partial^2}{\partial n^2} 2^{1-n}\left(1 - 2^{2-n}\right)\Gamma(n)\zeta(n-1)\right]_{n=1} = 1. \tag{12}$$

Here Γ and ζ denote Euler and Riemiann zeta functions, respectively. The Euler gamma function $\Gamma(z)$ is defined by the integral $\Gamma(z) \equiv \int_0^\infty dt t^{z-1} e^{-t}$. The Riemann zeta function $\zeta(s)$ is defined by the relation $\zeta(s) \equiv \sum_{k=1}^{\infty} k^{-s}$ (for $s > 1$) [18]. The parameter a is $a \equiv 2e^\gamma/\pi \simeq 1.13$, where γ is the Euler constant and

$$\phi_0 \equiv \ln\left(\frac{W}{\omega_D}\right) \ln\left(\frac{\sqrt{W\omega_D}}{b_2}\right). \tag{13}$$

After carrying out the elementary algebraic transformations in (10) , we obtain a simple expression for the transition temperature

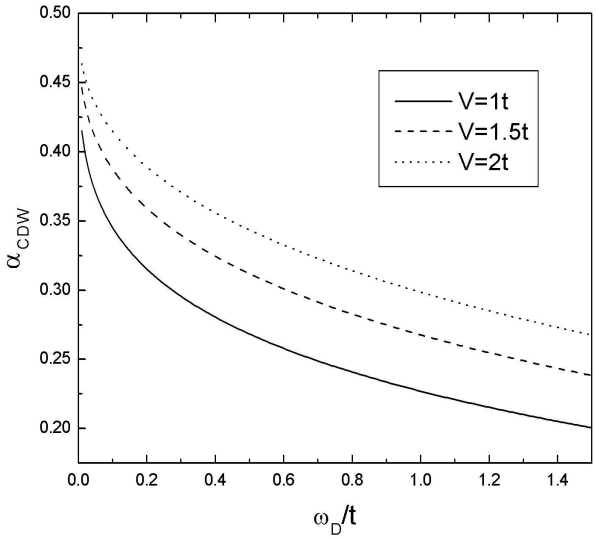

Fig. 1. The figure shows the isotope coefficient α_{CDW} as a function of the Debye phonon frequency ω_D for different values of the pairing potential V.

$$k_B T_{CDW} = a b_2 \exp\left(-\frac{1}{\lambda_1}\right), \tag{14}$$

where

$$\frac{1}{\lambda_1} \equiv \left[\ln^2\left(\frac{\omega_D}{b_2}\right) + \ln^2(2a) - 2 - \frac{2}{b_1 V\left(2 + b_1 V \phi_0\right)}\right]^{\frac{1}{2}}. \tag{15}$$

Here we shall study the dependence of the isotope coefficient α_{CDW} ,

$$\alpha_{CDW} \equiv \left(\omega_D / 2T_{CDW}\right) \frac{d}{d\omega_D} T_{CDW},$$

on the value of Debye phonon frequency ω_D and the pairing potential V. For many materials with phonon-mediated CDW, $T_{CDW} \sim M^{-\alpha_{CDW}}$, where M is the mass of the ions and it is assumed that $\omega_D \sim M^{-\frac{1}{2}}$. With the Balseiro-Falicov theory with a nearly constant $\rho(\varepsilon)$ near the Fermi level, $0.5 > \alpha_{CDW(BF)} > 0.39$. The isotope coefficient α_{CDW}, obtained from the Eq. (14), is

$$\alpha_{CDW} = \frac{\lambda_1}{2}\left[\frac{1}{\left(2 + b_1 V \phi_0\right)^2} - 1\right] \ln\left(\frac{\omega_D}{b_2}\right). \tag{16}$$

In Fig. 1 we show the isotope coefficient α_{CDW} as function of the Debye phonon frequency ω_D for different values of the pairing potential V. This is a very important point because it shows that the isotope coefficient α_{CDW} is in fact smaller than the isotope coefficient $\alpha_{CDW(BF)}$ in the standard BF model.

For $T = 0$ the integrals on the right-hand side of Eq. (9) can be exactly evaluated [19]. Then

$$\begin{aligned} - & \frac{2}{b_1 V (2 + b_1 V \phi_0)} - Li_2(1) = \ln^2\left(\frac{G(0)}{2\omega_D}\right) \\ + & 2\ln\left(\frac{\omega_D}{b_2}\right)\ln\left(\frac{G(0)}{2\omega_D}\right), \end{aligned} \tag{17}$$

where $G(0)$ is CDW-order parameter at zero temperature, $Li_n(z)$ is the polylogarithmic function given by $Li_n(z) \equiv \sum_{k=1}^{\infty} z^k/k^n$. The dilogarithm $Li_2(z)$ satisfies $Li_2(z) = \int_z^0 dt \ln(1-t)/t$ and $Li_2(1) = \pi^2/6$ [20]. We can evaluate the equation (17) analytically and obtain following expression for the CDW order parameter at the zero temperature.

$$G(0) = 2\omega_D \exp\left(-\frac{1}{\lambda_2}\right), \tag{18}$$

where

$$\begin{aligned} \frac{1}{\lambda_2} & \equiv \ln\left(\frac{\omega_D}{b_2}\right) \\ & + \left[\ln^2\left(\frac{\omega_D}{b_2}\right) - \frac{2}{b_1 V (2 + b_1 V \phi_0)} - \frac{\pi^2}{6}\right]^{\frac{1}{2}}. \end{aligned} \tag{19}$$

We are also interested in the CDW–gap-to-T_{CDW} ratio

$$\frac{2G(0)}{k_B T_{CDW}} = \frac{4\omega_D}{a b_2} \exp\left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2}\right). \tag{20}$$

The ratio $2G(0)/k_B T_{CDW}$ varies little from the constant electronic density of the states value of 3.52. Figure 2 shows the ratio of the CDW gap parameter and the CDW transition temperature as the function of the pairing potential V .

In order to calculate the temperature dependence of the order parameter $G(T)$ close to the transition temperature we follow the standard procedure discussed in Ref. [21]. With the help of the fermionic Matsubara frequencies, $\omega_n \equiv (\pi/\beta)(2n+1)$, one can rewrite Eq. (9) in the form

$$\begin{aligned} 1 & = [2 + \frac{V}{\beta}\sum_n (\int_{-W}^{\omega_D} + \int_{-\omega_D}^{W}) d\varepsilon \frac{\rho(\varepsilon)}{\omega_n^2 + E^2}] \\ & \times \frac{V}{\beta}\sum_n \int_{-\omega_D}^{\omega_D} d\varepsilon \frac{\rho(\varepsilon)}{\omega_n^2 + E^2}. \end{aligned} \tag{21}$$

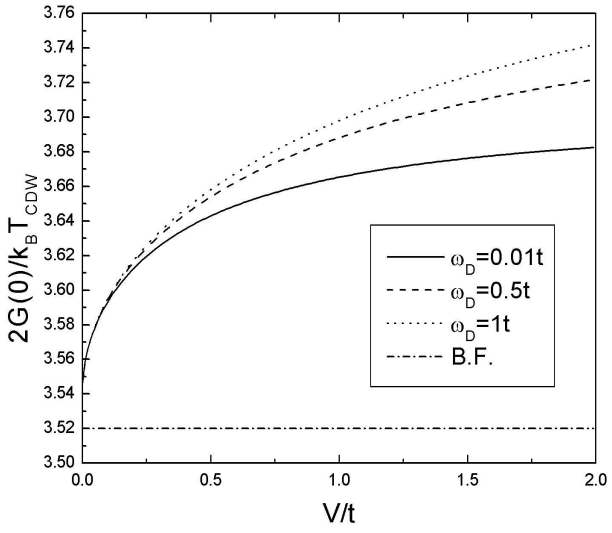

Fig. 2. The ratio $\frac{2G(0)}{k_B T_{CDW}}$ as a function of the pairing potential V. The horizontal line indicates the value obtained within the standard Balseiro-Falicov (BF) approach with the constant density of states.

The Taylor expansion around T_{CDW} provides us with the following equations:

$$\frac{1}{\omega_n^2 + E^2} \simeq \frac{1}{\omega_n^2 + \varepsilon^2} - \frac{G^2(T)}{\left(\omega_n^2 + \varepsilon^2\right)^2}. \tag{22}$$

By substituting Eq. (22) for Eq. (21), the temperature dependence of the order parameter near T_{CDW} is found to be

$$\begin{aligned} \tfrac{2G^2(T)}{\beta} \quad & \sum_n \int_0^{\omega_D} d\varepsilon \frac{\rho(\varepsilon)}{\left(\omega_n^2 + \varepsilon^2\right)^2} = b_1 \left(1 - \frac{T}{T_{CDW}}\right) \\ \times \quad & \left[\frac{T - T_{CDW}}{2T_{CDW}} + \ln\left(\frac{k_B T_{CDW}}{a b_2}\right)\right]. \end{aligned} \tag{23}$$

Up to this point we can see that the weak-coupling approximation $\omega_D / k_B T_{CDW} \to +\infty$ gives the result for the $G(T)$ as [22]

$$G(T) = \pi k_B T \left(\frac{8}{7\zeta(3)}\right)^{\frac{1}{2}} \left(1 - \frac{T}{T_{CDW}}\right)^{\frac{1}{2}} M r_1(T), \tag{24}$$

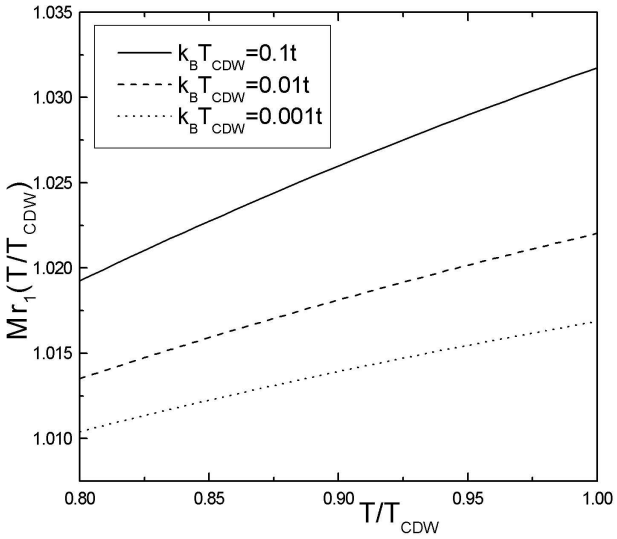

Fig. 3. Mr_1 as a function of temperature T for different values of the CDW transition temperature T_{CDW}.

where

$$Mr_1(T) \equiv \left[\frac{\ln\left(\frac{k_B T_{CDW}}{a b_2}\right) - \frac{T - T_{CDW}}{2T_{CDW}}}{\ln\left(\frac{\pi k_B T}{b_2}\right) - \frac{d}{ds}\left[\ln\zeta(s)\right]_{s=3} - 1.1} \right]^{\frac{1}{2}}. \tag{25}$$

Figure 3 shows Mr_1 as the function of T/T_{CDW}. The CDW gap function near T_{CDW} is very close to that derived in Balseiro-Falicov model. We can see that $Mr_1 \simeq 1$.

Thermodynamic properties depend on the potential difference $\Delta\Omega_{CDW} \equiv \Omega_C - \Omega_N$ between the CDW and normal states. The subscript C (N) refers to the CDW (Normal) state. The integral form of the $\Delta\Omega_{CDW}$ can be presented as

$$\Delta\Omega_{CDW} = \int_0^G dG' \left(G'\right)^2 \frac{d\left(\frac{1}{V}\right)}{dG'}. \tag{26}$$

In the presence of the logarithmic singularity the integral (26) can be rewritten as

$$\begin{aligned} \Delta\Omega_{CDW} &= -\frac{1}{2}\left(\pi k_B T\right)^2 \left(\frac{8}{7\zeta(3)}\right)\left(1 - \frac{T}{T_{CDW}}\right)^{\frac{1}{2}} \\ &\times \quad Mr_2(T), \end{aligned} \tag{27}$$

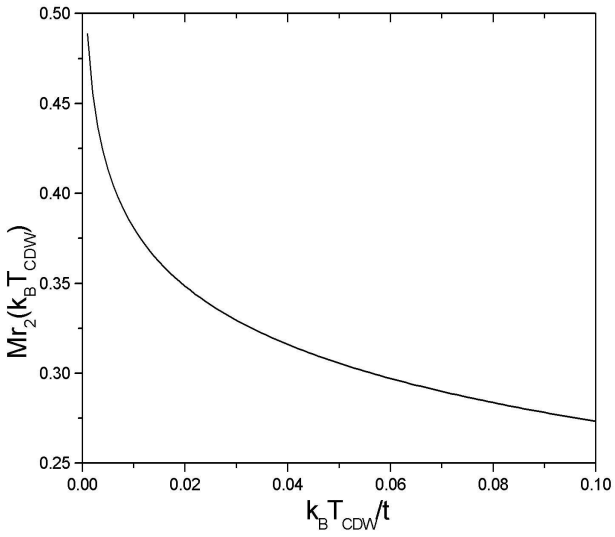

Fig. 4. Mr_2 as a function of the transition temperature T_{CDW}.

where

$$Mr_2\left(T\right) \equiv b_1 \frac{\left[\ln\left(\frac{k_B T_{CDW}}{a b_2}\right) - \frac{T - T_{CDW}}{2T_{CDW}}\right]^2}{\ln\left(\frac{\pi k_B T}{b_2}\right) - \frac{d}{ds}\left[\ln\zeta\left(s\right)\right]_{s=3} - 1.1}. \tag{28}$$

The potential difference function $\Delta\Omega_{CDW}$ has been used to study the specific heat jump ΔC_{CDW}. The specific heat jump is related to the thermodynamic potential difference by the general relation $\Delta C_{CDW} \equiv C_C - C_N = \left[-T\left(\frac{\partial^2 \Delta\Omega_{CDW}}{\partial T^2}\right)_N\right]_{T_{CDW}}$ which gives

$$\Delta C_{CDW} = Mr_2\left(T_{CDW}\right) \frac{8}{7\zeta\left(3\right)} \left(\pi k_B\right)^2 T_{CDW}. \tag{29}$$

Here, Mr_2 represents a deviation from the linear dependence between ΔC_{CDW} and T_{CDW} which can be obtained with a constant density of states. In Fig. 4 , the solid line represents the value of Mr_2 as a function of the critical temperature T_{CDW}. Equation (29) is one of more important results of our theory. In the standard BF formulation the ratio $\Delta C_{CDW}/T_{CDW}$ does not depend on the model parameters. Our exact results show that the ratio $\Delta C_{CDW}/T_{CDW}$ decreases with the increase of the critical temperature.

3 Conclusions

In the present work the BF weak-coupling model of CDW in the van Hove scenario is used to derive exact formulas for the transition temperature T_{CDW}, the isotope coefficient α_{CDW}, the CDW order parameter at zero temperature $G(0)$, the temperature dependence of the order parameter $G(T)$ near T_{CDW} and the specific heat jump ΔC_{CDW} at T_{CDW}. Within this simple approach the transition temperature T_{CDW} is strongly enhanced from the Balseiro-Falicov value. The isotope coefficient α_{CDW} can become very small in comparison with $0.5 > \alpha_{CDW(BF)} > 0.39$ for the Balseiro-Falicov model despite the fact that CDW originates from phononic mechanism. Experimental data e.q. nuclear magnetic resonance (NMR) [23] and nuclear quadrupole resonance (NQR) [24], show very small isotope shift ΔT^*; this is in agreement with our theory. The exact expression for $G(0)$ together with the exact T_{CDW} formula gives a gap-to-T_{CDW} ratio $2G(0)/k_BT_{CDW}$ deviating very little from the Balseiro-Falicov value of 3.52. Our maximum value of the ratio is $[2G(0)/k_BT_{CDW}]_{max} = 3.74$. The experiments have indicated that the pseudogap Δ^* and the crossover temperature T^* decrease with doping, holding the relation of $\Delta^*/k_BT^* \approx 10$ [25]. The values of the ratio $2G(0)/k_BT_{CDW}$ are thus definitely smaller than experimental. Probably the strong-coupling approach can generate larger values of the ratio $2G(0)/k_BT_{CDW}$, the non-negligible role play also (s+d) wave symmetry of the order parameter [26].

Our results show that within a weak-coupling approach the ratio $\Delta C_{CDW}/T_{CDW}$ decreases with the increase of the critical temperature. For superconductors, in the framework of the weak-coupling theory, the ratio $\Delta C_{SC}/T_{SC}$, where ΔC_{SC} is the superconducting specific heat jump at critical temperature T_{SC}, have the similar temperature dependence, in the presence of the logarithmic singularity [20].

Our results should be confirmed by a more reliable method e.q. Eliashberg's formalism. These problems will be under our investigation in the next step.

Acknowledgement: The authors would like to express this gratitude to Prof. M. B. Zapart and Prof. W. Zapart for creating excellent working conditions.

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