Electron-phonon interaction in charge-density-wave superconductors

S. N. Behera and S. G. Mishra
Institute of Physics, Bhubaneswar 751005, India
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Using a canonical transformation we derive an effective electron-phonon interaction for a system undergoing a lattice distortion followed by a superconducting (SC) transition. The relevance of this interaction in interpreting the Raman scattering observation of the SC gap mode in layered charge-density-wave and $A15$-compound superconductors is discussed.

In recent years two different theories[1,2] have been proposed to explain the Raman scattering observation[3] of superconducting (SC) gap excitations in the layered charge-density-wave (CDW) superconductor 2H-$NbSe_2$. Both of these assume the existence of a coupling between the CDW-amplitude-mode (CDW-AM) phonon and the SC electrons and interpret the experimental results in terms of the phonon self-energy effects. The Balseiro-Falicov[1] (BF) model assumes the usual electron-phonon type of coupling, where a phonon decays by emitting an electron-hole pair of same spin. On the other hand, Littlewood and Varma[2] (LV) propose a new mechanism of coupling where the oscillations of the CDW amplitude produces a variation in the electronic density of states at the Fermi surface which in turn changes the SC energy gap. The later mechanism corresponds to an interaction term where a phonon decays by emitting two electrons or two holes of opposite spins and momenta. Neither of these models has been derived from first principles, and the coupling constants remain as unknown parameters. Moreover, the characteristics of the CDW state do not enter the models explicitly. As a result, these theories do not forbid the observation of SC gap excitations by Raman scattering in normal superconductors, for which there is no experimental evidence to date.

In this paper we give a first principles derivation of a residual electron-phonon interaction in the CDW-SC state. Starting from a normal interacting electron-phonon system, we perform a canonical transformation which results in an effective electron-electron interaction and a residual electron-phonon interaction. The effective electron-electron interaction is known to be responsible for the BCS and the CDW condensate states. On the other hand, the residual electron-phonon interaction which involves two phonons and an electron-hole pair when treated in the mean field approximation produces an effective electron-phonon interaction. The coupling constant of this interaction explicitly involves the CDW order parameter, i.e., the Fourier component of the lattice distortion corresponding to the wave vector $\vec{Q}$. Using this effective interaction we recover the BF result for the phonon self-energy in the SC state.

The Hamiltonian of the interacting electron-phonon system in the metallic state is given by

$$H=H_0+H_{e\text{-ph}} \tag{1a}$$

$$=\sum_{\vec{k}\sigma}\epsilon_{\vec{k}}C^{\dagger}_{\vec{k}\sigma}C_{\vec{k}\sigma}+\sum_{\vec{q}}\omega_{\vec{q}}b^{\dagger}_{\vec{q}}b_{\vec{q}}$$

$$+\vec{g}\sum_{\vec{k}\vec{q}\sigma}C^{\dagger}_{\vec{k}+\vec{q},\sigma}C_{\vec{k}\sigma}(b_{\vec{q}}+b^{\dagger}_{-\vec{q}})\,, \tag{1b}$$

where $C^{\dagger}_{\vec{k}\sigma}(C_{\vec{k}\sigma})$ creates (annihilates) an electron with spin σ having energy $\epsilon_{\vec{k}}$, $b^{\dagger}_{\vec{q}}(b_{\vec{q}})$ creates (annihilates) a phonon with wave vector $\vec{q}$ having frequency $\omega_{\vec{q}}$ and g is the electron-phonon coupling constant. We perform a canonical transformation:[4]

$$\tilde{H}=e^{-S}He^{S}\,, \tag{2}$$

which eliminates $H_{e\text{-ph}}$ to lowest order in g. The generator S is determined by

$$H_{e\text{-ph}}=[S,H_0] \tag{3}$$

and the transformed Hamiltonian to $O(g^2)$ is

$$\tilde{H}=H_0+\tfrac{1}{2}[H_{e\text{-ph}},S] \tag{4a}$$

$$=H_0+\tilde{H}_{e\text{-}e}+\tilde{H}_{e\text{-ph}}\,, \tag{4b}$$

where

$$\tilde{H}_{e\text{-}e}=\sum_{\substack{\vec{k}\vec{k}'\vec{q}\\ \sigma\sigma'}}V_{\vec{k}',\vec{q}}C^{\dagger}_{\vec{k}'-\vec{q},\sigma'}C^{\dagger}_{\vec{k}+\vec{q},\sigma}C_{\vec{k}\sigma}C_{\vec{k}'\sigma'}\,, \tag{5}$$

with

$$V_{k,\vec{q}}=\frac{|g|^2\omega_{\vec{q}}}{[(\epsilon_{\vec{k}-\vec{q}}-\epsilon_{\vec{k}})^2-\omega^2_{\vec{q}}]} \tag{6}$$

and

$$\tilde{H}_{e\text{-ph}}=\sum_{\vec{k}\vec{q}\vec{q}'\sigma}[\tilde{V}_{-}(\vec{k},\vec{q},\vec{q}')C^{\dagger}_{\vec{k}+\vec{q},\sigma}C_{\vec{k}-\vec{q}',\sigma}$$

$$\times(b_{\vec{q}}+b^{\dagger}_{-\vec{q}})b_{\vec{q}'}$$

$$+\tilde{V}_{+}(\vec{k},\vec{q},\vec{q}')C^{\dagger}_{\vec{k}+\vec{q},\sigma}C_{\vec{k}-\vec{q}',\sigma}$$

$$\times b^{\dagger}_{\vec{q}'}(b_{\vec{q}}+b^{\dagger}_{-\vec{q}})] \tag{7}$$

with

$$\tilde{V}_{\mp}(k,\vec{q},\vec{q}')=-\tfrac{1}{2}|g|^2\left[\frac{1}{\epsilon_{\vec{k}}-\epsilon_{\vec{k}-\vec{q}'},\mp\omega_{\vec{q}'}}-\frac{1}{\epsilon_{\vec{k}+\vec{q}}-\epsilon_{\vec{k}+\vec{q}-\vec{q}'},\mp\omega_{\vec{q}'}}\right]. \tag{8}$$

In writing Eqs. (4)—(8) we have ignored the terms which renormalize the electron energies. It is well known that $\tilde{H}_{e\text{-}e}$ gives rise to the SC and CDW states in the mean field approximation. The residual interaction $\tilde{H}_{e\text{-ph}}$ couples two phonons with an electron-hole pair. This interaction can be further reduced in the mean field approximation to

$$[\tilde{H}_{e\text{-ph}}]_{\mathrm{MF}}=\tilde{H}^{1}_{e\text{-ph}}+\tilde{H}^{2}_{e\text{-ph}}\,, \tag{9a}$$

where

$$\tilde{H}^{1}_{e\text{-ph}}=\sum_{\vec{k}\vec{q}\sigma}\tilde{V}(\vec{k},\vec{q},\vec{Q})\langle b_{\vec{Q}}\rangle C^{\dagger}_{\vec{k}+\vec{Q},\sigma}C_{\vec{k}-\vec{q},\sigma}\times(b_{\vec{q}}+b^{\dagger}_{-\vec{q}}) \tag{9b}$$

and

$$\tilde{H}^{2}_{e\text{-ph}}=\sum_{\vec{k}\vec{q}\sigma}[\tilde{V}_{-}(\vec{k},\vec{q},\vec{Q}-\vec{q})\langle C^{\dagger}_{\vec{k}\sigma}C_{\vec{k}-\vec{Q},\sigma}\rangle\times(b_{\vec{q}}+b^{\dagger}_{-\vec{q}})b_{\vec{Q}-\vec{q}}+\tilde{V}_{+}(\vec{k},\vec{q},\vec{Q}-\vec{q})\langle C^{\dagger}_{\vec{k}\sigma}C_{\vec{k}-\vec{Q},\sigma}\rangle\times b^{\dagger}_{-\vec{Q}+\vec{q}}(b_{\vec{q}}+b^{\dagger}_{-\vec{q}})] \tag{9c}$$

with

$$\tilde{V}(\vec{k},\vec{q},\vec{Q})=-2|g|^2\left[\frac{(\epsilon_{\vec{k}}-\epsilon_{\vec{k}-\vec{q}})}{(\epsilon_{\vec{k}}-\epsilon_{\vec{k}-\vec{q}})^2-\omega^2_{\vec{q}}}+\frac{\epsilon_{\vec{k}}}{4\epsilon^2_{\vec{k}}-\omega^2_{\vec{Q}}}-\frac{\epsilon_{\vec{k}-\vec{q}}}{4\epsilon^2_{\vec{k}-\vec{q}}-\omega^2_{\vec{Q}}}\right]. \tag{9d}$$

In writing Eqs. (9) we have explicitly assumed that the system is in the CDW state and has undergone periodic lattice distortion, the CDW wave vector being $\vec{Q}$. Consequently $\langle C^{\dagger}_{\vec{k}\sigma}C_{\vec{k}-\vec{Q}\sigma}\rangle\neq 0$ and also $\langle b_{\vec{Q}}\rangle=\langle b^{\dagger}_{\vec{Q}}\rangle\neq 0$. However, care should be taken in evaluating these averages as the canonical transformation renormalizes the electron and phonon energies. Furthermore, the nesting property (electron-hole symmetry)

$$\epsilon_{\vec{k}\pm\vec{Q}}=-\epsilon_{\vec{k}} \tag{10}$$

which is essential for the formation of the CDW state, has also been used in simplifying Eq. (9d). Since $\vec{Q}$ is a reciprocal-lattice vector, Eq. (9c) essentially describes Umklapp scattering of phonons in the CDW state, which is irrelevant in the present context.

The interaction $\tilde{H}^{1}_{e\text{-ph}}$ is similar in structure to that of the BF model, however, its strength explicitly involves the lattice distortion. As a result, for a normal SC such an interaction does not exist. It is evident from Eq. (9d) that $\tilde{V}(\vec{k},\vec{q},\vec{Q})=0$ for $\vec{q}=0$, which signifies the fact that the optical phonons in the normal state will not couple to the electrons. This is confirmable with the deformation-potential theorem which states that $g(\vec{q}=0)=0$. Similarly, for $\vec{q}=\vec{G}$ (a reciprocal-lattice vector) again the coupling $\tilde{V}$ vanishes because of the lattice periodicity. On the other hand, when the system is in the CDW state, for $\vec{q}=\vec{Q}$, because of Eq. (10), the coupling

$$\tilde{V}(\vec{k},\vec{Q})=-8|g|^2\frac{\epsilon_{\vec{k}}}{(4\epsilon^2_{\vec{k}}-\omega^2_{\vec{Q}})}\,, \tag{11}$$

is finite, and since $\vec{Q}$ can be zone folded to $\vec{q}=0$, the opticlike CDW phonons (i.e., the CDW amplitude modes) will interact with the electrons in the SC state through $\tilde{H}^{1}_{e\text{-ph}}$. In what follows we shall approximate $\tilde{V}(\vec{k},\vec{Q})$ by a constant λ' keeping in mind the fact that λ' is of $O(g^2)$ and hence will be of the same order of magnitude as the BCS coupling constant. But the effective coupling constant $\lambda=\lambda'\langle b_{\vec{Q}}\rangle$ will be enhanced for systems having a higher Peierl's transition temperature. In $\tilde{H}^{1}_{e\text{-ph}}$ the CDW wave vector $\vec{Q}$ enters explicitly through the electron operators. It is worth remarking that to $O(g^2)$ a LV-type interaction cannot be generated from Eq. (7). However, the possibility of generating such an interaction cannot be ruled out if one considers terms to $O(g^4)$, as a result it is expected that the processes associated with LV-type interaction will be an order of magnitude weaker and the coupling constant will depend explicitly on both the lattice distortion and the SC gap.

On calculating the phonon propagator using the mean field Hamiltonian with the effective coupling constant λ, we obtain

$$D^{-1}_{\vec{q}}(\omega)=D^{0-1}_{\vec{q}}(\omega)-4\pi^2\lambda^2\chi_{\vec{Q}}(\vec{q},\omega)\,, \tag{12}$$

where the free-phonon propagator:

$$D^{0}_{\vec{q}}(\omega)=\omega_{\vec{q}}/\pi(\omega^2-\omega^2_{\vec{q}}) \tag{13}$$

and the electron response function in the CDW-SC state:

$$\chi_{\vec{Q}}(\vec{q},\omega)=\sum_{\substack{\vec{k}\vec{k}'\\ \sigma\sigma'}}\langle\langle C^{\dagger}_{\vec{k}+\vec{Q},\sigma}C_{\vec{k}+\vec{q},\sigma};C^{\dagger}_{\vec{k}'+\vec{Q},\sigma'}C_{\vec{k}'-\vec{q},\sigma'}\rangle\rangle_{\omega}\,, \tag{14}$$

which should be evaluated in the coexistent CDW-SC state. Since we describe the CDW and SC states by the mean field Hamiltonians it is expected that to the lowest order in the approximation, the CDW phonons will be generated first, which will then couple to the SC electrons. Keeping this in mind we evaluate $\chi_{\vec{Q}}(\vec{q},\omega)$ in the SC

state using the BCS Hamiltonian and assume that the phonons entering $D_{\vec{q}}(\omega)$ are CDW-AM phonons corresponding to $\vec{q}=\vec{Q}$. Thus, we obtain

$$\chi_{\vec{Q}}(\vec{Q},\omega) = -(2\Delta^2/\pi)\sum_{\vec{k}} \tanh\left[\frac{\beta E_{\vec{k}}}{2}\right] \Big/ E_{\vec{k}}(\omega^2-4E_{\vec{k}}^2) , \tag{15}$$

where

$$E_{\vec{k}}=(\epsilon_{\vec{k}}^2+\Delta^2)^{1/2} \tag{16}$$

and 2Δ is the SC energy gap. In evaluating $\chi_{\vec{Q}}(\vec{Q},\omega)$ we have made use of the electron-hole symmetry [Eq. (10)] of the CDW state and assume that $\vec{k}\pm 2\vec{Q}=\vec{k}$. Equation (15) gives the phonon self-energy calculated by BF, which has a square-root singularity at $\omega=2\Delta$. However, because of the prefactor $\langle b_{\vec{Q}}\rangle^2$ in λ^2, the self-energy is nonvanishing only in the CDW state contrary to the predictions of the BF model.

It was pointed out by LV that within the random-phase approximation, the Coulomb corrections completely screen the electron-phonon interaction. However, recently it has been shown[5] that on making the theory consistent by including higher-order electron-phonon effects one recovers the 2Δ singularity in the phonon self-energy.

The following are the predictions of the present calculation: (1) Only those systems which undergo a lattice distortion (e.g., due to CDW formation, martensitic transition, etc.), before the SC phase transition will show a peak below 2Δ in the phonon spectral function.[6] (2) Because of the dependence of the coupling constant on the lattice distortion which is a temperature-dependent quantity, the intensity of the peak associated with the gap mode will show a temperature dependence. (3) The gap-mode frequency will also show a temperature dependence arising from that of both Δ and $\langle b_{\vec{Q}}\rangle$. (4) The temperature dependence of the gap-mode intensity will be strong and predominantly that of $\langle b_{\vec{Q}}\rangle$ provided that the SC and structural transition temperatures are close to each other.

The Raman scattering data on the layered compound CDW superconductor[3] 2H-$NbSe_2$ as well as the high-T_c A15-compound superconductor[7,8] V_3Si show evidence in support of the above predictions. In the former case it has been shown that a peak in the Raman spectrum appears near the SC gap (2Δ) upon cooling from the CDW to the coexistent CDW-SC phase. The effect of magnetic field[3] on the strength of this peak shows that it derives its Raman activity from the presence of a nearby CDW-AM phonon. So far, there is no report of the observation of temperature dependence in the Raman spectrum of this system. While the observation of the gap-mode peak follows from Eqs. (12) and (15) the absence of temperature dependence can be attributed to the fact that the Peierl's transition temperature ($T_p=33$ K) is much higher than the SC transition temperature ($T_c=7.2$ K).

In the case of V_3Si, undergoing a martensitic transformation[9] at $T_m=20.5$ K and then a SC transition at $T_c=16.9$ K a gap mode has been observed[7] around 41 cm^{-1}. There is clear evidence[7] of the coupling of the gap mode to an E_g symmetry phonon around 260 to 300 cm^{-1}. Both the frequency and intensity of the gap mode show strong temperature dependence. In contrast, no such behavior is seen for nontransforming samples of V_3Si. In the case Nb_3Sn which is also a high-T_c ($=18$ K) A15-compound superconductor undergoing a martensitic transformation[8] ($T_m=50.6$ K) the observed gap mode[7,8] does not show any temperature dependence, in spite of the evidence[7] for the coupling between the gap excitations and a phonon at 150 cm^{-1}. The reason for the latter behavior again being $T_m \gg T_c$.

In conclusion, a first-principle derivation of a model Hamiltonian for a system undergoing a lattice distortion followed by a SC transition is presented and its relevance to the Raman scattering observation of the SC gap mode is discussed. The theory applies to the cases where a coupling between the gap mode and a phonon exists. Clearly, the alternative mechanism for the appearance of the gap mode due to direct electronic Raman scattering[8,10] falls outside the scope of the present discussion.

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