Density of states of quasi-one-dimensional charge-density and spin-density waves

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Making use of the quasi-two-dimensional model of charge-density waves, we analyze the electron density of states of $NbSe_3$ observed by the electron tunneling technique. The model provides an excellent description of both the observed density of states and the temperature dependence of the energy gap.

In spite of the reasonable success of weak-coupling mean-field theory[1] in describing the condensate density[2] and the increase in the sound velocity[3] in charge-density waves (CDW's) in $NbSe_3$ and orthorhombic TaS_3 (Ref. 4) and in spin-density waves (SDW's) in $(TMTSF)_2PF_6$ (Ref. 5) (TMTSF=tetramethyltetraselenafulvalene) and more recently the temperature dependence of the threshold field[6] E_T in $NbSe_3$ (Ref. 7), there is one glaring discrepancy between the theory and the experimental observation. The quasiparticle energy gap Δ of two CDW's in $NbSe_3$ measured by the electron tunneling technique[8,9] is much larger than expected from the BCS theory; the observed $2\Delta/k_BT_c \simeq 11.4$–$14.4$ instead of 3.52, where T_c is the corresponding transition temperature. However, the optical absorption measurement of CDW's in $NbSe_3$ appears to give an energy gap consistent with weak-coupling theory.[10] This discrepancy is usually attributed to the strong fluctuation in the quasi-one-dimensional system.[11] In particular, much broader structures than those expected from the BCS theory observed in the tunneling experiments[8,9] appeared to favor this possibility.

In this Brief Report we propose an alternative model. We assume that the electron spectrum in $NbSe_3$ is two or three dimensional, though it is strongly anisotropic. For definiteness we consider the quasiparticle spectrum given by

$$E(\mathbf{p}) = -2t_a\cos(ap_1) - 2t_b\cos(bp_2) - 2t_c\cos(cp_3)\,, \quad (1)$$

with $t_a \gg t_b, t_c$.

Here we take the a direction as the chain direction (i.e., the most-conducting direction; in actual $NbSe_3$ our a, b, and c directions correspond to the b, a, and c axis). From the observed anisotropy in the electric conductivity[12] and the anisotropy in the upper critical field[13] in the superconducting region under high pressure ($P > 7$ kbar), we may take for $NbSe_3$ $t_a:t_b:t_c \simeq 5:1:0.5$ for example. A similar model has been considered by Yamaji[14] in order to interpret the phase diagram of $(TMTSF)_2PF_6$, though the most-conducting direction in the (TMTSF) salt is the a direction and $t_a:t_b:t_c \simeq 10:1:0.03$. The spin-density wave transition temperature decreases as the pressure increases and disappears abruptly for $P = 6$–7 kbar, then the superconductivity with $T_c \simeq 1.2$ K appears for higher pressure.[15] A very similar phase diagram under pressure is observed[16] in $NbSe_3$, which strongly suggests that a similar quasi-two- or three-dimensional model applies to CDW's in $NbSe_3$ as well.

The mean-field theory by Lee, Rice, and Anderson (LRA)[1] is easily generalized for the present model. For example, the electron Green's function is given by[17]

$$G^{-1}(\mathbf{p},\omega_n) = i\omega_n - \eta(\mathbf{p}) - \xi(\mathbf{p})\rho_3 - \Delta\rho_1\,, \quad (2)$$

where

$$\xi(\mathbf{p}) = v(|p_1| - p_F)\,,$$
$$\eta(\mathbf{p}) = \varepsilon_0(1+\alpha)^{-2}[\cos(2bp_2) + 4\alpha\cos(bp_2)\cos(cp_3) + \alpha^2\cos(2cp_3) - 2\alpha]\,, \quad (3)$$

and

$$\varepsilon_0(1+\alpha)^{-2} = -\tfrac{1}{4}t_b^2\cos(ap_F)[t_a\sin^2(ap_F)]^{-1}\,,$$
$$\alpha = t_c/t_b\,,$$

and the ρ_i's are the usual Pauli 2×2 matrices operating on the spinor space formed by the right-going electron and the left-going electron.

Then the gap equation which determines the temperature-dependent order parameter is given by

$$1 = \lambda\pi T\sum_n \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \frac{1}{(2\pi)^2}[(\omega_n - i\eta)^2 + \Delta^2]^{-1/2}\,, \quad (4)$$

with

$$\eta = \varepsilon_0[2(1+\alpha)^{-2}(\cos\phi_1 + \alpha\cos\phi_2)^2 - 1]\,, \quad (5)$$

and the frequency sum is cut off at $|\omega_n| \sim \varepsilon_F$, the Fermi energy and λ is the dimensionless electron-phonon coupling constant.

The electron density of states is given from Eq. (1) as

$$N(E)/N_0 = \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \frac{1}{(2\pi)^2}\,\mathrm{Re}\left[\frac{|E-\eta|}{[(E-\eta)^2-\Delta^2]^{1/2}}\right] = \int_{-\varepsilon_0}^{\varepsilon_0} d\eta\, F(\eta)\,\mathrm{Re}\left[\frac{|E-\eta|}{[(E-\eta)^2-\Delta^2]^{1/2}}\right], \quad (6)$$

where

$$F(\alpha,x)=\begin{cases}[2/\pi(1+\alpha)](1-x^2)^{-1/2}K\left(\dfrac{2\sqrt{2}\alpha}{1+\alpha}(1-x)^{-1/2}\right), & \text{for } -1<x<-\alpha(2-\alpha), \quad (7a)\\ [2\sqrt{2}/\pi^2(1+\alpha)\sqrt{\alpha}](1+x)^{-1/2}K\left(\dfrac{1+\alpha}{2\sqrt{2}\alpha}(1-x)^{1/2}\right), & \text{for } -\alpha(2-\alpha)<x<1. \quad (7b)\end{cases}$$

Here $K(z)$ is the complete elliptic integral.

In the two-dimensional system (i.e., $\alpha=0$), Eq. (6) further simplifies as

$$N(E)/N_0=\begin{cases}\dfrac{1}{\pi}(\Delta\varepsilon_0)^{-1/2}\left[(|E|+\Delta+\varepsilon_0)\Pi\left(-\dfrac{|E|-\Delta+\varepsilon_0}{2\Delta},r\right)-\Delta K(r)\right], & \text{for } \Delta-\varepsilon_0<|E|<\Delta+\varepsilon_0, \quad (8a)\\ \dfrac{1}{\pi}[E^2-(\Delta-\varepsilon_0)^2]^{-1/2}\left[(|E+\Delta+\varepsilon_0)\Pi\left(-\dfrac{2\varepsilon_0}{|E|+\Delta-\varepsilon_0},r_1\right)-\Delta K(r_1)\right], & \text{for } |E|>\Delta+\varepsilon_0, \quad (8b)\end{cases}$$

where

$$r=\frac{1}{2}\left[\frac{E^2-(\Delta-\varepsilon_0)^2}{\Delta\varepsilon_0}\right]^{1/2},$$

$$r_1=r^{-1},$$

and $\Pi(n,z)$ is the complete elliptic integral of the third kind.

We numerically evaluate Eq. (6) for $\varepsilon_0/\Delta_{00}=0.92$ (Δ_{00} is the gap at $T=0$ K) and for several values of α ($0\le\alpha\le0.2$) and plot the results in Fig. 1. Unlike the two-dimensional limit ($\alpha=0$, as shown in Fig. 2), the density of states is not symmetric about $E=0$. In particular the density of states has a logarithmic singularity at $E=-(\Delta+\varepsilon_0)$ and cusps at $E=-[\Delta-\varepsilon_0\alpha(2-\alpha)]$, $-(\Delta-\varepsilon_0)$, $\Delta-\varepsilon_0\alpha(2-\alpha)$, and $\Delta+\varepsilon_0$, and a finite jump at $E=\Delta-\varepsilon_0$.

Comparing this with the tunneling density of states observed by Ekino and Akimitsu[9] in the CDW state of $NbSe_3$, we may conclude the following. (1) The observed density of states is quite consistent with the two-dimensional model ($\alpha=0$). For the three-dimensional model the parameter α has to be less than 0.2. (2) The effective energy gap associated with the peak in the density of states should be $\Delta+\varepsilon_0$, but not Δ as originally assumed. Indeed, as shown in Fig. 3, the observed temperature dependence of the energy gap of the CDW with $T_c=149$ K is described very well by $\Delta(T)+\varepsilon_0$, with $\Delta(T)$ obtained from Eq. (4), and $\Delta_{00}=157$ meV $=(1821\text{ K})k_B$ and $\varepsilon_0=0.92\Delta_{00}$ for the two-dimensional model ($\alpha=0$). We obtain a similar agreement for the energy gap of the CDW with $T_c=59$ K, where we have to take $\Delta_{00}=70$ meV. (3) Further, the above choice is consistent with the observed pressure dependence of the CDW transition temperature T_c.[16]

Within the same model we calculate the tunneling conductance between two CDW's,

$$\sigma_{\text{CDW-CDW}}=\partial J_{\text{CDW-CDW}}/\partial E, \quad (9)$$

where

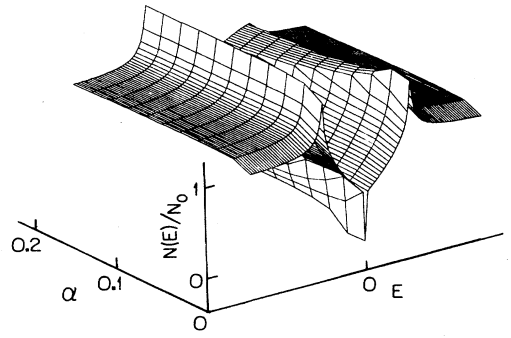

FIG. 1. Electron densities of states $N(E)$ of quasi-one-dimensional CDW are shown as functions of quasi-particle energy E and $\alpha=t_c/t_b$. In the two-dimensional limit ($\alpha=0$), $N(E)$ is symmetric [$N(-E)=N(E)$] at the origin, while an asymmetry develops for $\alpha\neq0$.

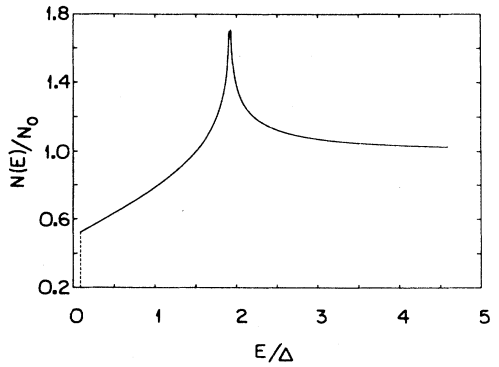

FIG. 2. Electron density of states $N(E)$ in the two-dimensional limit. We have shown only for $E>0$, since $N(-E)=N(E)$ in the present limit.

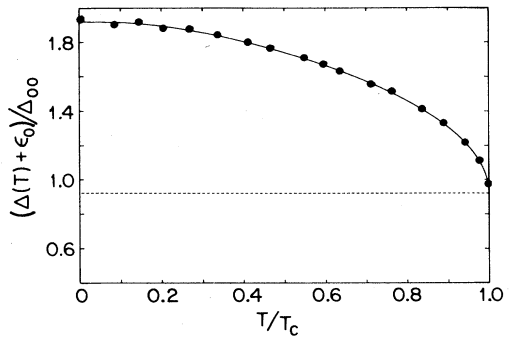

FIG. 3. We calculate the position of the logarithmic singularity (i.e., the effective energy gap $[\Delta(T)+\varepsilon_0]/\Delta_{00}$) in the density of states as a function of reduced temperature T/T_c, which is compared to the tunneling experiment by Ekino and Akimitsu (Ref. 9) (circles).

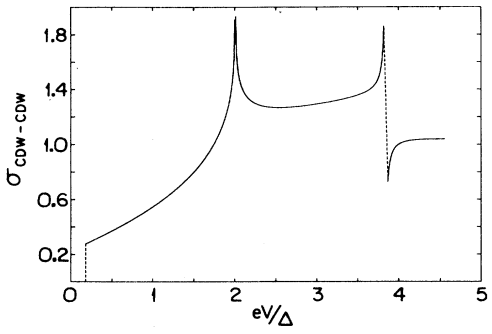

FIG. 4. The tunneling conductance between two CDW's in the two-dimensional limit is shown as a function of applied voltage V. Again the conductance is symmetric in V.

$$J_{\text{CDW-CDW}} = |T|^2 \int_{-\infty}^{\infty} dE' N(E') N(E-E') \left[\tanh\left(\frac{\beta}{2}E'\right) - \tanh\left(\frac{\beta}{2}(E'-E)\right) \right]. \tag{10}$$

$N(E)$ is the density of states defined in Eq. (6).

We show in Fig. 4 the tunneling conductance at $T=0$ K, since the temperature dependence is rather insignificant for $T \leq 0.1\Delta_{00}/k_B$. Unlike the experimental results,[9] which has a broader peak around $E=2(\Delta+\varepsilon_0)$, the numerical result exhibits a logarithmic singularity at $E=2\Delta$ and a jump with a weaker singularity at $E=2(\Delta+\varepsilon_0)$. However, the present result appears to be still more consistent than that expected from the BCS theory.

In summary, making use of the quasi-two-dimensional model of CDW's, we analyzed the electron tunneling data. The present model describes consistently both the observed feature of the tunneling electron density of states and the temperature dependence of the energy gap. Further, the present model is consistent with the observed pressure dependence of T_c. Finally, the discrepancy between the optical measurement and the tunneling experiment is easily resolved since the former experiment measures $2\Delta(T)$, while the latter is most sensitive to $\Delta(T)+\varepsilon_0$ as we have shown here.

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