

Comment on "Electron-Phonon Coupling and Superconductivity in Alkali-Intercalated C₆₀ Solid"

Recently, Schlüter *et al.* [1] proposed an intramolecular electron-phonon (IEP) mechanism for superconductivity in alkali-doped C₆₀. A similar analysis was proposed by Varma *et al.* [2]. We would like to point out some difficulties (1) with their analysis of the electron-phonon interaction as embodied in the traditional Coulomb pseudopotential parameter μ^* , and (2) with their analysis of the Raman scattering experiments [3].

Note that μ^* is given by $\mu^* = \mu/[1 + \mu \ln(\omega_c/\omega_{ph})]$, where $\mu = NV_c$; N is the density of states, V_c is the Coulomb matrix element, ω_c is a high-frequency cutoff of order the Fermi energy, and ω_{ph} is of order the Debye energy. This formula is valid as long as Migdal's theorem is applicable and as long as electron-electron vertex corrections can be ignored. The situation in doped C₆₀ is somewhat special. The Fermi energy resides in a narrow band of width not much greater than ω_{ph} , while there are a number of additional bands of moderate width separated by a few electron volts. Therefore, in addition to fundamental concerns regarding the importance of vertex corrections, the question arises as to what ω_c should be. In IEP theories ω_c is taken to be of the order of the overall bandwidth ~ 10 eV. We argue that ω_c should be the width of the narrow band, so $\mu \sim \mu^*$. Thus, we conclude, in agreement with Anderson [4], that IEP theories cannot account for the high transition temperatures observed in these materials.

Consider the following model in which the Fermi energy sits in a narrow band, but in addition there exists a wide band (the extension to several bands is straightforward) [2]. We define K to be the Coulomb matrix element which scatters an electron pair from one band to the other and V_c (narrow band), V'_c (wide band) to be the intraband Coulomb matrix elements. With these definitions, a self-consistent analysis within the ladder approximation yields the effective Coulomb interaction:

$$V_{\text{eff}} = \frac{V_c + (V_c V'_c - K^2)L_2}{1 + V_c L_1 + V'_c L_2 + (V_c V'_c - K^2)L_1 L_2}, \quad (1)$$

where $L_1 = N_1 \ln(\omega_1/\omega_{ph})$, and $L_2 = \frac{1}{2} N_2 \ln(\omega_3/\omega_2)$. Here $2\omega_1$ is the width of the narrow band and $\omega_3 - \omega_2$ is the width of the wide band; N_1 and N_2 are the respective densities of states. Thus, if $K^2 \ll V_c V'_c$, then $V_{\text{eff}} = V_c/(1 + V_c L_1)$. It is important to realize that in deriving this result we impose *no* restrictions on the logarithms.

To illustrate that K is typically quite small [5], consider a model of the screened Coulomb interaction which consists of an atomic-scale repulsion U between two electrons on the same C atom, and a repulsion on the scale of a molecule, V , between two electrons anywhere on the same molecule. The orthonormal Wannier functions cor-

responding to each band are essentially localized on a single molecule because the two bands are separated by a substantial gap. It is now simple to show that $V_c \approx V'_c \approx U/60 + V$ and $K \approx U/60$. Therefore, K is small as long as $V \gg U/60$, which is reasonable for the problem at hand ($U \approx 5-10$ eV, $V \approx 0.5-1$ eV) [6].

Consider now the Raman scattering experiments [3] in which all but one of the H_g intramolecular phonon modes are absent in both K₃C₆₀ and Rb₃C₆₀, while they are prominent in C₆₀, K₆C₆₀, and Rb₆C₆₀. According to Refs. [1,2], the absence of the Raman peaks is a result of the broadening of these H_g phonons due to the strong electron-phonon coupling. However, one-phonon Raman scattering probes phonons with wave vector $\mathbf{q} \approx 0$, as light has a wavelength much larger than the size of a single molecule. It is easy to see from Fermi's "golden rule" that a $\mathbf{q} = 0$ phonon of frequency ω_0 (> 0) cannot decay by particle-hole pair production, hence the absence of *one-phonon* Raman peaks cannot be due to the damping purportedly calculated by these authors. Umklapp scattering does not change this conclusion, provided that ω_0 is less than a critical energy of order the Fermi energy. Therefore, any broadening is due to disorder or some other effect present in the experimental samples.

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[1] M. Schlüter *et al.*, Phys. Rev. Lett. **68**, 526 (1992).

[2] C. Varma *et al.*, Science **254**, 989 (1991).

[3] S. Duclos *et al.*, Science **254**, 1625 (1991).

[4] P. W. Anderson (to be published).

[5] For estimates of similar *matrix elements*, see J. W. Garland, Phys. Rev. Lett. **11**, 111 (1963); **11**, 114 (1963).

[6] We have also calculated $K^2/V_c V'_c$ for the Coulomb interaction using the molecular orbitals calculated previously [S. Chakravarty and S. Kivelson, Europhys. Lett. **16**, 751 (1991)]. The largest ratio $K^2/V_c V'_c = 0.066$ is between the t_{1u} and t_{1g} states. All other ratios are an order of magnitude smaller.