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Electron-Phonon Interaction in Transition Metals

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We point out that an expression for the electron-phonon matrix element in transition metals recently derived by Barisic, Labbé, and Friedel from a "Hubbard-Hamiltonian" formulation, and of particular interest in understanding the superconducting properties of these materials, follows from the more basic "modified-tight-binding" approximation of Fröhlich and Mitra.

In a recent publication Barisic, Labbé, and Friedel[1] have indicated that the order of magnitude of the electron-phonon interaction required to explain the superconducting properties of transition metals can be obtained by considering the electron-phonon coupling between d-band states. Barisic *et al.* have used a Hubbard-Hamiltonian formulation in which the electron-phonon coupling arises from the dependence on interatomic distance of a "hopping" or overlap integral as encountered in tight-binding band theory. Here we wish to point out that their expression for the electron-phonon interaction is not limited to the Hubbard-Hamiltonian model, but rather follows from the assumption that the electron wave function rigidly follows the motion of the ions, an assumption in the spirit of the tight-binding approximation. In particular, their result for the electron-phonon matrix element can be rederived by considering instead the matrix elements of the electron-phonon operator between modified-tight-binding wave functions as introduced by Fröhlich[2] and used by Mitra.[3]

Fröhlich's assumption is that the tight-binding wave function corresponding to the ions in static-displaced positions a distance $\vec{X}_\mu$ from their equilibrium-lattice positions $\vec{R}_\mu$ can be written in a modified-tight-binding form

$$\psi(\vec{r}) = \sum_\mu e^{i\vec{k}\cdot\vec{R}_\mu}\,\phi(\vec{r}-\vec{R}_\mu-\vec{X}_\mu)\;, \tag{1}$$

where $\phi(\vec{r})$ is the localized orbital from which the tight-binding band arises. Using the Born-Oppenheimer formulation of the electron-phonon interaction leads to the electron-phonon matrix element [Eq. (2.18) of Ref. 3]

$$g^{\nu}_{kq} = M_1 + M_2\;, \tag{2}$$

where

$$M_2 = i\left(\frac{\hbar}{2MN\omega^0_{q\nu}}\right)^{1/2} \times \vec{\epsilon}^{\,\nu}_q\cdot\sum_{\vec{u}} \nabla J(\vec{u})\,[\sin\vec{k}\cdot\vec{u} - \sin(\vec{k}+\vec{q})\cdot\vec{u}\,] \tag{3}$$

in the notation of Ref. 1. Here M_1 involves degenerate three-center integrals, ignored by Barisic *et al.* (We note that these terms are not obviously negligible, since in the Garland-Bennemann[4] theory of the electron-phonon interaction they yield the principal contribution, although it should be noted that the latter have employed the Bloch rather than the Born-Oppenheimer viewpoint.)

Applying Eq. (3) to the case considered by Barisic *et al.*, in which the near-neighbor environment is orthorhombic, and using the expression of Ref. 1 for ∇J, we obtain

$$g^{\nu}_{kq} \cong M_2 = 2iq_0\left(\frac{\hbar}{2NM\omega^0_{q\nu}}\right)^{1/2} \times \sum_\alpha J(\vec{a}_\alpha)\,\frac{\vec{a}_\alpha\cdot\vec{\epsilon}^{\,\nu}_q}{a_\alpha}\,[\sin k_\alpha a_\alpha - \sin(\vec{k}+\vec{q})_\alpha a_\alpha\,]\;, \tag{4}$$

which is just the result of Barisic *et al.* [see Eq. (6) of Ref. 1].

In conclusion we note that this more basic foundation for the electron-phonon matrix element to some extent reinforces the validity of the Barisic *et al.* calculation, and also indicates clearly its extension to a more realistic, degenerate d-band case.

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