MAR17-2016-020070

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Electronic properties with and without electron-phonon coupling

PHILIP ALLEN[1], Stony Brook University

To decent approximation, electronic properties P of solids have a temperature dependence of the type $\Delta P(T) = \Sigma (dP/d\omega_i)[n_i(T)+1/2]$, where ω_i is the frequency of the i^{th} vibrational normal mode, and n_i is the Bose-Einstein equilibrium occupation of the mode. The coupling constant $(dP/d\omega_i)$ comes from electron-phonon interactions. At T=0, the "1/2" gives the zero-point electron-phonon renormalization of the property P, and at $T>\Theta_D$, the total shift ΔP becomes linear in T, extrapolating toward $\Delta P=0$ at T=0. This form of T-dependence arises from the adiabatic or Born-Oppenheimer approximation, where electrons essentially "don't notice" the time-dependence of thermal lattice fluctuations. In other words, the leading order theory for P is $\Delta P(T) = \Sigma (d^2P/du_i du_j)<u_i u_j>$, responding to the thermal average mean square lattice displacement, as if it were static. There are two situations where non-adiabatic effects alter things. (1) In metals at low T, the thermal smearing k_BT of the sharp Fermi edge gets small ($\omega_i << k_BT$). Then non-analyticity of k-integrals requires phonon energy to be included in perturbative denominators. (2) In insulators with polar phonons, Froehlich polaron effects enter, and k-integrals diverge unless phonon energies are kept. Most non-adiabatic effects become unimportant by room temperature, but the low T consequences can be very interesting (e.g. superconductivity.) This talk will discuss the confusing history and predict some future developments in this field.

[1]invited session: "Predictive Modeling of Electron-Phonon Coupling in Condensed-Matter Physics" My talk will be coordinated with that of Xavier Gonze. It would be best to schedule them back-to-back.