Electron-Phonon Interaction with Electron and Lattice Wannier Functions and Superconductivity in Boron-doped Diamond

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The electron-phonon interaction plays a crucial role in a variety of physical phenomena, ranging from conventional superconductivity to polaronic transport in organic materials. While experimental investigations of the manifestation of electron-phonon interaction in the excitation spectra of electrons and phonons have witnessed impressive advances in recent years, first-principles calculations of the electron-phonon coupling still remain computationally demanding for simple systems, and lie beyond the reach of current capabilities for most complex systems. In this talk I will present a first-principles methodology which we have recently developed for carrying out robust and effective calculations of the electron-phonon interaction with millions of k points in the Brillouin zone. This technique consists in evaluating the electron-phonon vertex in the electronic and lattice Wannier representation, and then using the result to obtain the vertex for arbitrary electron and phonon momenta in the Bloch representation. I will demonstrate this methodology by discussing the phonon self energy and the pairing mechanism in superconducting boron-doped diamond. We modeled boron-doped diamond by considering both a virtual crystal approximation and a large supercell containing boron, and by sampling the Brillouin zone with a million of k points. Our calculations indicate that the localized vibrational modes associated with the boron atoms are crucial to the superconducting pairing insofar they enable scattering processes with large momentum transfer. I will show that a dense Brillouin zone sampling is essential for a correct interpretation of the pairing mechanism in boron-doped diamond. This work was done in collaboration with J. R. Yates, I. Souza, M. L. Cohen, and S. G. Louie at the University of California, Berkeley.