Numerical Study of the Holstein Polaron

Bayo Lau, **Mona Berciu**, and **George Sawatzky**

Department of Physics and Astronomy
The University of British Columbia

The Holstein Hamiltonian models tight-binding electrons with local phonon excitations. Numerical calculations were performed to study the Hamiltonian in the single-electron-many-phonon Fock space. A numerical scheme due to Bonca, *et. al.* was employed to setup a matrix, from which low-energy eigenpairs were computed by Lanczos-type method. Calculation was performed for the 1D and 2D square lattice at different momentum and for different coupling strength. Numerically, the results of the ground state agree with previous calculations; however, the result of the first excited state differs from the result of quantum Monte-Carlo with analytical continuation in 1D. For the 2D case, the low-energy spectrum was computed, and the spatial symmetries of the wavefunctions were characterized.

This numerical scheme exploits translational symmetry of the Hamiltonian and the locality of the phonon excitations, but the size of the problem is still very big. The numerical result shows a continuum of eigenstates above $E_{GS} + \omega_{phonon}$; however, the majority of such states do not have the same symmetry as the pure-electron wavefunction, and thus do not have any spectral weight. The aforementioned numerical scheme is then confined into the S-symmetric basis in 2D. This reduces the matrix size and allows the computation of spectral weight for a broader energy range with better accuracy.

References

Bonca, *et. al.*, PRB, **60**, 1633 (1999)