Possibility of a Metallic Phase in the Half-Filled Hubbard-Holstein Model

For the last few decades, the competition between the phonon-mediated electron-electron attraction and the local Coulomb repulsion has been discussed in various contexts of condensed matter physics. Initially the problem was raised in relation to the quasi-one dimensional organic charge-transfer salts. In recent years, it has also become an important issue in studying the perovskite oxides such as cuprates and manganites.

Theoretically the Hubbard-Holstein (HH) model serves as a useful framework to investigate the competition. In addition to the kinetic-energy term represented by t the nearest-neighbor electron hopping integral, it consists of two interaction parts. One is the term describing the electron correlation effects through U the on-site Coulomb repulsion as in the Hubbard model. The other is the term to couple an electron with local phonons as in the Holstein model, leading to $\alpha\omega_0$ the polaron stabilization energy with α the non-dimensional electron-phonon coupling constant and ω_0 the optic phonon energy.

For this model, there have already been many previous works using various methods. These studies have revealed that the HH model can afford interesting phase diagrams due to the competition among charge-density wave (CDW), spin-density wave (SDW), and superconductivity as we change the parameters involved in the system, *i.e.*, U, α, t, ω_0, and n the electron filling. Roughly speaking, the CDW (SDW) nature manifests itself in the ground state at half filling (n=1), if the effective electron-electron interaction $U_{\rm eff}$ (~ U-2$\alpha\omega_0$) is negative (positive).

However, the detail of the CDW-SDW transition is not known well. In fact, the appearance of a superconducting phase is suggested [1] in the exact-diagonalization study on the two-site HH model. Thus we carefully consider the transition region at half-filling by approaching the HH model from the antiadiabatic region (t<<ω_0) where the variable displacement Lang Firsov canonical transformation is useful. In order to avoid any error that might enter through the approximations involved in dealing with the Coulomb correlation term, we have investigated the one-dimensional system so that the exact solution of Lieb and Wu can be taken advantage of. By determining the displacement variationally, we have obtained fairly accurate results for the properties of the ground state. [2]

In Fig. 1, we show the obtained phase diagram in the (α,U) plane at t=0.2ω_0. The metallic phase characterized by the local spin moment L_0 ~ 3/8 and a small effective mass of polarons appears along the line of U = 2$\alpha\omega_0$, namely, in the CDW-SDW crossover region. This phase seems to continuously convert into the superconducting phase in the attractive Hubbard model (or the system with α=0 and U<0).

We do not believe that this behavior is specific to one dimension (1D); a similar metallic behavior will be seen in higher dimensions as well, as long as $|U_{\rm eff}|$ is less than the polaron bandwidth in the crossover region. We may even conjecture that such a metallic phase will be realized more easily in higher dimensions in which we can avoid unusual phenomena specific to 1D like the Mott transition at U=0 irrespective of t in the 1D Hubbard model.

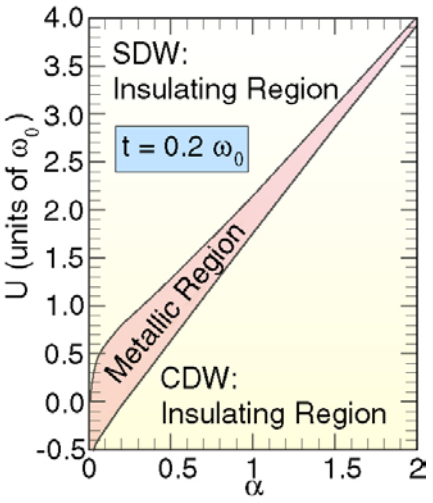

Fig. 1. Phase diagram in the (α,U) plane for the half-filled Hubbard-Holstein model.

It is not known for sure whether this kind of a metallic phase has already been observed in actual materials or not, but it has been pointed out [3,4] that physical properties including superconductivity in the alkali-doped fullerenes A_3C_{60} can be reproduced in a unified way in terms of this picture. For example, the superconducting transition temperature T_c in the HH model with suitably chosen parameters is obtained as a function of the lattice constant a_0 as shown in Fig. 2.

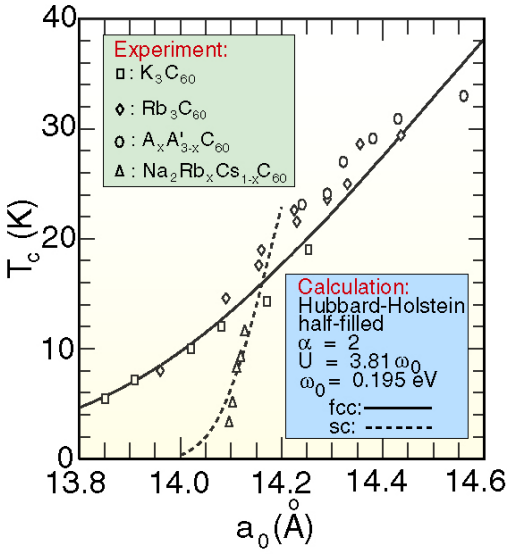

Fig. 2. T_c as a function of the lattice constant a_0 in A_3C_{60} and its dependence on the crystal structure in comparison with experimental results.

References

[1]Y. Takada, *J. Phys. Soc. Jpn.* **65**, 1544 (1996).
[2]Y. Takada and A. Chatterjee, *Phys. Rev. B* **67**, 081102(R) (2003).
[3]Y. Takada, *J. Phys. Soc. Jpn.* **65**, 3134 (1996).
[4]Y. Takada and T. Hotta, *Int. J. of Mod. Phys. B* **12**, 3042 (1998).

Authors

Y. Takada and A. Chatterjee[a]
[a]University of Hyderabad.