Visualization of quantum electronic and lattice fluctuations by using the resonating Hartree-Fock method

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Abstract. Large quantum fluctuations in the strongly correlated electron systems as well as electron-phonon coupled systems are visualized by the resonating Hartree-Fock (HF) method. We show that in the two-dimensional Hubbard model, doped holes form topological defects called polarons. It is also shown that the quantum fluctuations drastically change the lattice structures in the Su-Schrieffer-Heeger model.

1. Introduction

Visualization of large quantum fluctuations has been a challenging issue in not only condensed matter physics but also nuclear physics. Recent progress in computer science has made it possible to describe the many-body effects efficiently. Density matrix renormalization group (DMRG)[1], quantum[2] and variational[3] Monte Carlo simulations are well established numerical methods. Furthermore, we have even the exact solution, such as Lieb-Wu solution for the one-dimensional Hubbard model. In spite of such progress or even the exact solutions, we cannot usually see physics behind the many-body effects intuitively.

In this paper, we introduce an alternative numerical approach, called a resonating Hartree-Fock (HF) method, in which a many-fermion wave function is constructed by superposition of non-orthogonal Slater determinants (S-dets). The orbitals in all the S-dets, as well as the superposition coefficients, are simultaneously optimized. As we mention details in the following sections, the resonating HF method describes the many-body effects efficiently. In addition, this method can make it possible to reveal physics behind the complicated many-body effects by analyzing the structures of the S-dets generating the resonating HF wave function. We apply the method to the two-dimensional (2D) Hubbard model on a square lattice. More recently, we have developed to describe the quantum lattice fluctuations by superposition of coherent states of phonons. By using this approach, we investigate the quantum lattice fluctuations in Su-Schrieffer-Heeger (SSH) model. The paper is organized as follows, In §2, we introduce the resonating HF method and coherent state representation of phonons. Results and discussions are given in §3. Brief summary is given in §4.
2. Method and model

Generally speaking, a many-fermion wave function is exactly constructed by superposition of S-dets. In spite of recent progress in computer ability, however, it is impossible to obtain the exact wave functions for more than 30 interacting fermions. When we approximate the exact wave function by a single S-det, it is called a HF approximation. To include the large correlations, the resonating HF method has been developed, where the wave function is constructed by superposition of non-orthogonal S-dets.[4, 5] Non-orthogonality is important because one S-det includes the complete excitation effects from other S-dets automatically. As a result, large correlation effects can be included quite efficiently. A wave function is explicitly given by

\[ |\Psi> = \sum_{n=1}^{N_S} \sum_G C_n^{G} |\psi_n> |G>, \]

where \( N_S \) denotes the number of S-dets generating the resonating HF wave function. The molecular orbitals of all the constituting S-dets \( |\psi_n> \), as well as the superposition coefficients \( C_n \), are variationally determined. To incorporate the correlation effects from symmetry broken states, the DODS (different orbitals for different spins)-type S-dets are employed in the resonating HF method. Therefore, we adopt symmetry projections for each constituting S-det to recover the original symmetry of the system, which are symbolically denoted by \( P^G \) in eq. (1).

We should note that one of the most important features of the resonating HF method is that we can visualize quantum fluctuations by analyzing the structures of S-dets. In the next section, the method is applied to the 2D Hubbard model, whose Hamiltonian is given by

\[ H = - \sum_{<i,j>\sigma} t(i,j)(a_{i,\sigma}^\dagger a_{j,\sigma} + a_{j,\sigma}^\dagger a_{i,\sigma}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}, \]

where \( t(i, j) = t \) for the electron hopping to the nearest-neighbor sites, while \( t(i, j) = t' \) for the hopping to the next nearest-neighbor sites. \( U \) and \( N \) represent an on-site Coulomb repulsion and a system size, respectively.

Recently, we have extended the method to include the quantum lattice fluctuation effects. A coherent state representation of phonons is used for this purpose, which is given by

\[ |z> = e^{-\frac{1}{2}z^2} e^{z b^\dagger} |0>, \]

where \( b^\dagger = (b_1^\dagger, b_2^\dagger, ...) \) represents the set of creation operators of phonons. \( z = (z_1, z_2, ...) \) are determined by the lattice structure, such as

\[ z_k = \sqrt{\frac{m\omega_k}{2N\hbar}} \sum_{n=0}^{N-1} <z|q_n|z> \exp\{-\frac{2\pi ink}{N}\}, \]

where \( q_n \) denotes the lattice displacement from the equilibrium position. Thus, the extended form of the resonating HF wave function is written by

\[ |\Psi> = \sum_{n=1}^{N_S} \sum_G C_n^{G} |\psi_n> |z_n>. \]

Ideally, we should optimize these \( z_n \)'s of the coherent states, and in fact, we can carry out the optimization when we employ a single coherent state. However, at the present stage, it is complicated to optimize plural coherent states. Therefore, in the following calculations, we put the coherent states by hand. We choose the coherent states from the optimized result for a single
coherent state. On the other hand, the S-dets are optimized by the resonating HF procedures. In the next section, we apply the method to the Su-Schrieffer-Heeger (SSH) model for the 1D electron-phonon coupled system. SSH Hamiltonian is given as

\[
H = -t \sum_{l} \left\{ 1 + \alpha (q_{l+1} - q_{l}) \right\} \left( \hat{a}_{l+1}^{\dagger} \hat{a}_{l+1} + \hat{a}_{l}^{\dagger} \hat{a}_{l} \right) + \sum_{l} \left\{ \frac{1}{2m} p_{l}^2 + \frac{k}{2} (q_{l+1} - q_{l})^2 \right\}.
\]

In this model, the lattice displacement affects the electron transfer of the first term. We will investigate the quantum lattice fluctuation effects on this model beyond the adiabatic and classical approximation.

3. Results and Discussion

One of the most interesting problems in the copper-oxides is what carriers are. To answer the question, we calculate the resonating HF wave function for the 2D doped Hubbard model with the parameters of \(U/t = 8\) and \(t'/t = -0.32\). Figure 1 shows the structures of a typical Slater determinants generating the resonating HF wave function for \(N = 16 \times 16\) and \(N_e = 208\). We can see many dips, where the anti-ferromagnetic ordering is suppressed and the charge density wave ordering is raised. These are kinds of topological defects and called polarons. As also seen in Fig.1, polarons have net charges and spins. Other S-dets, which are not shown here to save space, also have many polarons with different relative configurations. Our results indicate that the doped holes become polarons in the 2D Hubbard model.[6] Another interesting question is whether an attractive interaction works between polarons. Figure 2 shows the HF and projected HF energies of the states having two polarons. We change distance between polarons, which is shown as a horizontal axis. For the projected HF state, symmetry projections are adopted to the HF S-dets and no further orbital optimizations are carried out. From Fig.2, we can see that the attractive interaction works between polarons, when we partially incorporate the electron correlation effects by adopting the symmetry projections. Thus, the electron correlation effects cause the attractive interaction between polarons. Our results strongly suggest that doped holes become polarons and they can be carriers of superconductors.

![Figure 1. Structures of a typical S-det for \(N = 256\) and \(N_e = 208\).](image-url)
Next, we investigate the lattice fluctuation effects in the SSH model. We show in Fig.3 $x$-dependence of the lowest state energies. The system size is $N = 98$. Black circles represent the energy of the state with single coherent state of phonons having the uniform dimerization. On the other hand, a red circle represents the energy of the lowest state with 5 coherent states of phonons. We do not have enough space to show the lattice structures, but soliton-like defects, which convert the dimerization pattern from long-short-long-short to short-long-short-long or vice versa, do not stabilize the ground state. This indicates that the dimerization is very strong in the half-filled ground state. In the case of doped system with $N_e = 90$ electrons (or 8 holes), a single coherent state of phonons indicates the equidistant lattice, as shown by black circles in Fig.3(b). On the other hand, when we increase the number of coherent states, the dimerized lattice becomes still the lowest state. But, its dimerization amplitude is very small, as shown by a red circle in Fig.3(b).

![Figure 2](image1.png)

**Figure 2.** Energy of UHF and pHF states with a single pair of polarons.

![Figure 3](image2.png)

**Figure 3.** Dimerization amplitude($q$)-energy relation for the half-filled (a) and 8% doped (b) systems.

When the number of electrons is reduced to $N_e = 86$, the ground state has the equidistant lattice, even if we increase the number of coherent states. In the classical approximation, the soliton lattice is always the lowest state in any doping regimes. Therefore, the present results show that quantum fluctuations destabilizes the soliton lattice state.

### 4. Summary

We have visualized the quantum fluctuations in the 2D doped Hubbard model and SSH model by using the resonating HF method. Quantum lattice fluctuation effects have been described by superposition of coherent states of phonons. We have shown that doped holes form polarons in the 2D Hubbard model. It has been suggested that an attractive interaction works between two polarons when the electron correlation is partially incorporated within the framework of the projected HF approximation. These results have strongly suggested that polarons could be carriers of high-temperature superconductors.

Then, it has been shown that the dimerization is very strong in the SSH model at a half-filling. On the other hand, quantum fluctuations due to lattice solitons stabilize the ground state energies in the lightly doped systems, though the dimerization decreases with the increase of doping. Finally, the ground state has an equi-distant lattice beyond 12% doping.

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### References

[1] S. R. White, Phys. Rev. Lett. 69, 2863(1992).
[2] *Quantum Monte Carlo Method in Condensed Matter Physics*, edited by M. Suzuki(World Scientific, Singapore, 1993).
[3] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. 56, 3582(1987).
[4] H. Fukutome, Prog. Theor. Phys. 80, 417(1988).
[5] N. Tomita, Phys. Rev. B69, 045110(2004).
[6] N. Tomita and S. Watanabe, Phys. Rev. Lett. 103, 116401(2009).