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Electronic structure of BaBiO₃: QMC CT-INT algorithm

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Abstract. The continuous time quantum Monte Carlo algorithm with interaction expansion is implemented for Hubbard-Holstein model. Algorithm is approbated on the Bethe lattice with exact diagonalization technique and then is applied to calculate the self-energy of the BaBiO₃ compound.

1. Introduction

Perovskite compounds based on bismuth are a special case of high-temperature superconductive (HTSC) materials. Noteworthy, that superconductivity in these compounds doped with lead (BPBO) with transition temperature $T_c = 13K$ was discovered in 1975 [1], earlier than in cuprates. Later, in 1988, superconductivity has been revealed with potassium doping at $T_c = 34K$ [2]. Until now, the mechanism of superconductivity in these materials is still not known [3]. There are plenty of unique properties of bismuth-based HTSC which still have not accurate explanations [4].

Because of the lack of free electron carriers, there is a suggestion that bipolaron conductivity could be an adequate explanation of superconductivity mechanism, and the local electronic structure of bismuth-based compounds doped with potassium (BKBO) could can be interpreted in terms of existence of spatial-distributed fermi-bose liquid [5]. This concept relies on the assumption of presence of a new quantum state in such compounds, pair density wave (PDW). This situation has an analogy with cuprate HTSC, where the presence of two electron components on the Fermi level was predicted theoretically [6] and then proved experimentally [7]. PDW phase is formed due to a double-well potential, which emerges because of local structure distortions. Parameters of this potential were obtained experimentally [8] for various compounds of BKBO and BPBO types. Recently, the validity of the theory of [5] was confirmed by DFT calculations [9].

Electron-phonon coupling plays a crucial role in these materials. The Holstein model is the simplest microscopic model which includes such interaction. The model can describe a complex phase diagram covering charge-density wave (CDW) and superconductivity (SC) phases. Coulomb repulsion between electrons is not included in the Holstein model; to account for the direct interaction between electrons, the Hubbard-Holstein model should be used instead of the Holstein model.



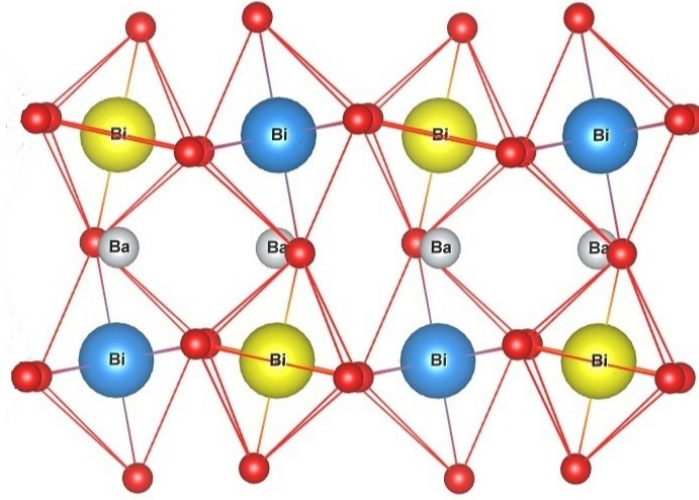


Figure 1. Structure of BaBiO₃ in the ground state has simple cubic lattice with two different types of octahedra BiO₆ that tilted to each other by 11 degrees.

The aim of this work is to develop the QMC CT-INT algorithm for effective solving Hubbard-Holstein model, testing this algorithm on the Bethe lattice and compute electron properties of BaBiO₃ by means of computing Green function and self-energy $\Sigma(i\omega_n)$.

2. Method

2.1. Hubbard-Holstein model

In this work we use Hubbard-Holstein model:

$$H = \sum_{i,j,\sigma} t_{i,j} c_{i,\sigma}^+ c_{j,\sigma} + U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) + g \sum_i (b_i^+ + b_i)(n_i - 1) + \omega_0 \sum_i b_i^+ b_i + \mu \sum_i n_i, \quad (1)$$

where $c_{i,\sigma}^+$ ($c_{i,\sigma}$) is creation (annihilation) operator for the electron with spin σ at a lattice site i ; $n_i = n_{i,\uparrow} + n_{i,\downarrow}$ is particle number operator; b_i^+ (b_i) is the boson operator of creation (annihilation); $t_{i,j}$ is the amplitude of electron hopping between lattice sites i and j ; g is the constant of electron-phonon coupling; U corresponds to Coulomb repulsion between electrons on one site; ω_0 is the phonon frequency.

One of the most effective methods of studying tight-binding models such as Hubbard-Holstein is the Dynamical Mean-Field Theory (DMFT). The method is based on independence of the self-energy Σ of electrons in the limit of infinite dimensions ($d \rightarrow \infty$) on the momentum \mathbf{k} . Then the single-site Green's function of the system takes the form:

$$G = \sum_{\mathbf{k}} (i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma(i\omega_n))^{-1}, \quad (2)$$

where $i\omega_n$ are Matsubara frequencies, μ is the chemical potential, and $\epsilon_{\mathbf{k}}$ is the kinetic energy of electrons. Due to this fact, it is possible to reduce the many-body problem on the lattice to an effective single-impurity model, for which there are various ways of numerical solution. One of such methods is the quantum Monte Carlo algorithm (QMC).

2.2. QMC CT-INT

There are various realizations of QMC depending on the system under study [11], e.g., auxiliary field method (CT-AUX), hybridization expansion (CT-HYB) or interaction expansion (CT-INT). For Hubbard-Holstein model, the latter is the most stable among the others, because it can take account of the interaction of more general type than CT-AUX and has better scaling of the system than CT-HYB. Another advantage of CT-INT algorithm is a simplicity of including the phonon degrees of freedom: phonons can be represented as the effective retarded interaction between electrons. In that case, the partition function become

$$Z = \int D(c^+, c) \exp \{-S_{kin} [c^+, c] - S_U [c^+, c]\} \times \\ \times \int D(b^+, b) \exp \{-S_{eph} [c^+, c, b^+, b]\}. \quad (3)$$

According to [12], the action is divided into three parts: S_{kin} corresponds to the kinetic energy of free electrons, S_U reflects the Hubbard interaction, and S_{eph} responds to electron-phonon coupling,

$$S_{kin} = - \sum_{\sigma} \int_0^{\beta} d\tau d\tau' c_{\sigma}^{\dagger}(\tau) G_{\sigma}^0(\tau - \tau')^{-1} c_{\sigma}(\tau'); \quad (4)$$

$$S_U = \frac{U}{2} \int_0^{\beta} d\tau \sum_{i,s} \prod_{\sigma} [n_{i,\sigma}(\tau) - \alpha_{\sigma}(s)]; \quad (5)$$

$$S_{eph} = - \frac{g^2}{4k} \int_0^{\beta} d\tau d\tau' \sum_{i,\sigma\sigma'} \sum_{s=\pm 1} P(\tau - \tau') [n_{i\sigma}(\tau) - \alpha_{+}(s)] \times \\ \times [n_{i\sigma'}(\tau') - \alpha_{+}(s)]. \quad (6)$$

Here, $P(\tau)$ is the phonon propagator:

$$P(\tau) = \frac{\omega_0}{2(1 - e^{-\beta\omega_0})} \left(e^{-|\tau|\omega_0} + e^{-(\beta-|\tau|)\omega_0} \right). \quad (7)$$

In CT-INT, calculation of integrals (5), (6) is carried out by sampling vertex configurations

$$V(\tau) = \{i, \tau, \sigma, \tau', \sigma', s, b\}, \quad (8)$$

where V describes interaction between two electrons with spins σ, σ' at times τ, τ' on site i , and b is equal to 0 or 1, which corresponds to the Hubbard or Holstein case, respectively. To avoid the sign problem, we choose $\alpha_{+}(s) = 1/2 + s\delta$ with $\delta = 0.51$, where s is spin variable of auxiliary Ising field.

As showed in [13], the partition function can be expressed in the following way:

$$\frac{Z}{Z_0} = \sum_{C_n} W(C_n) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^{\beta} d\tau_1 \sum_{V_1(\tau_1)} w[V_1(\tau_1)] \dots \\ \dots \int_0^{\beta} d\tau_n \sum_{V_n(\tau_n)} w[V_n(\tau_n)] \left\langle T \hat{H}[V_1(\tau_1)] \dots \hat{H}[V_n(\tau_n)] \right\rangle_0. \quad (9)$$

To satisfy the condition of ergodicity, only two updates are needed: addition and removing of vertices. The full probability of the system to move to a new configuration is

$$P_{C \rightarrow C'} = \min \left(\frac{T_{C' \rightarrow C}^0 W(C')}{T_{C \rightarrow C'}^0 W(C)}, 1 \right), \quad (10)$$

where the transition probability coefficients are the following:

$$T_{C_n \rightarrow C_{n+1}}^0 = \frac{P_U}{2(n+1)L\beta} + \left(\frac{1}{2}\right)^3 \frac{(1-P_U)P(\Delta\tau)}{(n+1)L\beta}, \quad (11)$$

$$T_{C_n \rightarrow C_{n-1}}^0 = \frac{1}{n}. \quad (12)$$

The first part in (11) expresses the coefficient for addition of Hubbard vertex with probability P_U , and the second term corresponds to the coefficient of Holstein type vertex, which is chosen with $1 - P_U$ probability.

3. Results

The algorithm was tested on Bethe lattice in the limit of an infinite number of neighbors $z \rightarrow \infty$ with a semi-elliptic density of electronic states $\rho = \sqrt{4t^2 - \epsilon^2}/\pi t^2$ $|\epsilon| \leq 2t$ in the DMFT approximation. Due to the fact that the DMFT equations in this case are greatly simplified, there are a number of analytical and numerical data related to the solution of this problem.

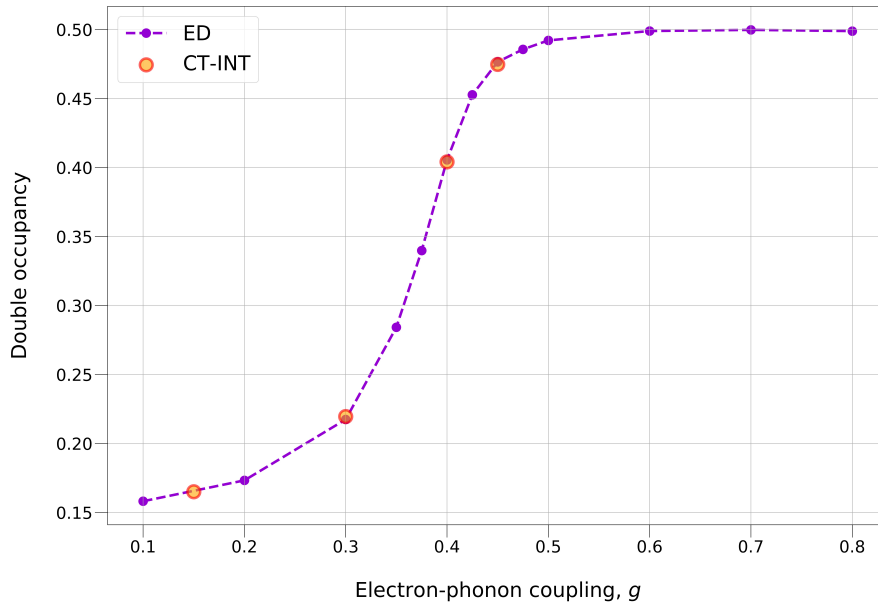


Figure 2. Double occupancy $D = \langle n_{\uparrow} n_{\downarrow} \rangle$ obtained by exact diagonalization (dashed line) and by CT-INT (big circles).

After testing, QMC CT-INT was applied to the Hubbard-Holstein model within the dynamical mean-field on the Bethe lattice with the $U/t = 2$, $\omega_0/t = 0.4$, $\mu = 0$ and $\beta t = 5$. The choice $\mu = 0$ corresponds to the half-filling. The double occupancy $D = \langle n_{\uparrow} n_{\downarrow} \rangle$ as a function of the electron-phonon coupling g was calculated and is shown in figure 2 in comparison with the data obtained by exact diagonalization method (ED) method. The obtained results show an

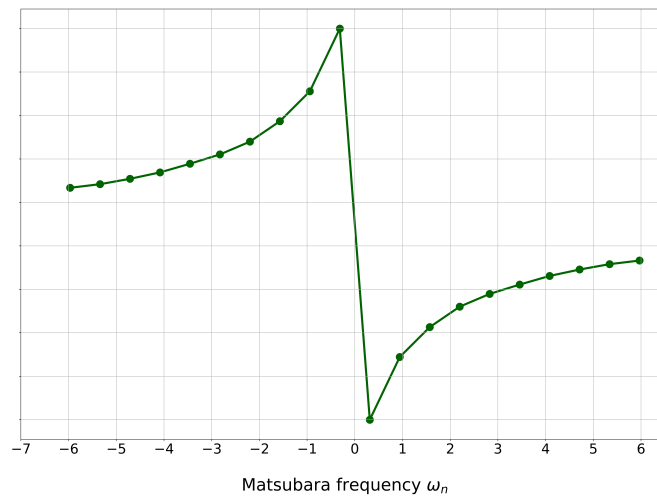


Figure 3. Imaginary part of the self-energy $\Sigma(i\omega_n)$ for the ground state of BaBiO_3 has a divergence at small Matsubara frequencies that corresponds to insulator phase.

excellent agreement; for both methods the critical electron-phonon coupling for the transition to the bipolaronic insulator is $g_c \approx 0.4t$. As stated above, the chemical potential $\mu = 0$ corresponds to half-filling which means that the the average particle number $\rho = 1$, but it oscillates strongly between an empty or double occupied states. When the values of the electron-phonon interaction are greater than $g_c \approx 0.4t$ it becomes increasingly hard to guarantee a symmetric histogram of ρ corresponding to the particle-hole symmetry of the model, and the simulation freezes in the doubly occupied or empty state.

The initial state of BaBiO_3 is an insulator with a transport gap $\approx 0.25eV$ [5]. The presence of a gap can be detected using the self-energy $\Sigma(i\omega_n)$ or Green's function of the system $G(i\omega_n)$ in Matsubara frequencies.

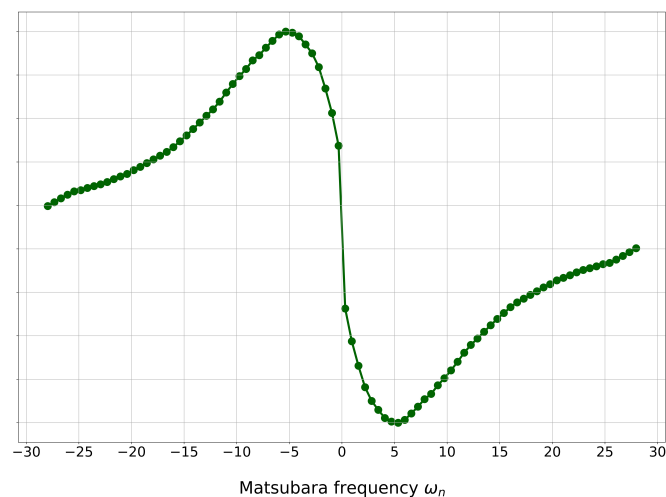


Figure 4. Imaginary part of the Green function for the ground state of BaBiO_3 has a continuous dependence with an extremum near small Matsubara frequencies, which indicates insulator phase.

In [10], the parameters of the tight-binding model (1) were obtained by fitting the results of

ab-initio calculations:

$$t_1 = -0.45, t_2 = -0.09, t_4 = 0.10,$$

$$\mu = 0.13, g = 0.4321, \beta = 10.0, \omega_0 = 0.07,$$

where the amplitudes t_{ij} are hopping parameters: $t_{ij} = (t_1, t_2, t_4)$ for sites at distances a , $a\sqrt{2}$ and $2a$ respectively, where a is the lattice parameters (all units are in eV). The self-energy $\Sigma(i\omega_n)$ and Green's function $G(i\omega_n)$ were calculated with the use of CT-INT. The self-energy shows a divergence (figure 3), and the Green's function has an extremum at small $i\omega_n$ (figure 4) which characterizes the presence of an insulator phase in the system. This result can also be concluded based on the dependence of the green function on imaginary time (figure 5). In particular, the value of the Green function at the point $\beta/2$ corresponding to $G(\beta/2) \approx -0.0028$ makes it possible to conclude that there is an insulator phase.

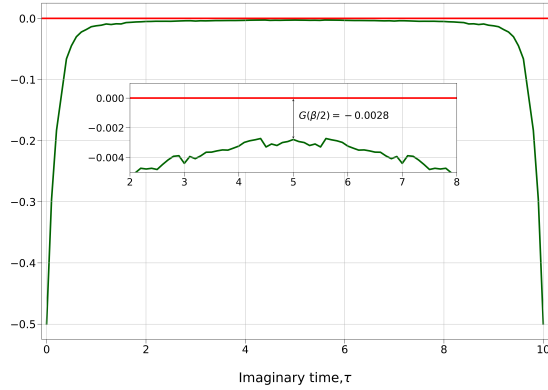


Figure 5. Dependence of the Green function on imaginary time, which indicates insulator phase.

4. Conclusions

In this work, we developed the QMC CT-INT algorithm that was successfully tested on the Bethe lattice. For BaBiO₃ ground state we obtained the insulator phase by computing the self-energy $\Sigma(i\omega_n)$ and Green's function $G(i\omega_n)$. In the future, the algorithm will be applied to obtain the phase diagram of BaBi_{1-x}K_xO₃ compound.

Acknowledgments

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