Quantum Monte-Carlo simulation of polaron tunneling

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Polaron tunneling is a prominent example of a task with the different energy scales, for which using the standard quantum Monte-Carlo methods faces a slow-down problem. We construct a path-integral quantum Monte-Carlo method which is free from this issue and apply it to study an impurity interacting with a one-dimensional Bose-Einstein condensate and simultaneously trapped in an external double-well potential. Our scheme works for an arbitrary coupling between the particle and condensate and, at the same time, allows for an account of tunneling effects. We observe two distinct quasi-particle peaks associated, respectively, with the phonon-assisted tunneling and the self-trapping of the impurity, which are in a crossover regime for the system modelled. While increasing the coupling strength in the Frohlich-Bogoliubov model, we observe changes in the peak’s weights and their spectral positions (or, equally, effective masses of the quasi-particles). Possible experimental realizations with cold atoms are discussed.

I. INTRODUCTION

A single mobile impurity, interacting with a reservoir, is one of the fundamental problems in condensed matter physics. Originally, this so-called polaron model was introduced to describe the coupling between electrons and lattice phonons in a dielectric crystal. Today polaronic effects have been extensively studied for impurities in the Bose-Einstein condensates (BECs) where tunable interaction between impurities and host atoms via Feshbach resonance goes beyond the parameter range relevant for solid. However, theoretical techniques based on perturbation theory and variational approaches predict different phenomena in the strongly interacting regime even for one-dimensional polarons. Nevertheless, this model became a sound benchmark for various many-body techniques, with an unprecedented opportunity for their experimental testing. Research of this kind of problems is crucial for the understanding of physical processes not only in BECs, but also in neutral atoms in optical traps and quantum dots which is important in a quantum computational context.

Generally, the incoherent tunneling effect with a nonlinear coupling is hard to study with analytical and numerical approaches. Tunneling particle interacting with a bath has at least two different energy scales – a barrier height (related to tunneling energy splitting) and interaction strength. The path-integral quantum Monte-Carlo (QMC) methods could be applied because they usually are used to study the complex quantum impurity model. However, the straightforward application of the QMC algorithm for the simulation of tunneling is limited by the exponential growth of the computation time. This slow-down problem is related to a complex energy landscape for Feynman trajectories in the path-integral.

In this manuscript, we propose a special modification of the QMC method for quantum tunneling and apply it to the polaron problem. We investigate tunneling of a single impurity immersed in a one-dimensional BEC and trapped in a double-well potential. Our method is based on a separation of path-integral computation into two independent parts – the first one corresponds to the particle tunneling in a double-well, which can be efficiently estimated, and the second one is a retarded interaction with a bath. We consider a particle in a double-well potential numerically exact, and BEC-excitation are determined by integrating out the bosonic modes. The method relies on the assumption that the typical energy of a BEC-impurities interaction is comparable with the tunnel splitting but much smaller than the barrier height. By analytical continuation of the computed impurity’s correlation functions, we calculate the density of states for different interaction strength at the low-temperature limit. Using the proposed QMC method, we demonstrate the resonance many-body effects in the BEC-impurity system, such as the phonon-assisted tunneling for weak coupling regimes and self-trapping in a strong interaction case. These phenomena can be observed in the existing experimental setups with the addition of two close harmonic optical dipole traps for impurity atoms.

The paper is organized as follows. In Sec. II we discuss a general formalism, model, and the proposed method. Section III contains details of the QMC scheme for BEC-polaron tunneling in the case of the two-mode bath, comparison with the exact diagonalization and results for a model with the continuous spectrum of the bath. We provide conclusions in Sec. IV.

II. MODEL AND METHOD

A. Frohlich-Bogoliubov model

We use the Frohlich Hamiltonian, which describes the impurity in a Bose-Einstein condensate in the Bogoliubov
Here $\hat{p}$ and $\hat{x}$ are momentum and position operators of the impurity atom with mass $m_I$, $\hat{b}_k^\dagger$ is the creation operator of the Bogoliubov excitation with momentum $k$ and frequency $\omega_k$, $V_k$ is interaction strength of phonon modes with the impurity atom, $c$ and $\xi$ is the speed of sound in BEC and its healing length respectively, $a_{IB}$ is the boson-impurity scattering length, $n_0$ is the BEC-density, and $M^{-1} = m_B^{-1} + m_I^{-1}$, where $m_B$ is the mass of a host atom.

To study equilibrium properties of the polaron tunneling we consider an impurity in the double-well potential:

$$\hat{H} = \hat{H}_{FB} + \kappa \left( -\frac{\hat{x}^2}{2} + \frac{\hat{x}^4}{4} \right)$$

where we set $\hbar, e, d$ to unity ($e = c/\xi$ is energy in polaronic units, $2d$ is a distance between $\xi$ of the double-well potential).

B. Quantum Monte-Carlo method

The Feynman path-integral defines the transition amplitude as the sum of all possible paths between the given initial and final configurations of a quantum system. The standard path-integral QMC utilizes this idea in a sampling of a large number of discrete trajectories in imaginary time. On every step of the algorithm, the current trajectory is changed according to the Metropolis condition. The more steps of the method are applied, the better result converges to the numerically exact one. However, QMC simulation of the tunneling problem requires a lot of computational time to sample valuable trajectories. This issue becomes even more demanding for tunneling problems with interaction since the application of the standard QMC scheme leads to the exponential growth of computational time. The root of the QMC failure is that the tunneling time is much larger than the time scale of interaction, for example, for BEC this gives $M/a_{IB}\sqrt{n_0} \ll \Delta E^{-1}$ ($\Delta E$ is tunneling energy splitting) and as the consequence, a simulation requires a very fine grid for trajectories.

To overcome this problem, we proposed the following modification of the quantum Monte-Carlo method. Our method separates path-integral computation into two parts. The impurity tunneling in a double-well contribution is accounted through a numerically exact calculation of its propagator. BEC-excitations are integrated out at the low-temperature limit, which results in the following retarded action

$$Z = \int \mathcal{D}[\hat{b}] e^{-S[\hat{b}]} = \int \mathcal{D}[x] e^{-S_I[x]} e^{-S_R[x]}$$

where $S_I[x]$ is the action of the impurity in a double-well potential, $S_B[x]$ is the action related to the impurity in the BEC, $S_R[x]$ is the retarded polaronic action:

$$S_R = -2 \sum_{k \neq 0} V_k^2 \sum_{\tau,\tau'} e^{-\delta\tau k(x(\tau) - x(\tau'))} \times e^{-\omega_k((\tau-\tau') + \beta(\tau - \tau'))} \frac{1}{1-e^{-\omega_k\beta}} \delta\tau\delta\tau'$$

where $\Theta(\tau)$ is the Heaviside step function, $\beta$ is inverse temperature, $\delta\tau$ is a time-slice.

Now we discuss the algorithm of our QMC procedure in more detail:

1) an explicit calculation of the propagator – probability amplitude for non-interacting impurity, which moves from $x$ to $x'$ during time interval $\delta\tau$ – for tunneling particle without considering the condensate influence. We exactly diagonalize Hamiltonian for the impurity in the

![FIG. 1. Correlation functions and spectral densities of states (a) $\rho(\omega)$ and (b) $\langle x(\tau) \rangle$ for different values of scattering length: $a_{IB} = 0.0$, $a_{IB} = 0.08$, $a_{IB} = 0.34$. Dashed and dotted lines correspond to quantum Monte-Carlo simulation with $10^{10}$ steps, solid lines are the exact diagonalization results, $\beta = 100, \xi = 2.5$.](image-url)
double-well and obtain eigenfunctions and eigenvalues \( \phi_i, E_i \) to estimate propagator in a numerically exact way

\[
K(x, x', \delta \tau) = \sum_i \phi_i^*(x) \phi_i(x') e^{-E_i \delta \tau} \tag{5}
\]

2) an explicit calculation of the retarded action integrated over the bosonic field \( S_R \).

3) a QMC simulation of the impurity’s trajectories with calculated data of \( K(x', x, \tau), S_R \) according with equation (3).

This scheme enables us to use a coarse time grid with the step \( \delta \tau \sim \Delta E^{-1} \) for QMC sampling. We apply this algorithm to find the correlation functions of the impurity in imaginary time. Using QMC data, we obtain a response or spectral functions on the real axis through a Fourier transform:

\[
\langle x_0 x_\tau \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left( e^{-\omega \tau} + e^{-\omega (\beta - \tau)} \right) \rho(\omega) d\omega \tag{6}
\]

The main difficulty of this approach is that small fluctuations of the QMC data \( \langle x_0 x_\tau \rangle \) lead to large fluctuations of the spectral function \( \rho(\omega) \). To solve this problem, we have to define the regularization parameters and boundary conditions from physical guesses and they are not universal (except, most likely, the non-negativity of \( \rho(\omega) \)).

In this work we use a standard maximum entropy method (MaxEnt) for obtaining the density of states from correlation function.

### III. RESULTS

First, we benchmark the proposed quantum Monte Carlo algorithm on the model (2) with two resonance modes of Bogoliubov excitations. We solve this problem by the exact diagonalization (ED) and the QMC scheme for different coupling strengths or equivalently boson-impurity scattering length \( a_{IB} \) (see Fig. 1). QMC correlation functions \( \langle x_0 x_\tau \rangle \) were transformed into a density of states (DOS) by the MaxEnt method. While exact diagonalization provides delta-function peaks for this problem, our MaxEnt procedure uses Gaussian approximation for DOS peaks with the width defined through both MaxEnt and QMC accuracy. Nevertheless, the significant features of density of states, namely a peak position and its amplitude, can be obtained without any restrictions on the boson-impurity scattering length \( a_{IB} \).

For a very small interaction in the two-mode case, we find a single peak in DOS, corresponding to the impurity tunneling (Fig 1 a). At the small coupling, this peak splits into two DOS peaks. As interaction grows, the right peak shifts to higher frequencies and its amplitude decreases, while the left DOS peak grows up and shifts leftward (Fig 1 b). Finally, this peak dominates for strong coupling, which might indicate a self-trapping of the impurity (Fig 1 c). We note, that for any value of \( a_{IB} \) our QMC results are in a good agreement with the exact diagonalization.

Now let us discuss QMC results for the model (2) with the continuous bosonic spectrum, which does not allow ED treatment. Fig. 2 shows the obtained spectral density of states from the QMC data. The DOS behavior is qualitatively similar to the two-mode problem.

For a small interaction strength (scattering length \( a_{IB} < 0.05 \)), the tunneling DOS-peak shifts to the right, and another DOS-peak appears. When the interaction strength grows, the amplitude of the right DOS-peak decreases, and its position continues to move to higher frequencies, indicating the decrease of tunneling time. Simultaneously, the left DOS-peak grows and shifts to the left. After the scattering length \( a_{IB} > 0.07 \), this peak exceeds the tunneling peak, which means that tunneling time increases.

For obtained QMC data MaxEnt method does not provide any change in the widths of the DOS-peaks, which

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![Diagram](image-url)

**FIG. 2.** Spectral densities of states for \( ^{89} \text{K} \) tunneling impurity, which interacts with continuous spectra of the Bogoliubov excitations in \( ^{87} \text{Rb} \) condensate; \( \beta = 100, \kappa = 10.24, k_{\text{max}} = 0.805 \), \( \xi = 2.5 \), \( 10^{10} \) QMC steps

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![Diagram](image-url)

**FIG. 3.** Effective mass of quasiparticles in \( ^{87} \text{Rb} \) condensate; red dots correspond right quasiparticle’s peaks, blue dots - left quasiparticle’s peaks, circle marks are lower DOS-peaks, \( \beta = 100, \kappa = 10.24, k_{\text{max}} = 0.805, \xi = 2.5 \)
continue to be narrow. Therefore, we can interpret them as the well-defined quasiparticle peaks. To illustrate this, we show an estimated effective mass for each peak as a function of scattering length in Fig. 3. For a given double-well potential (with $\kappa = 10.24$ in our case), we can employ exact diagonalization to obtain a dependence of tunneling splitting $\Delta E$ on a particle mass. Now we can use this dependence to estimate an effective mass for each DOS peak. We see that for a small interaction, which we refer to as a phonon-assisted tunneling region, the effective mass decreases (red dots in Fig. 3). For a large coupling, we observe an increase of the effective mass, which indicates that the impurity is localized in this regime (blue dots in Fig. 3). In the intermediate case, there is a crossover region, where two DOS peaks have nearly the same amplitude and the two phenomena coexist.

In Fig. 4 we also show sampled imaginary-time trajectories for different scattering lengths. For a small interaction, the impurity freely tunnels from one well to another and can be located in each well (Fig. 4 a). As interaction increases, the impurity tunneling starts to lessen (Fig. 4 b). For strong coupling, tunneling fades out almost completely, which results in the self-trapping of impurity in one of the wells (Fig. 4 c).

**IV. CONCLUSIONS**

In the present work, we propose a special modification of the QMC method for tunneling problems in an external environment, which can simulate equilibrium dynamics beyond perturbation theory. We apply this approach to study the tunneling of BEC-impurity for weak, intermediate, and strong coupling regimes in Frohlich-Bogoliubov approximation. The method was verified by employing the exact diagonalization for a model bath with only two modes of the bosonic field. We note that the accuracy of our algorithm does not depend on a number of bath excitations, which is valuable for the investigation of various many-body effects. We used an analytic continuation of the impurity’s correlation functions at low temperatures to calculate the density of states. We found that for BEC-impurity tunneling there is a crossover between the phonon-assisted tunneling for weak coupling and self-trapping for a strong interaction case. These phenomena might be observed in the resent experiment playground with the addition of two close harmonic optical dipole traps for impurity. Spectral response of the tunneling impurity in the BEC on radio-frequency pulses might be used for observation of transition between phonon-assisted tunneling and self-trapping regimes.

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1. L. Landau and S. Pekar, Zh. Eksp. Teor. Fiz. 18, 419 (1948).
2. F. Cucchietti and E. Timmermans, Phys. Rev. Lett. 96, 210401 (2006).
3. K. Sacha and E. Timmermans, Physical Review A 73, 063604 (2006).
4. J. Levinsen, M. M. Parish, and G. M. Bruun, Physical Review Letters 115, 125302 (2015).
5. F. Grusdt and M. Fleischhauer, Physical review letters 116, 053602 (2016).
6. M. Drescher, M. Salmhofer, and T. Enss, Physical Review A 99, 023601 (2019).
7. S. P. Rath and R. Schmidt, Physical Review A 88, 053632 (2013).
8. R. S. Christensen, J. Levinsen, and G. M. Bruun, Physical Review Letters 115, 125302 (2015).
9. J. Tempere, W. Casteels, M. Oberthaler, S. Knoop, E. Timmermans, and J. Devreese, Phys. Rev. B 80, 184504 (2009).
10. W. Casteels, J. Tempere, and J. Devreese, Physical Review A 86, 043614 (2012).
11. J. Catani, G. Lamporesi, D. Naik, M. Gring, M. Inguscio, F. Minardi, A. Kuntian, and T. Giamarchi, Physical Review A 85, 023623 (2012).
12. F. Grusdt, Y. E. Shchadilova, A. N. Rubtsov, and E. Demler, Scientific reports 5, 12124 (2015).
13. Y. E. Shchadilova, R. Schmidt, F. Grusdt, and E. Demler, Phys. Rev. Lett. 117, 130002 (2016).
14. A. Volosniev and H.-W. Hammer, Physical Review A 96, 031601 (2017).
15. F. Grusdt, G. E. Astrakharchik, and E. Demler, New Journal of Physics 19, 103035 (2017).
16. N. B. Jorgensen, L. Wacker, K. T. Skalmstang, M. M. Parish, J. Levinsen, R. S. Christensen, G. M. Bruun, and J. J. Arlt, Phys. Rev. Lett. 117, 055302 (2016).
17. M.-G. Hu, M. J. Van de Graaff, D. Kedar, J. P. Corson, E. A. Cornell, and D. S. Jin, Phys. Rev. Lett. 117, 055301 (2016).
18. D. Frese, B. Ueberholz, S. Kuhr, W. Alt, D. Schrader, V. Gomer, and D. Meschede, Physical review letters 85, 3777 (2000).
19. H. Bernien, S. Schwartz, A. Keesling, H. Levine, A. Omran, H. Pichler, S. Choi, A. S. Zibrov, M. Endres, M. Greiner, et al., Nature 551, 579 (2017).
20. T. Stauber, R. Zimmermann, and H. Castella, Physical Review B 62, 7336 (2000).
21. D. Loss and D. P. DiVincenzo, Physical Review A, 120 (1998).
22. U. Weiss, H. Grabert, P. Hänggi, and P. Riseborough, Physical Review B 35, 9535 (1987).
23. S. V. Isakov, G. Mazzola, V. N. Smelyanskiy, Z. Jiang, S. Boixo, H. Neven, and M. Troyer, Physical review letters 117, 180402 (2016).
24. E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, and P. Werner, Reviews of Modern Physics 83, 349 (2011).
25. F. Lingua, B. Capogrosso-Sansone, A. Safavi-Naini, A. Jahangiri, and V. Penna, Physica Scripta 93, 105402 (2018).
26. T. Parolini, E. Inack, G. Giudici, and S. Pilati, Physical Review B 100, 214303 (2019).
27. E. Inack, G. Giudici, T. Parolini, G. Santoro, and S. Pilati, Physical Review A 97, 032307 (2018).
28. N. Nemec, Physical Review B 81, 035119 (2010).
29. D. Oberli, J. Shah, T. Damen, J. Kuo, J. Henry, J. Lary, and S. M. Goodnick, Applied physics letters 56, 1239 (1990).
30. V. Vargas-Calderón and H. Vinck-Posada, Physics Letters A 384, 126076 (2020).
31. A. Myasnikova, Physical Review B 52, 10457 (1995).
32. N. Metropolis and S. Ulam, Journal of the American statistical association 44, 335 (1949).
33. R. Levy, J. LeBlanc, and E. Gull, Computer Physics Communications 215, 149 (2017).
34. K. Ghanem and E. Koch, Verhandlungen der Deutschen Physikalischen Gesellschaft (2016).