

QUANTUM MONTE-CARLO SIMULATION OF POLARON TUNNELING

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Theoretical investigation of polaron effects in ultracold gasses became justified due to the latest experimental results [1, 2] with tunable interaction between impurities and surrounding bosonic field via Feshbach resonance. Investigation of tunneling effects in such systems is of great interest in condensed matter physics. In the present work, for considering the dynamics of tunneling effect in the polaron task we used Frohlich Hamiltonian [3]. We study a single impurity interacting with bosonic field and its tunneling in a double-well potential. As a practical application, this system can be considered as one of the implementations of a quantum qubits [4, 5].

Since the existing theoretical techniques cannot describe the strong interacting regimes between the impurity and the surrounding condensate [6], we used numerical quantum Monte-Carlo method in terms of path integrals [7]. Nevertheless, the straightforward application of this algorithm for the simulation of polaron tunneling is limited by the exponential growth of the calculation time. This problem originates from the differences between a time scale of the polaron dynamics and the tunneling time of the particle. Therefore, we proposed the new modification of the QMC method. The main idea of the modification is to divide the calculations into two parts: at first, we integrate the action over bosons and then calculate the propagator for impurity in a double-well potential.

The modified quantum Monte-Carlo method was verified by employing the exact diagonalization in the case of the impurity interacting with two modes of BEC. For this, we used an approximation of the impurity correlation functions at low temperatures by exponents, which lets to find the tunnel splitting. The new algorithm allows considering multimode regimes beyond the limitations on the coupling constant (i.e. on the interaction between an impurity and surrounding bosonic field) given by analytical approach.

Chertkova Anastasia acknowledges the financial support from the Foundation for the advancement of theoretical physics and mathematics BASIS.

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