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Holstein and Fröhlich bipolarons

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Abstract

We explore the properties of the bipolaron in a simplified one-dimensional (1D) Fröhlich–Hubbard model in comparison with results in the Holstein–Hubbard model, where the former has a longer range electron–phonon interaction. We solve the model with an exact diagonalization method on an infinite 1D lattice. In the strong coupling regime, the effective mass of the Fröhlich bipolaron is much smaller than the Holstein bipolaron mass. In contrast to the Holstein model where only a singlet bipolaron is bound, in the Fröhlich model, a triplet bipolaron can also form a bound state.

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There is a growing evidence that electron–phonon coupling plays an important role in determining exotic properties of novel materials such as high-T_c compounds [1] and colossal magnetoresistance materials [2]. Motivated by the recent discovery of a mobile small polaron in a Fröhlich model by Alexandrov and Kornilovitch [3], we investigate a simplified version of their model in the case of two electrons with opposite spins

$$H = -t\sum_{js}(c^{\dagger}_{j+1,s}c_{j,s} + \text{h.c.}) - \omega g_0 \sum_{jls} f_l(j) c^{\dagger}_{j,s}c_{j,s}(a_l + a^{\dagger}_l) + \omega\sum_j a^{\dagger}_j a_j + U\sum_j n_{j\uparrow}n_{j\downarrow}, \tag{1}$$

where $c^{\dagger}_{j,s}$ creates an electron of spin s and $a^{\dagger}_j$ creates a phonon on site j. The second term represents the coupling of an electron on site j with an ion on site l with g_0 being the dimensionless electron–phonon coupling constant.

While in general long range electron–phonon coupling $f_l(j)$ is considered [3,4], we further simplify this model by placing ions on the interstitial sites located between Wannier orbitals. In this case it is natural to investigate a simplified model, where an electron, located on site j couples only to neighboring ions, i.e. $l = j \pm 1/2$ (we set the lattice constant to 1). We describe such a coupling with $f_{j\pm 1/2}(j) = 1$ and 0 otherwise and refer to this model as a Fröhlich–Hubbard model (FHM). Even though in a true FHM electron–phonon coupling is long range, we would like to stress that in one-dimensional (1D), the long-range version of FHM [3,4] gets 99.2% of the polaron energy on the first two sites. In the case when $f_l(j) = \delta_{l,j}$, the model in Eq. (1) maps onto a Holstein–Hubbard

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model (HHM). An essential difference between the two models comes from comparing polaron energies $\epsilon_p = g_0^2 \sum_l f_l(0)^2$ which gives $\epsilon_p = 2\omega g_0^2$ and $\epsilon_p = \omega g_0^2$ for the FHM and HHM respectively.

In this work we use a recently developed numerical technique [5,6] to study FHM bipolaron (FB) and HHM bipolaron (HB). To achieve sufficient numerical accuracy (error bars are smaller than line-widths, results are valid in the thermodynamic limit), we have used up to 3×10^6 variational states. We have set the bare hopping constant to $t = 1$. We have calculated the binding energy $\Delta = E_{bi} - 2E_{po}$ where E_{bi} is the ground state energy of FB or HB and E_{po} is the ground state energy of a single polaron. We have searched for bound states of bipolarons in a spin-singlet and a spin-triplet state. From binding energies we have determined the phase diagram $(U_c, \lambda \equiv \epsilon_p/2t)$ of the FB (filled circles) and HB (open circles), presented in Fig. 1(a). Three different regimes exist in the case of FB. For small λ and large U we find a state of separated polarons. With increasing λ there is a phase transition into a bound singlet bipolaron state. For λ larger than $\lambda_c \sim 0.76$ (vertical dashed line), a triplet bipolaron becomes bound in the FHM. The critical λ_c is U-independent since the wave function of the spin-triplet bipolaron has a node if particles occupy the same Wannier orbital. For comparison we include the phase boundary determining the stability of the HB (open circles) [6]. Note that only singlet bipolarons exist in the HHM.

In Fig. 1(b) we present the bipolaron effective mass near the strong coupling regime, $\lambda = 1.45$ as a function of the Coulomb interaction U. The effective mass of the FB is almost two orders of magnitude smaller than the HB when $U = 0$.

We have shown that a light FB exists even in the strong coupling regime with an effective mass that can be a few orders of magnitude smaller than the HB effective mass. The effect of the Coulomb interaction U on the FB effective mass is much smaller than the effect on the HB effective mass, which strongly decreases with increasing U. As we have shown in our previous work [6], HB becomes very light with increasing U close to the transition into two unbound polarons $U = U_c$. In the regime of a light HB its binding energy substantially diminishes and reaches $\Delta = 0$ at the transition point U_c. In contrast, FB has a small effective mass almost independently of U and remains bound even in the limit when $U \to \infty$ with substantial binding energy that in the strong coupling regime approaches $\Delta = -\epsilon_p/2$. The difference between the binding energies of spin-singlet and the spin-triplet bipolaron is proportional to $1/U$.

The existence of a singlet and a triplet Fröhlich bipolaron state has important implications in the case of finite doping. As was established in our previous work [6], there is no phase separation in

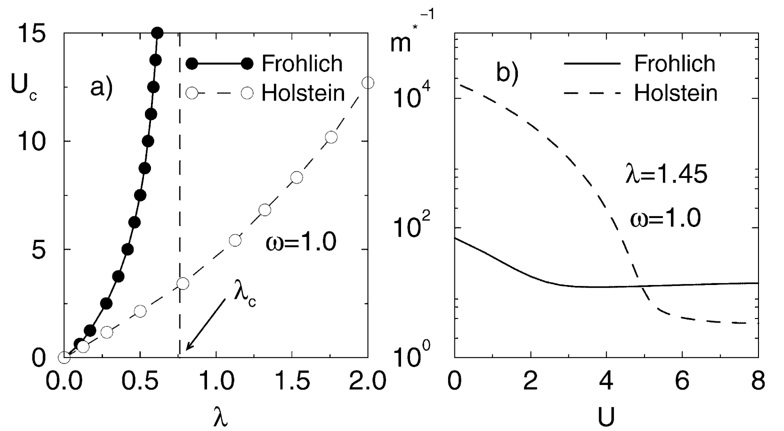

Fig. 1. (a) Phase diagram of the FB (●) and the HB (○) for the case of two electrons calculated at $\omega = 1$, and (b) inverse effective mass m^{*-1} vs. U.

the low-density limit of the HHM despite a substantially renormalized bandwidth. The reason is in part that a triplet bipolaron is always unstable. The lack of phase separation in the low-density limit and in the strong coupling regime has a simple intuitive explanation: a third particle, added to a bound singlet bipolaron, introduces a triplet component to the wave function. The opposite is true in the strong coupling limit of FHM where singlet and triplet bipolarons coexist. In this case, the third added particle simply attaches to the existing singlet bipolaron and thus gains in the potential energy. We therefore expect that the FHM phase separates in the case of finite doping for λ sufficiently large. The system is unstable with respect to phase separation into a fully spin-polarized state, with unpolarized states even lower in energy.

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