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Abstract

The stability criteria of quasi-two-dimensional dimensional bipolarons have been studied within the framework of strong coupling and path-integral theories. It is shown that the critical values of the electron-phonon coupling constant (α), and the ratio of dielectric constants ($\eta = \epsilon_\infty/\epsilon_0$) exhibit some non-trivial features as the effective dimensionality is tuned from three to two.

1. Introduction

Two electrons in an ionic or polar crystal may form a bound state, provided that the phonon-mediated attractive forces between them are strong enough to counterbalance the Coulomb repulsion. Such a quasiparticle, consisting of two electrons and a common cloud of virtual phonons is termed a bipolaron. The properties of the bipolaron state and the critical conditions for its formation have been studied extensively [1-7]. The aim of the present work is to investigate the stability criteria of bipolarons in a quasi-two-dimensional (Q2D) medium.

For the bipolaron formation to be favorable, one should have: $E_{\rm g} < 2E_{\rm g}^{(1)}$, where $E_{\rm g}$ and $E_{\rm g}^{(1)}$ are respectively, the bipolaron and one-polaron ground state energies which are calculated within identical frameworks. On this purpose, we will borrow the one-polaron energy values from the relevant works [8,9].

2. Theory

The Hamiltonian describing the confined electron–pair coupled to LO-phonons is

$$\mathsf{H} = H_e + \sum_Q a_Q^\dagger a_Q + \sum_{j=1,2}\sum_Q V_Q \left(a_Q e^{i\vec{Q}\cdot\vec{r}_j} + a_Q^\dagger e^{-i\vec{Q}\cdot\vec{r}_j} \right) , \tag{1}$$

$$H_e = \sum_{j=1,2} \left(\frac{1}{2} p_j^2 + V_{\rm conf}(z_j) \right) + \frac{U}{|\vec{r}_1 - \vec{r}_2|} . \tag{2}$$

Here we use dimensionless units for which $m^\star = \hbar = \omega_{LO} = 1$. In the above, a_Q and $a_Q^\dagger$ denote the phonon operators, and $\vec{r}_j = (\vec{\rho}_j, z_j)$, $(j = 1, 2)$, are the positions of the electrons in cylindrical coordinates. Similarly, $\vec{p}_j$ denote the respective momenta of the electrons. The Fröhlich interaction amplitude is related to the phonon wavevector $\vec{Q} = (\vec{q}, q_z)$ through $V_Q = (2\sqrt{2}\pi\alpha)^{1/2}|\vec{Q}|^{-1}$. The coupling constant is given, in terms of the high frequency and static dielectric constants of the material, by $\alpha = e^2\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)/\sqrt{2}$ in terms of which the unscreened Coulomb repulsive amplitude is $U = e^2/\epsilon_\infty = \alpha\sqrt{2}/(1-\eta)$, where $\eta = \epsilon_\infty/\epsilon_0 < 1$. For the confining potential we use a harmonic oscillator profile with adjustable barrier slopes, i.e., we set $V_{\rm conf}(z) = \frac{1}{2}\Omega^2 z^2$, in which the dimensionless frequency Ω serves for the measure of the degree of confinement of the electrons. When tuned from zero to infinity, it yields a unifying display of the phase stability of the bipolaron as a function of the effective dimensionality ranging from three to two.

2.1. Strong Coupling Theory

In the limit of strong α, it is convenient to use the adiabatic Pekar theory, where one assumes a separable form for the phonon and the particle coordinates of the bipolaron state,

$$\Psi_{\rm bipol} = \Phi(\vec{R}, \vec{r})\, e^{\mathcal{U}}|0\rangle \tag{3}$$

where $|0\rangle$ is the phonon vacuum state, and $e^{\mathcal{U}}$ is the operator of optimal displaced-oscillator transformation with $\mathcal{U} = \sum_Q f_Q\,(a_Q - a_Q^\dagger)$. For the particle part, we assume a variational form which is separable in the center of mass, $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$, and the relative, $\vec{r} = \vec{r}_1 - \vec{r}_2$, coordinates, i.e. $\Phi(\vec{R}, \vec{r}) = \phi(\vec{R}) \times \varphi(\vec{r})$. We choose the following oscillator type anisotropic waveforms

$$\phi(\vec{R}) = N_R\, \exp\left\{-\frac{1}{2}\kappa_1^2(R_\varrho^2 + \mu_1^2 R_z^2)\right\} \qquad \varphi(\vec{r}) = N_r\, r^\gamma\, \exp\left\{-\frac{1}{2}\kappa_2^2(r_\varrho^2 + \mu_2^2 r_z^2)\right\}\ . \tag{4}$$

The bipolaron ground state energy is calculated by optimizing of $E_{\rm g}^{\rm (SC)} \equiv \langle\Psi_{\rm bipol}|\mathsf{H}|\Psi_{\rm bipol}\rangle$, with respect to the variational parameters $\{\kappa_i, \mu_i\}$, $(i = 1, 2)$, contained in the wavefunction, with γ taken as either 0 or 1.

2.2. Path Integral Formulation

Feynman's path integral formulation of the polaron systems, is also a variational technique, but it provides the lowest energy upper bounds and it is reasonably valid for all values of the electron-phonon coupling constant.

Following the standard formulation [2,9,10], after the elimination of the phonon variables, the partition function of the system can be written as a path integral,

$$\mathcal{Z} = \prod_{i=1,2}\left(\int d\vec{r}_0 \int_{\vec{r}_i(0)=\vec{r}_0}^{\vec{r}_i(\beta)=\vec{r}_0} \mathcal{D}\vec{r}_i(\lambda)\right)\ e^{\mathcal{S}[\vec{r}_1(\lambda),\vec{r}_2(\lambda)]}\ . \tag{5}$$

Here, β is the inverse temperature and $\mathcal{S}$ is the action expressed in imaginary time variables ($t \rightarrow -i\lambda$):

$$\mathcal{S} = -\frac{1}{2}\int_0^\beta d\lambda \sum_{i=1,2}\left(\dot{\vec{r}}_i^{\,2}(\lambda) + \Omega^2 z_i^2(\lambda)\right) - \int_0^\beta d\lambda \frac{U}{|\vec{r}_1(\lambda) - \vec{r}_2(\lambda)|} + \mathcal{S}_{\mathrm{e-p}} \ , \qquad (6)$$

$$\mathcal{S}_{\mathrm{e-p}} = \frac{1}{2}\sum_{i=1,2}\sum_{j=1,2}\sum_{Q} V_Q^2 \int_0^\beta d\lambda \int_0^\beta d\lambda' \, G_{(\omega_{\mathrm{LO}}=1)}(\lambda - \lambda') \, e^{i\vec{Q}\cdot[\vec{r}_i(\lambda) - \vec{r}_j(\lambda')]} \ . \qquad (7)$$

In the above $G_\omega(u)$ is the Green's function of a harmonic oscillator with frequency ω. The introduction of a trial action $\mathcal{S}_0$ provides us with a convenient variational upper bound to the ground state energy, led by the Jensen-Feynman inequality

$$E_{\mathrm{g}}^{(\mathrm{PI})} \leq E_0 - \lim_{\beta\rightarrow\infty} \frac{1}{\beta} \langle \mathcal{S} - \mathcal{S}_0 \rangle_{\mathcal{S}_0} \qquad (8)$$

where the notation $\langle ... \rangle_{\mathcal{S}_0}$ denotes a path-integral average with density function $e^{\mathcal{S}_0}$, and E_0 is the trial ground state energy corresponding to $\mathcal{S}_0$. For the trial action, we choose the same model, which was successfully applied previously to similar polaron or bipolaron problems [2,9,10], where the electrons are considered to be in harmonic interaction with fictitious masses.

3. Results

The Q2D-bipolaron ground state energies $E_{\mathrm{g}}^{(\mathrm{SC})}$ and $E_{\mathrm{g}}^{(\mathrm{PI})}$ are calculated numerically, and comparing them to twice the corresponding one-polaron energies [8,9], the critical η and α values are obtained as functions of the degree of confinement. The work by Verbist *et al.* [3] on bipolarons reveals that the strong coupling theory does not provide information on any critical value of α; and the value of η_{c} strongly depends on the form of the wavefunction adopted. For instance, choosing $\gamma = 0$ for the relative coordinate part of the wavefunction, one gets $\eta_{\mathrm{c}} = 0.079$ in both 3D and 2D [3]. On the other hand for $\gamma = 1$, those values are 0.131 and 0.158 for 3D and 2D, respectively. Our strong coupling results indicate that η_{c} smoothly varies from the bulk to the 2D limit values as the effective dimensionality is tuned from three to two (Fig.1(a)). It is intersting to note that η_{c} experiences a relative decrease when the size of the external potential becomes comparable to the effective size of (bi)polaron ($\Omega/\alpha^2 \sim 1$). The results of the more powerful theory, path integral (PI) formalism, however have explicit dependence on α, and in Fig.1(a) it is also seen how PI results confirm to the SC results with $\gamma = 0$. It is reported previously that the bipolaron formation is more favourable in 2D than it is in bulk [2,5,6]. The statement is true if one considers the two extreme limits, with $\eta = 0$. However in the transition region ($10 \leq \Omega \leq 10^4$), for non-zero η, α_{c} can be much larger than its bulk value (c.f. Fig.1(b)). For example, choosing $\eta = 0.065$, the bulk value is $\alpha_{\mathrm{c}} = 15.0$ and its 2D value is $\alpha_{\mathrm{c}} = 6.6$; but α_{c} can be as high as 35.3 for $\Omega = 10^3$. These salient features observed for Q2D bipolarons arise from the dependence of the competing

counter-effects (phonon mediated atractive forces and the repulsive Coulomb forces) on the degree of confinement.

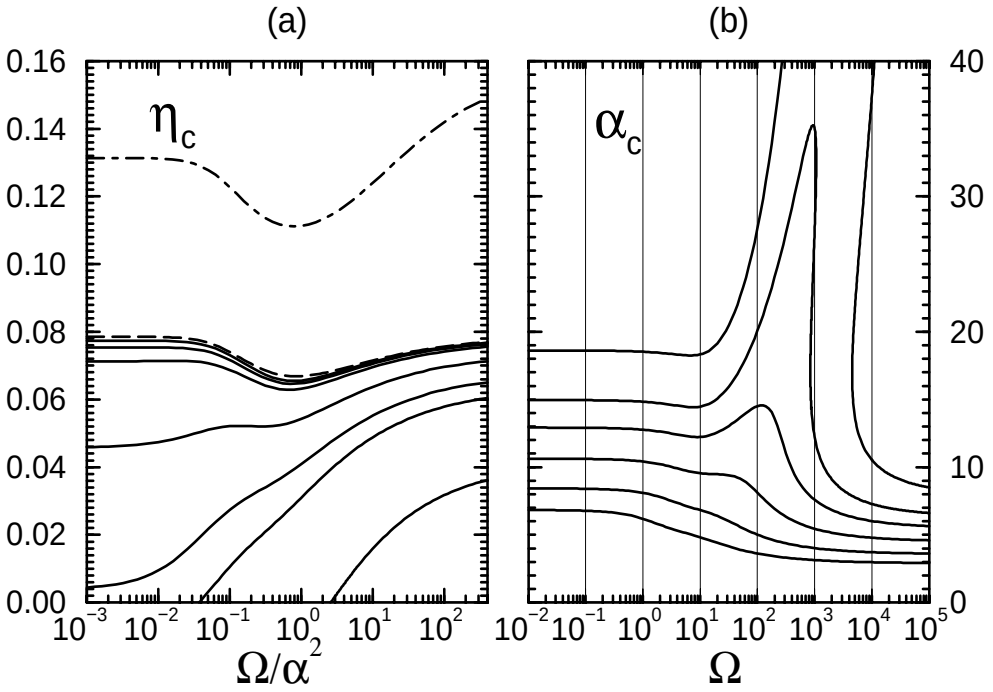

Figure 1. (a) The critical value of ratio of dielectric constants below which the bipolarons can form. The solid curves are path integral results for $\alpha = 4, 6, 7, 10, 20, 30, 50$ (from bottom to top). The strong coupling results for the wavefunction with $\gamma = 0$ (dashed) and $\gamma = 1$ (dot-dashed) are also given. (b) The path integral results for the critical α values over which the bipolarons exist. The curves are for $\eta = 0, 0.03, 0.05, 0.06, 0.065, 0.07$ (from bottom to top) respectively.

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