Stability of Quasi-Two-Dimensional Bipolarons

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Received 01.03.1999

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 ($\alpha$), 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: $E_\text{g} < 2E_{\text{g}}^{(1)}$, where $E_\text{g}$ and $E_{\text{g}}^{(1)}$ 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

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

$$H_c = \sum_{j=1,2} \left( \frac{1}{2} \mathbf{p}_j^2 + V_{\text{conf}}(z_j) \right) + \frac{U}{|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (2)$$
Here we use dimensionless units for which \( m^* = h = \omega_{LO} = 1 \). In the above, \( a_Q \) and \( a_Q^\dagger \) denote the phonon operators, and \( \vec{r}_j = (\vec{p}_j, z_j) \), \( (j = 1, 2) \), 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

\[
\alpha = \frac{e^2}{\epsilon_\infty - 1} = \frac{\eta}{\epsilon_\infty/\epsilon_0 < 1}
\]

For the confining potential we use a harmonic oscillator profile with adjustable barrier slopes, i.e., we set \( V_{\text{conf}}(z) = \frac{1}{2} \Omega^2 z^2 \), in which the dimensionless frequency \( \Omega \) 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 \( \alpha \), 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,

\[
\Psi_{\text{bipol}} = \Phi(\vec{R}, \vec{r}) \, e^{iU(0)} \tag{3}
\]

where \( |0\> \) is the phonon vacuum state, and \( e^{iU} \) is the operator of optimal displaced-oscillator transformation with \( U = \sum Q f_Q (a_Q - a_Q^\dagger) \). 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

\[
\phi(\vec{R}) = N_R \exp \left\{ -\frac{1}{2} \kappa_1^2 (R^2 + \mu_1^2 R_z^2) \right\} \quad \varphi(\vec{r}) = N_r r^\gamma \exp \left\{ -\frac{1}{2} \kappa_2^2 (r^2 + \mu_2^2 r_z^2) \right\} \tag{4}
\]

The bipolaron ground state energy is calculated by optimizing of \( E_{\text{bipol}}^{(\text{SC})} = \langle \Psi_{\text{bipol}} | H | \Psi_{\text{bipol}} \rangle \), with respect to the variational parameters \( \{ \kappa_i, \mu_i \}, (i = 1, 2) \), contained in the wavefunction, with \( \gamma \) 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,

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

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

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

$$S_{e-p} = \frac{1}{2} \sum_{i=1,2} \sum_{j=1,2} \sum_Q V^2 Q \int_0^\beta d\lambda \int_0^\beta d\lambda' G_{(\omega L \Omega=1)}(\lambda - \lambda') e^{iQ[\vec{r}_i(\lambda) - \vec{r}_j(\lambda')]} . \quad (7)$$

In the above $G_\omega(u)$ is the Green’s function of a harmonic oscillator with frequency $\omega$. The introduction of a trial action $S_0$ provides us with a convenient variational upper bound to the ground state energy, led by the Jensen-Feynman inequality

$$E^{(\text{PI})}_g \leq E_0 - \lim_{\beta \rightarrow -\infty} \frac{1}{\beta} \langle S - S_0 \rangle_{S_0} . \quad (8)$$

where the notation $\langle \cdots \rangle_{S_0}$ denotes a path-integral average with density function $e^{S_0}$, and $E_0$ is the trial ground state energy corresponding to $S_0$. 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 $E_g^{(\text{SC})}$ and $E_g^{(\text{PI})}$ are calculated numerically, and comparing them to twice the corresponding one-polaron energies [8,9], the critical $\eta$ and $\alpha$ values are obtained as functions of the degree of confinement. The work by Verbist et al. [3] on bipolarnon reveals that the strong coupling theory does not provide information on any critical value of $\alpha$; and the value of $\eta$, strongly depends on the form of the wavefunction adopted. For instance, choosing $\gamma = 0$ for the relative coordinate part of the wavefunction, one gets $\eta_c = 0.079$ 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 $\eta_c$ 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 $\eta_c$ 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 $\alpha$, 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 $\eta$, $\alpha_c$ can be much larger than its bulk value (c.f. Fig.1(b)). For example, choosing $\eta = 0.065$, the bulk value is $\alpha_c = 15.0$ and its 2D value is $\alpha_c = 6.6$; but $\alpha_c$ can be as high as 35.3 for $\Omega = 10^5$. These salient features observed for Q2D bipolarons arise from the dependence of the competing
counter-effects (phonon mediated attractive forces and the repulsive Coulomb forces) on the degree of confinement.

![Graph](image)

**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 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.

**References**


