Eur. Phys. J. B **36**, 65–73 (2003)
DOI: 10.1140/epjb/e2003-00317-x

THE EUROPEAN PHYSICAL JOURNAL B

Ground state features of the Fröhlich model

G. De Filippis[a], V. Cataudella, V. Marigliano Ramaglia, C.A. Perroni, and D. Bercioux

Coherentia-INFM and Dipartimento di Scienze Fisiche, Università degli Studi di Napoli "Federico II", Complesso Universitario Monte Sant'Angelo, Via Cintia, 80126 Napoli, Italy

Received 2 July 2003
Published online 19 November 2003 –

Abstract. Following the ideas behind the Feynman approach, a variational wave function is proposed for the Fröhlich model. It is shown that it provides, for any value of the electron-phonon coupling constant, an estimate of the polaron ground state energy better than the Feynman method based on path integrals. The mean number of phonons, the average electronic kinetic and interaction energies, the ground state spectral weight and the electron-lattice correlation function are calculated and successfully compared with the best available results.

PACS. 71.38.Fp Large or Fröhlich polarons

1 Introduction

In recent years a large amount of experimental results has pointed out that the electron-phonon (e-ph) interaction plays a significant role in determining the electronic and magnetic properties of new materials as the high T_c superconductors and the colossal magneto-resistance manganites [1]. The experimental data have given rise to a renewed interest in models of the e-ph coupled system. In this paper we investigate the polaronic features of the Fröhlich model within a variational approach [2]. Here the picture is the following. When an electron in the conduction band of a polar crystal moves through the crystal, its Coulomb field produces in its neighborhood an ionic polarization that will influence the electron motion. Then the particle must carry this polarization with it during its motion through the crystal. The quasi-particle formed by the electron and the induced polarization charge is called polaron. Within the Fröhlich model: 1) the optical modes have the same frequency; 2) the dielectric is treated as a continuum medium; 3) in the undistorted lattice the electron moves as a free particle with a quadratic dispersion relation (effective band mass approximation).

The problem of finding the ground state energy of the Fröhlich Hamiltonian attracted the interest of a lot of researchers mainly in the period 1950–1955. Numerous mathematical techniques have been used to solve this problem: from the perturbation theory in the weak coupling regime [3] to the strong coupling theory [4], from the linked cluster theory [5] to variational [6] and Monte Carlo approaches [7,8]. The weak coupling regime is well described within the Lee, Low and Pines (LLP) approach [9]. Here, after the dependence of the Hamiltonian on the electron coordinates has been eliminated, an upper bound for the polaron ground state energy is obtained by using a variational wave function which is based on the physical assumption that successive virtual phonons are emitted independently. In the opposite regime, when the e-ph interaction is very strong, a good description of the polaron features has been obtained by Landau and Pekar [10]. Their theory, based on a variational calculation, stems from the idea that, for very large values of the e-ph coupling constant, the electron can follow adiabatically the quantum zero-point fluctuations of the polarization field. In their first papers the electron is localized with a Gaussian wave function. Next, the method has been improved by Hohler [11] by constructing an eigenstate of the total wave number by superposing Landau-Pekar states localized at different points of the lattice. In any case the validity of LLP and Hohler approaches is restricted, respectively, to weak and strong e-ph coupling regimes.

An excellent approximation, that is accurate at all couplings, has been introduced by Feynman [12]. His approach provides a variational estimate of the electron self-energy based on the path integrals and the Feynman-Jensen inequality. After the phonon variables have been eliminated exactly, Feynman introduces a model Hamiltonian which describes approximatively the interaction of the electron with the lattice. This Hamiltonian is that of an electron coupled to another particle with a harmonic oscillator coupling. The trial action for the system is obtained by eliminating the coordinates of the fictitious particle simulating the phonon degrees of freedom. The mass M of the fictitious particle and the spring constant

[a] e-mail: giuliode@na.infn.it

are the two variational parameters within the Feynman approach. The Monte Carlo study [7,8] of the Fröhlich model has demonstrated the remarkable accuracy of the Feynman method to the electron self-energy.

In this paper we use a variational technique, within an Hamiltonian approach, to investigate the polaronic features of the Fröhlich model. It is based on linear superposition of two translationally invariant wave functions that provide a very good description of the weak and strong e-ph coupling regimes. These wave functions are built assuming as starting points the LLP [9] and Hohler [11] variational approaches. First, we improve these methods obtaining a better upper bound for the polaron ground state energy in the two asymptotic regimes of weak and strong e-ph interaction. Then, we use a linear superposition of these two wave functions. The comparison of our results with the Feynman [12] and Monte Carlo data [7] shows that the proposed method provides an excellent description of the polaron ground state energy for any value of the e-ph coupling. Within our variational approach, the estimate of the electron self-energy turns out systematically lower than one of the Feynman method. In particular, unlike the Feynman approach, the ground state energy shows the exact dependence on the e-ph coupling constant in the strong coupling regime. Next, we calculate the mean number of phonons present in the virtual phonon cloud surrounding the electron, the average electronic kinetic and interaction energies, the ground state spectral weight and the induced ionic polarization charge density. These quantities are successfully compared with Monte Carlo [8] and Feynman results [13].

The proposed method has the advantage to exhibit, first to the author's knowledge, a wave function that gives the correct behavior in both weak and strong coupling limits and provides an interpolation between them with results at least accurate as those of the Feynman approach [12].

2 The model

The Fröhlich model [2] is described by the Hamiltonian:

$$\begin{aligned} H &= H_{el} + H_{ph} + H_{e-ph} \\ &= \frac{p^2}{2m} + \sum_{\vec{q}} \hbar\omega_0 a_{\vec{q}}^{\dagger} a_{\vec{q}} + \sum_{\vec{q}} (M_q e^{i\vec{q}\cdot\vec{r}} a_{\vec{q}} + \text{h.c.}). \end{aligned} \quad (1)$$

In equation (1) m is the band mass of the electron, $\hbar\omega_0$ is the longitudinal optical phonon energy, $\vec{r}$ and $\vec{p}$ are the position and momentum operators of the electron, $a_{\vec{q}}^{\dagger}$ represents the creation operator for phonons with wave number $\vec{q}$ and M_q indicates the e-ph matrix element. In the Fröhlich model [2], M_q assumes the form:

$$M_q = i\hbar\omega_0 \frac{R_p^{1/2}}{q} \sqrt{\frac{4\pi\alpha}{V}}\ , \quad (2)$$

where α, dimensionless quantity, is the e-ph coupling constant, $R_p = \sqrt{\frac{\hbar}{2m\omega_0}}$ and V is the volume of the system.

3 The strong coupling regime

3.1 The adiabatic approximation

When the value of α is very large ($\alpha \gg 1$) the electron can follow adiabatically the lattice polarization changes and it becomes self-trapped in the induced polarization field. The idea of Landau and Pekar [10], in the first works on polarons, is to use, as trial wave function for the e-ph coupled system, a product of normalized variational wave functions $|\varphi\rangle$ and $|f\rangle$ depending, respectively, on the electron and phonon coordinates:

$$|\psi\rangle = |\varphi\rangle|f\rangle. \quad (3)$$

The expectation value of the Hamiltonian (1) on the state (3) gives:

$$\begin{aligned} \langle\psi|H|\psi\rangle = \langle\varphi|\frac{p^2}{2m}|\varphi\rangle \\ + \langle f| \sum_{\vec{q}} \left[\hbar\omega_0 a_{\vec{q}}^{\dagger} a_{\vec{q}} + \rho_{\vec{q}} a_{\vec{q}} + \rho_{\vec{q}}^{*} a_{\vec{q}}^{\dagger}\right] |f\rangle \end{aligned} \quad (4)$$

with

$$\rho_{\vec{q}} = M_q \langle\varphi|e^{i\vec{q}\cdot\vec{r}}|\varphi\rangle. \quad (5)$$

The variational problem with respect to $|f\rangle$ leads to the following lowest energy phonon state:

$$|f\rangle = e^{\sum_{\vec{q}}\left[\frac{\rho_{\vec{q}}}{\hbar\omega_0} a_{\vec{q}} - \text{h.c.}\right]} |0\rangle. \quad (6)$$

The minimization of the corresponding energy with respect to $|\varphi\rangle$ leads to a non-linear integro differential equation that has been solved numerically by Miyake [14]. The result for the polaron ground state energy in the strong coupling limit is:

$$E = -0.108513\alpha^2\hbar\omega_0. \quad (7)$$

The Landau-Pekar [10] Gaussian ansatz for $|\varphi\rangle$:

$$|\varphi_{lp}\rangle = e^{-\left(\frac{m\omega}{\hbar}\right)\frac{r^2}{2}} \left(\frac{m\omega}{\hbar\pi}\right)^{3/4}, \quad (8)$$

after the minimization of the expectation value of the Hamiltonian (1) on this state, with respect to the variational parameter ω, provides an estimate of the ground state energy:

$$E = -\frac{\alpha^2}{3\pi}\hbar\omega_0 \simeq -0.106103\alpha^2\hbar\omega_0 \quad (9)$$

that is very close to the exact result (7). The best value for ω turns out:

$$\omega = \frac{4\alpha^2}{9\pi}\omega_0. \quad (10)$$

An excellent approximation for the true energy (7) is obtained by using a trial wave function similar to that one introduced by Pekar [10]:

$$|\varphi_p\rangle = N e^{-\gamma r}\left[1 + b\,(2\gamma r) + c\,(2\gamma r)^2\right] \quad (11)$$

with N normalization constant and b, c and γ variational parameters. The minimization of $\langle\varphi_p|H|\varphi_p\rangle$ leads to:

$$E = -0.108507\alpha^2\hbar\omega_0. \tag{12}$$

This upper bound for the energy differs from the exact value less than 0.01%.

3.2 Path integral method versus Hamiltonian approach

At this point we recall the result of the Feynman [12] variational calculation when the approximating action is represented by a fixed harmonic binding potential:

$$E = \left[-\frac{\alpha^2}{3\pi} - 3\log 2\right]\hbar\omega_0, \qquad \alpha \to \infty. \tag{13}$$

It is given by the sum of two terms. The first one corresponds to use a Gaussian wave function in the Landau and Pekar's method (Eq. (8)). The last one does not depend on the e-ph coupling constant α. The origin of this contribution in Feynman's expansion of the polaron energy has been discussed by Allcock [15] by using the perturbation theory in the strong coupling limit. Our first aim is to put this result on variational basis. This will allow us to characterize the terms that one has to introduce in the trial wave function to improve the Landau and Pekar's ansatz. To this aim, starting from equations (3) and (6), we apply the following unitary transformation:

$$H_1 = e^{S_1} H e^{-S_1} \tag{14}$$

with

$$S_1 = -\sum_{\vec{q}} \left[\frac{\alpha_{\vec{q}}}{\hbar\omega_0} a_{\vec{q}} - \text{h.c.}\right]. \tag{15}$$

The transformed Hamiltonian assumes the form:

$$H_1 = H_0 + H_I \tag{16}$$

with

$$H_0 = \frac{p^2}{2m} + \sum_{\vec{q}} \hbar\omega_0 a^\dagger_{\vec{q}} a_{\vec{q}} - \sum_{\vec{q}} \left[\left(M_q e^{i\vec{q}\cdot\vec{r}} - \alpha_{\vec{q}}\right)\frac{\alpha^*_{\vec{q}}}{\hbar\omega_0} + \text{h.c.}\right] - \sum_{\vec{q}} \frac{|\alpha_{\vec{q}}|^2}{\hbar\omega_0} \tag{17}$$

and

$$H_I = \sum_{\vec{q}} \left[\left(M_q e^{i\vec{q}\cdot\vec{r}} - \alpha_{\vec{q}}\right) a_{\vec{q}} + \text{h.c.}\right]. \tag{18}$$

One recognizes immediately that the Landau-Pekar approach corresponds to use as trial wave function for H_1:

$$|\psi\rangle^{(0)} = |0\rangle|\varphi_{lp}\rangle \tag{19}$$

with $|\varphi_{lp}\rangle$ given by equation (8) and $\alpha_q = M_q\langle\varphi_{lp}|e^{i\vec{q}\cdot\vec{r}}|\varphi_{lp}\rangle$. In other words, in this approach, one approximates the lowest energy state of H_0 with a Gaussian wave function containing the variational parameter ω, that represents the characteristic oscillation of the electron in the induced lattice polarization. The next order term is obtained assuming H_I as perturbation and approximating the eigenstates of H_0 with those of an harmonic oscillator. At the first order of the perturbation theory the wave function is:

$$|\psi\rangle^{(1)} = |\psi\rangle^{(0)} - \int_0^1 t^{\left[\frac{\omega_0}{\omega}-1\right]} \sum_{\vec{q}} h^*_{\vec{q}}(\vec{r},t) a^\dagger_{\vec{q}}|0\rangle|\varphi_{lp}\rangle dt \tag{20}$$

where

$$h_{\vec{q}}(\vec{r},t) = \frac{M_q}{\hbar\omega} e^{i\vec{q}\cdot\vec{r}t} e^{\frac{q^2}{2}\frac{\hbar}{2m\omega}(t^2-1)} - \frac{\alpha_{\vec{q}}}{\hbar\omega}\,. \tag{21}$$

This expression has been got using the generating function of the Hermite polynomials. Finally we note that $|\psi\rangle^{(1)}$ can be obtained from

$$|\psi\rangle = e^{-S_2}|\varphi_{lp}\rangle|0\rangle \tag{22}$$

with

$$S_2 = -\int_0^1 t^{\left[\frac{\omega_0}{\omega}-1\right]} \sum_{\vec{q}} \left[h_{\vec{q}}(\vec{r},t) a_{\vec{q}} - \text{h.c.}\right] dt\,, \tag{23}$$

by expanding the exponential e^{-S_2} and truncating the expansion at the first order. Taking into account also the unitary transformation in equation (14), the previous considerations lead us to assume as trial wave function for the Fröhlich Hamiltonian in the strong coupling limit:

$$|\psi_{\text{F}}\rangle = e^{-S_{\text{F}}}|\varphi_{lp}\rangle|0\rangle, \tag{24}$$

with

$$S_{\text{F}} = -\int_0^1 t^{\left[\frac{\omega_0}{\omega}-1\right]} \times \sum_{\vec{q}} \left[\frac{M_q}{\hbar\omega} e^{i\vec{q}\cdot\vec{r}t} e^{\frac{q^2}{2}\frac{\hbar}{2m\omega}(t^2-1)} a_{\vec{q}} - \text{h.c.}\right] dt\,. \tag{25}$$

We have indicated this coherent state with "F" since it is easy to show that the expectation value of the Fröhlich Hamiltonian on the state (25) gives:

$$E = \frac{3}{4}\hbar\omega - \alpha\hbar\omega_0\sqrt{\frac{\omega_0}{\omega}}\frac{\Gamma(\frac{\omega_0}{\omega})}{\Gamma(\frac{\omega_0}{\omega}+\frac{1}{2})}\,, \tag{26}$$

i.e. the Feynman result when the approximating action is represented by a fixed harmonic binding potential [12]. In equation (26) $\Gamma(x)$ is the Gamma function. In particular the minimization of E with respect to the variational parameter ω and the asymptotic expansion for $\alpha \to \infty$ restore equation (13). Then, the order beyond the Landau and Pekar's theory is due to the lattice fluctuations and to the consequent change in the electron wave function.

3.3 Improvements of the Feynman result

The next step is to try to improve the Feynman result. To this aim, we note that is possible to obtain an excellent approximation of the polaron ground state energy in equation (26) substituting in equation (25) $S_{\rm F}$ with:

$$S = -\sum_{\vec{q}} \left[\left(v_{\vec{q}} e^{i\vec{q}\cdot\vec{r}\eta} + u_{\vec{q}} e^{i\vec{q}\cdot\vec{r}} \right) a_{\vec{q}} - \text{h.c.} \right] \tag{27}$$

where

$$v_{\vec{q}} = \frac{M_q}{\hbar\omega} \int_0^a t^{\left[\frac{\omega_0}{\omega}-1\right]} e^{\frac{q^2}{2}\frac{\hbar}{2m\omega}(t^2-1)} \tag{28}$$

and

$$u_{\vec{q}} = \frac{M_q}{\hbar\omega} \int_a^1 t^{\left[\frac{\omega_0}{\omega}-1\right]} e^{\frac{q^2}{2}\frac{\hbar}{2m\omega}(t^2-1)} \ . \tag{29}$$

Here a and η are two variational parameters. In other words, we obtain the main contribution to the Feynman estimate of the electron self-energy approximating $S_{\rm F}$ as sum of two terms: the first one stems from the observation that the electron moves very fast in the induced potential well; the second one takes into account the lattice fluctuations and the possibility that they can follow instantaneously the electron motion. In order to improve the Feynman result, the Pekar's approach (Eq. (11)) and the previous analysis suggest us to try the following ansatz:

$$|\psi\rangle = e^{-\sum_{\vec{q}} \left[\left(s_{\vec{q}} e^{i\vec{q}\cdot\vec{r}} + l_{\vec{q}} e^{i\vec{q}\cdot\vec{r}\eta} \right) a_{\vec{q}} - \text{h.c.} \right]} |0\rangle |\varphi_p\rangle \tag{30}$$

with $|\varphi_p\rangle$ given by equation (11), η variational parameter and $l_{\vec{q}}$ and $s_{\vec{q}}$ functions to be determined by minimizing the expectation value of the Fröhlich Hamiltonian on this state. This last quantity turns out:

$$\begin{aligned} \langle\psi|H|\psi\rangle =& \langle\varphi_p|\frac{p^2}{2m}|\varphi_p\rangle + \sum_{\vec{q}} \left[\hbar\omega_0 \left(|l_{\vec{q}}|^2 + |s_{\vec{q}}|^2 \right) \right. \\ & \left. + \frac{\hbar^2 q^2}{2m} \left(\eta^2 |l_{\vec{q}}|^2 + |s_{\vec{q}}|^2 \right) \right] \\ & + \sum_{\vec{q}} \left[\left(\hbar\omega_0 + \frac{\hbar^2 q^2}{2m}\eta \right) \left(r_{\vec{q}} s_{\vec{q}} l^*_{\vec{q}} + \text{h.c.} \right) \right. \\ & \left. - \left(M_q s^*_{\vec{q}} + M_q r_{\vec{q}} l^*_{\vec{q}} + \text{h.c.} \right) \right] \end{aligned} \tag{31}$$

with

$$r_{\vec{q}} = \langle\varphi_p| e^{i\vec{q}\cdot\vec{r}(1-\eta)} |\varphi_p\rangle. \tag{32}$$

Making $\langle\psi|H|\psi\rangle$ stationary with respect to arbitrary variations of the functions $l_{\vec{q}}$ and $s_{\vec{q}}$, we obtain two, easily solvable, algebraic equations. The minimization and the asymptotic expansion of the ground state energy, for $\alpha \to \infty$, provide:

$$E = \left[-0.108507\alpha^2 - 1.89 \right] \hbar\omega_0. \tag{33}$$

The electron self-energy shows the exact dependence on α^2 in the strong coupling regime together with a good estimate of the e-ph coupling constant independent contribution due to the lattice fluctuations. This allows to obtain, for $\alpha \geq 8.7$, an upper bound for the polaron ground state energy better than the Feynman approach when the approximating action is represented by a fixed harmonic binding potential (Eq. (26)). On the other hand, both these methods give the same result for $\alpha \leq 6$, i.e. $E = -\alpha\hbar\omega_0$. However, both the methods show a discontinuity in the transition from the weak to strong coupling regime.

To overcome this difficulty one has to take into account the translational invariance. We construct an eigenstate of the total wave number by taking a superposition of the localized states (30) centered on any point of the lattice in the same manner in which one constructs a Bloch wave function from a linear combination of atomic orbitals:

$$|\psi_{(sc)}\rangle = \int \psi(\vec{r} - \vec{R}) d^3R \ . \tag{34}$$

The minimization, with respect to the variational parameters, of the expectation value of the Fröhlich Hamiltonian on this state, that accounts for the translationally symmetry, and the asymptotic expansion for $\alpha \to \infty$ provide:

$$E = \left[-0.108507\alpha^2 - 2.67 \right] \hbar\omega_0. \tag{35}$$

This upper bound is lower than the variational Feynman estimate which for large values of α assumes the form [12]:

$$E = \left[-\frac{\alpha^2}{3\pi} - 3\log 2 - \frac{3}{4} \right] \hbar\omega_0. \tag{36}$$

4 The weak coupling regime

When the value of α is very small the lattice follows adiabatically the electron. A good physical description of the polaron features in this regime is provided by the LLP approach [9]. The starting point is the observation that the total momentum operator:

$$\vec{P}_t = \vec{p} + \sum_{\vec{q}} \hbar\vec{q} a^\dagger_{\vec{q}} a_{\vec{q}} \tag{37}$$

is a motion constant, i.e. it commutes with the Hamiltonian. The conservation law of the total momentum is taken into account through the unitary transformation:

$$U = e^{i(\vec{Q} - \sum_{\vec{q}} \vec{q} a^\dagger_{\vec{q}} a_{\vec{q}})\cdot\vec{r}} \ , \tag{38}$$

where $\hbar\vec{Q}$ is the eigenvalue of $\vec{P}_t$. In this paper we are interested in the ground state properties of the e-ph coupled system, so that we will restrict ourselves to the case $\vec{Q} = 0$. The transformed Hamiltonian does not contain the electron variables and it is given by:

$$\begin{aligned} H_1 =& U^{-1} H U \\ =& \sum_{\vec{q}} \left(\hbar\omega_0 + \frac{\hbar^2 q^2}{2m} \right) a^\dagger_{\vec{q}} a_{\vec{q}} + \sum_{\vec{q}} (M_q a_{\vec{q}} + \text{h.c.}) \\ & + \frac{\hbar^2}{2m} \sum_{\vec{q}_1, \vec{q}_2} \vec{q}_1 \cdot \vec{q}_2 a^\dagger_{\vec{q}_1} a^\dagger_{\vec{q}_2} a_{\vec{q}_2} a_{\vec{q}_1}. \end{aligned} \tag{39}$$

The LLP wave function is:

$$|\psi\rangle = e^{\sum_{\vec{q}}\left(f_{\vec{q}}a_{\vec{q}}-\text{h.c.}\right)}|0\rangle, \tag{40}$$

where $|0\rangle$ is the phonon vacuum state and $f_{\vec{q}} = M_q/\left(\hbar\omega_0 + \frac{\hbar^2 q^2}{2m}\right)$. In other words $|\psi\rangle$ is the lowest energy state of the first two terms of the transformed Hamiltonian H_1. The use of this wave function is based on the physical assumption that, when the e-ph interaction is weak, there is not correlation among the emission of successive virtual phonons by the electron. This assumption restricts the validity of this approach to the regime characterized by small values of α. The ground state energy turns out $E = -\alpha\hbar\omega_0$. In other words, this method puts the results of the perturbation theory on variational basis.

To improve the LLP approximation [9], one has to introduce in the trial wave function a better description of the recoil effect of the electron, effect present only on average in LLP approach. This can be done using the following ansatz:

$$|\psi_{(wc)}\rangle = e^{\sum_{\vec{q}}\left(g_{\vec{q}}a_{\vec{q}}-h.c.\right)}\left[|0\rangle + \sum_{\vec{q}_1,\vec{q}_2} d_{\vec{q}_1,\vec{q}_2}a^{\dagger}_{\vec{q}_1}a^{\dagger}_{\vec{q}_2}|0\rangle\right], \tag{41}$$

that takes into account the correlation between the virtual emission of pairs of phonons [16]. In this paper we will choose:

$$g_{\vec{q}} = \frac{M_q}{\left(\hbar\omega_0 + \frac{\hbar^2 q^2}{2m}\epsilon^2\right)} \tag{42}$$

and

$$d_{\vec{q}_1,\vec{q}_2} = \gamma\hbar\omega_0\frac{\hbar^2}{2m}\vec{q}_1\cdot\vec{q}_2\frac{M_{q_1}}{\left(\hbar\omega_0 + \frac{\hbar^2 q_1^2}{2m}\delta^2\right)}\frac{M_{q_2}}{\left(\hbar\omega_0 + \frac{\hbar^2 q_2^2}{2m}\delta^2\right)}. \tag{43}$$

Here γ, δ and ϵ are three variational parameters that have to be determined by minimizing the expectation value of the Hamiltonian (1) on the state (41). This procedure provides as upper bound for the polaron ground state energy at small values of α:

$$E = -\alpha\hbar\omega_0 - 0.0123\alpha^2\hbar\omega_0, \quad \alpha \to 0\ , \tag{44}$$

i.e. the same result, at this order, of the Feynman approach [12]. We stress that, at the α^2 order, the result for the electron self-energy is:

$$E = -\alpha\hbar\omega_0 - 0.0159\alpha^2\hbar\omega_0 \tag{45}$$

as found by Hohler and Mullensiefen [17], Larsen [16] and Roseler [18].

5 All couplings

A careful inspection of the wave function (34) shows that is able to interpolate between strong and weak coupling regimes. On the other hand, for small values of α a better description of the polaron ground state features is provided by the wave function (41). Moreover, in the weak and intermediate e-ph coupling, $\alpha \leq 7$, these two solutions are not orthogonal and have non zero off diagonal matrix elements. This suggests that the lowest state of the system is made of a mixture of the two wave functions that give an accurate description of weak and strong e-ph coupling regimes. Then the idea is to use a variational method to determine the ground state energy of the Hamiltonian (1) by considering as trial state a linear superposition of the two previously discussed wave functions:

$$|\psi\rangle = \frac{A|\overline{\psi}_{(wc)}\rangle + B|\overline{\psi}_{(sc)}\rangle}{\sqrt{A^2 + B^2 + 2ABS}}, \tag{46}$$

where

$$|\overline{\psi}_{(wc)}\rangle = \frac{|\psi_{(wc)}\rangle}{\sqrt{\langle\psi_{(wc)}|\psi_{(wc)}\rangle}}, \quad |\overline{\psi}_{(sc)}\rangle = \frac{|\psi_{(sc)}\rangle}{\sqrt{\langle\psi_{(sc)}|\psi_{(sc)}\rangle}}, \tag{47}$$

and S is the overlap factor:

$$S = \frac{\langle\overline{\psi}_{(wc)}|\overline{\psi}_{(sc)}\rangle + \text{h.c.}}{2}. \tag{48}$$

In equation (46) A and B are two additional variational parameters that provide the relative weight of the two solutions in the ground state of the system. In this paper we perform the minimization procedure in two steps. First, the expectation values of the Fröhlich Hamiltonian on the two trial wave functions in equations (41) and (34) are minimized and the variational parameters are determined. Then, the minimization procedure discussed in the present section is carried out. This way to proceed simplifies significantly the computational effort and makes all described calculations accessible on a personal computer. An approach, similar to that one described in this section, has been successfully used for the Holstein model [19].

The procedure of minimization of the quantity $\langle\psi|H|\psi\rangle$ with respect to A and B gives for the polaron ground state energy

$$E = \frac{E_m - SE_c - \sqrt{\left(E_m - SE_c\right)^2 - \left(1-S^2\right)\left(E_{(wc)}E_{(sc)} - E_c^2\right)}}{1-S^2} \tag{49}$$

and for the ratio of the two parameters A and B

$$\frac{A}{B} = \frac{E_c - ES}{E - E_{(wc)}}\ . \tag{50}$$

Here $E_{(wc)} = \langle\overline{\psi}_{(wc)}|H|\overline{\psi}_{(wc)}\rangle$, $E_{(sc)} = \langle\overline{\psi}_{(sc)}|H|\overline{\psi}_{(sc)}\rangle$, $E_m = \left(E_{(wc)} + E_{(sc)}\right)/2$ and $E_c = \left(\langle\overline{\psi}_{(wc)}|H|\overline{\psi}_{(sc)}\rangle + \text{h.c.}\right)/2$.

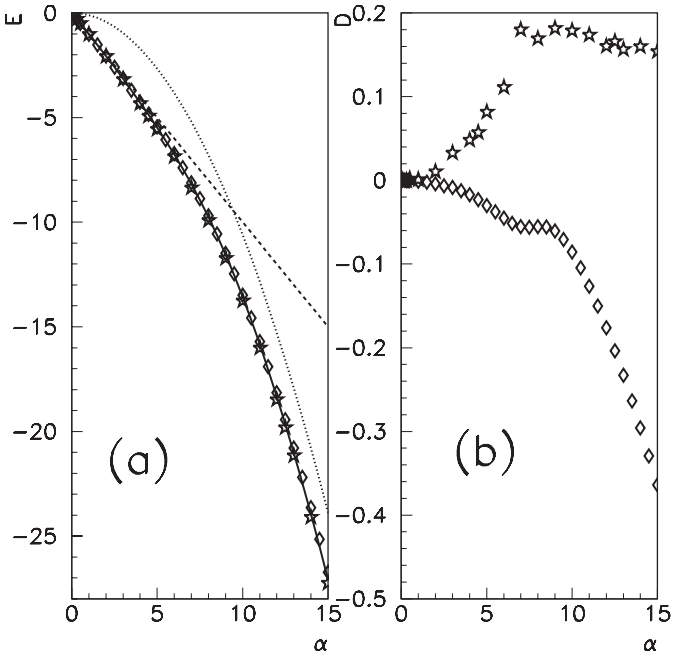

Fig. 1. (a) The polaron ground state energy, E, is reported as function of α in units of $\hbar\omega_0$. The data (solid line), obtained within the approach discussed in this paper, are compared with the results (diamonds) of the Feynman approach, $E_{\rm F}$, and the results (stars) of the diagrammatic Quantum Monte-Carlo method, $E_{\rm MC}$, kindly provided by A.S. Mishchenko. (b) The differences: $E - E_{\rm F}$ (diamonds) and $E - E_{\rm MC}$ (stars) are reported as function of α.

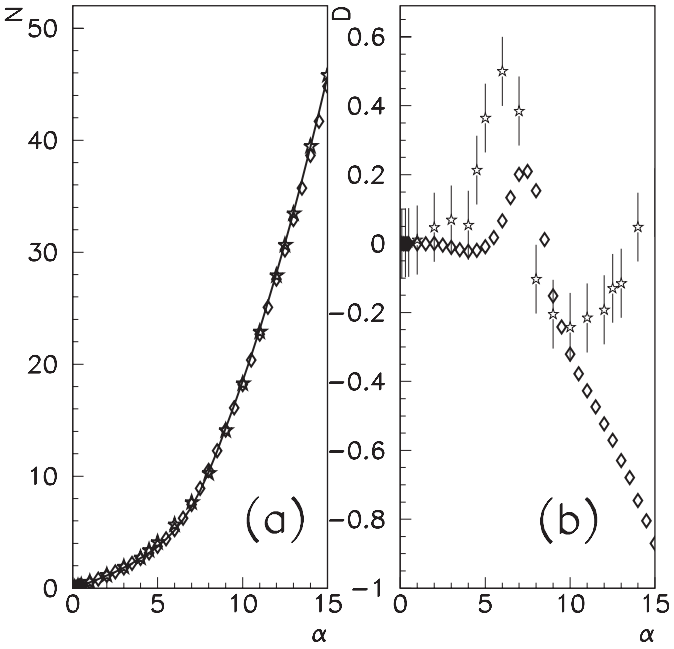

Fig. 2. (a) The mean number of phonons, N, is plotted as function of α. The data, obtained within the approach discussed in this paper (solid line), are compared with the results of the Feynman approach, $N_{\rm F}$ (diamond), and the results of the diagrammatic Quantum Monte-Carlo method, $N_{\rm MC}$ (stars), extracted from Figure 8 of reference [7]. (b) The differences: $N_{\rm F} - N$ (diamonds) and $N_{\rm MC} - N$ (stars) are reported as function of α. The error bars are due to uncertainty in the procedure used to extract the numerical values from Figure 8.

6 Numerical results

In Figure 1 we plot the polaron ground state energy, obtained within our approach, as a function of the e-ph coupling constant α. The data are compared with the results of the variational treatments due to Lee, Low and Pines [9], Pekar [10], Feynman [12] and with the energies calculated within a diagrammatic Quantum Monte-Carlo method [7]. As it is clear from the plots, our variational proposal recovers the asymptotic result of the Feynman approach in the weak coupling regime, improves the Feynman's data particularly in the opposite regime, characterized by values of the e-ph coupling constant $\alpha \gg 1$, and it is in very good agreement with the best available results in literature, obtained with the Quantum Monte Carlo calculation [7]. This agreement indicates that the true ground state wave function is very close to a superposition of the above introduced functions, that provide a very good description of the two asymptotic regimes. Within our approach we have also calculated the mean number of phonons present in the virtual phonon cloud surrounding the electron, N, the average electronic kinetic and interaction energies, K and I. These quantities are reported, respectively, in Figures 2, 3 and 4 where are compared with the same properties obtained in the Feynman's variational treatment based on path integrals [13]. As for the ground state energy, our variational ansatz is able to recover all the expected behaviors. For small values of α, $N \to \alpha/2$, $K \to \alpha\hbar\omega_0/2$, $I \to -2\alpha\hbar\omega_0$ as predicted by the LLP approach [9] and the weak coupling perturbation theory [17]. In the opposite regime the electron follows adiabatically the lattice polarization changes. The values $N = \frac{2\alpha^2}{3\pi}$, $K = \frac{\alpha^2}{3\pi}\hbar\omega_0$, $I = -\frac{4\alpha^2}{3\pi}\hbar\omega_0$ obtained within the Landau and Pekar's variational treatment (see Eq. (8)), based on the electron self-trapping with a Gaussian wave function, represent very accurate estimates of these quantities when they are calculated within the Feynman's approach. On the other hand, the values $N = 2{\times}0.108507\alpha^2$, $K = 0.108507\alpha^2\hbar\omega_0$, $I = -4 \times 0.108507\alpha^2\hbar\omega_0$ obtained within the Pekar's variational treatment (see Eq. (11)) represent very good approximations for the same quantities calculated within our approach. Then the variational Feynman's and our methods differ mainly in the strong coupling regime as it turns out from the plots in Figures 1, 2, 3 and 4. We stress that, in this range of values of α, our approach provides a better estimate of the polaron ground state energy than the Feynman's method [12].

Another physical quantity of interest is $\rho(\vec{r})$, i.e. the average ionic polarization charge density induced at a distance r by the electron. This quantity is related to the static correlation function between the electron

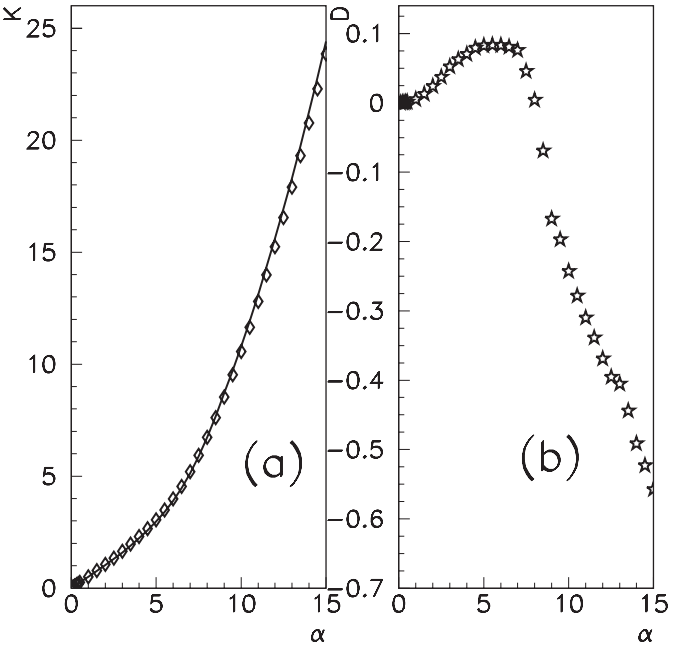

Fig. 3. (a) The average electronic kinetic energy, K, is plotted as function of α in units of $\hbar\omega_0$. The data (solid line), obtained within the approach discussed in this paper, are compared with the results (diamonds) of the Feynman approach, $K_{\rm F}$. (b) The difference: $K_{\rm F} - K$ (stars) is reported as function of α.

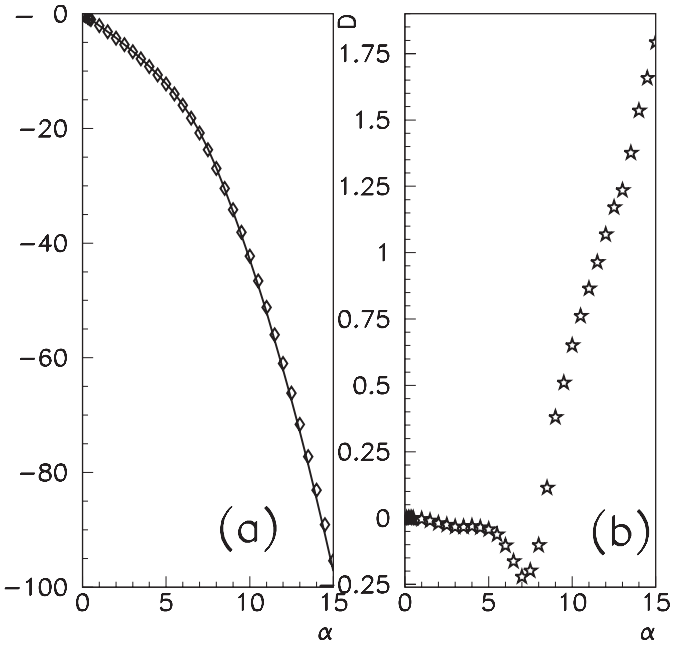

Fig. 4. (a) The average electronic interaction energy, I, is plotted as function of α in units of $\hbar\omega_0$. The data (solid line), obtained within the approach discussed in this paper, are compared with the results (diamonds) of the Feynman approach, $I_{\rm F}$. (b) The difference: $I_{\rm F} - I$ (stars) is reported as function of α.

position $\vec{r_e} = 0$ and the oscillator displacement at $\vec{r}$:

$$\rho(\vec{r}) = -\left(\frac{1}{4\pi e}\right)\langle\psi(\vec{r_e}=0)|\sum_{\vec{q}}(M_q e^{i\vec{q}\cdot\vec{r}}q^2 a_{\vec{q}} + \text{h.c.})|\psi(\vec{r_e}=0)\rangle. \tag{51}$$

It easy to show, analytically, that the exact sum rule for the total induced charge [20]:

$$\int \rho(\vec{r})d^3r = e\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right) \tag{52}$$

is satisfied within our variational approach. Figure 5 shows $\rho(\vec{r})/\int\rho(\vec{r})d^3r$ as a function of r for different values of the e-ph matrix element α corresponding to weak, intermediate and strong coupling regimes. Our data are compared with results obtained within the Feynman's method [13] and a path integral Monte Carlo scheme [20]. If the e-ph coupling is weak, the lattice deformation is not able to trap the charge carrier. The extension of the polaron is large compared with the characteristic length $\sqrt{\frac{\hbar}{2m\omega_0}}$. The situation is different in the opposite regime where the lattice deformation is localized around the electron. In any case also this correlation function, evaluated within our approach, is in agreement with the best data available in literature.

Finally Figure 6 shows the ground state spectral weight:

$$Z = |\langle\psi|c^\dagger_{\vec{k}=0}|0\rangle|^2, \tag{53}$$

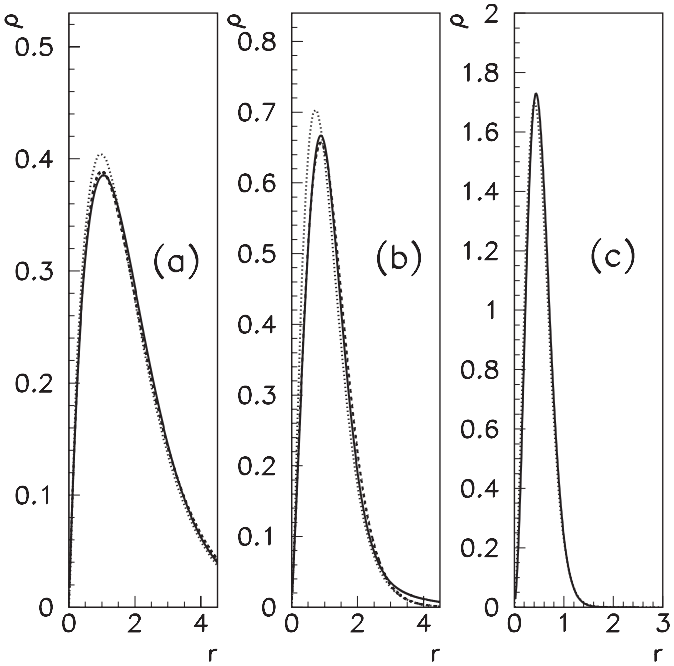

Fig. 5. The average normalized ionic polarization charge density, induced at a distance r by the electron, is reported for three different values of α: (a) $\alpha = 1$; (b) $\alpha = 6$; (c) $\alpha = 12$. The data (solid line), obtained within the approach discussed in this paper, are compared with the results (dashed line) of the Feynman approach and the results (dotted line) of the Monte-Carlo method, kindly provided by S. Ciuchi. The distance r is measured in units of R_p.

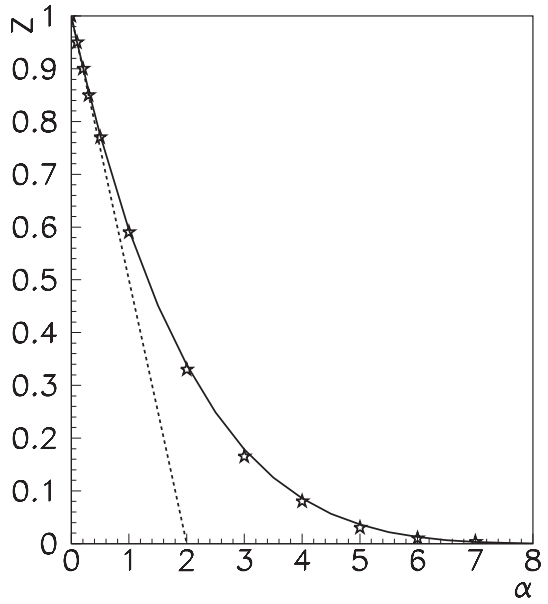

Fig. 6. The ground state spectral weight, Z, is plotted as function of α. The data (solid line), obtained within the approach discussed in this paper, are compared with the results (stars) of of the diagrammatic Quantum Monte-Carlo method. The result of the weak coupling perturbation theory (dashed line) is also indicated.

where $|0\rangle$ is the electronic vacuum state containing no phonons and $c^{\dagger}_{\vec{k}}$ is the electron creator operator in the momentum space. Z represents the renormalization coefficient of the one-electron Green's function and gives the fraction of the bare electron state in the polaron trial wave function. This quantity is compared with that one obtained in the diagrammatic Quantum Monte Carlo method [7]. The result of the weak coupling perturbation theory is also indicated: $Z = 1 - \alpha/2$. For small values of α the main part of the spectral weight is located at energies that correspond approximatively to the bare electronic levels. Increasing the e-ph interaction, the spectral weight decreases very fast and becomes practically zero in the strong coupling regime. Here the most part of the spectral weight is located at excited states. The diagrammatic Quantum Monte Carlo study [7] of the Fröhlich polaron has pointed out that there is no stable excited states in the energy gap between the ground state energy and the continuum. There are, instead, several many phonon unstable states at fixed energies: $E_f - E_0 \simeq 1, 3.5$ and $8.5\hbar\omega_0$. These results seem to be contrary to the data about the optical absorption of large polarons [21], which show, for large values of α, the presence of a very narrow peak corresponding to the electronic transitions from the ground state to the first relaxed excited state (RES). The nature of the excited states and the optical absorption of polarons in the Fröhlich model require further study which is beyond the scope of this paper.

In conclusion, in this paper, a variational approach has been developed to investigate the features of the Fröhlich model. It has been shown that a linear superposition of two wave functions, that describe the two asymptotic regimes of weak and strong e-ph coupling, provides an estimate of the polaron ground state energy which is in very good agreement with the best available results for any value of the e-ph matrix element. All the evaluated ground state properties show that the crossover between the two asymptotic regimes is very smooth. On the other hand the transfer of spectral weight from the polaron ground state to the higher energy bands turns out very fast. We stress that, to the best of our knowledge, it is the first time that a variational wave function, able to interpolate between the weak and strong e-ph coupling regimes, at least carefully as the Feynman method [12], is exhibited for the Fröhlich model.

References

1. A. Damascelli, Z. Hussain, Z.X. Shen, Rev. Mod. Phys. **75**, 473 (2003); S. Lupi, P. Maselli, M. Capizzi, P. Calvani, P. Giura, P. Roy Phys. Rev. Lett. **83**, 4852 (1999); A.J. Millis, Nature London, **392**, 147 (1998)
2. H. Fröhlich et al., Philos. Mag. **41**, 221 (1950); H. Fröhlich, in *Polarons and Excitons*, edited by C.G. Kuper, G.A. Whitfield (Oliver and Boyd, Edinburg, 1963), p. 1; for a review see: J.T. Devreese, *Polarons*, in: *Encyclopedia of Applied physics*, edited by G.L. Trigg (VCH, New York, 1996), Vol. 14, p. 383, and references therein
3. G. Höhler, A.M. Mullensiefen, Z. Physik **157**, 159 (1959); D.M. Larsen, Phys. Rev. **144**, 697 (1966); G.D. Mahan, in *Polarons in Ionic Crystals and Polar Semiconductors* (North-Holland, Amsterdam, 1972), p. 553; M.A. Smondyrev, Teor. Mat. Fiz. **68**, 29 (1986)
4. L.D. Landau, Phys. Z. Sowjetunion **3**, 664 (1933) [English translation: *Collected Papers* (Gordon and Breach, New York, 1965), pp. 67–68]; L.D. Landau, S.I. Pekar, J. Exptl. Theor. Phys. **18**, 419 (1948); S.I. Pekar, Zh. Eksp. i Theor. Fiz. **19**, 796 (1949); N.N. Bogoliubov, S.V. Tiablikov, Zh. Eksp. i Theor. Fiz. **19**, 256 (1949); S.I. Pekar, *Research in Electron Theory of Crystals* (Gostekhizdat, Moscow, 1951) [English translation: *Research in Electron Theory of Crystals*, US AEC Report AEC-tr-5575 (1963)]; S.V. Tiablikov, Zh. Eksp. i Theor. Fiz. **21**, 377 (1951); S.V. Tiablikov, Abhandl. Sowj. Phys. **4**, 54 (1954); G.R. Allcock, Adv. Phys. **5**, 412 (1956); G. Höhler in *Field Theory and the Many Body Problem*, edited by E.R. Caianiello (Accademic Press, 1961), p. 285; E.P. Solodovnikova, A.N. Tavkhelidze, O.A. Khrustalev, Teor. Mat. Fiz. **11**, 217 (1972); V.D. Lakhno, G.N. Chuev, Physics-Uspekhi **38**, 273 (1995)
5. D. Dunn, Can. J. Phys. **53**, 321 (1975)
6. T.D. Lee, F. Low, D. Pines, Phys. Rev. **90**, 297 (1953); M. Gurari, Phil. Mag. **44**, 329 (1953); E.P. Gross, Phys. Rev. **100**, 1571 (1955); G. Höhler, Z. Physik **140**, 192 (1955); G. Höhler, Z. Physik **146**, 372 (1956); R.P. Feynman, Phys. Rev. **97**, 660 (1955); Y. Osaka, Prog. Theor. Phys. **22**, 437 (1959); T.D. Schultz, Phys. Rev. **116**, 526 (1959); T.D. Schultz, in *Polarons and Excitons*, edited by C.G. Kuper, G.A. Whitfield (Oliver and Boyd, Edinburg, 1963), p. 71; D.M. Larsen, Phys. Rev. **172**, 967 (1968); J. Roseler, Phys. Stat. Sol. **25**, 311 (1968)

7. A.S. Mishchenko, N.V. Prokof'ev, A. Sakamoto, B.V. Svistunov, Phys. Rev. B **62**, 6317 (2000); N.V. Prokof'ev, B.V. Svistunov, Phys. Rev. Lett. **81**, 2514 (1998)
8. J.T. Titantah, C. Pierleoni, S. Ciuchi, Phys. Rev. Lett. **87**, 206406 (2001)
9. T.D. Lee, F. Low, D. Pines, Phys. Rev. **90**, 297 (1953)
10. L.D. Landau, Phys. Z. Sowjetunion **3**, 664 (1933) [English translation: *Collected Papers* (Gordon and Breach, New York, 1965), pp. 67–68]; L.D. Landau, S.I. Pekar, J. Exptl. Theor. Phys. **18**, 419 (1948); S.I. Pekar, *Research in Electron Theory of Crystals* (Gostekhizdat, Moscow, 1951) [English translation: *Research in Electron Theory of Crystals*, US AEC Report AEC-tr-5575 (1963)]
11. G. Höhler, Z. Physik **140**, 192 (1955); G. Höhler, Z. Physik **146**, 372 (1956)
12. R.P. Feynman, Phys. Rev. **97**, 660 (1955)
13. F.M. Peeters, J.T. Devreese, Phys. Stat. Sol. **115**, 285 (1983); F.M. Peeters, J.T. Devreese, Phys. Rev. B **31**, 4890 (1985)
14. S.J. Miyake, J. Phys. Soc. Jpn **38**, 181 (1975); S.J. Miyake, J. Phys. Soc. Jpn **41**, 747 (1976)
15. G.R. Allcock, Adv. Phys. **5**, 412 (1956)
16. D.M. Larsen, Phys. Rev. **172**, 967 (1968)
17. G. Höhler, A.M. Mullensiefen, Z. Physik **157**, 159 (1959)
18. J. Roseler, Phys. Stat. Sol. **25**, 311 (1968)
19. V. Cataudella, G. De Filippis, G. Iadonisi, Phys. Rev. B **60**, 15163 (1999); V. Cataudella, G. De Filippis, G. Iadonisi, Phys. Rev. B **62**, 1496 (2000)
20. S. Ciuchi, J. Lorenzana, C. Pierleoni, Phys. Rev. B **62**, 4426 (2000)
21. F.M. Peeters, J.T. Devreese, Phys. Rev. B **28**, 6051 (1983)