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STRONG-COUPLING LIMIT FOR ONE-DIMENSIONAL POLARONS IN A FINITE BOX

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I. INTRODUCTION

The one-dimensional polaron problem attracted attention because of its relevance in semiconductor physics, where it becomes possible to confine electrons in one direction[1] (i.e., quantum wires), and in linear polymers[2,3]. In the present paper we will focus on large polarons considering an extreme case of complete confinement into one dimension. Besides, there exist systems with anomaly high values of the electron-phonon coupling constant. Between those should be mentioned, e.g., protein globules[4] and solvated electrons in liquid ammonia[5]. This is why we consider here the strong-coupling limit.

In this limit the adiabatic approximation leads to a basic equation which describes the 1D polaron and is the known non-linear effective Schrödinger equation[6] relevant to many problems of non-linear physics such as self-trapping phenomena in nonlinear optics, Langmuir waves in plasmas, Ginzburg-Landau theory of superconductivity etc. (see Ref. 7 and references quoted herein). Usually it is solved on an infinite axis but in practice we never deal with systems of infinite size. Most of the numerical calculations use also a box with a large but finite length a to approximate the problem. So it is interesting to study the limit of an infinitely large box starting from a box with finite length. On the other hand, in the limit of small boxes one obtains the characteristics of a quantum dot which are the same as the one of a quantum particle in a box. Therefore we investigate the features of 1D polarons confined to external potentials such as 1) a δ-function potential (which imitates the Coulomb interaction in 1D) and 2) an infinitely deep potential well with finite size a.

Dealing with polarons in mentioned potentials we can find the so-called relaxed excited states (RES), which are the self-consistent solutions to the non-linear effective Schrödinger equation. The ionic polarization is then adapted to the final electronic configuration. The ground state and each RES generate an effective potential well in which different excited states can exist. For those excited states the polarization remains to the initial electronic configuration. The main goal of the present paper is to find all these states and the corresponding energy levels for 1D polarons. Besides, it could give us some estimates on polaron characteristics in 2D and 3D.

The paper is organized as follows. In Sec. III we obtained the characteristics of the 1D polaron in a δ-function potential using the results for the free 1D polaron (Sec. II). In Sec. IV we consider the excited states in the corresponding effective potential. The ground state and excited states of the 1D polaron in an infinite deep potential well are treated in Sec. V and Sec. VI, respectively.

II. STRONG COUPLING LIMIT AND THE SOLUTION FOR A FREE 1D-POLARON

The Hamiltonian of a polaron confined in a one-dimensional structure is of the form:

$$H = \frac{p^2}{2m} + \hbar \sum_k \omega_k a_k^\dagger a_k + U(z) + \sum_k \left[V_k a_k e^{ikz} + V_k^* a_k^\dagger e^{-ikz} \right]. \qquad (2.1)$$

Here z and p are the position and momentum operators of the electron, m is the electron band mass and ω_k is the frequency of the phonons with a wave vector k. In what follows we consider different external potentials $U(z)$. To start we choose $U(z) = U\,\delta(z)$ which corresponds to the conventional 3D Coulomb potential confined to a one-dimensional structure. Here we took its coupling constant U so that the case $U > 0$ corresponds to a repulsive potential.

As is well known[8] a ground state in the strong coupling limit is described by the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi(z)}{\partial z^2} + V_{eff}(z)\phi(z) = E\,\phi(z) \qquad (2.2)$$

with the effective potential

$$V_{eff}(z) = U\delta(z) + \sum_k |V_k|^2 \frac{|\rho_k|^2}{\hbar\omega_k} - \sum_k \frac{|V_k|^2}{\hbar\omega_k}\left[\rho_k^* e^{ikz} + \rho_k e^{-ikz}\right], \qquad (2.3)$$

where

$$\rho_k = \int_{-\infty}^{\infty} dz\, |\phi(z)|^2 e^{ikz}. \qquad (2.4)$$

In the case of an electron interacting with LO-phonons we have $\omega_k = \omega$ and

$$V_k = -i\hbar\omega \left(\frac{2\alpha'}{L}\sqrt{\frac{\hbar}{2m\omega}}\right), \qquad (2.5)$$

where α' is the dimensionless electron-phonon coupling constant and L is a size of the sample. It is convenient to introduce the dimensionless coupling constant U':

$$U = \hbar\omega\sqrt{\frac{\hbar}{m\omega}}\,U', \qquad (2.6)$$

as well as the ratio of the coupling constants

$$g = \frac{U'}{\alpha'}. \qquad (2.7)$$

Performing the scaling

$$z \to \frac{z}{\alpha'}\sqrt{\frac{\hbar}{m\omega}}, \qquad \phi\left(\frac{z}{\alpha'}\sqrt{\frac{\hbar}{m\omega}}\right) \to \left(\alpha'\sqrt{\frac{\hbar}{m\omega}}\right)^{1/2}\phi(z), \qquad (2.8)$$

we arrive at the Schrödinger equation in dimensionless units:

$$-\frac{1}{2}\frac{\partial^2\phi(z)}{\partial z^2} + V_{eff}(z)\phi(z) = \epsilon\,\phi(z), \qquad (2.9)$$

with

$$V_{\rm eff}(z) = g\delta(z) + \sqrt{2}\int_{-\infty}^{\infty} dz\,|\phi(z)|^4 - 2\sqrt{2}\,|\phi(z)|^2, \qquad (2.10)$$

and

$$\epsilon = E/\hbar\omega\alpha'^2. \qquad (2.11)$$

Equation (2.9) is the basic relation of the present paper. At $g = 0$ it is known as the time-independent non-linear Schrödinger equation[6].

Let us first remind its solution at $g = 0$ (free 1D polaron in the strong coupling limit). Eq. (2.9) is then of the form:

$$-\frac{1}{2}\phi'' + \sqrt{2}B\,\phi - 2\sqrt{2}\,\phi^3 - \epsilon\,\phi = 0 \qquad (2.12)$$

where

$$B = \int_{-\infty}^{\infty} dz\,\phi^4(z). \qquad (2.13)$$

Here we suppose $\phi(z)$ being a real function keeping in mind that the solution is defined up to the constant phase factor $\exp(i\chi)$.

The first integral (the energy conservation) of Eq. (2.12) can be obtained readily:

$$-\frac{1}{4}\phi'^2 + \frac{1}{\sqrt{2}}\,\phi^2\left(A - \phi^2\right) = C, \qquad (2.14)$$

where we used the notation

$$A = B - \frac{\epsilon}{\sqrt{2}}. \qquad (2.15)$$

The integration constant C should be equal to zero because the wave function $\phi(z)$ and its first derivative should disappear at infinity. Note that

$$0 \le \phi^2(z) \le A. \tag{2.16}$$

The solution of Eq. (2.14) is then of the form

$$\phi(z) = \frac{\sqrt{A}}{\cosh\left[2^{3/4}\sqrt{A}(z-r)\right]}, \tag{2.17}$$

where r is an arbitrary constant. Its presence here is related to the translation invariance of the system. The integrals in the normalization condition and the definition of the parameter B are calculated readily:

$$N = \int_{-\infty}^{\infty} \phi^2(z)dz = 2^{1/4}\sqrt{A},$$
$$B = \int_{-\infty}^{\infty} \phi^4(z)dz = \frac{2}{3}2^{1/4}A^{3/2}, \tag{2.18}$$

where from the results for A, B and the ground state ϵ follows [see Eq. (2.15)]:

$$A = \frac{1}{\sqrt{2}}, \qquad B = \frac{\sqrt{2}}{3}, \qquad \epsilon = -\frac{1}{3}. \tag{2.19}$$

With Eq. (2.19) and Eq. (2.10) one can find the analytical expression for the effective potential at $g = 0$:

$$V_{\rm eff}^{(0)}(z) = \frac{2}{3} - \frac{2}{\cosh^2\left[\sqrt{2}(z-r)\right]}. \tag{2.20}$$

The result $E = -\hbar\omega\alpha'^2/3$ for the 1D polaron ground state energy was found by Gross[8] (see also Ref. 9. This is the unique solution under the discussed assumptions. One can search for excited states in the given potential (2.20). Except of the continuous spectrum there is only a non-normalized kink-like solution

$$\phi_{ex}(z) = D\,\tanh[\sqrt{2}(z-r)] \tag{2.21}$$

with a positive energy $\epsilon_{ex} = 2/3$ which corresponds to the asymptotical value of the effective potential (2.20).

III. POLARON IN A δ-FUNCTION POTENTIAL

The solution of the previous Section for a free polaron can be used for regions which include at least one of the infinitely distant points $z = \pm\infty$. As an example

we consider now the case $g \neq 0$. In the regions to the right and to the left from the δ-function potential we have the same equation (2.12). Because one of the infinitely far points is included to each of these regions the integration constant C should be equal to zero for the same reasons. Thus the solution can be represented in the form

$$\phi(z) = \theta(z)\phi_{\rm R}(z) + \theta(-z)\phi_{\rm L}(z), \tag{3.1}$$

where $\phi_{\rm R}$ and $\phi_{\rm L}$ are of an analogous form as Eq. (2.17), perhaps, with different constants r. The wave function should be continuous at the point $z = 0$

$$\phi_{\rm R}(0) = \phi_{\rm L}(0) = \phi(0), \tag{3.2}$$

and its first derivative has a jump

$$\phi'_{\rm R}(0) - \phi'_{\rm L}(0) = 2g\phi(0). \tag{3.3}$$

The wave function $\phi(z)$ should be either a symmetrical or an antisymmetrical function of z which determines the relation between the functions $\phi_{\rm R}$ and $\phi_{\rm L}$:

$$\phi(-z) = \pm\phi(z) \rightarrow \phi_{\rm L}(z) = \pm\phi_{\rm R}(-z). \tag{3.4}$$

Using Eq. (2.17) we arrive at the solution for the symmetrical wave function

$$\phi(z) = \frac{\sqrt{A}}{\cosh\left[2^{3/4}\sqrt{A}(|z|-r)\right]}. \tag{3.5}$$

Note that the continuity condition (3.2) is already satisfied. Note also that the antisymmetrical solution is trivial ($\phi \equiv 0$). The constant A satisfies the same equation (2.15), where from one can find the ground state energy ϵ. But the constant r is not arbitrary any more: both A and r have to be defined from the normalization condition and the jump of the first derivative (3.3). The latter gives us the relation

$$\tanh\left(2^{3/4}\sqrt{A}r\right) = \frac{g}{2^{3/4}\sqrt{A}}. \tag{3.6}$$

From the normalization condition using Eq. (3.6) we arrive at the result

$$\sqrt{A} = \frac{\sqrt{2}-g}{2^{3/4}}, \qquad g < \sqrt{2}. \tag{3.7}$$

The expression for the constant r is then:

$$r = -\frac{\ln(1-g\sqrt{2})}{2(\sqrt{2}-g)}. \tag{3.8}$$

The integral defined as the constant B can then be calculated and therefore also the ground state energy:

$$B = \frac{\sqrt{2}}{3} - \frac{g}{2}, \qquad \epsilon = -\frac{1}{3} + \frac{g}{\sqrt{2}} - \frac{g^2}{2}. \tag{3.9}$$

With these results we obtain the effective potential

$$V_{\text{eff}}(z) = g\,\delta(z) + \frac{2}{3} - \frac{g}{\sqrt{2}} - \frac{(\sqrt{2}-g)^2}{\cosh^2\left[(\sqrt{2}-g)(|z|-r)\right]}, \tag{3.10}$$

where r is defined by Eq. (3.8).

Some analytical results we obtained are shown in Fig. 1-4. In Fig. 1 the polaron ground state energy is plotted versus the coupling constant g. As it follows from Eq. (3.8) the physical region is defined as $g \le 1/\sqrt{2}$, and the scaled energy reaches the value $\epsilon = -1/12$ in this limiting point which corresponds also to the maximum of $\epsilon(g)$. If $g > 1/\sqrt{2}$ the repulsion potential becomes so strong that it destroys the polaron state. The solution does not exist in this case. At large negative values of the coupling constant the energy behaves as $O(-g^2/2)$ that is as the energy of a quantum-mechanical particle in an attractive δ-function potential, which is strong enough to dominate over the electron-phonon interaction[10].

Fig. 2 shows the dependence of the parameter r on the coupling constant g. At positive values of g (repulsive potential) the constant r is positive [cfr. Eq. (3.8)]. It plays the role of the (dimensionless) distance between 'two parts' of the polaron as is clear from expression (3.5) for the wave function. When the coupling constant g reaches its limiting value $1/\sqrt{2}$ the parameter r becomes infinitely large. In the opposite limiting case $g = 0$ the parameter r also tends to zero. It becomes negative for the attractive potentials.

At $g > 0$ the polaron, that is the electron surrounded by a cloud of virtual phonons, can be found with the same probability on both sides of the δ-function potential. In this sense we can consider it as a quasi-bipolaron formed by two quasi-polarons attracted via phonons exchange and repulsed by the potential. The limiting case of infinitely separated quasi-polarons leads to the energy $\epsilon = -1/12$, that is the expression $\epsilon_1 = -1/24$ can be interpreted as the energy of a free quasi-polaron. Then the ground state energy ϵ of the Eq. (3.9) can be considered as the energy of a quasi-bipolaron. At $g = 0$, that is in the absence of the repulsion, it reaches the value $\epsilon_2 = -1/3$. The same relation $\epsilon_2 = 2^3\epsilon_1$ is valid also[11] for the energies of real free polarons and the energy of a real bipolaron when the Coulomb repulsion is "switched off". Thus the problem of a polaron in a δ-function potential indeed has common features with the problem of a bipolaron formed of two real polarons.

The effective potential for the case of the repulsion is shown in Fig. 3 for two values of the coupling constant g. The ground state energy, which is very close to $-1/12$ for both potentials, are shown also. When the absolute value of g decreases the barrier of this double well potential becomes lower and will disappear at $g = 0$.

Fig. 4 represents the effective potential for the case of an attractive δ-function potential. Again two different values of g are chosen and the corresponding ground state energies are shown. At large enough absolute values of g the polaron energy is lower than the bottom of the nonsingular part of the potential — polaron "occupies" the region of the δ-function.

Note that the effective potential is closely connected with the squared polaron wave function [see Eq. (2.10)]. So, there is no need to plot the latter.

IV. FRANCK-CONDON STATE IN A δ-FUNCTION POTENTIAL

Here we find excited states in the potential well (3.10). From symmetry properties it follows that symmetrical and antisymmetrical solutions can be represented, respectively, as

$$\phi^s(z) = \phi_R(|z|), \qquad \phi^a(z) = \text{sgn}(z)\,\phi_R(|z|), \tag{4.1}$$

where $\phi_R(z)$ are solutions at $z > 0$. The continuity conditions (3.2), (3.3) can be written in terms of this function:

$$\phi_R'(0) = g\,\phi_R(0) \quad \text{for symmetrical solutions,} \tag{4.2a}$$

$$\phi_R(0) = 0 \quad \text{for antisymmetrical solutions.} \tag{4.2b}$$

A function $\phi_R(z)$ is a solution of the Schrödinger equation in a modified Pöschl-Teller potential well. Therefore it can be written as a superposition of two basic solutions (hypergeometric functions)[12]. The wave function $\phi_R(z)$ should tend to zero for $z \to \infty$. The superposition where exponentially increasing terms are cancelled is as follows:

$$\phi_R(z) = N\frac{\pi}{2}\left[1+S^2(z)\right]\left[\kappa\,{}_2F_1\!\left(1-\frac{\kappa}{2}, 1+\frac{\kappa}{2}; \frac{1}{2}; -S^2(z)\right)\right.$$
$$\left.+(1-\kappa^2)\,S(z)\,{}_2F_1\!\left(\frac{3-\kappa}{2}, \frac{3+\kappa}{2}; \frac{3}{2}; -S^2(z)\right)\right] \tag{4.3}$$

with

$$S(z) = \sinh[(\sqrt{2} - g)(z - r)] \tag{4.4}$$

and where the 'mean separation' r is defined by Eq. (3.8) and the constant N is to be defined from the normalization condition. A parameter $\kappa > 0$ is related to the energy through the equation

$$\epsilon = \frac{2}{3} - \frac{g}{\sqrt{2}} - \kappa^2 \frac{(\sqrt{2} - g)^2}{2}. \tag{4.5}$$

As is seen the value $\kappa = 0$ corresponds to the asymptotical value of the effective potential (3.10) at infinity $(2/3 - g/\sqrt{2})$ and the value $\kappa = 1$ corresponds to the ground state energy (3.9). Substituting Eq. (4.3) into the continuity condition (4.2) one finds the parameter κ as a function of the coupling constant g and the subsequent energy levels if they exist. In what follows we will need the expression for $S(z)$ at the point $z = 0$:

$$S = S(0) = -\frac{g\sqrt{2}}{2\sqrt{1 - g\sqrt{2}}}. \tag{4.6}$$

For the numerical calculations it is convenient to use the integral representations of the hypergeometric functions in Eq. (4.3):

$$\phi_R(z) = N\,[1 + S^2(z)]\,\left\{\sin\frac{\pi\kappa}{2}\,I_1(z) + \cos\frac{\pi\kappa}{2}\,I_2(z)\right\} \tag{4.7}$$

with

$$I_1(z) = \int_0^1 dt \left(\frac{1-t}{t}\right)^{\kappa/2} \frac{1 - 4\,S^2(z)\,t(1-t)}{[1 + 4\,S^2(z)\,t(1-t)]^2},$$

$$I_2(z) = \int_0^1 dt \left(\frac{1-t}{t}\right)^{\kappa/2} \frac{4\,S(z)\,\sqrt{t(1-t)}}{[1 + 4\,S^2(z)\,t(1-t)]^2}. \tag{4.8}$$

Using those formulae we found the following results: There is only one symmetrical solution which is obtained from Eq. (4.2a) at $\kappa = 1$ and arbitrary coupling constant $g < 1/\sqrt{2}$. It coincides with the one described by Eq. (3.5), (3.7), (3.8), (3.9) and corresponds to the ground state. Besides, at $g > 0$ (that is, for the repulsive potential) there exists an antisymmetrical solution, which corresponds to the Franck-Condon excited state. When $g \to 0$ we have $\kappa \to 0$ and the antisymmetrical solution tends to the kink-like solution (2.21) for a free particle. When $g \to 1/\sqrt{2}$ the two potential wells are infinitely separated and the tunnelling between them becomes impossible. The energy of the excited state tends to the same limit as the ground state energy (that is, the level becomes twice degenerated). The energy of the Franck-Condon excited state is also plotted in Fig. 1.

V. POLARON IN AN INFINITE DEEP POTENTIAL WELL

In the preceding Section we exploit the solution for the 1D polaron on a half axis. The main goal of this Section is to find symmetrical and antisymmetrical solutions $\phi^{s(a)}(z)$ of Eq. (2.12) for a free polaron on a finite segment which does not include infinitely distant points $z = \pm\infty$. That is, we consider an infinitely deep potential well of width l:

$$U(z) = \begin{cases} \infty, & |z| > \dfrac{a}{2}, \\ 0, & |z| \le \dfrac{a}{2}, \end{cases} \qquad l = \frac{a}{\alpha'}\sqrt{\frac{\hbar}{m\omega}}. \tag{5.1}$$

In this potential we can't consider the constant C in Eq. (2.14) being equal to zero, which makes the solutions more complicated. We'll see that they can be represented as different Jacobian elliptic functions [see Ref. 13, ch. 16].

Let us introduce the notations for new parameters:

$$\sqrt{2}\,C = \Phi_1\,\Phi_2, \qquad A = \Phi_1 + \Phi_2 \tag{5.2}$$

Because of the symmetry we can always consider $\Phi_2 \ge \Phi_1$. Then Eq. (2.14) can be written in a form

$$\phi'^2(z) = 2\sqrt{2}\,(\phi^2(z) - \Phi_1)\,(\Phi_2 - \phi^2(z)). \tag{5.3}$$

We have to distinguish the cases:

$$\begin{aligned} &\textbf{Case 1}: \quad 0 \le \Phi_1 < \Phi_2, \\ &\textbf{Case 2}: \quad \Phi_1 = -|\Phi_1| \le 0. \end{aligned} \tag{5.4}$$

Let us consider first case 1. Evidently any solution takes its values between the constants Φ_1 and Φ_2. It follows then that the antisymmetrical solution which is equal to zero at $z = 0$ does not exist in this case. The integration of Eq. (5.3) gives us two symmetrical solutions

$$\phi^s_{1a}(z) = \sqrt{\Phi_1}\,\mathrm{nd}(2^{3/4}\sqrt{\Phi_2}\,z\,|m), \tag{5.5a}$$

$$\phi^s_{1b}(z) = \sqrt{\Phi_2}\,\mathrm{dn}(2^{3/4}\sqrt{\Phi_2}\,z\,|m), \tag{5.5b}$$

$$m = 1 - \frac{\Phi_1}{\Phi_2}, \qquad 0 < m \le 1. \tag{5.5c}$$

The parameter m is the modulus of the Jacobian elliptic functions, and both wave functions of Eq. (5.5a) and Eq. (5.5b) are periodical in z with a period $2^{1/4}\mathbf{K}(m)\sqrt{\Phi_2}$, where $\mathbf{K}(m)$ is the complete elliptic integral of the first kind:

$$\mathbf{K}(m) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - m\sin^2\theta}}. \tag{5.6}$$

The written functions can be obtained one from another by shifting with a half period.

Let us turn now to case 2. Then Eq. (5.2) can be written as follows:

$$\phi'^2(z) = 2\sqrt{2}\left(\phi^2(z) + |\Phi_1|\right)\left(\Phi_2 - \phi^2(z)\right). \tag{5.7}$$

Evidently any solution takes its values in the interval $[-\Phi_2, \Phi_2]$. There is a symmetrical solution

$$\begin{aligned} \phi_2^s(z) &= \sqrt{\Phi_2}\,\mathrm{cn}(2^{3/4}\sqrt{|\Phi_1| + \Phi_2}\,z\,|M), \\ M &= \frac{\Phi_2}{|\Phi_1| + \Phi_2}, \quad 0 < M \le 1. \end{aligned} \tag{5.8}$$

This solution is periodical in z with a period equal to $2^{5/4}\mathbf{K}(M)/\sqrt{|\Phi_1| + \Phi_2}$. Note that the modulus of this elliptic function is equal now to M.

Shifting the solution (5.8) by a quarter of the period we arrive at the antisymmetrical solution

$$\begin{aligned} \phi_2^a(z) &= -\sqrt{\frac{|\Phi_1|\Phi_2}{|\Phi_1| + \Phi_2}}\,\mathrm{sd}(2^{3/4}\sqrt{|\Phi_1| + \Phi_2}\,z\,|M) \\ &= \sqrt{\Phi_2}\,\mathrm{cn}(2^{3/4}\sqrt{|\Phi_1| + \Phi_2}\,z + \mathbf{K}(M)\,|M). \end{aligned} \tag{5.9}$$

It has the same period in z as the solution presented by Eq. (5.8)

Now we remind the definitions of different Jacobian elliptic functions being used in the present Section. They are given by the relations[13]:

$$\mathrm{sn}(u|m) = \sin\phi, \tag{5.10a}$$

$$\mathrm{cn}(u|m) = \cos\phi, \tag{5.10b}$$

$$\mathrm{dn}(u|m) = \left(1 - m\,\mathrm{sn}^2(u|m)\right)^{1/2}, \tag{5.10c}$$

$$\mathrm{nd}(u|m) = \left(1 - m\,\mathrm{sn}^2(u|m)\right)^{-1/2}, \tag{5.10d}$$

$$\mathrm{sd}(u|m) = \frac{\mathrm{sn}(u|m)}{\left(1 - m\,\mathrm{sn}^2(u|m)\right)^{1/2}}, \tag{5.10e}$$

where the amplitude ϕ is defined by the relation

$$u = \int_0^{\phi} \frac{d\theta}{\sqrt{1 - m\sin^2\theta}}. \tag{5.11}$$

We presented the complete set of solutions of Eq. (2.14) on a finite segment. They describe so called cnoidal waves, that is, the periodical excitations which can be found, e.g., in a book by Davydov[14]. Here we use them to find the wave-functions in an infinite deep potential well (5.1). Then one has to satisfy the boundary conditions

$$\phi(-a/2) = \phi(a/2) = 0. \tag{5.12}$$

Wave functions (5.5) do not satisfy these conditions. It follows from Eq. (5.12) and solutions (5.8), (5.9) that the potential width should be equal to an integer number of half waves (odd for the symmetrical and even for the antisymmetrical solutions):

$$a\sqrt{|\Phi_1| + \Phi_2} = n\,2^{1/4}\,\mathbf{K}(M), \quad n = 1, 2, \ldots . \tag{5.13}$$

Then we use the normalization condition which can be represented in the form [see Ref. 13, formulae (16.25), (16.26)]:

$$\begin{aligned} \int_{-a/2}^{a/2} dz\;\phi_2^{s(a)}(z)^2 &= \frac{2^{1/4}\,\Phi_2\,n}{\sqrt{|\Phi_1| + \Phi_2}} \int_0^{\mathbf{K}(M)} dz\;\mathrm{cn}^2(z|M) \\ &= \frac{\Phi_2\,a}{M}\left[\frac{\mathbf{E}(M)}{\mathbf{K}(M)} + M - 1\right] = 1. \end{aligned} \tag{5.14}$$

Here we used Eq. (5.13) which allowed us to reduce the integration over the width of the potential to that over a quarter of the period. The complete elliptic integral of the second kind with modulus M is defined as follows:

$$\mathbf{E}(M) = \int_0^{\pi/2} d\theta\sqrt{1 - M\sin^2\theta}. \tag{5.15}$$

Eq. (5.13) and (5.14) allow us to find the parameters $|\Phi_1|$ and Φ_2 and to obtain then the parameter $A = \Phi_2 - |\Phi_1|$. It is convenient to use as independent parameters M [see Eq. (5.8)] and Φ_2. Then $|\Phi_1| = \Phi_2(1 - M)/M$ and $A = \Phi_2(2M - 1)/M$.

To obtain the energy $\epsilon = \sqrt{2}(B - A)$ [see Eq. (2.15)] one has to calculate the parameter B of Eq. (2.13) which can be done using Ref. 15, formula (5.131):

$$B = \int_{-a/2}^{a/2} dz\, \phi_2^{s(a)}(z)^4 = \frac{2^{1/4}\,\Phi_2^2\, n}{\sqrt{|\Phi_1| + \Phi_2}} \int_0^{\mathbf{K}(M)} dz\, \mathrm{cn}^4(z|M)$$
$$= \frac{\Phi_2^2\, a}{3M^2}\left[(1-M)(2-3M) + 2(2M-1)\,\frac{\mathbf{E}(M)}{\mathbf{K}(M)}\right]. \qquad (5.16)$$

Introducing the notation

$$x = \frac{n^2}{a} \qquad (5.17)$$

and exploiting Eq. (5.13) to find Φ_2 we arrive at the equation for the parameter M as a function of x:

$$\sqrt{2}\,\mathbf{K}^2(M)\left[\frac{\mathbf{E}(M)}{\mathbf{K}(M)} + M - 1\right] = \frac{1}{x}. \qquad (5.18)$$

In these notations the energy is represented via a universal function F:

$$\epsilon_n = \frac{1}{n^2} F\left(\frac{n^2}{a}\right), \qquad (5.19)$$

where the expression for $F(x)$ follows from Eq. (5.16):

$$F(x) = \frac{\sqrt{2}}{3}\,(x\,\mathbf{K}(M))^2 \times \left[2M(1-M)\,x\,\mathbf{K}^2(M) - \sqrt{2}\,(2M-1)\right]. \qquad (5.20)$$

The function $F(x)$ is plotted in Fig. 5 as well as the dependence of the modulus M on x. The solutions and energy levels can be calculated with the help of those functions. Because the obtained solutions are self-consistent solutions of the non-linear effective Schrödinger equation, we obtain here the ground state ($n = 1$) and the RES states ($n = 2, 3, \ldots$) together with their energies. In Fig. 6, 7 the energy levels (arrows) as well as the corresponding effective potentials are shown for the ground state and the first two RES states for a box with length $a = 6$ and $a = 25$ respectively.

Let us discuss two limiting cases. When a is infinitely small, that is $x \to \infty$, we obtain from Eq. (5.18) that $x\,M \to 4\sqrt{2}/\pi^2$. Inserting this to Eq. (5.20) we arrive at the result

$$\lim_{x\to\infty} F(x) = \frac{\pi^2}{2}x^2. \qquad (5.21)$$

Taking into account that the energy here is given in units of $\hbar\omega\alpha'^2$ and the width of the potential $l = a\sqrt{\hbar/m\omega\alpha'^2}$ we arrive at the result for the quantum-mechanical particle in an infinitely deep potential:

$$\epsilon_n = \frac{\pi^2 n^2}{2\,a^2}, \qquad E_n = \frac{\hbar^2\pi^2 n^2}{2ml^2}. \qquad (5.22)$$

The interpretation of this limit is obvious: the interaction with the potential well is so strong that the electron-phonon interaction can be neglected even in the strong-coupling limit. The same is also true for higher excited states with large $n \gg 1$.

When $x \to 0$ that is the potential width becomes infinitely large, the parameter M tends to unity:

$$\mathbf{E}(1) = 1, \quad \mathbf{K}(M)_{M\to 1} \approx \frac{1}{2}\ln\left(\frac{16}{1-M}\right),$$
$$M \approx 1 - 16\exp\left(-\frac{\sqrt{2}}{x}\right). \qquad (5.23)$$

It follows then that $x\,\mathbf{K}(M) \to 1/\sqrt{2}$. Eq. (5.20) provides us then

$$\lim_{x\to 0} F(x) = -\frac{1}{3}, \qquad \epsilon_n = -\frac{1}{3n^2}. \qquad (5.24)$$

Thus, we obtained energy levels with a Coulomb like dependence on the quantum number n. The parameter $\Phi_1 \to 0$ in this limit so we are dealing with the frontier value between cases 1 and 2 of Eq. (5.4). When the modulus $M \to 1$ the period of the wave functions which is proportional to $\mathbf{K}(M)$ becomes infinitely large. The solution ϕ_2^s of Eq. (5.8) for the ground state ($n = 1$) then takes the form (note that $\Phi_2 \to A$)

$$\sqrt{A}\,\mathrm{cn}(2^{3/4}\sqrt{A}\,z\,|1) = \frac{\sqrt{A}}{\cosh(2^{3/4}\sqrt{A}\,z)}. \qquad (5.25)$$

This is the solution of the free 1D-polaron on an infinite axis with the energy $\epsilon_1 = -1/3$, which is reproduced by Eq. (5.24). For a large box with length a the solutions (5.8) and (5.9) with $n \neq 1$ can be considered as a superposition of n solutions of the type of Eq. (2.17) being infinitely separated from each other:

$$\phi_2(z) = \frac{1}{n2^{1/4}} \sum_{l=0}^{n-1} \frac{(-1)^l}{\cosh[\frac{\sqrt{2}}{x}(n\frac{z}{a} + \frac{n-1}{2} - l)]}. \qquad (5.26)$$

The limiting energy $\epsilon_n = -1/(3n^2)$ corresponding to the functions of Eq. (5.26) can be obtained from the known ground state solution in the single well by the following arguments. The normalization condition $N = 1$ [see Eq. (2.18)] has to be replaced by $n\,N = 1$ where from $A \to A_n = 1/(\sqrt{2}n^2)$ which is in agreement with Eq. (5.26). In a similar way the parameter B of Eq. (2.18) has to be replaced by

$B_n = n\,2^{5/4}A^{3/2}/3 = \sqrt{2}/(3\,n^2)$. Using A_n and B_n instead of the values of Eq. (2.19) leads us to the energies described by Eq. (5.24). Thus, these energies correspond to the ground state energies in a potential constructed of n independent Pöschl-Teller wells.

Note, that these solutions look like n quasi-particles. For example, the antisymmetrical solution at $n = 2$ reproduces in this limit the solution for the δ-function potential with a coupling constant $g = 1/\sqrt{2}$. The energy is in both cases $\epsilon_2 = -1/12$. These solutions did not appear in Sec. 2 while considering the free 1D-polaron on an infinite axis due to the boundary conditions. But taking into account that, in practice, we never deal with infinite sizes we can conclude that the energy levels (5.24) have physical meaning.

Comparing Fig. 6 and Fig. 7 we see that in Fig. 7 the energy levels for a box length $a = 25$ are already very good approaching the above result of Eq. (5.24), while they do not in Fig. 6 for $a = 6$. Therefore, a box with $a = 25$ can already be considered as a large box.

Applying the scaling relation[16,17]

$$E_{3D}(\alpha) \approx 3\,E_{1D}(\alpha/3), \tag{5.27}$$

we can *estimate* the subsequent energy levels for three-dimensional polarons ($\alpha = \alpha'$ in 3D case). Then we obtain from Eq. (5.24) and Eq. (5.27) for the 3D-polarons:

$$\epsilon_{3D,n} = E_{3D,n}/\hbar\omega\alpha^2 = -\frac{1}{9\,n^2}. \tag{5.28}$$

These values can be compared with the numerical calculations performed by the Pushchino-Dubna collaboration [see, e.g., Ref. 18]. From Table I we can see that the presented numerical values are rather close to each other which reveals the origin of the excited states reported in Ref. 18. For the completeness we estimate also the energy levels of the two-dimensional polaron ($\alpha' = \alpha(\pi/2)$ in this case):

$$E_{2D}(\alpha) \approx \frac{2}{3}E_{3D}\left(\frac{3\pi}{4}\alpha\right),$$
$$\epsilon_{2D,n} = E_{2D,n}/\hbar\omega\alpha^2 \approx -\frac{\pi^2}{24\,n^2} = -\frac{0.4112}{n^2}. \tag{5.29}$$

The direct calculation of the ground state energy gives the result[16] $\epsilon_{2D,1} = -0.4047$, which differs from our estimate by 1.6% only.

VI. THE COMPLETE SET OF EXCITED STATES IN AN INFINITE DEEP POTENTIAL WELL

To obtain the complete set of possible excited states for the 1D polaron confined to a box with length a, we should also investigate the excited states in the potential generated, e.g., by the ground state. In what follows we use the quantum number $n' \geq 1$ to enumerate those excited states, therefore $\epsilon_{n,n'}$ will be the energy of the n'-th state in a potential generated by the n-th solution corresponding to the quantum number n, found in the preceding Section.

To obtain those excited states numerical calculations are used. We expand the wave function in a Fourier series with unknown parameters a_k:

$$\phi(z) = \sum_{k=1}^{K} a_k \sin\frac{k\pi(z + a/2)}{a}, \tag{6.1}$$

restricting ourselves to K terms. Using this expansion and the Hamiltonian of Eq. (2.9) we calculate the Hamilton-matrix

$$H_{ij} = \int_{-a/2}^{a/2} dz\, \sin\frac{i\pi(z + a/2)}{a}\hat{H}\sin\frac{j\pi(z + a/2)}{a}. \tag{6.2}$$

The diagonalization of this matrix to the parameters a_k delivers us the eigen-energies and (after normalization) the corresponding wave functions of the ground state and $K - 1$ excited states. The larger is K the more accurate solutions will be obtained. The wavefunction of the ground state or RES by which the effective potential is generated can be compared with the analytical result of the same expansion (6.1) using formulae 16.23 of Ref. 13 for the wavefunctions in Eq. (5.8) and Eq. (5.9). The coefficients a_k (up to the common sign) are

$$a_{n(2l+1)} = (-1)^l \frac{2^{5/4}\pi n}{a}\frac{q^{l+1/2}}{1 + q^{2l+1}} \tag{6.3}$$

with

$$q = \exp\left(-\pi\frac{\mathrm{K}(1 - M)}{\mathrm{K}(M)}\right). \tag{6.4}$$

Here n is the same number as in Eq. (5.13). All other a_k in the expansion (6.1) are equal to zero. Thus, an exact expansion for the wave function corresponding to the quantum number n is of the form:

$$\phi = \frac{2^{5/4} n\pi}{a} \sum_{l\geq 0} (-1)^l \frac{q^{l+1/2}}{1+q^{2l+1}} \sin \frac{n(2l+1)\pi(z+a/2)}{a}. \qquad (6.5)$$

With n and a being given we obtain from Eq. (5.17), (5.18) the corresponding M which is used to calculate q. For example, we obtain for the ground state ($n = 1$) $q = 0.315$ and $q = 0.756$ for $a = 6$ and $a = 25$, respectively. The exact expansion shows us how fast the convergence of the series is. Therefore, we can calculate the Fourier series (6.5) and derive the number of terms needed to obtain results within a certain accuracy.

In Table II we present, as an example, the energies $\epsilon_{n,n'}$ for $n = 1 \div 5$ and $n' = 1 \div 5$ for a 1D-polaron in a box with length $a = 6$. The diagonal elements $\epsilon_{n,n}$ are nothing more than ϵ_n of the preceding Section, three of which are shown in Fig. 6. Indeed, let us consider the potential generated by the relaxed excited state corresponding to n. The corresponding wave function found in the preceding Section is "itself" the solution to the effective Schrödinger equation with this very potential. It has $n-1$ zeros and corresponds therefore to the energy level with $n' = n$ ($\epsilon_{n,n}$). Below it are the levels $\epsilon_{n,1}$, $\epsilon_{n,2}, \ldots, \epsilon_{n,n-1}$. Some of them could have a rather low energy. For instance, one can see from Table II that the ground state energy ($n' = 1$) and the first excited state ($n' = 2$) in a potential generated by the first relaxed excited state ($n = 2$) have lower energies than the first excited state ($n' = 2$) in a potential generated by the ground state ($n = 1$).

When the box size a becomes larger, the energy levels of the excited states in potentials generated by the ground state or a RES are becoming less separated. This is demonstrated in Fig. 8 for the six excited states ($n' = 1 \div 6$) in a potential generated by the second RES ($n = 3$). Their energies are plotted vs. the size of the box in the range $a = 5 \div 90$. We notice that only two limiting energy levels exist for a large box, namely: 1) the energy of the second excited state in this potential, which corresponds to the second relaxed excited state; all the underlying states converge to the same energy (therefore we have in this case a degeneracy of 3); 2) the energy of the excited states above the second excited state are all tending to the energy of the kink-like solution, that is, to the asymptotical value of the potential well ($\epsilon_{ex,3} = \sqrt{2}B_3 = 2/27$).

These numerical results can be explained as follows. It was found that $\epsilon_{n,n} \to -1/3n^2$ when the box is infinitely large. It was demonstrated also that the ground state energy $\epsilon_{n,1}$ also tends to the same limit. Thus, when the box becomes infinitely large all the states with $1 \leq n' \leq n$ tend to the same limiting energy $-1/3n^2$. In this case we deal with n infinitely separated wells without tunnelling between them.

n	1	2	3	4
ϵ_n	- 0.1085	- 0.0206	- 0.0083	- 0.0045
$\epsilon_{3D,n}$	- 0.1111	- 0.0278	- 0.0123	- 0.0069
$\epsilon_{2D,n}$	- 0.4112	- 0.1028	- 0.0457	- 0.0257

TABLE I. Four first energy levels for 3D-polarons taken from Ref. 18 (1st row) and estimated with the help of the scaling relation (2nd row). The estimates for 2D polarons are presented in the 3rd row.

n \ n'	1	2	3	4	5
1	- 0.332	0.905	1.516	2.444	3.662
2	- 0.031	0.180	1.197	2.129	3.354
3	0.039	0.399	0.874	2.119	3.336
4	0.017	0.419	1.092	1.836	3.339
5	0.015	0.425	1.107	2.056	3.071

TABLE II. The five first energy levels ($n' = 1 \div 5$) in potentials generated by the five first relaxed excited states ($n = 1 \div 5$) for a 1D polaron in a box of the size $a = 6$. Diagonal elements are the energies $\epsilon_{n,n}$ of the corresponding relaxed excited states.

So the resulted energy level indeed will be n times degenerated.

On the other hand, the only excited state in a single potential well is the kink-like solution (2.21) with an energy equal to the asymptotical value of the effective potential. If we deal with n infinitely separated potential wells the only difference is the dependence of this asymptotics on n (cfr. the parameter B_n in the preceding Section). Thus, the energies of all excited states with $n' > n$ should tend to the asymptotical value of the effective potential at infinity, namely to $\epsilon_{ex,n} = \sqrt{2}B_n = 2/(3n^2)$.

To conclude, we presented exact and numerical calculations for the 1D polaron, resp., in a δ-function potential and in an infinite deep potential well. We considered both relaxed excited states and excited states in the potentials generated by the ground state or a RES, and studied the limit of an infinitely large box. This limit demonstrates the existence of the whole set of energy levels which do not appear while solving the problem on an infinite axis.

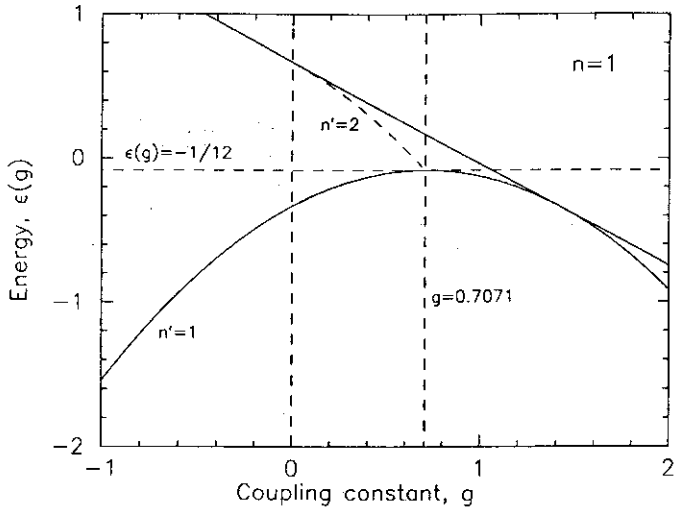

FIG. 1. A polaron energy vs. the scaled coupling constant (a solid curve). The physical region is defined as $g \leq 1/\sqrt{2} \approx 0.7071$, and the scaled ground state energy reaches the value $\epsilon = -1/12$ in the limiting point. The energy of the Franck-Condon excited state which exists at $0 < g < 1/\sqrt{2}$ is shown by the dashed curve. At $g = 1/\sqrt{2}$ it takes the same value as the ground state energy. At $g = 0$ it reaches the asymptotic value $2/3$ of the effective potential. The solid line shows this asymptotics at different values of g.

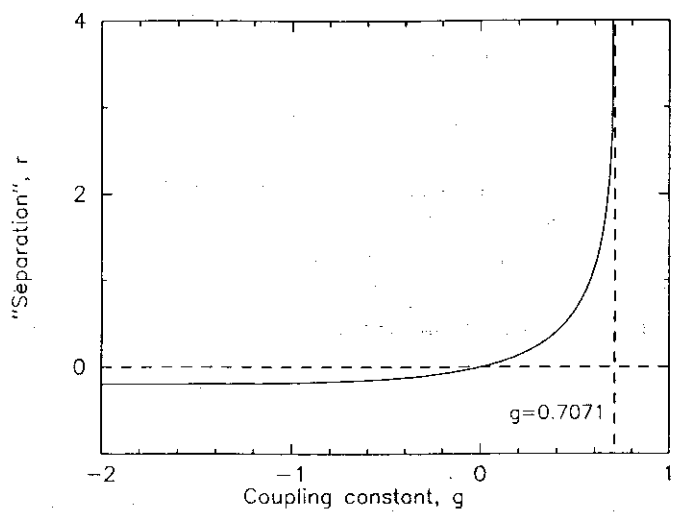

FIG. 2. A 'mean separation' of the polaron parts vs. the scaled coupling constant. When g is positive the parameter r indeed plays a role of a distance between 'two parts' of a polaron. It becomes infinitely large at $g = 1/\sqrt{2} \approx .7071$. When $g < 0$ (attractive δ-function potential) the parameter r becomes negative.

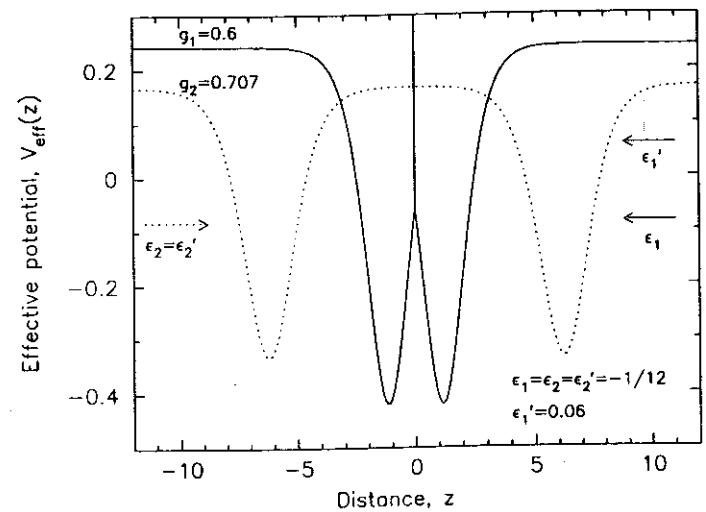

FIG. 3. Effective potentials for two different values g_a and g_b of the coupling constant $g > 0$ in the case of the repulsive δ-function. The arrows represent the energy levels. The ground state energies ϵ_a and ϵ_b of the corresponding potentials are very close to each other. For $g_b = 0.707$ the energy ϵ_b' of the Franck-Condon excited state has almost the same value as the ground state energy ϵ_b because g_b approaches the critical value $1/\sqrt{2}$.

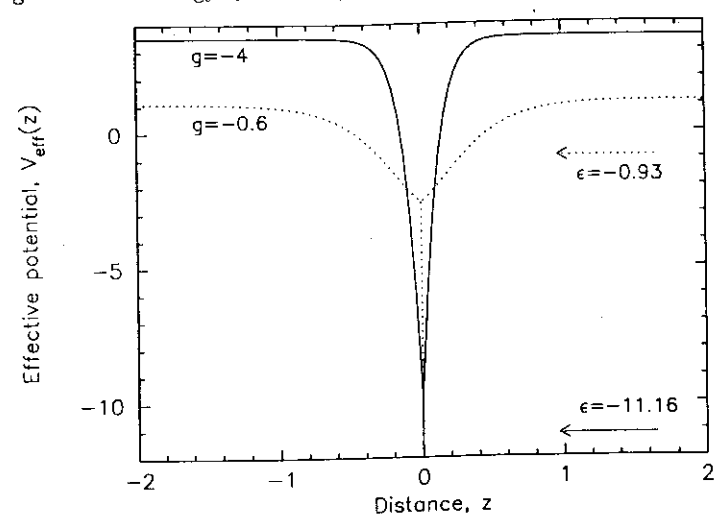

FIG. 4. Effective potentials for two different values g_a and g_b of the coupling constant $g < 0$ in the case of an attractive δ-function. The arrows represent the ground state energy levels, one of which lays below the bottom of the non-singular part of the potential. In this state a particle is located in the δ-function well.

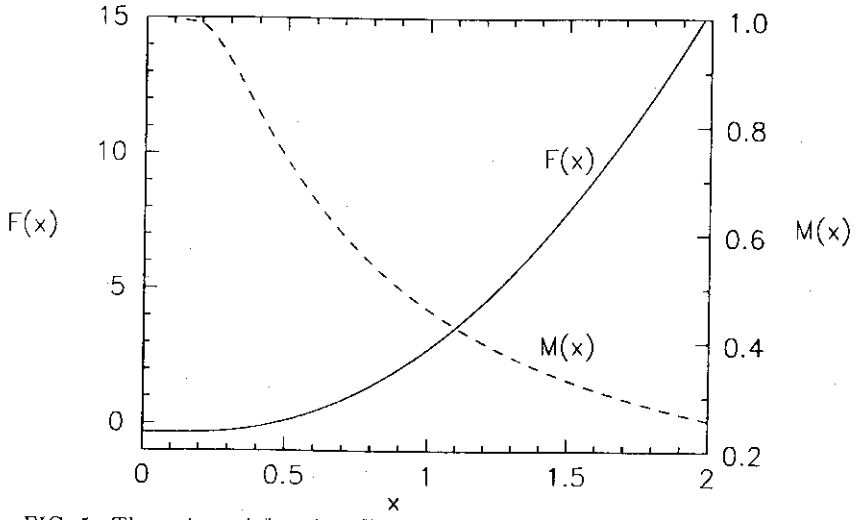

FIG. 5. The universal function $F(x)$, describing polaron energy levels in a infinitely deep potential well, is plotted vs. $x = n^2/a$ (solid line). At $x \to 0$ which corresponds to the limit of a free polaron, it tends to the value -1/3. At large x the asymptotic behavior is described by the same parabola which is characteristic for a quantum-mechanical particle. The dependence of the parameter M on x is shown also (dashed line).

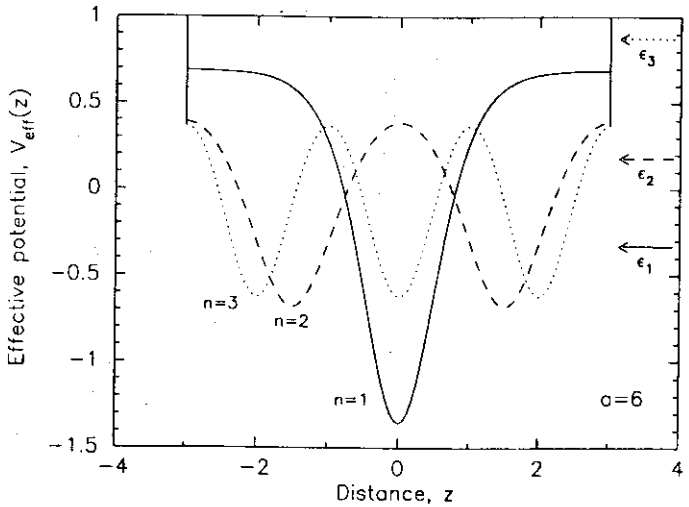

FIG. 6. The effective potentials are shown for the first three polaron states with $n = 1 \div 3$ in a box with length $a = 6$ (resp. the solid, the dashed and the dotted curve). The ground state energy (solid arrow) almost reaches its asymptotic value -1/3, the energy of the first (dashed arrow) and second (dotted arrow) relaxed excited states have positive energies and exceed their corresponding asymptotical value.

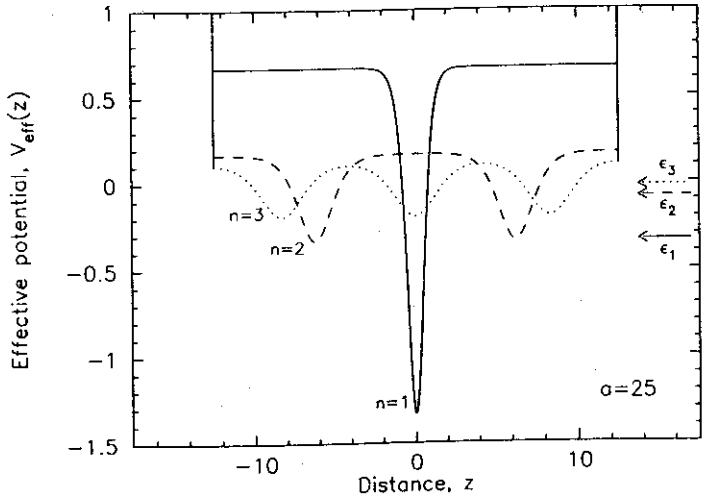

FIG. 7. The effective potentials are shown in this figure for the same states as in Fig. 6 but for $a = 25$ (resp. the solid, the dashed and the dotted curve). For larger values of a more levels have negative energies approaching their asymptotical values $-1/(3n^2)$. All three levels (see arrows) have negative energies and the first two of them practically coincide with -1/3 and -1/12, respectively.

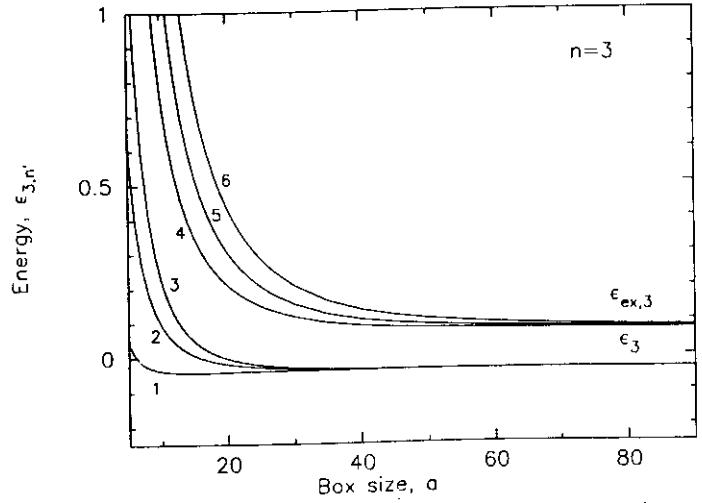

FIG. 8. The energies of the ground state ($n' = 1$) and of the five lowest excited states ($n' = 2 \div 6$) in the potential generated by the second relaxed excited state ($n = 3$) are plotted vs. the length of the box a . The relevant numbers n' are printed near the corresponding curves. Three of them tend to the limiting value $\epsilon_3 = -1/27$, all others to the asymptotical value $\epsilon_{ex,3} = 2/27$ of the effective potential at infinity.

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