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The Optical Polaron in a Slab-Like Confinement
البولارون الضوئي في شريحة كمية

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Abstract

The problem of a polaron in a quantum slab-like confinement is retrieved using a modified LLP approach. The proposed modification is intended to interpolate between the strong and weak-coupling limits of the problem. It is found that the binding energy increases with decreasing thickness of the slab as well as with increasing coupling constant. The polaronic effect becomes more important with decreasing thickness of the slab.

ملخص

درست مسألة البلارون في شريحة كمية باستخدام طريقة معدلة لنظريةLLP. التعديل المقترح يهدف إلى أن تكون النظرية صالحة لجميع قيم ثابت الربط بين الإلكترون و الفونون (حالة الربط الضعيفة وحالة الربط القوية). لقد وجد أن طاقة الربط تزيد مع نقصان سماكة الشريحة وزيادة قوة الربط البولاروني. كما أن التأثير البولاروني يكون أكثر أهمية كلما قلة سماكة الشريحة.

1. Introduction

Recent advances in microfabrication techniques have made the fabrication of low- dimensional structures possible and have therefore, tend to a great of work on the effect of the electron-phonon interaction in reduced dimensionality [1-6].

The problem of a polaron confined in a quantum dot has been studied extensively [7-14]. The common conclusion is that the phonon contribution to the binding energy is dependent on the size of the quantum dot as well as of the impurity in the quantum dot.

The problem of a polaron in quantum slab confinement has also been investigated using different approach [15].

Huang et al. [16] studied the energy and the effective mass as functions of the coupling constant and the thickness of the slab using the strong-coupling approximation.

Hai el al. [17] investigated the polaron effect on the cyclotron mass using a variational approach [18]. The temperature dependence on the properties of the strong coupling polaron in a slab of polar crystal was considered by Bao, E. and Xiao J.L [16]. They all found the binding energy decreases rapidly with increasing of slab thickness [15].

In this paper we revisit the problem of a polaron confined in a slab-like confinement, using modified LLP-theory. The modification we propose is intended to cover all the values of the coupling constant. A test of well-known limits of the problem is made.

2. Theory

The usual Fröhlich polaron Hamiltonian describing an electron confined in 2D and interacting with the optical phonon with a parabolic potential $V(z)$ is [5]

$$H = p^2 + \frac{1}{4}\omega^2 z^2 + \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q \left[a_Q e^{(i\vec{q}\cdot\vec{\rho})} + a_Q^\dagger e^{(-i\vec{q}\cdot\vec{\rho})}\right] , \quad (1)$$

H_e representing the electronic Hamiltonian:

$$H_z = p^2 + \frac{1}{4}\omega^2 z^2 \quad , \tag{2}$$

where $\vec{p}$ represents the momentum of the electron, and ω represents the strength of the quantum well potential that serves as a measure of the degree of confinement of the electrons:

$$\omega = (k/m\omega_{LO}^2)^{1/2} \quad ,$$

in which κ denotes the force constant, and $2m = \omega_{LO} = 1$ [in Fröhlich units]. m being the effective mass of the electron, and ω_{LO} the frequency of the the longitudinal optical phonons (LO). (Note that the thickness of the slab is proportional to the reciprocal of ω).

H_{ph} represents the phonon Hamiltonian, written as [19]

$$H_{ph} = \sum_Q a_Q^{\dagger} a_Q \tag{3}$$

Here $a_Q^{\dagger}(a_Q)$ are the creation (annihilation) operators for LO phonons of wave-vector $\vec{Q} = (\vec{q}, q_z)$, and V_Q is the amplitude of the electron-phonon interactions given [19]

$$V_Q = -i(\frac{\hbar\omega_{LO}}{Q})(\frac{4\pi\alpha}{V})^{1/2}(\frac{\hbar}{2m\omega_{LO}})^{1/4} \quad , \tag{4}$$

where $\hbar\omega_{LO}$ is the energy of the phonons, V is the volume of the crystal taken as a unit, and α is the standard dimensionless coupling constant of the electron-phonon interaction, given as [19]

$$\alpha = \frac{e^2}{2\hbar\varepsilon_0}\sqrt{\frac{2m}{\hbar\omega_{LO}}}(\frac{\varepsilon_0}{\varepsilon_\infty} - 1) \quad , \tag{5}$$

$\varepsilon_\infty(\varepsilon_0)$ being the high frequency (static) dielectric constant of the medium.

For the mixed-coupling approximation to be adopted for such a problem, we propose a modification to the first LLP-transformation. Our proposed U_1 is [14]

$$U_1 = \exp[i(\vec{P}_\rho - \vec{\Pi}_\rho).b\vec{\rho}] \quad , \tag{6}$$

where U_1 is the unitary transformation related to the electron operator: this transformation eliminates the electron operators from the electron-phonon part of the Hamiltonian, $\vec{P}_\rho$ is the total-momentum operator of the polaron in 2D:

$$\vec{P}_\rho = \vec{p}_\rho + \Sigma_Q \vec{q} a_Q^\dagger a_Q \quad . \tag{7}$$

$\vec{\Pi}_\rho$ represents the momentum of phonons

$$\vec{\Pi}_\rho = \Sigma_Q \vec{q} a_Q^\dagger a_Q \quad . \tag{8}$$

The modification made here is the insertion of another variational parameter b in Eq.(6). This parameter is proposed to trace the problem from the strong-coupling limit $(b = 0)$ to the weak-coupling limit $(b = 1)$.

The second transformation is of the form:

$$U_2 = \exp[\Sigma_Q u_Q (a_Q^\dagger - a_Q)] \quad . \tag{9}$$

u_Q is treated as a variational function. This transformation is called the displaced oscillator and is related to the phonon operators via Eq.(9). The phonon wave function is

$$\Phi_{ph} = U_2|0_{ph}\rangle \quad , \tag{10}$$

where the ket $|0_{ph}\rangle$ is the phonon vacuum state, so called because at low temperature $(K_B T << \hbar\omega_{LO})$, there will be no effective phonons, (K_B is Boltzmann's constant and T the absolute temperature) [19], [20]. The ground-state energy of the polaron can be obtained as [14]

$$E_g = \langle 0_{ph}|\langle 0_e|U_2^{-1}U_1^{-1}HU_1U_2|0_e\rangle|0_{ph}\rangle \tag{11}$$

$$= \langle 0_{ph}|\langle 0_e|U_2^{-1}H'U_2|0_e\rangle|0_{ph}\rangle \quad ,$$

where

$$H' \rightarrow U_1^{-1}HU_1 \quad ,$$

and $|0_e\rangle$ is the electron state [21].

Applying the first LLP transformation to each part of the Hamiltonian, we get [3]

$$H' = p^2 + b^2(P_\rho - \Pi_\rho)^2 + 2bp_\rho(P_\rho - \Pi_\rho) + \frac{1}{4}\omega^2 z^2 \tag{12}$$

$$+ \sum_Q a_Q^\dagger a_Q + \sum_Q V_Q\left[a_Q e^{i(1-b)\vec{q}\cdot\vec{\rho}} + a_Q^\dagger e^{-i(1-b)\vec{q}\cdot\vec{\rho}}\right] \quad .$$

From Eq.(12) it is clear that when $b = 1$, the terms $e^{\pm(1-b)\vec{q}\cdot\vec{\rho}}$ will be eliminated, leading to the weak-coupling approach. Now, applying the second LLP-transformation U_2 of Eq.(9), one can transform the Hamiltonian of Eq.(12) transforms as [14]

$$H'' = p_\rho^2 + p_z^2 + \frac{1}{4}\omega^2 z^2 + b^2(P_\rho - \Pi_\rho)^2 + b^2[\Pi_\rho^{(0)}]^2 + \Sigma_Q\ a_Q^\dagger a_Q \tag{13}$$

$$+\sum_Q u_Q^2 + b^2(\Pi_\rho^{(1)} - 2\Pi_\rho)\Pi_\rho^{(1)} + 2b^2(P_\rho - \Pi_\rho^{(0)})\Pi_\rho^{(1)} + 2b^2\Pi_\rho^{(0)}\Pi_\rho - 2b^2 P_\rho \Pi_\rho^{(0)}$$

$$\Sigma_Q\ V_Q u_Q [e^{i(1-b)\vec{q}.\vec{\rho}} + e^{-i(1-b)\vec{q}.\vec{\rho}}] + 2bp_\rho(P_\rho - \Pi_\rho + \Pi_\rho^{(1)} - \Pi_\rho^{(0)})$$

$$+\Sigma_Q\ [V_Q e^{i(1-b)\vec{q}.\vec{\rho}} - u_Q]a_Q + \Sigma_Q\ [V_Q\, e^{-i(1-b)\vec{q}.\vec{\rho}} - u_Q]a_Q^\dagger \quad .$$

where $\overleftarrow{\Pi}$ is given in Eq.(8), and

$$\overleftarrow{\Pi}_\rho^{(1)} = \Sigma_Q\ \vec{q} u_Q (a_Q^\dagger + a_Q) \quad , \tag{14}$$

$$\overleftarrow{\Pi}_\rho^{(0)} = \Sigma_Q\ \vec{q} u_Q^2 \quad . \tag{15}$$

The ground-state energy can be obtained as

$$E_g = \langle 0_e|p^2|0_e\rangle + \langle 0_e|\frac{1}{4}\omega^2 z^2|0_e\rangle + b^2 P_\rho^2 - 2b^2 P_\rho \Pi_\rho^{(0)} \tag{16}$$

$$+b^2[\Pi_\rho^{(0)}]^2 + \sum_Q u_Q^2(1 + b^2 q^2) + \langle 0_e|\langle 0_{ph}|2bp_\rho(P_\rho - \Pi_\rho + \Pi_\rho^{(1)} - \Pi_\rho^{(0)})|0_{ph}\rangle|0_e\rangle$$

$$-\Sigma_Q\ V_Q u_Q \langle 0_e|e^{-i(1-b)\vec{q}.\vec{\rho}}|0_e\rangle - \Sigma_Q\ V_Q u_Q \langle 0_e|e^{i(1-b)\vec{q}.\vec{\rho}}|0_e\rangle \quad .$$

or

$$E_g = \varepsilon_k + b^2 P_\rho^2 - 2b^2 P_\rho \Pi_\rho^{(0)} + b^2[\Pi_\rho^{(0)}]^2 \tag{17}$$

$$+\Sigma_Q\ u_Q^2(1 + b^2 q^2) - 2\Sigma_Q\ V_Q u_Q S_q \quad ,$$

where ε_k is

$$\langle 0_e | p_\rho^2 + p_z^2 + \frac{1}{4}\omega^2 z^2 | 0_e \rangle \quad , \tag{18}$$

and S_q is

$$\langle 0_e | e^{\pm i(1-b)\vec{q}\cdot\vec{r}} | 0_e \rangle \quad . \tag{19}$$

Expressing the coordinates and momenta of the electron as [22]

$$p_\mu = \lambda_1^{\frac{1}{2}}(\sigma_\mu + \sigma_\mu^\dagger) \quad . \tag{20}$$

$$x_\mu = i/\lambda_1^{-\frac{1}{2}}(\sigma_\mu - \sigma_\mu^\dagger) \tag{21}$$

$$p_z = \lambda_2^{\frac{1}{2}}(\sigma_z + \sigma_z^\dagger) \quad . \tag{22}$$

$$z = i/\lambda_2^{-\frac{1}{2}}(\sigma_z - \sigma_z^\dagger) \quad , \tag{23}$$

where the index μ refers to the x and y directions, λ_1, λ_2 are variational parameters, and $\sigma^\dagger(\sigma)$ are the creation (annihilation) operators for the electron. Performing some straightforward calculations, we obtain the ground-state energy of the polaron as

$$E_g = \varepsilon_k + b^2 P_\mu^2 - 2b^2 P_\mu \Pi_\rho^{(0)} + b^2 [\Pi_\rho^{(0)}]^2 \tag{24}$$

$$+ \sum_Q u_Q^2 (1 + b^2 q^2) - 2\sum_Q V_Q u_Q S_q \quad .$$

Minimizing Eq.(24) with respect to the variational function u_Q, we get

$$[1 - 2b^2(P_\rho - \Pi_\rho^{(0)})q + b^2 q^2]u_Q - V_Q S_q = 0 \quad , \tag{25}$$

where $\vec{\Pi}_\rho^{(0)}$ differs from the total momentum by a scalar factor:

$$\vec{\Pi}_\rho^{(0)} = \eta \vec{P}_\rho \quad . \tag{26}$$

So we can write u_Q as

$$u_Q = \frac{S_q V_Q}{1 - 2b^2(1-\eta)qP_\rho + b^2 q^2} \quad , \tag{27}$$

in which the unknown scalar η is determined by

$$\vec{\Pi}_\rho^{(0)} = \sum_Q \vec{q} u_Q^2$$

$$\eta P_\rho = \frac{q S_q^2 V_Q^2}{[1 - 2b^2(1-\eta)qP_\rho + b^2 q^2]^2} \quad . \tag{28}$$

Then

$$E_g = \varepsilon_k + \sum_Q \frac{S_q^2 V_Q^2 (1 + b^2 q^2)}{[1 - 2b^2(1-\eta)qP_\rho + b^2 q^2]^2}$$

$$-2\sum_Q \frac{S_q^2 V_Q^2}{[1 - 2b^2(1-\eta)qP_\rho + b^2 q^2]} + b^2(1-\eta)^2 P_\rho^2 \quad . \tag{29}$$

But E_g may be well represented by the first two terms of a power series expansion in P^2 as [20]

$$E_g(P) = E_g(0) + cP^2/2 + O(P^4) + \ldots \tag{30}$$

The effective mass of the polaron is then c^{-1}.

By comparing equations (29) and (30), we conclude that the expression for the ground-state energy is [14]

$$E_g(0) = \varepsilon_k - \sum_Q \frac{S_Q^2 V_Q^2}{[1+b^2 q^2]} \quad , \tag{31}$$

and the mass of the polaron is

$$m_p = \frac{1}{2[b^2(1-\eta)^2]} \quad . \tag{32}$$

Then, ε_K and S_q are found to be

$$\varepsilon_k = \frac{\omega^2}{4\lambda_2} + \frac{\lambda_1}{2} + \frac{\lambda_2}{4} \quad . \tag{33}$$

$$S_q = e^{-(1-b)^2 q^2 / 2\lambda_1} \quad , \tag{34}$$

where λ_1, λ_2 are two variational parameters.

So, E_g can be written as

$$E_g = \frac{\omega^2}{4\lambda_2} + \frac{\lambda_1}{2} + \frac{\lambda_2}{4} - \sum_Q V_Q^2 \frac{e^{-(1-b)^2 q^2 / \lambda_1}}{[1+b^2 q^2]} \quad . \tag{35}$$

This last equation gives the general formula for the ground-state energy of the confined polaron. This formula enables us to find the binding energy of the 2D polaron in both weak- and strong-coupling ranges. The calculations depend on the values of b.

The binding energy of the 2D polaron is given as

$$\varepsilon_p = \frac{\omega}{2} - E_g \quad . \tag{36}$$

3. Results and Discussions

First, let us test our theory for some limiting cases. In the limit $b \to 0$, the ground-state energy of Eq.(35) becomes

$$E_g = \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \Sigma_Q V_Q^2 e^{-q^2/\lambda_1} \quad . \tag{37}$$

In the strict 2D limit, $\lambda_2 = \omega \to \infty$, therefore the value of λ_1 which minimizes E_g can be obtained numerically as

$$\lambda_1 = \frac{\pi\alpha^2}{4} \quad .$$

Projecting out the $\vec{Q}$-summation in Eq.(37), we obtain

$$\varepsilon_p^{(2D)} = \frac{\pi\alpha^2}{8} \quad . \tag{38}$$

This result agrees with the result obtained in [22] using the strong-coupling theory.

Also, in the limit $b \to 1$, the ground-state energy describes the case of weak-coupling as

$$E_g = \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \Sigma_Q \frac{V_Q^2}{[1+q^2]} \quad . \tag{39}$$

In the strict 2D limit, $\lambda_2 = \omega \to \infty$, therefore the value of λ_1 which minimizes E_g can be obtained numerically as $\lambda_1 = 0$.

Projecting out the $\vec{Q}$-summation in Eq.(39), we finally obtain

$$\varepsilon_p^{(2D)} = \frac{\pi}{2}\alpha \quad . \tag{40}$$

This is the weak-coupling 2D-result, and it agrees with the result obtained in [23] using perturbation theory.

Letting the values of the parameter b be determined variationally, together with the parameters λ_1 and λ_2, the formula given in Eq.(35) is supposed to describe the ground-state energy of the problem for all values of the coupling constant.

From the numerical calculations, we see that b varies from 0 to 1 as α changes from small values to large values, respectively.

To show the effect of the slab thickness on the energy we display in Figs. 1 and 2 the binding energy ε_p as a function of the degree of confinement ω, and as a function of the slab thickness D(remember that the thickness $D \propto \frac{1}{\omega}$). The figures are plotted for three values of $\alpha(\alpha = 0.5, 1.0, 5.0)$. As is clear from the figures, the binding energy decreases sharply with increasing thickness (decreasing degree of confinement). The effect of the electron-phonon interaction (through α) is more important for small values of the slab thickness. This is understandable because, for small values of D, the problem becomes more confined and this, in turn, enhances the importance of the polaronic effect.

When $\omega \to 0$, the result goes to the 3D limit. While for large values of ω, the result approaches the 2D-limit (see Figure 1).

To study the effect of the coupling constant on the energy explicitly, we plot in Fig.3 ε_p versus α for two values of $\omega(\omega = 1.0, \omega = 10)$. As expected, the binding energy increases with increasing α as well as with increasing ω. The two curves coincide for large values of α due to the fact that in that limit the polaronic effect is dominant over the effect of the degree of confinement. It should be noted that, by increasing the degree of confinement, the polaronic effect increases implicitly and this means that α and ω do not inter the problem independently but rather in an interrelated manner.

4. Conclusion

A modification to the LLP approach has been proposed for studying the polaron problem in a quantum slab-like confinement. and for interpolating between the strong- and weak-coupling limits of the problem.

It is found that the binding energy increases with increasing degree of confinement as well as increasing coupling constant α.

The polaronic effect is found to be more pronounced for large values of degree of confinement.

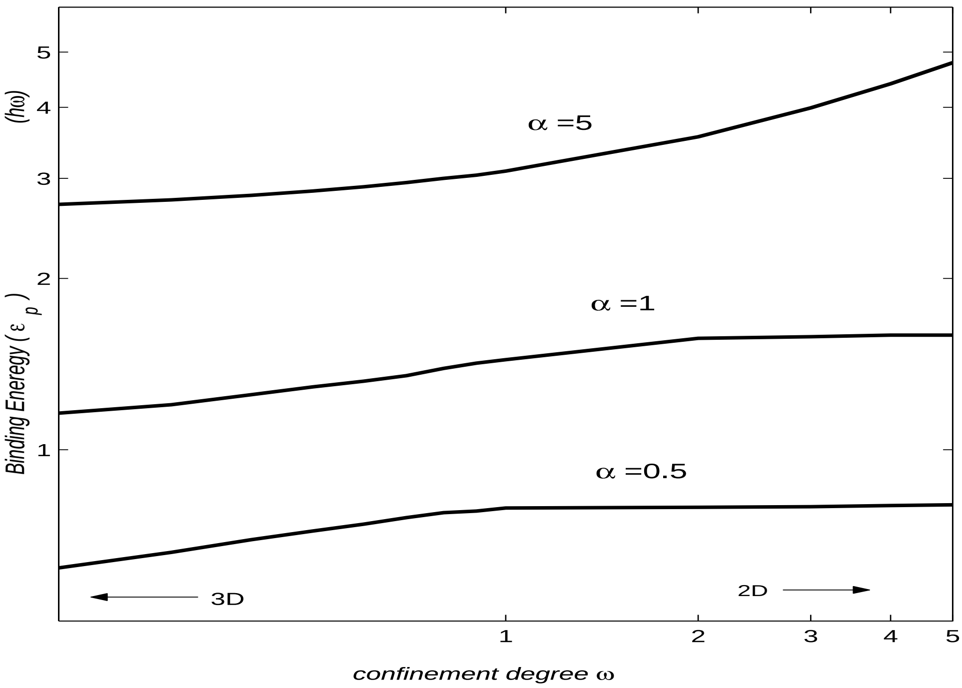

Fig. (1): The binding energy ε_p versus the confinement degree ω at coupling constant $(\alpha = 0.5, 1.0, 5.0)$ in units of $\hbar\omega$.

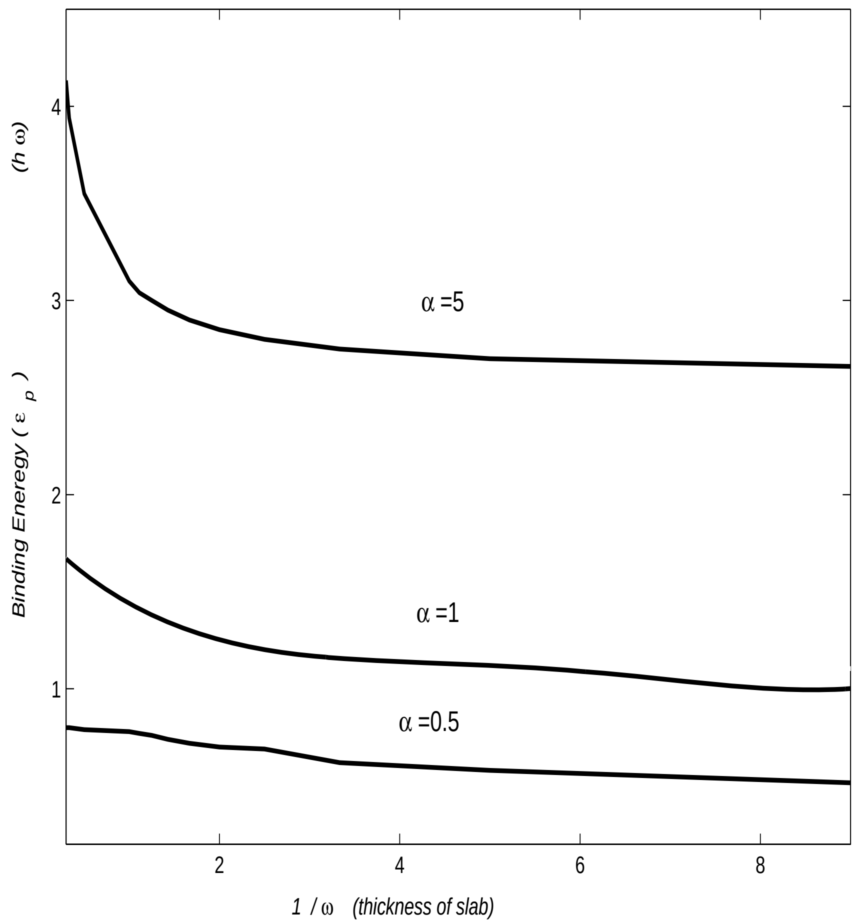

Fig. (2): The binding energy ε_p versus the thickness of slab $(1/\omega)$ in units of $\hbar\omega$.

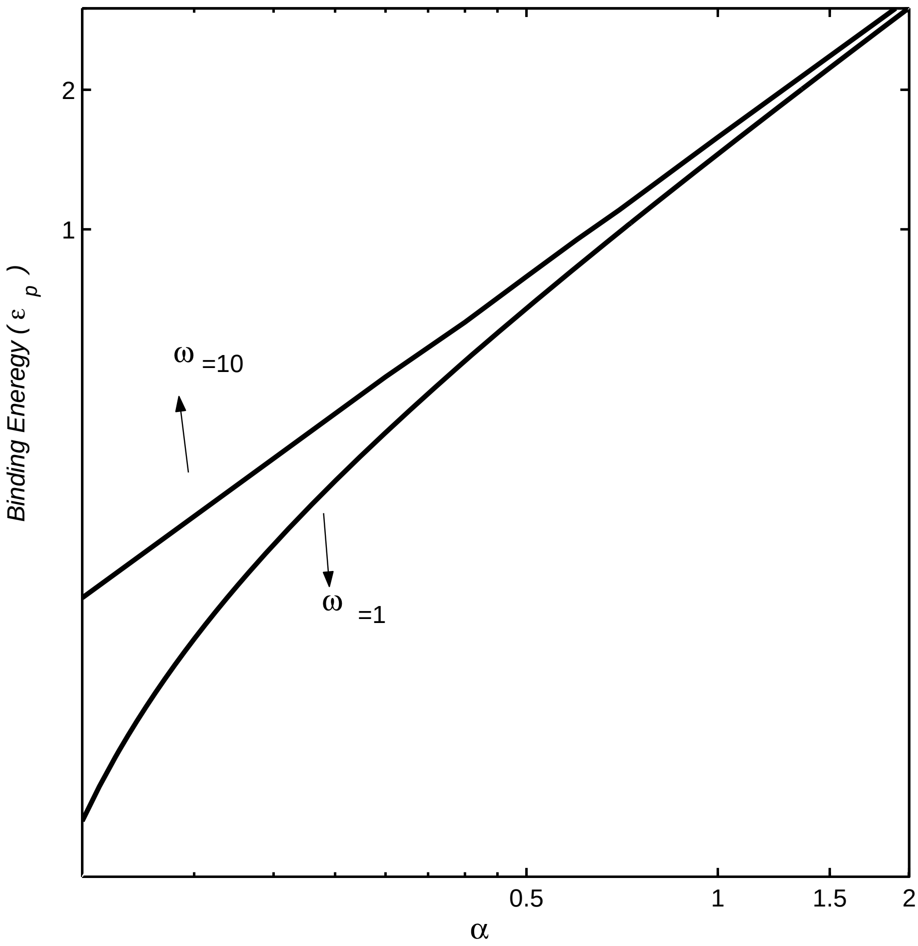

Fig. (3): The binding energy ε_p versus the coupling constant α at confinement degree $\omega = 10, 1.0$ in units of $\hbar\omega$.

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