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A Nearly Free Nano Particle in an Electromagnetic Field

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Abstract

The role of nano particles (NPs) behavior in an electromahnetic (EM) field will increase in the future due to the advent of quantum electronic devices which is assisted by the increasing sophistication of fabrication technology. Knowing this behavior in an EM becomes also necessary for modeling structural properties of nano structured devices. To understand and predict the physical properties of such devices, new theoretical view is required.We show how the modified Hamiltonian of the interactions imposed by the simplified approaches based on envelop function approximation. Indeed, the aim of this work is a mathematically rigorous foundation of new approach together with an investigation of the involved operators ultimately the development of methods for describing the dynamics of the NPs in an EM.

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1 Introduction

The theoretical description of semiconductor nanostructures is of crucial importance since it allows us both to investigate fundamental physics and to optimize nanostructure-based devices [1, 2]. Modern applications push nanostructures to dimensions and geometries where the Independent Nano particle

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Approximation (INA) may not be as accurate as necessary [3]. For example, this is the case of nanometre-scale silicon metal-oxide semiconductor field effect transistors (MOSFETs) [4, 5, 6]. In this case, oxide dimension, channel thickness and channel length are such that the application of the INA is highly questionable. Moreover, the advent of molecular electronics also requires more sophisticated approaches which treat systems where electrons are well localized [7, 8, 9, 10, 11, 12].

However NP behavior in an EM has been a topic of great interest in recent years. This is due to the unique physical properties of NPs such as carbon nanotubes, quantum dots, and oxide nanorods and their potential for use in novel devices such as sensors and circuit elements. We should consider that the description of a realistic nanostructure requires an amount of atoms in the interaction volume which is related to the dimensionality of the problem. Typically, a few hundred atoms are needed for systems confined in one dimension, such as quantum wells, resonant tunneling diodes, etc, and up to millions of atoms for three-dimensional (3D) confined (dots) nanostructures. Similarly, for organic structures such as carbon nanotubes, typically 100-1000 atoms need to be taken into account. Such a high-level description, however, requires many-body system and the interaction between NPs, which is suitable for routine device simulation. It is worth noting that the single orthogonal wavefunction has a longer range than the atomic orbitals. Thus, interactions between NP sites have a shorter range (typically a few nearest-neighbor shells) when many body interactions are taken into account. We indeed studied the dynamics of these NPs and also modified the Hamiltonian for better describing of NPs in an EM.

2 Theory

Traditionally, nanostructures are studied via INA approaches in the context of the envelope function approximation (EFA) [13, 14]. In this case, only the envelope of the nanostructure wavefunction is described, regardless of many body interaction details.

Since NPs and nanocrystals lose translational symmetry in all directions, calculations of electronic and magnetic properties of these nanostructures need to consider the whole dimension of the system. As in the case of nano structured materials, the large number of NPs present in an EM has favored NP assemblies investigations. The most promising approach for NPs in an EM has been proposed by Maxwell and Schrödinger, but these approaches include

equations for the envelope functions and approaches in terms of the single Hamiltonian. We firstly start with the simplest ortognal plane wave description for NPs in terms of

$$\hat{H} = -t\sum_{\lambda}[\hat{a_\lambda}^{\dagger}e^{\frac{ie}{\hbar c}\delta_i A}\hat{a}_{\lambda+\delta} + c.c.], \tag{1}$$

where t is the nearest neighbor interaction parameter, $\hat{a}^{\dagger}$ and $\hat{a}$ are rising and lowering operators of NPs, respectively. The vector potential A is introduced by means of the Peierls substitution [3] as follow

$$\hat{a_\lambda}^{\dagger}\hat{a_\lambda} \rightarrow \hat{a_\lambda}^{\dagger}e^{(\frac{-ie}{\hbar c}\int_m^n Adr)}\hat{a}_\lambda, \tag{2}$$

It indicates the phase factor $e^{\frac{ie}{\hbar c}\delta_i A}$ in the interacting term. We keep Plank constant $\hbar$ and the velocity of light C, but set $K_B = 1$.

By expanding the Hamiltonian and neglecting some higher order in the vector potential, one has accordingly conclude that the Hamiltonian acquires the familiar form as follow

$$\hat{H} = \sum_{\lambda}\hbar\omega_\lambda\left(\hat{a_\lambda}^{\dagger}\hat{a}_\lambda + \frac{1}{2}\right), \tag{3}$$

where

$$\hat{a_\lambda}^{\dagger} = \sqrt{\frac{\mu_0 c^2}{2\hbar}\omega_\lambda}\left[\hat{P_\lambda}^{\dagger}(t) + \frac{i\omega_\lambda}{\mu_0 c^2}\hat{A_\lambda}^{\dagger}(t)\right], \tag{4}$$

$$\hat{a_\lambda}^{\dagger} = \sqrt{\frac{\mu_0 c^2}{2\hbar}\omega_\lambda}\left[\hat{P_\lambda}(t) - \frac{i\omega_\lambda}{\mu_0 c^2}\hat{A_\lambda}(t)\right], \tag{5}$$

the λ subscript indicates the polarization of the electromagnetic field and the frequency ω_λ is given by

$$\omega_\lambda = c|\vec{k}_\lambda|, \tag{6}$$

However, to overcome the limitations of EFA, such as parametrization, transferability, distance dependence of matrix elements, etc, it would be better to calculate the matrix elements by starting from the knowledge of the localized orbitals and the Hamiltonian of NPs. For a given k, the eigenenergies E are calculated by solving the secular equation

$$H|E,k\rangle = (H+V)|E,k\rangle = E|E,k\rangle, \tag{7}$$

where H is the system Hamiltonian and V is the Hartree potential, which can represent an externally applied potential or the internal potential due to charge interactions. In the Bloch sum expansion, considering orthonormalized basis functions, the secular equation reduces to

$$\sum_{R',\alpha'} H_{R,\alpha;R',\alpha'} C_{R',\alpha'} = E C_{R',\alpha'}, \tag{8}$$

which needs to be solved with appropriate boundary conditions.

We know the lagrangian (L) and Hamiltonian (H) operators, in that the conjugate momentum P is

$$P(r,t) = \frac{\partial L}{\partial \dot{q}(r,t)}, \tag{9}$$

where $q(r,t)$ is the continues coordinate as function of space and time, and the Hamiltonian for the full system can be described as follow

$$H = P(r,t)\dot{q}(r,t) - L, \tag{10}$$

We define the field equations by using Lagranges equation

$$\frac{\partial L}{\partial q} - \sum_{i=1}^{4} \frac{\partial}{\partial x_i} \left[\frac{\partial L}{\partial \frac{\partial q}{\partial x_j}} \right] = 0, \tag{11}$$

Therefore

$$L = \frac{1}{2\mu_0} \int \left(\frac{|\hat{A}(r,t)|^2}{c^2} + |\nabla \hat{A}(r,t)|^2 \right) d^3 r, \tag{12}$$

where

$$[(x_1, x_2, x_3, x_4)] = (x, y, z, t), \tag{13}$$

Having defined the H and P, the momentum of the system p can be written as

$$p = -\int d^3 r P(r,t) \nabla q(r,t), \tag{14}$$

where p describing the dynamics of the NPs in an EM. This momentum operator can be derived from Eq.9. The obvious normal modes can thus written as

$$A(r,t) = \sum_{\lambda} A_\lambda(t) \vec{e}_\lambda e^{i k_\lambda \cdot r}, \tag{15}$$

$$P(r,t) = \sum_{\lambda} P_{\lambda}(t)\vec{e}_{\lambda}e^{ik_{\lambda}.r}, \tag{16}$$

However, an alternative way to write the Hamiltonian of a NP in an EM is obtained by using polorization vector. This method also allows us to introduce many body interactions mechanism. Let us first write again the Hamiltonian of system as follow

$$H_{NP} = \frac{1}{2m}\left(p - \frac{eA}{c}\right)^2, \tag{17}$$

this in turn can be expand to give

$$H_{NP} = \frac{|\vec{p}|^2}{2m} + \frac{e^2|\vec{A}|^2}{2mc^2} - \frac{e}{2mc}(\vec{p}.\vec{A} + \vec{A}.\vec{P}) = H_{free} + H_{int}, \tag{18}$$

which gives

$$\left[\hat{P}_{\lambda}, \hat{A}_{\lambda'}\right] = \frac{\hbar}{i}\delta_{\lambda,\lambda'}, \tag{19}$$

substituting we have

$$\hat{H} = \frac{1}{2}\sum_{\lambda}\left[c^2\mu_0 P_{\lambda}(t)P^{\dagger}_{\lambda}(t) + \frac{\omega^2_{\lambda}}{\mu_0 c^2}\hat{A}_{\lambda}(t)\hat{A}^{\dagger}_{\lambda}(t)\right], \tag{20}$$

The effect of electric fields in nanostructures has been widely described from internal polarizations. In this sprit, it is helpful to define an internal polarization vector so that

$$\vec{A}(r,t) = \vec{e}A_e\left(\vec{r},t\right), \tag{21}$$

where $A_e\left(\vec{r},t\right)$ is the scaler generalized coordinate. Therefore, the generalized momentum $P\left(\vec{r},\vec{t}\right)$ becomes

$$\vec{P}\left(\vec{r},t\right) = \frac{\partial L}{\partial A^{\circ}} = \frac{A^{\circ}_e}{\mu_0 c^2}, \tag{22}$$

and the Hamiltonian can now be expressed as

$$H = \frac{1}{2\mu_0}\int\left(|P(r,t)|^2\mu_0^2c^2 + |\nabla A(r,t)|^2\right)d^3r, \tag{23}$$

or

$$H = \frac{1}{2}\sum_{\lambda}\left[P_{\lambda}(t)P_{-\lambda}(t)c^2\mu_0 + \frac{k^2_{\lambda}}{\mu_0}A_{\lambda}(t)A_{-\lambda}(t)\right], \tag{24}$$

quantization is obtained from

$$\left[\hat{H}(r,t),\vec{A}(r,t)\right]=\frac{\hbar}{i}\delta(r-r'), \tag{25}$$

Due to the presence of large fields, the bending of the bands are such that NPs are confined in a narrow region and this, as for the thin layer perturbation, calls for a direct use of multi-band treatment. Therefore, the total Hamiltonian consist of two parts, the Hamiltonian of the individual component and the interaction Hamiltonian H_{int}. Now from Eqs. 4 and 5, we have

$$\hat{a}^{\dagger}_{\lambda}-\hat{a}_{\lambda}=\sqrt{\frac{\mu_0c^2}{2\hbar\omega_{\lambda}}}\frac{2i\omega_{\lambda}}{\mu_0c^2}(2A_{\lambda}(t)) \tag{26}$$

$$A_{\lambda}(r,t)=A^{*}_{-\lambda}(r,t), \tag{27}$$

$$\sum A_{\lambda}(t)e_{\lambda}e^{ik.r}=\sum A^{*}_{-\lambda}(t)e_{-\lambda}e^{ik.r}, \tag{28}$$

$$k_{\lambda}=-k_{-\lambda},e_{\lambda}=e_{-\lambda},A_{\lambda}=A^{*}_{-\lambda}, \tag{29}$$

$$a^{\dagger}_{-\lambda}-a_{\lambda}=\frac{1}{\sqrt{\mu_0c^2}}\frac{i}{\sqrt{\hbar}}\sqrt{2\omega_{\lambda}}+A_{\lambda}(t)=i\sqrt{\frac{2\omega_{\lambda}}{\hbar\mu_0c^2}}A_{\lambda}(t), \tag{30}$$

we can thus write the interaction, remembering that in free space the polarization $\vec{e}_{\lambda}$ is perpendicular to the direction of propagation (in the $\vec{k}_{\lambda}$ direction)

$$\hat{H}_{int}=-\frac{e}{2mc}(\vec{p}.\vec{A}+\vec{A}.\vec{P})=\sum\hbar\vec{k}_{\lambda}(a^{\dagger}_{\lambda}a_{\lambda}+\frac{1}{2}).\frac{1}{i}\sqrt{\frac{\hbar\mu_0c^2}{2\omega_j}}(a^{\dagger}_{-j}-a_j)+\frac{1}{i}\sqrt{\frac{\hbar\mu_0c^2}{2\omega_j}}(a^{\dagger}_{-j}-a_j).\hbar\vec{k}_{\lambda}(a^{\dagger}_{\lambda}a_{\lambda}). \tag{31}$$

Here, H_{int} is the Hamiltonian matrix which describes the interaction between NP and EM. This interaction phenomenon causes a transmission of NPs to the higher levels with energy given by the transmission matrix $(H_{mm}-EI)$

$$\Gamma_m=\begin{pmatrix} H^{-1}_{m,m+1}(H_{m,m}-EI) & H^{-1}_{m,m+1}(H_{m,m-1}) \\ I & 0 \end{pmatrix}, \tag{32}$$

Where H_{mm} is a Hamiltonian matrix for a NP at (m,m) energy level and I is a unitary matrix. Therefore, the Schrödinger equation (32) can be expressed as

$$\begin{pmatrix} C_{m+1} \\ C_m \end{pmatrix}=\Gamma_m\begin{pmatrix} C_m \\ C_{m-1} \end{pmatrix}, \tag{33}$$

Where C is discussed in Eq.8. And the coefficients of the TB expansion at a point where NPs meet each other, we can write

$$\begin{pmatrix} C_{N+2} \\ C_{N+1} \end{pmatrix} = \prod_{m=N+1}^{0} \Gamma_m \begin{pmatrix} C_m \\ C_{m-1} \end{pmatrix}, \tag{34}$$

The main advantage of this approach is the reduction to the solution of a very small linear system independent of the size of the problem.

3 Conclusion

We could give new and more accurate approach for describing the behavior of NPs in an EM. The obtained results indicate that the single Hamiltonian operator can not describe the behavior of NP in an EM. The present modified Hamiltonian can be used for more details of NP behavior in an EM. We thus suggest to use this approach for studying the ultra thin film, nano clusters and NPs interactions.

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