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Dynamics of 2-D one electron quantum dots in periodically fluctuating confinement potential: Influence of size and anharmonicity

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ABSTRACT

We explore the dynamics of harmonically confined single electron quantum dots as a function of dot size under periodically fluctuating confinement potential. The system of interest is a 2-D system in the presence of a perpendicular magnetic field. We show that for given strengths of the magnetic field and effective mass, a periodic variation in the strength of the confinement potential could invite interesting features in the dynamics of the system. Also, the pattern of time evolution of eigenstates of the unperturbed system reveals significant size-dependence. The fluctuation in the confinement potential from its initial value is found to modulate the dynamical aspects in a prominent way. The presence of cubic anharmonicity in the confining field brings in new features in the dot dynamics.

1. Introduction

In recent years, significant progr ess has been made in the fabrication of low-dimensional structures thereby reducing the effective dimensions from 3-D bulk materials, to quasi 2-D quantum wires, and even to quasi 0-D quantum dots [1–3]. The quantum confinement effects in such systems of reduced space dimensions have attracted considerable attention. Maksym and Chakraborty [4,5] worked out the energy levels and found an incredibly rich structure. In quantum dots the electron energy levels are quantized and the behavior is similar to that of an atom. The presence of discrete energy levels, and even the manifestations of the shell structure which was predicted [6–9] and experimentally observed [10] for quantum dots, give grounds for treating them as *artificial atoms* [4,11].

The advantage of studying the quantum dot system is that the properties of artificial atom can be extensively controlled by the external applied field. The cyclotron frequency (a measure of externally applied magnetic field strength), and confinement potential are two important system parameters that demand discussion. The effect of magnetic field on the energy spectrum of quantum dot is especially interesting. External electric and magnetic fields can be added to generate new static and dynamical effects in nanostructures [12–15]. The electronic structure of quantum dots in magnetic fields displays a rich scenario of different phases in the ground state. An overwhelming amount of literature on this topic has been published. It has been found that high magnetic field energetically favors the population build up in only the lowest states sequentially with single-particle angular momenta, and the energy increases monotonically with *B*.

The confinement potentials in quantum dots can be exploited to describe [4,5] typical features of transport processes [15–19] and spin oscillations in magnetic field [20,21]. The main components responsible for the formation of the confinement potential in a quantum dot include the external voltage applied to the layered nanostructure and properties of contacts having various geometries and connecting the quantum dot with ambience [1,22]. Quantum mechanical effects play a significant role in the description of the mechanism of quantum dot formation. However, the form of the confinement potential may be strongly affected under certain experimental conditions. For example, the description of experiments involving photoemission [23] in a quantum dot requires the introduction of anharmonic corrections [24,25] to the parabolic confinement potential. Dineykhan et al. showed how a change in the shape of

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confinement potential from that of parabolic dot can be achieved based on an assumption that considers existence of an image charge [26]. Kwaśniowski et al. showed the effect of confinement potential shape on exchange interaction in coupled quantum dots by a CI method using confinement potentials of different profiles [27]. Xie et al. analyzed two interacting electrons in a Gaussian confinement potential quantum dot under the influence of a perpendicular magnetic field [28].

Quantum dots are now realizable in various shapes and sizes and device applications are being made. For making further progress it is necessary that we can correlate the dynamical aspects of the dot with dot size. As the physical dimensions of the dot approach the nanometer scale, size effect begins to play an important role, leading to drastic changes in the measured properties [29]. In the last few years, semiconductor quantum dots with tunable size have attracted a great deal of attention, particularly in the 1.3–1.55 μm range of optical communications [30–33]. In consequence, of late, we investigated the influence of size, on the optical properties of the quantum dot [34,35], and also on its electronic structure and dynamics (under external sinusoidal electric field) [36].

Above discussions raise some natural questions concerning the outcome of the time-dependent modulation of the form of confinement potential and its interplay with the dot size. What will happen if the form of the confinement potential changes with time? How such a change can be monitored? How anharmonicity can influence such a change? etc. Thus, it would be interesting to investigate the dynamics of the dot under a time-dependent confinement potential. Such a time-dependence could be effectively modeled by introducing a potential $V(t)$ to the dot Hamiltonian. The problem now boils down to following the dynamics of the dot in the time-dependent potential. In the present paper $V(t)$ is so chosen that the confinement potential varies sinusoidally with time about its initial value (i.e. at $t=0$). The size of the fluctuation could now influence the characteristic parameters of dot dynamics viz. $E(t)$ vs. t profile and population distribution among the various eigenstates quite prominently. Added to this, the dot size plays an anchoring role in modulating the above dynamical aspects. The present paper is an attempt to address these features.

2. Method

We assume that the electron in the dot atom has an effective mass m^* and has been confined by a harmonic potential $[V_0(x,y)=\frac{1}{2}m^*\omega_0^2(x^2+y^2)]$ in the simultaneous presence of a static perpendicular magnetic field B $(=\nabla\times A)$, A being the vector potential. For the perpendicular magnetic field ($B_x=B_y=0$), and Landau gauge used for A, the motion along z-axis is continuous while the motion in the $x-y$ plane is quantized and the quantized energy levels are obtainable from the following energy eigenvalue equation (in Cartesian coordinate system):

$$H_0\psi_n(x,y)=E_n\psi_n(x,y), \tag{1}$$

where

$$H_0=\left[-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+\frac{1}{2}m^*\omega_0^2x^2+\frac{1}{2}m^*(\omega_0^2+\omega_c^2)y^2-i\hbar\omega_c y\frac{\partial}{\partial x}\right], \tag{2}$$

$\omega_c=eB/m^*c$ is the cyclotron frequency. Introducing $\Omega^2=\omega_0^2+\omega_c^2$ we have Eq. (2) transformed into an energy eigenvalue equation of a pair of interacting harmonic oscillator Hamiltonian H_x and H_y with harmonic frequencies ω_0 and Ω, respectively, the interaction operator given by

$$\hat{V}_{int}=-i\hbar\omega_c y\frac{\partial}{\partial x}.$$

That is, our problem reduces to modeling the energy eigenvalues and eigenvectors of the 2-D Hamiltonian H_0:

$$H_0(x,y,\omega_c,\omega_0)\psi_n(x,y)\equiv\left[H_x(\omega_0)+H_y(\Omega)-i\hbar\omega_c y\frac{\partial}{\partial x}\right]\psi_n(x,y)$$
$$=E_n\psi_n(x,y). \tag{3}$$

Here we mention that the quantum properties of circular dots are well understood in terms of Fock–Darwin states which provide a complete orthonormal basis. In that case the symmetric gauge is more suitable than the Landau gauge. Also the matrix elements could have been analytically calculated in that basis. However, since we also investigate the dynamical aspects of the system under anharmonic perturbations $V_1(x,y)$ present in the confinement potential, and since exact solution is not possible in such case, we explore a variational approach that can handle the problem with or without anharmonic perturbation, on equal footing. Thus, we write the trial wave function as a superposition of the product of harmonic oscillator eigenfunctions. With this basis the matrix elements are much simpler to determine than with the Fock–Darwin basis.

Eq. (3) reduces to the energy eigenvalue equation of a 2-D harmonic oscillator as ω_c (i.e. B)$\to 0$. It would be natural, therefore, to seek diagonalization of $H(x,y,\omega_c,\omega_0)$ in the direct product basis of eigenfunctions of $H_x(\omega_0)$ and $H_y(\Omega)$. In order to investigate the size-dependent properties, the spatial extension of the dot wave function must be truncated at some finite value. Thus, in this case the spatial extension of the wave function ranges from $-L$ to $+L$ (instead of $\pm\infty$) where L represents the dot size. Accordingly the basis functions $\phi_n(x)$ and $\phi_m(y)$ have to be modified. The normalized, but non-orthogonal basis functions for the finite-sized dot in the x-direction reads

$$\phi_n(x)=a_nH_n(x)\exp\left(-\frac{x^2}{2}\right), \tag{4}$$

where a_n is the normalization constant of the basis function $\phi_n(x)$ for the finite-sized dot. Analogously, we have the basis function for the y-direction. The normalization constant a_n is given by the following expression [34–36]:

$$a_n=\left(\frac{1}{I_{nn}}\right)^{1/2}, \tag{5}$$

where

$$I_{nn}=\sum_{r=0}^{[n/2]}\sum_{s=0}^{[n/2]}(-1)^{r+s}(2)^{2n-2(r+s)}\frac{(n!)^2}{(n-2r)!(n-2s)!r!s!}$$
$$\times\exp(-L^2)L^{2n-2(r+s)+1}\left[\sum_{k=0}^{\infty}\frac{\Gamma\left(\frac{2n-2(r+s)+1}{2}\right)}{\Gamma\left(\frac{2n-2(r+s)+1}{2}+1+k\right)}L^{2k}\right]. \tag{6}$$

We may represent the trial wave function $\psi(x,y)$ for the finite dot as a superposition of the product of fixed basis functions $\phi_n(x)$ and $\phi_m(y)$, respectively, leading to

$$\psi(x,y)=\sum_{n,m}C_{n,m}\phi_n(x)\phi_m(y). \tag{7}$$

When anharmonicity (V_1) in the confinement potential is added, we have

$$H=H_0+V_1. \tag{8}$$

The various matrix elements in the direct product basis $\{\phi_n(x)\phi_m(y)\}$ can be worked out once the form of V_1 has been specified. We have chosen $V_1=\lambda(x^3+y^3)$ as the symmetry breaking anharmonicity. The general expressions for the matrix