Anharmonic oscillator model of a quantum dot nanostructure

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The energy level spacings observed recently in resonant tunneling through an axially symmetric double-barrier quantum dot structure are reproduced by an isotropic two-dimensional anharmonic oscillator model. We propose that the extent of the depletion region in such a device effectively controls the possible angular momentum states of those electrons contributing to the current-voltage curve.

There is much current interest in electron devices which utilize resonant tunneling through quantum wells as the dominant mode of electron transport. 1-3 Resonant tunneling devices offer the prospect of fast frequency responses 4-5 and the possibility of fabrication at nanometer length scales. In particular, it has become possible to fabricate structures, termed quantum dots, in which an electron is confined in all three spatial dimensions. As a consequence of three-dimensional confinement, one would expect discrete electron energy levels. Indeed, discrete energy levels have recently been observed 6 in resonant tunneling through an axially symmetric quantum dot consisting of GaAs-AlGaAs barriers and an InGaAs quantum well. A simple model of the electron-potential considered in Ref. 6, which explains the discreteness of the energy levels, consists of a vertical (z) quantum well potential imposed by the heterojunctions, together with a fabrication-imposed laterally confining, axially symmetric component Φ(r), extending from r = 0 to r = R (see Fig. 1), where r = (x^2 + y^2)^1/2. Basically Φ(r) arises from the Fermi level pinning at the (microfabricated) cylindrical outer surface of exposed GaAs/AlGaAs/InGaAs at the physical radius of the device, r = R. From the spectrum of levels, it was argued in Ref. 6 that Φ(r) is well approximated by a parabola, at least for values of r exceeding a core radius, denoted by r_c, in the following. However, certain features of the spectrum, notably the ground-state level, could not be explained by a purely parabolic form.

In this letter we present possible quantum dot confining potentials whose energy levels agree with the observed 6 energy level spectrum. These consist of a one-parameter infinite family of anharmonic potentials, all exhibiting considerable modifications to parabolicity within the inner core of the quantum well, yet each potential of the family reproduces the energy level spacings of Ref. 6. A detailed microscopic calculation of Φ(r), described below and currently in progress, should serve to select a unique member of this family of possible potentials.

Five discrete energy levels have been identified from the measured 6 I-V curves. The upper four levels appear to be uniformly spaced with a 25 meV spacing, while the ground-state level lies some 40 meV below the first excited level. In the absence of Φ, the quantum well potential would give rise to a sequence of isolated subbands. With Φ(r) imposed, each subband is replaced by a series of discrete energy levels. These levels become observable if their spacings are large compared to k_B T. At the same time, one would like the splittings to be much smaller than the separation between the unperturbed subbands so as to avoid possible ambiguities in the interpretation of the spectrum. The observation of equally spaced excited levels suggests that Φ is approximately parabolic within the depletion region, 7 Φ(r) = Φ(R)(r - r_c)/W^2 for r_c < r < R, where the core radius is given by r_c = R - W and where W is the depletion depth. The value of Φ(R) can be estimated from measurements of the Fermi level pinning. The criteria for unambiguously ob-

![Graph of energy levels](image)

**FIG. 1.** Schematic illustration of quantum dot of Ref. 6, consisting of laterally confined InGaAs quantum well ("quantum dot"), AlGaAs tunnel barriers, and GaAs contacts. Structure has radius R and is cylindrically symmetric about the vertical (z) axis. Current (I) flows through central undepleted core of radius r_c = R - W, where W is the depletion depth. In this letter we propose nonparabolic modifications to the lateral confining potential Φ(r) for r < r_c to account for the observed 6 energy levels.
serving discrete subband splittings are summarized by the inequalities
\[
\left(\frac{k_n T}{\hbar}\right)^2 M^* W^2 < \Phi(R) \frac{W^2}{a^2} M^* a^2,
\]
where \( M^* \) is the electron effective mass in the InGaAs quantum well and \( a \) is the well width. For the quantum dot structure studied in Ref. 6, these inequalities are well obeyed at liquid-nitrogen temperatures.

Whereas a parabolic form for \( \Phi(r) \) explains the uniform spacing of the excited levels, a major deviation from parabolicity is required for \( r < r_e \) in order to account for the measured ground-state energy. In recent years several different methods have been developed for constructing families of confining potentials all of which correspond to a given set of discrete eigenvalues. Although a given confining potential gives rise to a unique discrete spectrum of eigenvalues, the converse is decidedly false! Of particular interest to us here, vast families of anharmonic potentials have been identified which give rise to an infinite ladder of equally spaced levels, usually thought to be unique to the familiar harmonic oscillator potential. Moreover, techniques are available for altering the harmonic oscillator potential to produce a given level spectrum. The simplest case and the one most relevant for our purposes consists of inserting a new ground state at an arbitrary energy beneath an existing ladder of equally spaced levels. We now outline such a procedure for constructing anharmonic potentials which fit the data of Ref. 6.

We briefly recall that the energy eigenvalues of a two-dimensional isotropic oscillator, described by the Hamiltonian
\[
H = -\hbar^2/(2M^*) (\partial_x^2 + \partial_y^2) + \frac{1}{2} M^* \omega^2 (x^2 + y^2),
\]
when separated using polar coordinates are given by \( E_n = n\hbar \omega \), where \( n = 2n_x + m + 1 \), \( n_x \) is a positive integer or zero, and \( m = 0, \pm 1, \pm 2, \ldots \). The degeneracy of the level \( E_n \) is given by \( n \). The Hamiltonian commutes with the operator describing the \( z \) component of orbiral angular momentum and \( m \) is the corresponding quantum number. As pertains to the quantum dot system, we contend that the only electrons contributing with an appreciable probability to the \( I-V \) characteristics have zero orbital angular momentum \((m = 0)\) with respect to the \( z \) axis. This is because of the existence of a narrow central conduction-path core through the device arising from the fact that \( W \) is only slightly smaller than \( R \). That is, the narrow undepleted inner core effectively filters out states of higher angular momentum. The viability of this contention is discussed below.

We therefore consider the subset of energy eigenvalues \( 1, 3, 5, 7, \ldots \) (henceforth all energies will be given in units of \( \hbar \omega \)), associated with \( m = 0 \). This subset of states is of special importance in that these are the states for which there is an appreciable probability of occupying the undepleted central core. We employ the Abraham–Moses procedure, with which we have generalized for two-dimensional systems, so as to create a new spectrum associated with these \( m = 0 \) states, with eigenvalues \( E_{G,1}, 3, 5, 7, \ldots \). The sole limitation that needs to be placed on the value of \( E_{G,1} \) is that \( E_{G,1} < 1 \). To make contact with the observed data, we make the identification that \( 2\hbar \omega \) corresponds to the \( 25 \text{ meV} \) spacing between excited levels, and that \((1 - E_{G,1})\hbar \omega \) corresponds to 40 meV, i.e., \( E_{G,1} = -2.2 \). We state without proof that such a spectrum is reproduced by the family of potentials of the form
\[
\Phi(r, \xi) = \frac{1}{2} M^* \omega^2 r^2 - \hbar \omega \frac{d^2}{dt^2} \ln[1 + \xi I(t)],
\]
where
\[
I(t) = \frac{1}{2} \int_0^t dt e^{-t} \left[ F_1 \left( \frac{1}{2} (1 - E_{G,1}); 1; u \right) \right]^2,
\]
where \( I = r/r_0 \) is a dimensionless distance, and \( r_0 = (\hbar/ M^* \omega)^{1/2} \) is the characteristic length for the oscillator. For the quantum dot system of Ref. 6, \( r_0 \approx 100 \text{ Å} \). Here, \( F_1(a; c; u) \) denotes the standard confluent hypergeometric function \((1) \) and \( \xi \) is an arbitrary real positive number which parameterizes the family. Note that the second term on the right-hand side of (1) is the anharmonic modification to the original isotropic oscillator potential.

We have numerically evaluated Eqs. (1) and (2) for \( E_{G,1} = -2.2 \), and some of our results, corresponding to different values of \( \xi \), are shown in Fig. 2 in units of \( \hbar \omega \). We stress that irrespective of \( \xi \), all the potentials given by Eqs. (1) and (2) fit the data of Ref. 6 and, furthermore, give rise to states of zero angular momentum. Note that the deviations from parabolicity are restricted to only the small \( r \) region. This is in accord with the expected parabolicity within the preponderance of the depletion regime. All members of the family tend asymptotically to the displaced parabola \((1/2)(r/r_0)^2 - 2 \). Also shown is the original harmonic oscillator potential (upper solid line). Shown are the potentials which result for \( \xi = 10 \) (dashed line), \( \xi = 6 \) (dotted line), \( \xi = 2 \) (dash-dot line), and \( \xi = \xi^* = 4.323 \) (lower solid line), which is chosen such that the coefficient of the quadratic term vanishes in the small \( r \) expansion of \( \Phi(r) \). The significance of \( \Phi(r, \xi^*) \) is discussed below.

To support our claim that the electrons contributing to the resonant tunneling current have angular momentum \( m = 0 \), we note that two-dimensional oscillator eigenstates associated with angular momentum \( m \) are peaked at a dis-
tance of order $|m|^{1/2}r_0$. Thus, if the radius $r_c$ of the undepleted conduction path core is small compared to $r_0$, clearly only $m = 0$ states will participate in the tunneling current. Previously $^9 r_c$ has been estimated to be about 65 Å. However, this value may be imprecise since it does not assume any localization corrections to the barrier-limited impedance. As we stated above, one requires additional physical criteria to select from among the family of isospectral potentials, $\Phi(r_0g)$. Requiring that the quantum dot be undepleted in the center of the device would suggest a potential of the form given by $\xi = \xi_0 g^{-n}$ in Fig. 2, which is seen to be essentially flat out to $r \approx 30$ Å. We note that this length (30 Å) is comparable in magnitude to the experimental estimate for $r_c$, and that both are less than the characteristic length $r_0$. Thus, it is indeed quite plausible that the observed data are consistent with our proposal regarding the angular momentum of the participating electrons. It would be extremely useful to attempt to control the value of $r_c$ and thereby put our proposal to a decisive test. Specifically, we propose that as $r_c$ is decreased the characteristics of the quantum dot energy spectrum remain essentially unchanged. (Of course, caution must be exercised so as to avoid pinching off the central core.) On the other hand, if $r_c$ were to be increased, we anticipate that new levels, associated initially with $|m| = 1$, will begin to appear in the measured spectrum if the linewidths are resolvable.

The argument that the higher angular momentum eigenstates are peaked in a depleted region and therefore cannot contribute appreciably to the tunneling current, begs the question as to the actual distribution of electrons under the operating conditions of the device. Based as it is upon the Schrödinger equation alone, the present treatment obviously cannot specify the distribution of carrier densities and hence the extent to which the system is depleted under bias. One requires a microscopic simulation of $\Phi(r)$ determined self-consistently with the charge distribution using Poisson's equation to obtain a more realistic estimate of the depletion width. This treatment should take into account the distribution of carriers and dopants, band structure discontinuities, applied bias, and surface states necessary to support Fermi level pinning.

In the simplest scenario, the Fermi level would be constant in the lateral direction with the device undepleted in the center. Of course suggests a potential of the form of $\Phi(r_0g^*)$ in Fig. 2. It will be noted, however, that for all $\xi$ the potentials possess two inflection points, which from Poisson's equation implies two changes in sign of the net charge distribution in the radial direction. We contend that such inflections are a necessary consequence of an observed depressed ground-state level. In general, to accommodate such a ground state it is necessary to add at small $r$ a negative nonparabolic component such that the total potential is substantially lowered vis-à-vis a parabolic form. It would appear then, that the observation of a depressed ground-state level necessarily implies that even a fully self-consistent solution of the coupled Schrödinger–Poisson equations would possess such inflections and, along with them, the implication of a radial "ring of charge." An alternative to this conclusion is that the usual interpretation of assigning to each peak in the $I-V$ curve a resonant tunneling level is oversimplified and that some more complicated spectroscopy $^9$ incurred by the lateral quantization is occurring. Such intriguing questions can be addressed only in the framework of a microscopic simulation. Such a calculation is currently in progress and the results will be presented elsewhere. $^11$

In summary, we have presented a continuous family of two-dimensional anharmonic potentials, all of which yield discrete energy levels coinciding with those reported in a recent tunneling experiment, $^9$ and which therefore serve as candidates for a model of the lateral confining potential of the quantum dot. Furthermore, the relevant eigenstates for this class of anharmonic potentials are states of zero angular momentum. We have argued that the narrow conduction path core of the quantum dot device in question effectively precludes all but the zero angular momentum states from appreciably contributing to the tunneling current and we have suggested procedures for testing this proposal. We have also listed the major questions to be addressed by a first principles theory, specifically, (1) elimination of the inherent ambiguity among the spectrally equivalent potentials, (2) ascertaining the angular momentum states which are able to occupy the central conduction channel, and (3) elucidation of the charge distribution. Successful modeling of $\Phi(r)$, and the detailed understanding of its origins and what controls it, should offer new insights and opportunities in device microfabrication and operation.

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$^7$The value of $W$ should be less than $\pi$ to preclude pinching off the central conduction path core.


$^{11}$M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions (Dover, New York, 1965), p. 504.

$^{12}$After this work was completed we received a preprint from G. Bryant which explores this possibility. This work has now appeared in print [Phys. Rev. B 39, 3145 (1989)].


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