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2001 J. Phys. A: Math. Gen. 34 2311

(http://iopscience.iop.org/0305-4470/34/11/322)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **34** (2001) 2311–2317 www.iop.org/Journals/ja PII: S0305-4470(01)14574-9

Integrable systems on a sphere as models for quantum dots

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Received 2 June 2000

Abstract

Model potentials for quantum dots with smooth boundaries, realistic in the whole range of energies, are introduced, starting from the integrable motion of a particle on a sphere under the action of an external quadratic field. We show that in the case of rotational invariant potentials, the associated 2D Schrödinger equation has exact zero-energy eigenfunctions, in terms of which the whole discrete spectrum can be characterized.

PACS numbers: 0230R, 7320D

A lot of interest is currently devoted to the physics of semiconductor nanostructures such as quantum dots [1]. These systems can be viewed as artificial atoms in two space dimensions [2] from which a significant amount of insight can be gained starting from their single-particle aspects. This is currently done by using harmonic confining potentials. Whilst these potentials give correct results at the bottom of the well, such as the prediction of correct magic numbers, etc, they are unsuitable for studying the valence single-electron states at the top of the potential.

In this paper we consider realistic confining potentials with finite asymptotic values and for which the zero-energy states of the corresponding 2D Schrödinger equation can be given in simple analytical forms. These potentials are qualitatively realistic for quantum dots with smooth boundaries, such as those produced by gating and shallow etching. Since every bound state in the well can be adiabatically obtained starting from a zero-energy state, this leads, from the knowledge of these states, to a complete characterization of the whole energy spectrum.

We start by considering the Neuman Hamiltonian describing the motion of a particle on a sphere under the action of a quadratic potential [3]:

$$H = \tfrac{1}{2}\sum_{i=0}^{3}(a_i q_i^2 - l_i^2). \tag{1}$$

0305-4470/01/112311+07$30.00

Here q_i are Cartesian coordinates, l_i are the components of angular momentum, and a_i are real constants. One can easily check that

$$H = \tfrac{1}{2}\sum_i^3 a_i F_i(q,l) \tag{2}$$

where F_i are the Uhlenbeck–Devani integrals of motion in involution, given by

$$F_k(q,l) = q_k^2 - \sum_{i\neq k}^3 \frac{l_k^2}{a_i - a_k} \qquad k = 1,\ldots,3. \tag{3}$$

As is well known, the dynamics of this system can be put in correspondence with the geodetic flow on an ellipsoid $\sum_i^3 \frac{q_i^2}{a_i} = 1$, by using the transformation $q' = l$, $l' = -q$, $a_i = a_i^{-1}$ [4]. In the following we shall construct confining 2D potentials by projecting Neuman's dynamics from the sphere to the plane (the sphere is seen as a one-point compactification of the plane). To this end it is suitable to include the constraint o $\sum_i^3 q_i^2 = 1$ directly into the equation of motion by means of the Lagrangian L

$$L(q_i,\dot q_i) = \tfrac{1}{2}\sum_{i=0}^3 (\dot q_i^2 - a_i q_i^2) + \lambda\left(\sum_i^3 q_i^2 - 1\right) \tag{4}$$

where λ is a Lagrange multiplier given by

$$\lambda = \tfrac{1}{2}\sum_i^3 (a_i q_i^2 - \dot q_i^2). \tag{5}$$

To project the dynamics to the plane we use the stereographic mapping

$$q_1 \equiv \tilde q_1 = \frac{2r\cos\varphi}{1+r^2} \tag{6}$$

$$q_2 \equiv \tilde q_2 = \frac{2r\sin\varphi}{1+r^2} \tag{7}$$

$$q_3 \equiv \tilde q_3 = \frac{1-r^2}{1+r^2} \tag{8}$$

in terms of which the Lagrangian (on the plane) becomes

$$L(r,\varphi,\dot r,\dot\varphi) = \frac{2}{(1+r^2)^2}[\dot r^2 + r^2\dot\varphi^2 - r^2(a_1\cos^2\varphi + a_2\sin^2\varphi + a_3(1-r^2))].$$

Introducing the conjugate momenta of r, φ respectively as

$$p_r = \frac{\delta L}{\delta \dot r} = \frac{4}{(1+r^2)^2}\dot r \tag{9}$$

$$p_\varphi = \frac{\delta L}{\delta \dot\varphi} = \frac{4r^2}{(1+r^2)^2}\dot\varphi \tag{10}$$

we have that the projected Uhlenbeck–Devani integrals can be written as

$$\tilde F_k(r,\varphi) = \tilde q_k^2 + \sum_{i\neq k}^3 \frac{\tilde l_k^2}{a_i - a_k} \tag{11}$$

where $\tilde q_i$ are given by equation (8) and $\tilde l_i$ denote the components of angular momentum mapped on the plane

$$\begin{aligned}
\tilde l_1 &= -p_r\sin\varphi\tfrac{1}{2}(1+r^2) - p_\varphi\frac{1-r^2}{2r}\cos\varphi\\
\tilde l_2 &= p_r\cos\varphi\tfrac{1}{2}(1+r^2) - p_\varphi\frac{1-r^2}{2r}\sin\varphi\\
\tilde l_3 &= p_\varphi.
\end{aligned} \tag{12}$$

The Hamiltonian of the system on the plane is then written as (see also [5])

$$\tilde{H}(r,\varphi) = \frac{1}{2}\sum_i^3 a_i \tilde{F}_i = -\frac{(1+r^2)^2}{4}\left\{p_r^2 + \frac{1}{r^2}p_\varphi^2 + V(r,\varphi)\right\} \tag{13}$$

where $V(r,\varphi)$ is the potential

$$V(r,\varphi) = -\frac{4}{(1+r^2)^4}[4r^2(a_1\cos^2\varphi + a_2\sin^2\varphi) + a_3(1-r^2)^2]. \tag{14}$$

It is worth remarking that on the zero-energy shell the common factor $\frac{(1+r^2)^2}{4}$ in front of the kinetic and potential parts in equation (13) is not relevant to the zero-energy trajectories in phase space, which coincide with those of the standard Hamiltonian

$$\tilde{H}(r,\varphi) = p_r^2 + \frac{1}{r^2}p_\varphi^2 + V(r,\varphi). \tag{15}$$

Note that for $a_1 = a_2 = \beta$, $a_3 = \alpha$ (with $\alpha \neq \beta$), the potential becomes rotationally invariant

$$V_r(r) = -\frac{4\alpha(1-r^2)^2 + 16\beta r^2}{(1+r^2)^4} \tag{16}$$

(on the plane the angular momentum is just l_z), and the corresponding dynamics are related to a free motion on a prolate or oblate ellipsoid of revolution (the particular case $\alpha = \beta$ in which the ellipsoid degenerates into a sphere (spherical case) was also considered in [6, 7]).

In the following we are interested in the quantum version of this system and in the characterization of its zero-energy states in the case of rotationally invariant potentials (16). To this end we introduce the operators

$$\begin{aligned}
\hat{l}_1 &= \mathrm{i}\left(\sin\varphi\tfrac{1}{2}(1+r^2)\frac{\partial}{\partial r} + \frac{1-r^2}{2r}\cos\varphi\frac{\partial}{\partial\varphi}\right)\\
\hat{l}_2 &= -\mathrm{i}\left(\cos\varphi\tfrac{1}{2}(1+r^2)\frac{\partial}{\partial r} - \frac{1-r^2}{2r}\sin\varphi\frac{\partial}{\partial\varphi}\right)\\
\hat{l}_3 &= -\mathrm{i}\frac{\partial}{\partial\varphi}
\end{aligned} \tag{17}$$

which generate the $so(3)$ algebra

$$[\hat{l}_i, \hat{l}_j] = \varepsilon_{ijk}\hat{l}_k. \tag{18}$$

These operators are essentially self-adjoint with respect to the L_2 product corresponding to the Lebesgue measure $4\alpha r\ (1+r^2)^{-2}\,\mathrm{d}r\,\mathrm{d}\varphi$ (with respect to which this is the Lie algebra of an $SO(3)$ group of measure-preserving transformations of the plane). The Uhlenbeck–Devani operators are then written as

$$\hat{F}_k(\hat{q},\hat{l}) = \hat{q}_k^2 - \sum_{i\neq k}^3 \frac{\hat{l}_k^2}{a_i - a_k} \qquad k = 1,\ldots,3 \tag{19}$$

and the Hamiltonian of the quantum system is written as

$$\hat{H} = \tfrac{1}{2}\sum_i^3 a_i\hat{F}_i(\hat{q},\hat{l}). \tag{20}$$

An explicit calculation shows that

$$\hat{H} = \frac{(1+r^2)^2}{4}\left\{\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2} - \hat{V}(r,\varphi)\right\} \tag{21}$$

from which the Schrödinger equation for the zero-energy states follows [5]:

$$\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}-\hat{V}(r,\varphi)\right)\Psi(r,\varphi)=0. \tag{22}$$

For rotational invariant potentials this equation can be easily solved by separation of variables. Indeed, by substituting $\Psi(r,\varphi)=\psi(r)\mathrm{e}^{\mathrm{i}l\varphi}$ into equation (22) (with $\hat{V}$ replaced by $\hat{V}_r$), we obtain the following radial equation:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}-\left(\frac{l^2}{r^2}-\frac{4\alpha}{(1+r^2)^2}+\frac{16(\alpha-\beta)r^2}{(1+r^2)^4}\right)\right]\psi=0.$$

It is remarkable that this equation can be mapped into the equation of the spheroidal harmonics

$$(1-\xi^2)\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2}-2\xi\frac{\mathrm{d}\psi}{\mathrm{d}\xi}+\left(\beta+c^2\xi^2-\frac{l^2}{1-\xi^2}\right)\psi=0 \tag{23}$$

by the transformation

$$\xi=\frac{1-r^2}{1+r^2} \tag{24}$$

of the half-line $[0,\infty]$ into the interval $[-1,1]$. In equation (23) l is an integer denoting the angular momentum, while the parameter $c^2\equiv\alpha-\beta$ is the oblateness parameter (in spite of the notation, c^2 can be positive or negative leading, respectively, to prolate or oblate eigenfunctions). Note that this equation has singular points in $\xi=\pm1$ while the physical solutions $\psi(\xi)$ must be regular at these points. This puts restrictions on the possible values that the parameter β can assume. More precisely, the eigenfunction $\psi_{n,l}(\xi,c^2)$ can be expressed in terms of infinite series of associated Legendre functions with coefficients satisfying complicated recursion relations. The zero-energy states will depend on the oblateness parameter and can be labelled by the integers n,l, with n given by $n=l+1,l+2,\ldots$. Corresponding to these eigenfunctions a fixed value $\beta_{n,l}(c^2)$ for β exists which can be expressed as a power series in the oblateness parameter with complicated coefficients. Although these recursion relations cannot be solved analytically, one has recourse to numerical tools (see below). For simplicity, in the following we will first restrict ourselves to the case of the zero-oblateness parameter $c^2=0$ (spherical case) for which it is possible to give explicit analytical results. In this case, indeed, equation (23) reduces to the well known associated Legendre equation so that the solution can be readily written as [6]

$$\Psi_{n,l}(r)=\left(\frac{r}{1+(r)^2}\right)^{|l|}\left(\frac{r^2+(-1)^{n-|l|}}{r^2+1}\right)\sum_{j=0}^{[\frac{n-|l|}{2}]}c_j(n,l)\left(\frac{r}{1+r^2}\right)^{2j} \tag{25}$$

where $c_j(n,l)$ are given by

$$c_j(n,l)=(-2)^j\prod_{i=0}^{j}\left[\frac{([\frac{n-|l|}{2}]+1-\mathrm{i})}{|l|+\mathrm{i}}\left(2\left(l+\mathrm{i}+\left[\frac{n-|l|}{2}\right]\right)+(-1)^{n-|l|-1}\right)\right]. \tag{26}$$

Here $[\frac{p}{2}]$ denotes the integer part of $\frac{p}{2}$ and $n-|l|$ is the number of nodes of the wavefunction in addition to the one in the origin. In this case the corresponding values of $\beta=\alpha$ are $\beta_{n,l}=n(n+1)$ with $n=|l|,|l|+1,|l|+2,\ldots$, with the integer n labelling successive eigenvalues. The degeneracy among states with identical principal quantum number n can be easily resolved by perturbation theory. From this it follows that the energy eigenvalues are increasingly ordered according to increasing values of n, and for one and the same n value, according to decreasing values of $|l|$. Thus (by extrapolation to $|l|\leqslant 1$) the energy eigenvalues at the top of the potential well, corresponding to the quantum numbers n,l, are

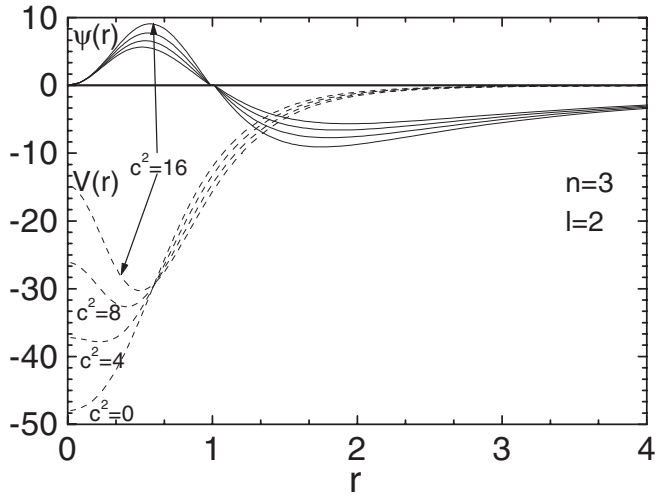

Figure 1. Zero-energy eigenfunctions (full curves) and potential profiles (dashed curves) for $n = 3$, $|l| = 2$ and different positive values of the oblateness parameter c^2.

ordered according to $\cdots < E_{\bar{n}-1,p} < E_{\bar{n}-1,s} < \cdots < E_{\bar{n},d} < E_{\bar{n},p} < E_{\bar{n},s}$ where the first index of E denotes the principal quantum number n, $\bar{n}$ being the maximum n value for the given deepness, while the second one denotes the orbital angular momentum in the usual atomic physics notation.

These results can be generalized to the case of the non-zero oblateness parameter by using numerical relaxation (path-following) methods which allow us to find the eigenfunctions and the corresponding values of β for $c^2 \neq 0$ by slowly increasing (decreasing) the oblateness parameter away from zero, starting from the wavefunctions of the spherical case. This is shown in figure 1 where the $n = 3$ and $|l| = 2$ zero-energy eigenfunctions and the corresponding potential profiles (dashed curves) are reported for different values of c^2. We see that as c^2 increases, the bottom of the potential is moved away from zero (i.e. in the plane we have a circle) with a potential barrier appearing in the origin. The height of the barrier increases with the oblateness parameter and for large values of c^2 the particles will be confined in a ring. This limit leads to a model potential for circular quantum wires.

The situation is quite different for the prolate case ($c^2 < 0$). In figure 2 we report the potential profiles and the zero-energy states for $n = 3$, $|l| = 2$ for negative values of c^2. We see that in this case the deepness of the potential increases as c^2 is decreased, and its bottom is always at the origin. We see that the wavefunctions have one node exactly at the position $r = 1$. It is indeed a general feature that all odd $n - |l|$ eigenfunctions vanish for $r = 1$. This can be understood by noting that $\xi = 0$ in equation (24) corresponds to $r = 1$ and the above solutions in terms of ξ are either even or odd polynomials in ξ according to the parity of $n - |l|$. It is of interest to remark that from the exact knowledge of the zero-energy eigenfunctions one can completely characterize the bound state spectrum in terms of the quantum numbers n, l. Indeed, when a new level appears in the spectrum as the depth of the potential is increased, it has exactly zero energy. This implies that from knowledge of the c^2 values for which normalizable zero-energy states exist one can determine the number of bound eigenfunctions for a given angular momentum as a function of c^2. The degeneracy among states with identical principal quantum number n can be easily resolved by perturbation theory. From this it follows that the

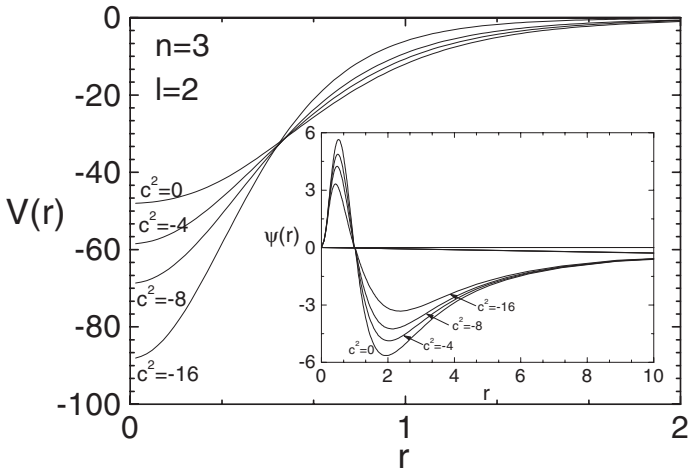

Figure 2. As for figure 1 but for negative values of c^2.

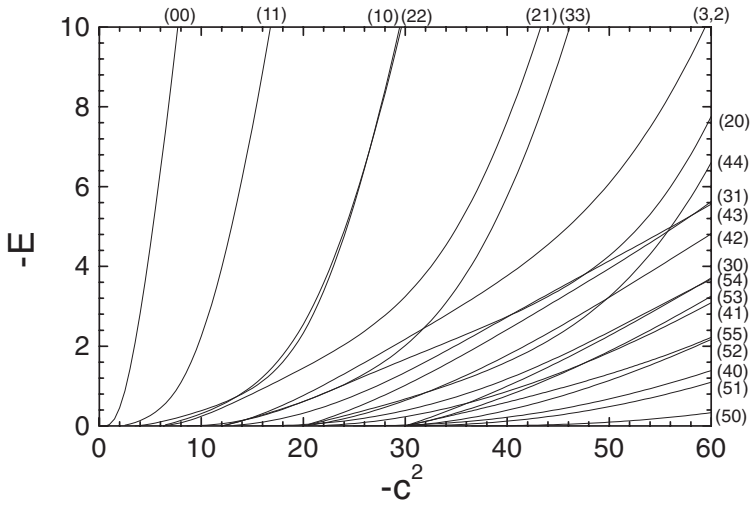

Figure 3. Energy spectrum of the potential in equation (16) for the prolate case as a function of the oblateness parameter c^2.

energy eigenvalues are increasingly ordered according to increasing values of n, and for one and the same n value, according to decreasing values of $|l|$. This is exactly true for the spherical case ($\alpha = \beta$), while in the general case the $n = l$ levels exhibit multiple-level crossing. This is shown in figure 3 where the energy spectrum is built for the prolate case using the path-following method starting from the spherical case with $\beta = n(n + 1)$ and c^2 decreasing from zero.

Before closing this paper, we wish to point out an interesting link existing between the 2D Schrödinger equation with the potential (16) with $\alpha = \beta$, and the Lax operator for the KdV equation [5, 7]. To be specific consider the following radial equation:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l^2}{r^2} + \frac{4\alpha}{(1+r^2)^2}\right]\psi(r) = 0. \tag{27}$$

One can easily check that this equation is transformed through the map of the half-line onto the entire real axis,

$$x = \tanh^{-1}\left(\frac{1-r^2}{1+r^2}\right) \tag{28}$$

into the equation

$$\left(\frac{1+\tanh(x)}{1-\tanh(x)}\right)\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} - l^2 + \alpha(1-\tanh^2(x))\right]\psi(x) = 0 \tag{29}$$

which, after multiplying by r^2, is readily recognized as the 1D spectral problem

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \alpha\,\mathrm{sech}^2(x)\right]\psi(x) = l^2\psi(x) \tag{30}$$

for the KdV equation. It is known that the potential $u(x) = \alpha\,\mathrm{sech}^2(x)$ becomes reflectionless for integer values of α given by

$$\alpha = n(n+1) \tag{31}$$

where n is just the number of bound states present in the 1D potential $u(x)$ (i.e. the number of solitons present in the solution of the KdV equation). On the other hand, equation (31) is also the relation between the total number n of nodes of the angular and radial part of the bound states $\Psi_{n,l}$ and the depth α of the 2D Schrödinger potential $\frac{-4\alpha}{(1+r^2)^2}$. This suggests that the above potentials could emerge as the soliton limit of the 2D periodic potentials related to finite gap solitons of the KdV equation.

In conclusion, we have used integrable models on the sphere to construct a realistic 2D model potential for quantum dots. The considered models allow complete control of the zero-energy states and of the number of bound states as a function of angular momentum for arbitrary parameter values. For a spherical potential ($\alpha = \beta$) it is possible to give analytical expressions for the zero-energy states and to show that the potential in this case is linked with the linear spectral problem associated with the n soliton solution of the KdV equation.

Acknowledgment

Financial support from the INFM, Unità di Salerno, is acknowledged.

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