

Bound states of a charged particle in the field of an electric quadrupole in two dimensions

Francisco M. Fernández

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Abstract The Schrödinger equation for a charged particle in the field of a nonrelativistic electric quadrupole in two dimensions is known to be separable in spherical coordinates. We investigate the occurrence of bound states of negative energy and find that the particle can be bound by a quadrupole of any magnitude. This result is remarkably different from the one for a charged particle in the field of a nonrelativistic electric dipole in three dimensions where a minimum value of the dipole strength is necessary for capture. Present results differ from those obtained earlier by other author.

Keywords Quadrupole field · Electron capture · Bound states · Separable Schrödinger equation

1 Introduction

Some time ago Alhaidari [1] discussed the problem of a charged particle in the field of a nonrelativistic electric quadrupole and calculated the minimum quadrupole strength that allows the particle to be bound by the charge distribution. The author chose the charge distribution of four fixed point charges with zero total charge and dipole moment. The first nonzero contribution to the multipole expansion is, therefore, the quadruple term. Since this term is inversely proportional to the square of the distance between the fifth charge and the origin of the distribution the Schrödinger equation is trivially separable in spherical coordinates.

In some ways that problem resembles the most widely studied one of a charged particle in the field of a nonrelativistic dipole moment in three dimensions [2] (and

F. M. Fernández (✉)

División Química Teórica, INIFTA (UNLP, CCT La Plata-CONICET), Blvd. 113 S/N,
Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina
e-mail: fernande@quimica.unlp.edu.ar

references therein). This simple model proved useful in nuclear as well as in molecular physics [2] (and references therein). In the latter field it has been used to predict the capture of an electron by a polar molecule to produce an anion. It has been known from long ago that the polar molecule cannot bind an electron unless the dipole is greater than some critical value [2] (and references therein). Camblong et al. [2] gave a simple and smart proof, based on dimensional scaling, of why the simple model is successful.

Alhaidari [1] arrived to a similar conclusion in the case of the particle in the field of an electric quadrupole in two dimensions. On revising his arguments we found that his conclusions may not be correct. Since the problem may be of physical interest we put forward our results in this paper. In Sect. 2 we solve the Schrödinger equation and derive the conditions for the capture of the charged particle by the electric quadrupole. We split the Schrödinger equation into the angular and radial parts in the usual way and show that the radial equation is different from the one derived by Alhaidari. We also show that the standard solution of the angular part yields results that are different from those obtained by that author. As a result we obtain conditions for the capture that considerably differ from those given earlier. In Sect. 3 we summarize the main results and draw conclusions.

2 Bound states

The dimensionless Schrödinger equation for a particle moving in a potential $V(\mathbf{r})$ is

$$\left[-\frac{1}{2}\nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}). \quad (1)$$

In two dimensions this equation is separable in spherical coordinates $0 < r < \infty$ and $0 \leq \theta < 2\pi$ when

$$V(\mathbf{r}) = V_r(r) + \frac{V_\theta(\theta)}{r^2}, \quad (2)$$

because it takes the particularly simple form

$$\left\{ -\frac{1}{2r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + V_r(r) + \frac{1}{r^2} \left[-\frac{1}{2} \frac{\partial^2}{\partial \theta^2} + V_\theta(\theta) \right] \right\} \psi(r, \theta) = E\psi(r, \theta). \quad (3)$$

For comparison purposes throughout this paper we follow the notation used by Alhaidari [1].

In order to separate the Schrödinger equation into two one-dimensional eigenvalue equations we write $\psi(r, \theta) = r^{-1/2}R(r)\Theta(\theta)$ where the angular factor is a solution to

$$\left[-\frac{1}{2} \frac{d^2}{d\theta^2} + V_\theta(\theta) \right] \Theta(\theta) = E_\theta \Theta(\theta), \quad (4)$$

with the boundary condition $\Theta(\theta + 2\pi) = \Theta(\theta)$. The remaining radial equation is

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} - \frac{1/4 - 2E_\theta}{2r^2} + V_r \right] R(r) = ER(r). \quad (5)$$

Note that the term $-1/(8r^2)$ is missing from the equation (1.4b) of Alhaidari's paper. As we will see below it has a dramatic effect on the condition for the existence of a bound state in the system.

When $V_r = 0$ Eq. (5) becomes the eigenvalue equation for an attractive square potential when $\alpha = 1/4 - 2E_\theta > 0$. It is well known that this operator is self-adjoint when $0 \leq \alpha \leq 1/4$ but it does not support negative eigenvalues for such values of the strength parameter [3]. On the other hand, when $\alpha > 1/4$ ($E_\theta < 0$) the operator is unbounded from below and exhibits a ground state with arbitrarily negative energy that is physically meaningless [3]. In-between there is a critical value $\alpha_c = 1/4$ that takes place when $E_\theta = 0$. The omission of the term $-1/(8r^2)$ led Alhaidari to the wrong critical condition $2E_\theta = -1/4$.

The charge distribution chosen by Alhaidari [1] exhibits zero total charge and zero dipole moment. The first nonvanishing contribution to the multipole expansion is the quadrupole term that he wrote in dimensionless form as

$$V_\theta(\theta) = -4\xi \sin(2\theta), \quad (6)$$

where ξ is proportional to the strength of the quadrupole. If we take into account that $\sin(2\theta - \pi/2) = -\cos(2\theta)$ we can rewrite the angular equation as

$$\Theta''(\theta) + [2E_\theta - 8\xi \cos(2\theta)] \Theta(\theta) = 0 \quad (7)$$

that has exactly the form of the Mathieu equation when $a = 2E_\theta$, $q = 4\xi$ [4]. The Mathieu equation exhibits four types of solutions that are relevant to our problem: even and odd and each one of period π and 2π . They can be obtained as Fourier series with coefficients that satisfy well-known three-term recurrence relations [4].

Alhaidari [1] also derived a three-term recurrence relation (Eq. 2.8). However, his basis set of polynomial functions $T_n(x)$ of $x = \sin(2\theta)$ can at most account for the solutions of period π . We verified that the eigenvalues given by that recurrence relation do not agree with those coming from the recurrence relations for the coefficients of the Fourier series [4].

In order to obtain the critical values of the quadrupole moment we just find the values of $q = q_c$ such that $a(q_c) = 0$. Since the lowest eigenvalue $a_0(q)$ is negative for all values of q and vanishes at $q = 0$ we conclude that there will be solutions to the Schrödinger equation with negative energy for all values of the quadrupole strength ξ . On the other hand, Alhaidari concluded that the minimum quadrupole parameter is $\xi \approx 0.2557$.

Table 1 shows the first critical values $\xi_c = q_c/4$ of the quadrupole moment obtained from the roots of the eigenvalues $a_m(q_c) = 0$ and $b_{m+1}(q_c) = 0$, $m = 0, 1, \dots$, of the Mathieu equation [4]. We observe the occurrence of pairs of close critical parameters that are due to the fact that $b_{m+1} - a_m$ vanishes exponentially $q \rightarrow \infty$ [4]. This

Table 1 First critical values ξ_c of the quadrupole moment

Eigenvalue	ξ_c
a_0	0
b_1	0.2270115834
a_1	1.878402574
b_2	1.894922593
a_2	5.324657803
b_3	5.325793406
a_3	10.48179309
b_4	10.48186048
a_4	17.35709457
b_5	17.35709827

behaviour is not found in the case of a charged particle in the field of a nonrelativistic electric dipole in three dimensions because the eigenvalues of the corresponding angular equation do not exhibit such pairing property [6].

3 Conclusions

In this paper we revisited the quantum-mechanical problem of a charged particle in the field of an electric quadrupole in two dimensions and obtained results that are quite different from those obtained some time ago by Alhaidari [1]. In the first place we found that a missing term in the radial equation has a considerable effect on the condition for the existence of negative eigenvalues. In the second place we showed that the solution of the angular part of the Schrödinger equation can be rewritten as a Mathieu equation which enables us to exploit all the analytical properties of such well-known equation. By means of the standard three-term recurrence relations for the coefficients of the Fourier expansions [4] we obtained the critical values of the quadrupole moment. Such recurrence relations may at first sight resemble the one derived by Alhaidari for the coefficients of the expansion in “improved ultraspherical Gegenbauer polynomials”. However, the latter recurrence relation fails to yield the well-known eigenvalues of the Mathieu equation that appear in the standard tables [4].

Our calculations show that there is no critical quadrupole-moment strength for the capture of the charge. This fact makes present quadrupole problem different from the charge in the field of an electric dipole in three dimensions where such critical value already exists [5].

Another important difference between the quadrupole and dipole problems is the occurrence of pairs of close critical quadrupole strengths that do not appear in the latter three-dimensional problem [6].

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