Schrödinger equations on $\mathbb{R}^3 \times \mathcal{M}$ with non-separable potential

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Abstract   We consider the problem of defining the Schrödinger equation for a hydrogen atom on $\mathbb{R}^3 \times \mathcal{M}$ where $\mathcal{M}$ denotes an m dimensional compact manifold. In the present study, we discuss a method of taking non-separable potentials into account, so that both the non-compact standard dimensions and the compact extra dimensions contribute to the potential energy analogously to the radial dependence in the case of only non-compact standard dimensions. While the hydrogen atom in a space of the form $\mathbb{R}^3 \times \mathcal{M}$, where $\mathcal{M}$ may be a generalized manifold obeying certain properties, was studied by Van Gorder (J Math Phys 51:122104, 2010), that study was restricted to cases in which the potential taken permitted a clean separation between the variables over $\mathbb{R}^3$ and $\mathcal{M}$. Furthermore, though there have been studies on the Coulomb problems over various manifolds, such studies do not consider the case where some of the dimensions are non-compact and others are compact. In the presence of non-separable potential energy, and unlike the case of completely separable potential, a complete knowledge of the former case does not imply a knowledge of the latter.

Keywords   Hydrogen atom · Schrödinger equation · Eigen value problem · Non-separable potential · Compact extra dimensions

1 Introduction

While there has been much interest concerning extra dimensions in theoretical physics, relatively little literature exists regarding atoms in higher spatial dimensions than three, particularly in the case in which the extra dimensions are compact. We should mention that some results for the higher dimensional Kepler problem do exist; see, e.g.,

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Mladenov and Tsanov [1]. Naturally, the case of non-compact extra dimensions have been more amenable to mathematical analysis. Some studies on the hydrogen-like atom over higher dimensional Euclidean space include [2–7], whereas studies of more complicated atomic structures appear in [8] and [9] for higher dimensional Euclidean space. Nouri describes coherent states for the d-dimensional Coulomb problem in [10], and problems in maintaining regularity of the wave functions for hydrogen atoms defined over higher dimensional Euclidean space are discussed in [11–13] whereas Burgbachera, Lämmerzahlb and Maciasc discuss a possible mathematical fix for this problem of regularity in [14].

Although more complicated, quantum mechanical problems can be considered on non-Euclidean space; indeed, "small" compact extra dimensions are a much more likely candidate for higher spatial dimensions than the full hyperspace $\mathbb{R}^n$. One physically realistic example of a candidate for any compact extra dimension would be Kähler manifolds. Examples of studies on mathematical physics problems taking Kähler manifolds or conifolds as the underlying space include [15–18]. Recently, Bellucci, Nersessian and Yeranyan [19] address a quantum mechanics model on a Kähler conifold, whereas Nersessian and Yeranyan [20] discuss the three-dimensional oscillator and Coulomb systems reduced from Kähler spaces, which is quite relevant to the hydrogen atom over Kähler spaces. In Van Gorder [21], a method of solving the Schrödinger equation for a hydrogen-like atom over a space $\mathbb{R}^3 \times \mathcal{M}$ was discussed, where $\mathcal{M}$ is a manifold or conifold which permits separability (that is, the Coulomb potential is taken to only depend on the radial coordinate in the $\mathbb{R}^3$ part of the space, which allows for separability).

We shall review the method discussed in Van Gorder [21] for obtaining solutions for wave functions governing a hydrogen-like atom over a space $\mathbb{R}^3 \times \mathcal{M}$ in the case of completely separable variable cases in Sect. 2. In such cases, the Coulomb potential depends only on the radial coordinate in $\mathbb{R}^3$, as was outlined in [21]. However, such an assumption of separability is unsatisfying, as it restricts the physical scenario too greatly. It is reasonable to consider cases in which the potential is influenced by the compact extra dimensions; indeed, it should be desirable to consider cases where the compact extra dimensions influence the potential in some manner, as this appears to be more physically plausible and may even lead to a detectability of extra dimensions through minute changes in expected values taken by the wave functions (although any such mechanism for this is beyond the scope of the present paper). Hence, in Sect. 3 we consider a potential depending on both the radial coordinate in $\mathbb{R}^3$ and on the position on the compact manifold, $\mathcal{M}$.

For illustrative purposes, in Sect. 4 we set $\mathcal{M} = S^m$, the m-sphere. Separating the Schrödinger equation as far as is possible, we obtain a partial differential equation in two variables, which is in analogy to the standard radial Schrödinger equation obtained in [21]. Relevant boundary conditions are also discussed, as is the normalization requirement. We introduce a coupling parameter, γ, which relates the strength of the contributions of both the radial coordinate and the coordinate on S^m to the potential. For small γ, we can discuss the first order perturbation theory for the model. We establish the dependence of the normalization coefficient on the coupling parameter, to first order.

We summarize the results in Sect. 5, and discuss how the method can be applied to more general situations where the Hydrogen-like atom is defined over spaces of the form $\mathbb{R}^n \times \mathcal{M}$ for well-behaved compact manifolds $\mathcal{M}$.

2 Review of the general solution method for the hydrogen atom on $\mathbb{R}^3 \times \mathcal{M}$ for separable potentials

Here we review the procedure given in [21]; while this material is covered in [21], it will be useful the review this material in order to contrast the solution method with that of the non-separable case considered in the next section. In order to find the wave function Ψ and associated energy spectrum E for the hydrogenic atom in higher dimensions than three, we consider the eigenvalue problem (a time-independent Schrödinger equation)

$$\hat{\mathcal{H}}\Psi = E\Psi, \quad \text{where} \quad \hat{\mathcal{H}} = -\frac{\hbar^2}{2\mu}\triangle + U, \tag{2.1}$$

over $\mathbb{R}^3 \times \mathcal{M}$, where $\hat{\mathcal{H}}$ is an elliptic operator, $\triangle$ is the Laplacian over $\mathbb{R}^3 \times \mathcal{M}$, U is the potential energy (we will, in general, assume a potential $U = U(r)$ for mathematical simplicity), and $\mathcal{M}$ is a generalized manifold over which we may perform separation of variables so that $\triangle = \triangle_{\mathbb{R}^3} + \triangle_{\mathcal{M}}$ with $\triangle_{\mathbb{R}^3}$ and $\triangle_{\mathcal{M}}$ denoting Laplacians over $\mathbb{R}^3$ and $\mathcal{M}$, respectively. (More accurately, $\triangle_{\mathcal{M}}$ denotes the *Laplace-Beltrami* operator over $\mathcal{M}$.) Then, assuming a separable solution to (2.1) of the form $\Psi = \Psi_1\Psi_2$, where $\Psi_1 : \mathbb{R}^3 \to \mathbb{C}$ and $\Psi_2 : \mathcal{M} \to \mathbb{C}$, we have that $\triangle\Psi = \Psi_2\triangle_{\mathbb{R}^3}\Psi_1 + \Psi_1\triangle_{\mathcal{M}}\Psi_2$, which allows us to write (2.1) as a system of coupled linear eigenvalue problems, to wit:

$$-\frac{\hbar^2}{2\mu}\triangle_{\mathbb{R}^3}\Psi_1 + (U - E - \Gamma_{\mathcal{M}})\Psi_1 = 0, \tag{2.2}$$

$$-\frac{\hbar^2}{2\mu}\triangle_{\mathcal{M}}\Psi_2 + \Gamma_{\mathcal{M}}\Psi_2 = 0, \tag{2.3}$$

where the spectrum $\Gamma_{\mathcal{M}}$ for Ψ_2 is obtained by the solution of the latter problem (2.3) over $\mathcal{M}$ and then placed into (2.2) in order to obtain Ψ_1 and hence the full wave function, Ψ. In principle, $\Gamma_{\mathcal{M}}$ provides us with the corrections to the standard energy spectra, E_N (for a hydrogen atom in $\mathbb{R}^3$), that are needed due to the assumption of extra dimensions which enter due to $\mathcal{M}$. Naturally, the spectrum $\Gamma_{\mathcal{M}}$ will depend strongly on the choice of $\mathcal{M}$. For now, we shall keep $\mathcal{M}$ arbitrary, and assume that a non-trivial solution Ψ_2 to the eigenvalue problem (2.3) exists and admits non-trivial spectrum $\{(\Gamma_{\mathcal{M}})_k\}_{k \in K}$ (where K is an index set). We then solve (2.2) subject to such an assumption, and obtain both the wave function and energy spectrum for a hydrogenic atom, in terms of Ψ_2 and the spectrum $\Gamma_{\mathcal{M}}$. Later, in Sect.3, we fix $\mathcal{M}$ so that we may obtain explicit expressions for the wave function Ψ_2 and spectrum $\Gamma_{\mathcal{M}}$ in some interesting cases.

Under such assumptions, (2.2) becomes

$$-\frac{\hbar^2}{2\mu}\triangle_{\mathbb{R}^3}\Psi_1 + \left(U - E - (\Gamma_{\mathcal{M}})_k\right)\Psi_1 = 0. \tag{2.4}$$

Assuming that Ψ_1 separates as $(\Psi_1)_l(r, \theta, \phi) = R(r)Y_l(\theta, \phi)$ where $R(r)$ is the radial component and $Y_l(\theta, \phi)$ is a spherical harmonic (here, the index ℓ runs as $\ell \in \mathbb{N}$). Taking the Laplacian $\triangle_{\mathbb{R}^3}$ to spherical coordinates, (2.4) results in the coupled eigenvalue problems

$$-\frac{\hbar^2}{2\mu}\left(\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\right) + r^2\left(U - E - (\Gamma_{\mathcal{M}})_k\right) = -\frac{\hbar^2}{2\mu}\lambda, \qquad (2.5)$$

$$\frac{\hbar^2}{2\mu}\left(\frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{Y\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right) = -\frac{\hbar^2}{2\mu}\lambda, \qquad (2.6)$$

where λ is a constant. It is well known that a solution $Y_\ell(\theta, \phi)$ to (2.6) results in eigenvalues $\lambda_\ell = \ell(\ell+1)$ (the square of the angular momentum) where $\ell \in \mathbb{N}$. Then, placing this expression into (2.5), we obtain the radial equation

$$-\frac{\hbar^2}{2\mu}\left(\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \ell(\ell+1)\right) + r^2\left(U - E - (\Gamma_{\mathcal{M}})_k\right) = 0. \qquad (2.7)$$

Setting U to the Coulomb potential (that is, $U = U(r) = -Ze^2/r$), defining constants $a_\ell = \ell(\ell+1)$, $b = -2\mu Ze^2/\hbar^2$, $c_k = -(2\mu/\hbar^2)(E + (\Gamma_{\mathcal{M}})_k)$ we obtain (making use of generalized Laguerre polynomials)

$$\Psi_{\ell,k}(r, \theta, \phi, \mathbf{w}) = \frac{(-1)^{2\ell+1}(2\sqrt{c_k}r)^\ell e^{-\sqrt{c_k}r}}{q!\binom{q}{2\ell+1}}L_q^{2\ell+1}(2\sqrt{c_k}r)Y_\ell(\theta, \phi)\Psi_{2,k}(\mathbf{w}), \quad (2.8)$$

where $\mathbf{w} \in \mathcal{M}$ and $q = \ell - \frac{b}{2\sqrt{c_k}}$. Now, as we require $\Psi_1 \in L^2(\mathbb{R}^3)$, the quantization condition $\ell + 1 + \frac{b}{2\sqrt{c_k}} = -m_r$, where $m_r \in \mathbb{N}$ is referred to as the radial quantum number, must hold (and hence $q = 2\ell + 1 + m_r \in \mathbb{N}^*$). Then, defining $N = m_r + \ell$, we have that the condition $-(2\mu/\hbar^2)(E + (\Gamma_{\mathcal{M}})_k) = c_k = \frac{b^2}{4(N+1)^2}$ holds and, in fact, yields the 'closed-form' expression for the energy spectrum for the hydrogenic atom over $\mathbb{R}^3 \times \mathcal{M}$, viz.,

$$E = E_{N,k} = -\frac{\mu(Ze^2)^2}{2\hbar^2(N+1)^2} - (\Gamma_{\mathcal{M}})_k. \qquad (2.9)$$

Clearly, for $(\Gamma_{\mathcal{M}})_0 = 0$, $E_{N,0}$ from (2.9) gives the standard energy spectrum for the hydrogen atom over $\mathbb{R}^3$. Thus, the term $(\Gamma_{\mathcal{M}})_k$ appears as a correction to the standard energy spectrum, to account for the additional dimensions inherent in the model due to the assumption of an underlying space of the form $\mathbb{R}^3 \times \mathcal{M}$. For precision, note that the indices in the above formulas run as $\ell \in \mathbb{N}$, $m_r \in \mathbb{N}$ and hence $N \in \mathbb{N}$.

3 The hydrogen atom on $\mathbb{R}^n \times \mathcal{M}$ for non-separable potentials

While the above analysis is useful when the potential U does not depend on $\mathcal{M}$ in any way, the above method of separation fails for reasonable choices of U which do

depend on $\mathcal{M}$. However, such situations may be more physically reasonable. This leads us to consider the case in which U depends on both the radial variable r and the position on $\mathcal{M}$.

Let us define a function $g : \mathcal{M} \to [0, 1]$, which we take to be some form of normalized distance on the compact manifold $\mathcal{M}$. For instance, taking $\mathcal{M}$ to be a sphere, we can take $g = 0$ at one pole, $g = 1$ at the other pole, and $0 < g < 1$ for all other points. We shall require that g be continuous. We then assume a potential which depends on g; that is, $U = U(r, g(\omega))$, where $\omega = (\omega_1, \omega_2, \dots, \omega_m) \in \mathcal{M}$. With such a choice of potential, we may still separate the ϕ and θ coordinates in $\mathbb{R}^3$, leaving a function which depends on $r \in [0, \infty)$ and $\omega \in \mathcal{M}$; we denote this effective wave function as $X(r, \omega)$, where $\Psi = X(r, \omega) Y(\phi, \theta)$. Under such an assumption, the function X is governed by an equation of the form

$$X_{rr} + \frac{2}{r} X_r + \frac{\mu_k}{r^2} X + \triangle_{\mathcal{M}} X + \frac{U(r, g(\omega))}{\kappa} X = \frac{E}{\kappa} X, \tag{3.1}$$

where $\kappa = -\frac{\hbar^2}{2\mu}$ is defined for brevity and μ_k is an eigenvalue of the spectral problem $\triangle_{\mathcal{S}^2} Y_k = \mu_k Y_k$ for the spherical harmonics Y_k. Note that

$$\triangle_{\mathcal{M}} X = X_{gg} \left(\sum_{j=1}^{m} \left(\frac{\partial g}{\partial \omega_j} \right)^2 \right) + X_g \left(\sum_{j=1}^{m} \frac{\partial^2 g}{\partial \omega_j^2} \right). \tag{3.2}$$

Picking g (which, recall, we are free to define in a convenient matter) to satisfy

$$\sum_{j=1}^{m} \left(\frac{\partial g}{\partial \omega_j} \right)^2 = F(g) \tag{3.3}$$

and

$$\sum_{j=1}^{m} \frac{\partial^2 g}{\partial \omega_j^2} = G(g), \tag{3.4}$$

we have that $\triangle_{\mathcal{M}} X = F(g) X_{gg} + G(g) X_g$ and hence Eq. (3.1) becomes

$$X_{rr} + \frac{2}{r} X_r + \frac{\mu_k}{r^2} X + F(g) X_{gg} + G(g) X_g + \frac{U(r, g)}{\kappa} X = \frac{E}{\kappa} X. \tag{3.5}$$

Then, provided such a $g = g(\omega)$ exists, the spectral problem becomes effectively two-dimensional. While any specific choice of $U(r, g)$ could be contested due to lack of explicit experimental support thus far for extra dimensions, we should note that there are certain requirements which must be met. For $g = 0$, we should recover the standard radial Schrödinger equation, and hence $U(r, 0) = -\frac{Ze^2}{r}$. Therefore, as $r \to 0$, we expect the potential to be singular. Potentials of this form would be, for

example, $U(r, g) = -\frac{Ze^2}{r+\gamma g}$ and $U(r, g) = -\frac{Ze^2}{r(1+\gamma g)}$. Here we have introduced a coupling parameter with which to scale the contribution of the manifold on the potential. Of course, far more complicated potentials are possible which satisfy the requirement $U(r, 0) = -\frac{Ze^2}{r}$.

For sake of demonstration, let us consider the latter example potential, $U(r, g) = \frac{U_0}{r(1+\gamma g)}$, where $U_0 = -Ze^2$. More generally, such potentials take the form $U(r, g) = \frac{U_0}{r}H(g)$. Under such an assumption, (3.5) takes the form

$$X_{rr} + \frac{2}{r}X_r + \frac{\mu_k}{r^2}X + F(g)X_{gg} + G(g)X_g + \frac{\tilde{U}_0}{r}H(g)X = \tilde{E}X. \quad (3.6)$$

where $\tilde{U}_0 = U_0/\kappa$ and $\tilde{E} = E/\kappa$. We thus have a coupled non-separable (due to the fact that the potential U depends on both r and g) linear partial differential equation for $X(r, g)$.

In principle, solving Eq. (3.6) is challenging due to the non-separability and the singular nature of the equation. Hence, in order to obtain any type of solution, further assumptions must be made. Making the reasonable assumption that g is normalized so that $g : \mathcal{M} \to [0, 1)$ and that $g \in C^2(\mathcal{M})$ (i.e., that g is twice continuously differentiable in all of it's variables), it makes sense to expand

$$F(g) = \sum_{j=0}^{\infty} F_j g^j \quad G(g) = \sum_{j=0}^{\infty} G_j g^j \quad H(g) = 1 + \sum_{j=1}^{\infty} H_j g^j. \quad (3.7)$$

Note that such representations are reasonable given the properties of g, assuming that such F and G exist. In fact, the series for F and G will terminate for most practical applications. To illustrate this, we consider two examples.

Example 1 Let $g(\omega) = \sum_{j=1}^{m} |\omega_j|$. Here, g is just the L^1-norm. Let us assume that the manifold $\mathcal{M}$ is defined so that $\omega_j \geq 0$ for all $j = 1, 2, \ldots m$. Then, $g(\omega) = \sum_{j=1}^{m} \omega_j$. From the definition of F and G we find that $F(g) = m$ while $G(g) = 0$.

Example 2 Let $g(\omega) = \exp\left(\sum_{j=1}^{m} |\omega_j|\right) - 1$. Assuming again that $\omega_j \geq 0$ for all $j = 1, 2, \ldots m$, we have $g(\omega) = \exp\left(\sum_{j=1}^{m} \omega_j\right)$. We then find that $F(g) = m \exp\left(2\sum_{j=1}^{m} \omega_j\right) = m(g+1)^2 = mg^2 + 2mg + m$. Likewise, $G(g) = m(g+1) = mg + m$.

Assuming that the compact manifold $\mathcal{M}$ is small, the we take the scaled quantity γ to be small (we can scale g to be on the order of the diameter of $\mathcal{M}$). Alternately, we can keep $g \in [0, 1]$, and introduce coupling parameter $\gamma > 0$. We then replace $F(g) \to F(\gamma g)$, $G(g) \to G(\gamma g)$ and $H(g) \to H(\gamma g)$ in (3.7) so that we obtain series in γ. Then, for the sake of preforming computations, we assume a solution of the form

$$X(r, g) = X_0(r, g) + \sum_{j=1}^{\infty} X_j(r, g)\gamma^j. \quad (3.8)$$

Under such an assumption, we iteratively obtain the partial differential equations

$$L[X_0] = 0\,, \tag{3.9}$$

$$L[X_j] = \sum_{i=1}^{j} \iota_i[X_{j-i}] \quad \text{for} \quad j \geq 1\,, \tag{3.10}$$

where we define the operators

$$L = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + F_0\frac{\partial^2}{\partial g^2} + G_0\frac{\partial}{\partial g} + \left(\frac{\mu_k}{r^2} + \frac{\tilde{U}_0}{r} - \tilde{E}\right), \tag{3.11}$$

$$\iota_i = -F_i\frac{\partial^2}{\partial g^2} - G_i\frac{\partial}{\partial g} - \frac{\tilde{U}_0}{r}H_i\,. \tag{3.12}$$

In order to determine the order zero term, X_0, let us note that $L[X_0] = 0$ is a separable PDE. Hence, we assume $X_0(r, g) = R(r)S(g)$, obtaining, through separation of variables,

$$\frac{R''(r)}{R(r)} + \frac{2}{r}\frac{R'(r)}{R(r)} + \left(\frac{\mu_k}{r^2} + \frac{\tilde{U}_0}{r} - \tilde{E}\right) = -\Lambda^0 = -\frac{F_0 S''(g) + G_0 S'(g)}{S(g)}\,. \tag{3.13}$$

Note that $\triangle_{\mathcal{M}} u(\omega) = \Lambda u(\omega)$ is a spectral problem on $\mathcal{M}$, admitting eigenfunctions u_j and corresponding spectrum Λ_j for $j \in J$ where J is an index set. Transforming $u(\omega) \rightarrow \hat{u}(g)$, note that $\triangle_{\mathcal{M}}\hat{u}(g) = F(g)\hat{u}''(g) + G(g)\hat{u}'(g) = \Lambda\hat{u}(g)$. If we replace $F(g)$ and $G(g)$ with $F(0) = F_0$ and $G(0) = G_0$, respectively, then we modify the spectral problem, obtaining modified spectra Λ_j^0. For each such $j \in J$, we thus have an eigenfunction $S_j(g)$ and associated eigenvalue Λ_j^0 such that $\triangle_{\mathcal{M}}S_j(g) = F_0 S_j''(g) + G_0 S_j'(g) = \Lambda_j^0 S_j(g)$. With such choice of eigenfunction and eigenvalue, the right hand equation in (3.13) is identically satisfied. Hence, the appropriate choice of the S_j's will lie in the structure of the compact manifold $\mathcal{M}$. What remains is to solve for $R(r)$. Note that $R(r)$ will depend on the index k (due to the hyperspherical harmonics Y_K and associated spectral parameter μ_k) and on the index j (due to the eigenfunctions S_j on the manifold $\mathcal{M}$ and associated spectral parameter Λ_j^0). Hence, we consider $R_{k,j}(r)$ satisfying the spectral problem

$$R_{k,j}''(r) + \frac{2}{r}R_{k,j}'(r) + \left(\frac{\mu_k}{r^2} + \frac{\tilde{U}_0}{r} - \Lambda_j^0\tilde{E}\right)R_{k,j}(r) = 0\,. \tag{3.14}$$

The solution to this equation is essentially that given for the radial factor in (2.8), replacing the energy spectra given in (2.9) with

$$E_{N,j} = -\frac{\mu(Ze^2)^2}{2\hbar^2(N+1)^2} - \Lambda_j^0. \tag{3.15}$$

From here, we sum over all possible eigenstates $j \in J$, obtaining for each k the function

$$X_0(r, g) = \sum_{j \in J} R_{k,j}(r) S_j(g), \qquad (3.16)$$

the zeroth order term in the perturbation solution for (3.6). Effectively, we have recovered the solution of Sect. 2 (for the completely separable case where U depends on r, alone) as the zeroth-order approximation to the solution to the problem in which the potential depends on both r and the position on the compact manifold $\mathcal{M}$.

We may continue in this manner, iteratively obtaining the higher order terms X_j. Upon attempting such calculations, one sees that the computations quickly become lengthy and complicated, with closed-form solutions either impossible or at the very least impractical. However, for sufficiently small g, a first order approximation will suffice. The equation governing $X_1(r, g)$ is

$$L[X_1] = \iota_1[X_0] = \iota_1 \left[\sum_{j \in J} R_{k,j}(r) S_j(g) \right] = \sum_{j \in J} R_{k,j}(r) \iota_1[S_j(g)], \quad (3.17)$$

as ι_1 is a differential operator in g alone (although r does make an appearance in ι_1 as a coefficient). Let us denote

$$\sum_{j \in J} R_{k,j}(r) \iota_1[S_j(g)] = -\sum_{j \in J} R_{k,j}(r) \left(F_1 S_j''(g) + G_1 S_j'(g) + \frac{\tilde{U}_0}{r} S_j(g) \right)$$

$$= \Xi_1(r, g). \qquad (3.18)$$

We may solve (3.17) by obtaining a Green's function $\mathcal{G}$ so that

$$X_1(r, g) = \int_0^\infty \int_0^{g_{max}} \mathcal{G}(r - r', g - g') \Xi_1(r', g') dg' dr'. \qquad (3.19)$$

As $\mathcal{M}$ is compact, g_{max}, the maximum value of g, is taken to be finite. For the "small" compact manifolds we are interested in, $g_{max} \ll 1$.

In order to obtain such a Green's function, we refer to the Fredholm theory. For the basis of eigenfunctions $\{R_{k,j}(r) S_j(g)\}_{j \in J}$ with associated eigenvalues $\tilde{E}_{k,j}$ which L admits, the Green's function for L may be constructed as

$$\mathcal{G}(r - r', g - g') = \sum_{j \in J} \frac{R_{k,j}^\dagger(r) R_{k,j}(r') S_j^\dagger(g) S_j(g')}{\tilde{E}_{k,j}}, \qquad (3.20)$$

where † denotes complex conjugation. Using (3.20) in Eq. (3.19), we obtain

$$X_1(r, g) = \sum_{j \in J} C_j^{[1]} R_{k,j}^\dagger(r) S_j^\dagger(g),$$ (3.21)

where we define the coefficients $C_j^{[1]}$ by

$$C_j^{[1]} = \int_0^\infty \int_0^{g_{max}} R_{k,j}(r') S_j(g') \Xi_1(r', g') dg' dr'.$$ (3.22)

More generally, employing the same process, we find that for integer $p \geq 1$

$$X_p(r, g) = \sum_{j \in J} C_j^{[p]} R_{k,j}^\dagger(r) S_j^\dagger(g),$$ (3.23)

where

$$C_j^{[p]} = \int_0^\infty \int_0^{g_{max}} R_{k,j}(r') S_j(g') \Xi_p(r', g') dg' dr',$$ (3.24)

and

$$\Xi_p(r, g) = \sum_{i=1}^p \iota_i [X_{p-i}(r, g)].$$ (3.25)

4 The hydrogen atom on $\mathbb{R}^n \times \mathcal{S}^m$: an illustrative case

The case of U depending on $\mathcal{M}$ and r is far more complicated than that addressed in [21]. To permit some tractability, we consider the special case $\mathcal{M} = \mathcal{S}^m$ for illustrative purposes. Here we take the non-compact dimensions $\mathbb{R}^n$; when $n = 3$, we obtain the most physically relevant solutions, though we shall keep n arbitrary for greater generality.

Let us define the Laplacians

$$\triangle_{\mathbb{R}^n} \equiv \frac{\partial^2}{\partial r^2} + \frac{n-1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \triangle_{\mathcal{S}^{n-1}},$$ (4.1)

$$\triangle_{\mathcal{S}^m} \equiv \frac{\partial^2}{\partial \omega_m^2} + (m-1) \cot(\omega_m) \frac{\partial}{\partial \omega_m} + \frac{1}{\sin^2(\omega_m)} \triangle_{\mathcal{S}^{m-1}}.$$ (4.2)

Then, for manifold $\mathcal{M}_\sigma = \mathbb{R}^n \times \mathcal{S}^m$ with m-sphere of radius $\sigma > 0$, the Laplacian over $\mathcal{M}_\sigma$ reads

$$\triangle_{\mathcal{M}_\sigma} = \frac{\partial^2}{\partial r^2} + \frac{n-1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\triangle_{\mathcal{S}^{n-1}} + \frac{1}{\sigma^2}\triangle_{\mathcal{S}^m}. \tag{4.3}$$

Defining the Hamiltonian

$$\hat{H} = \kappa\triangle_{\mathcal{M}_\sigma} + U, \tag{4.4}$$

the Schrödinger equation for the wave function, Ψ, becomes

$$\hat{H}\Psi = E\Psi. \tag{4.5}$$

Here the potential function U is in general a function of the $n+m$ variables. In Van Gorder [21], the case in which $U = U(r)$ was considered, as this case permits separability in the variables. However, under such an assumption, the potential is not influenced at all by the extra compact dimensions. In the present study, we will consider the case in which the potential is influenced by the compact extra dimensions. Along these lines, let us take $U = U(r, \omega_m)$, so that U depends on the space $\mathbb{R}^n$ radially (as is standard) while U depends on $\mathcal{S}^m$ azimuthally. Again, this is still a simplifying assumption, and we do not claim that this is the most physically relevant scenario. That said, this assumption does permit us to consider a non-separable case which is analytically tractable.

4.1 Separation of variables

Let us separate variables into three groups: those influencing the potential, those in $\mathbb{R}^n$ and not influencing the potential, and those in $\mathcal{S}^m$ and not influencing the potential. We then make the assumption

$$\Psi = X(r, \omega_n)Y(\phi, \theta_1, \ldots, \theta_{n-2})Z(\omega_1, \ldots, \omega_{m-1}). \tag{4.6}$$

To Y and Z we have the associated spectral problems

$$\triangle_{\mathcal{S}^{n-1}}Y = \mu_k Y \quad \text{and} \quad \triangle_{\mathcal{S}^{m-1}}Z = \nu_j Z \tag{4.7}$$

with respective spectra $\{\mu_k\}_{k\in\mathbb{K}}$ and $\{\nu_j\}_{j\in\mathbb{J}}$. Here $\mathbb{K}$ and $\mathbb{J}$ are the appropriate index sets.

Substituting (4.6) into (4.5), and applying (4.7) to remove the Y and Z terms, we find that

$$\kappa X_{rr} + \frac{\kappa(n-1)}{r}X_r + \frac{\kappa}{\sigma^2}X_{\omega_m\omega_m} + \frac{\kappa(m-1)}{\sigma^2}\cot(\omega_m)X_{\omega_m}$$
$$+ \left\{\frac{\kappa\mu_k}{r^2} + \frac{\kappa\nu_j}{\sigma^2\sin^2(\omega_m)} + U(r,\omega_m) - E\right\}X = 0. \tag{4.8}$$

In analogy to the standard potential over $\mathbb{R}^3$ we shall consider a potential of the form

$$U(r, \omega_m) = \frac{U_0}{r + \gamma \sigma g(\omega_m)}, \quad U_0 \equiv -Ze^2 \tag{4.9}$$

where $g(\omega_n)$ is a non-decreasing scaling function satisfying $g(0) = 0$ and $g(\omega_m) > 0$ for all $\omega_m \in [0, \pi]$. The parameter $\gamma \geq 0$ determines the strength of the contribution of ω_m relative to r. When $\gamma = 0$, we recover the standard potential discussed in Van Gorder [21].

4.2 Boundary conditions and normalization

Relevant boundary conditions for the partial differential equation (4.8) include

$$X(r, 0) = R(r), \tag{4.10}$$

(at $\omega_m = 0$ we recover the solution for the radial Schrödinger equation on $\mathbb{R}^n$)

$$X_r(0, \omega_m) = 0, \tag{4.11}$$

(the change in probability is zero at $r = 0$)

$$X(+\infty, \omega_m) = 0, \tag{4.12}$$

(the probability is zero "at infinite radius")

$$X_{\omega_m}(r, \pi) = 0, \tag{4.13}$$

(the change in probability is zero at "the top" of the sphere).

In addition to boundary conditions, one must be mindful of the normalization condition

$$\int_{\mathcal{A}} X d\mathcal{A} = 1 \tag{4.14}$$

due to conservation of probability, where $\mathcal{A} = \mathbb{R}^n \times S^m$. Assuming that the eigenfunctions $Y(\phi, \theta_1, \ldots, \theta_{n-2})$ and $Z(\omega_1, \ldots, \omega_{m-1})$ are appropriately normalized, the above implies that

$$\int_0^\infty \int_0^\pi X d\omega_m dr = 1. \tag{4.15}$$

4.3 PDE for $g(\omega_m) = \sin^2(\omega_m/2)$

Let us consider a potential U of the form

$$U(r, \omega_m) = \frac{U_0}{r + \gamma\sigma\sin^2(\omega_m/2)}, \tag{4.16}$$

and let us make the change of variable $\chi = \sin^2(\omega_m/2)$ along with the change of function

$$X(r, \omega) = \frac{1}{(1-\chi)\chi}\tilde{X}(r, \chi). \tag{4.17}$$

Upon placing the transformed quantities into (4.8), we obtain

$$\kappa\tilde{X}_{rr} + \frac{\kappa(n-1)}{r}\tilde{X}_r + \frac{\kappa}{\sigma^2}\tilde{X}_{\chi\chi} + \frac{\kappa(m-4)}{2\sigma^2}\frac{1-2\chi}{(1-\chi)\chi}\tilde{X}_\chi$$
$$+ \left\{\frac{\kappa\mu_k}{r^2} + \frac{\kappa}{4\sigma^2}\left[\frac{8(m-4)}{\chi} + \frac{\nu_j}{(1-\chi)^2\chi^2}\right] + \frac{U_0}{r+\gamma\sigma\chi} - E\right\}\tilde{X} = 0. \tag{4.18}$$

4.4 Perturbation expansion in γ

The partial differential equation (4.18) is non-separable, due to the form of the potential taken. However, small values of γ are physically reasonable, hence we shall discuss a perturbation solution which gives the first order perturbation for the solution $\tilde{X}$ to (4.18). To this end, consider

$$\tilde{X}(r, \chi) = X^{[0]}(r, \chi) + \gamma X^{[1]}(r, \chi) + O(\gamma^2). \tag{4.19}$$

Note that we shall make use of the expansion

$$U(r, \omega_m) = \frac{U_0}{r+\gamma\sigma\chi} = \frac{U_0}{r} - \gamma\frac{\sigma U_0\chi}{r^2} + O(\gamma^2), \tag{4.20}$$

for small γ. Separating the $O(1)$ and $O(\gamma)$ terms, we find that (4.18) yields

$$\kappa X_{rr}^{[0]} + \frac{\kappa(n-1)}{r}X_r^{[0]} + \frac{\kappa}{\sigma^2}X_{\chi\chi}^{[0]} + \frac{\kappa(m-4)}{2\sigma^2}\frac{1-2\chi}{(1-\chi)\chi}X_\chi^{[0]}$$
$$+ \left\{\frac{\kappa\mu_k}{r^2} + \frac{\kappa}{4\sigma^2}\left[\frac{8(m-4)}{\chi} + \frac{\nu_j}{(1-\chi)^2\chi^2}\right] + \frac{U_0}{r} - E\right\}X^{[0]} = 0, \tag{4.21}$$

$$\kappa X_{rr}^{[1]} + \frac{\kappa(n-1)}{r}X_r^{[1]} + \frac{\kappa}{\sigma^2}X_{\chi\chi}^{[1]} + \frac{\kappa(m-4)}{2\sigma^2}\frac{1-2\chi}{(1-\chi)\chi}X_\chi^{[1]}$$
$$+ \left\{\frac{\kappa\mu_k}{r^2} + \frac{\kappa}{4\sigma^2}\left[\frac{8(m-4)}{\chi} + \frac{\nu_j}{(1-\chi)^2\chi^2}\right] + \frac{U_0}{r} - E\right\}X^{[1]} = \frac{\sigma U_0\chi}{r^2}X^{[0]}. \tag{4.22}$$

4.5 Zeroth-order perturbation theory

Let us deal with $X^{[0]}$ first. Note that Eq. (4.21) is separable in r and χ, so let us assume a solution of the form $X^{[0]} = C\rho(r)\eta(\chi)$. Placing this into (4.21) we find that

$$\mathcal{L}_r\rho = \kappa\frac{\partial^2\rho}{\partial r^2} + \frac{\kappa(n-1)}{r}\frac{\partial\rho}{\partial r} + \left[\frac{\kappa\mu_k}{r^2} + \frac{U_0}{r} - E\right]\rho = -\lambda\rho \qquad (4.23)$$

and

$$\mathcal{L}_\chi\eta = \frac{\kappa}{\sigma^2}\frac{\partial^2\eta}{\partial\chi^2} + \frac{\kappa(m-4)}{2\sigma^2}\frac{1-2\chi}{(1-\chi)\chi}\frac{\partial\eta}{\partial\chi}$$
$$+ \frac{\kappa}{4\sigma^2}\left[\frac{8(m-4)}{\chi} + \frac{\nu_j}{(1-\chi)^2\chi^2}\right]\eta = \lambda\eta, \qquad (4.24)$$

where λ is a constant and $\mathcal{L}_r$, $\mathcal{L}_\chi$ denote differential operators for future reference. Note that solutions to (4.23) are of the form $\rho(r) = R^{[n]}(r)$, where R is the radial function described in [21] (in the three-dimensional $n = 3$ case; for $n > 3$ we lose regularity) which, as demonstrated in (2.8), may be written in terms of generalized Laguerre polynomials. Solutions to (4.24) must satisfy the boundary conditions $\eta(0) = 0$ and $\eta'(1) = 0$ (which follow from the change of variables $\omega_m \to \chi$) and must be regular. There are two independent HeunC type solutions (confluent hypergeometric functions), one of which fails regularity. The remaining solution is of the form

$$\eta(\chi) = \text{Constant} \times \exp\left(\sigma\sqrt{\frac{\lambda}{\kappa}}\chi\right)[x(1-x)]^{\frac{1}{4}\left[\sqrt{(m-6)^2-4\nu_j}-(m-6)\right]}$$
$$\times \text{HeunC}\left(2\sigma\sqrt{\frac{\lambda}{\kappa}}, \frac{\sqrt{(m-6)^2-4\nu_j}}{2}, \frac{\sqrt{(m-6)^2-4\nu_j}}{2}, 2m\right.$$
$$\left. -8, -\left(\frac{\nu_j}{2} + \frac{m^2}{8} + m - \frac{13}{2}\right), \chi\right), \qquad (4.25)$$

which always satisfies $\eta(0) = 0$. Furthermore, this solution has a regular derivative at $\chi = 1$ (and hence permits the boundary condition $\eta'(1) = 0$) provided that $\sqrt{(m-6)^2-4\nu_j} - (m-6) > 1$, i.e. as $\nu_j \geq 0$, we must have m is an integer satisfying $0 < m < 6$. Which this restriction on m is limiting, this is likely more due to the form of the toy model taken, than any physically meaningful bound on the dimension of the compact extra dimensions. The constant coefficient can be ignored, as we have already introduced a normalizing constant C.

With solutions to $\rho(r)$ and $\eta(\chi)$ we have now determined the order-zero perturbation contributions, which basically gives the wave function for the case where the potential is influenced only by the radial variable, r, and not by any variables in the space $\mathcal{S}^m$. The first order perturbation will then give an approximation to the dependence of the wave function on a potential which takes into account both r and ω_m.

4.6 First-order perturbation theory

In order to simplify the inhomogeneity present in (4.22), observe that we can write this equation as

$$(\mathcal{L}_r + \mathcal{L}_\chi)X^{[1]} = \frac{\sigma U_0 \chi}{r^2}\rho(r)\eta(\chi). \tag{4.26}$$

Making the substitution

$$X^{[1]}(r, \chi) = C\sigma U_0 \xi(r, \chi)\rho(r)\eta(\chi) \tag{4.27}$$

we find that using (4.23) and (4.24)) (4.26) reduces to

$$(\mathcal{L}_r + \mathcal{L}_\chi)\xi(r, \chi) = \frac{\chi}{r^2}. \tag{4.28}$$

While this equation is still inhomogeneous and non-separable, at least we have removed the dependence on $X^{[0]}$ from the right hand side. Inverting the linear operators subject to homogeneous boundary data, we would obtain

$$\xi(r, \chi) = (\mathcal{L}_r + \mathcal{L}_\chi)^{-1}\left[\frac{\chi}{r^2}\right]. \tag{4.29}$$

This solution, while difficult to write explicitly, can be determined numerically for fixed values of the physical parameters. In particular, let $\mathcal{G}(r, \hat{r}, \chi, \hat{\chi})$ be the Green's function for the linear differential operator $\mathcal{L}_r + \mathcal{L}_\chi$. Such a function $\mathcal{G}(r, \hat{r}, \chi, \hat{\chi})$ can be found via eigenfunction expansion in the standard way; this is messy, and we omit the specifics, however this method allows a constructive proof of the existence of such a function $\mathcal{G}(r, \hat{r}, \chi, \hat{\chi})$. We will then obtain

$$\xi(r, \chi) = \int_0^\infty \int_0^1 \mathcal{G}(r, \hat{r}, \chi, \hat{\chi})\frac{\hat{\chi}}{\hat{r}^2}d\hat{\chi}d\hat{r}. \tag{4.30}$$

The first order perturbation theory is then given by

$$\tilde{X}(r, \chi) = C\left(1 + \gamma\sigma U_0 \xi(r, \chi) + O(\gamma^2)\right)\rho(r)\eta(\chi). \tag{4.31}$$

Hence, the separable solution $C\rho(r)\eta(\chi)$ is perturbed by a variable coefficient $\xi(r, \chi)$ for positive values of the coupling parameter γ when we move to the non-separable case.

4.7 γ-dependent normalization

One now sees that the normalization coefficient should depend on the value of γ taken; i.e., $C = C(\gamma)$. When $\gamma = 0$, we obtain the normalization for the case discussed in

[21], whereas for $\gamma > 0$ the value of the normalization coefficient should change. Placing (4.31) into the normalization requirement (4.15), we obtain

$$C(\gamma) \int_0^\infty \int_0^1 (1 + \gamma \sigma U_0 \xi(r, \chi)) \frac{\rho(r)\eta(\chi) d\chi dr}{(x(1-x))^{3/2}} = 1.$$

(4.32)

It is then clear to see that $C(\gamma)$ scales as

$$C(\gamma) = C_0 - \left(\sigma U_0 C_0^2 \int_0^\infty \int_0^1 \frac{\xi(r, \chi)\rho(r)\eta(\chi)}{(x(1-x))^{3/2}} d\chi dr \right) \gamma + O(\gamma^2), \quad (4.33)$$

where C_0 is the normalization for the case in which the potential depends only on r (i.e., U_0/r) and is given by

$$C_0 = \frac{1}{\int_0^\infty \int_0^1 \frac{\rho(r)\eta(\chi)}{(x(1-x))^{3/2}} d\chi dr}.$$

(4.34)

5 Conclusions

What we have done here was derive a non-separable PDE describing the eigenvalue problem for a hydrogen-like atom over a space of the form $\mathbb{R}^n \times \mathcal{M}$. This serves as an extension of the methods and results discussed in Van Gorder [21], as we considered a case where the potential energy depends not only on r (which was the case considered in Van Gorder [21], as it permitted separability of the radial variable from all other variables) but also on the compact extra dimensions. In particular, when the dependence of the Coulomb potential on the compact extra dimensions is small (relative to the dependence of the Coulomb potential on r), a perturbation expansion and related first order perturbation solution shows that the qualitative form of the separable and non-separable solutions for the hydrogen wave functions agree up to a scale factor. In the case of the non-separable potential, this scale factor is variable; in particular, it depends on both the radial coordinate r and the coordinates considered from $\mathcal{M}$. For the special case $\mathcal{M} = \mathcal{S}^m$ considered in Sect. 4, the coordinate taken corresponded to ω_m, although if other variables, or more than one variable, were taken from $\mathcal{S}^m$, it is clear to see that the obtained scale factor would depend on any such variables which enter into the Coulomb potential.

Symbolically, when $\Psi_{\gamma=0}$ denotes the wave function for a hydrogen atom over $\mathbb{R}^n \times \mathcal{S}^m$ with Coulomb potential which scales as only a function of r (i.e., $U = U(r) \sim 1/r$), the wave function Ψ_γ for a hydrogen atom over $\mathbb{R}^n \times \mathcal{S}^m$ with a potential depending on r and one or more of the coordinates $\omega_1, \omega_2, \ldots, \omega_m$ (i.e., $U = U(r, \gamma\omega_1, \ldots, \gamma\omega_m)$) will take the form $\Psi_\gamma = (1 + \gamma F_1 + \gamma^2 F_2 + \cdots)\Psi_{\gamma=0}$ where the F_k's are higher order corrections which account for any dependence of U on the coordinates for $\mathcal{S}^m$. We may view $1 + \gamma F_1 + \gamma^2 F_2 + \cdots$ as the Taylor expansion of a function $\mathcal{F}(\gamma, r, \omega_1, \ldots, \omega_m)$ about $\gamma = 0$. Then, we have $\Psi_\gamma = \mathcal{F}\Psi_{\gamma=0}$.

As contributions of the compact extra dimensions in the potential are likely small (though doubtfully negligible), the perturbation expansion in the coupling parameter γ seems reasonable, and thus the first order perturbation theory is expected to be qualitatively realistic for the model considered.

Furthermore, for sufficiently well-behaved manifolds (i.e., the so-called "tame manifolds") describing the compact extra dimensions, we expect similar methods and derivations to hold. In other words, for a Hydrogen atom over $\mathbb{R}^n \times \mathcal{M}$ ($\mathcal{M}$ is a well-behaved manifold with $\dim(\mathcal{M}) = m$), if the Coulomb potential's dependence is $U = U(r, \overrightarrow{\omega}) = U_0 \left[r + \gamma g(\overrightarrow{\omega}) \right]^{-1}$ (where $\overrightarrow{\omega} \in \mathcal{M}$) then we may always (after separating the angular variables from $\mathcal{R}^n$) write the remaining parts of the Schrödinger operator as

$$\hat{\mathcal{L}}_r + \hat{\mathcal{L}}_{\overrightarrow{\omega}} + \frac{U_0}{r + \gamma g(\overrightarrow{\omega}))} \tag{5.1}$$

where $\hat{\mathcal{L}}_r$ and $\hat{\mathcal{L}}_{\overrightarrow{\omega}}$ are linear second order differential operators in the variables indicated by subscripts. Expanding $X(r, \overrightarrow{\omega})$, the multiplicative factor of the wave function governed by the variables $(r, \overrightarrow{\omega})$, in a γ-series as $X = X^{[0]} + \gamma X^{[1]} + \cdots$ we see that the Schrödinger operator (5.1) leads to a system of PDEs from which the $X^{[k]}$'s may be obtained. The order zero term corresponds to a solution of

$$\left(\hat{\mathcal{L}}_r + \hat{\mathcal{L}}_{\overrightarrow{\omega}} + \frac{U_0}{r} \right) X^{[0]} = 0 \,, \tag{5.2}$$

which is exactly separable, and, thus, admits closed-form solutions. Note that such solutions correspond to the type of solution discussed in [21]. The solution for the next term, $X^{[1]}$, is in general non-separable and gives the first order perturbation theory, which may be found in a manner similar to the methods discussed in Sect. 3. By such methods, one may construct the first order perturbation theory for Hyderogen-like atoms over $\mathbb{R}^n \times \mathcal{M}$ governed by Coulomb potentials of the form $U = U_0 \left[r + \gamma g(\overrightarrow{\omega}) \right]^{-1}$ or $U = U_0 \left[r(1 + \gamma g(\overrightarrow{\omega})) \right]^{-1}$.

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