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Variational Bound States of Screened Potentials

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Abstract A number of years ago, a calculational scheme was introduced by Stubbins [Phys. Rev. **A**48, 220 (1993)] to compute the energies of both the Hulthén and Yukawa potentials. The method introduces a particular ansatz for solving the Schrödinger equation with screened Coulomb type potentials. In this work, we wish to review the method of Stubbins and to show that it is, in fact, equivalent and a subset of a more systematic (and hence more useful) variational scheme [Zhou et al. Phys. Rev. **A**51, 3337 (1995)]. This variational approach involves the construction of a basis by taking derivatives of the variational parameters of the system. The eigenvalues of the Hamiltonian matrix are then minimized with respect to these parameters yielding a "best guess" upper bound on the energies.

Keywords Variational method · Screened potential

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1 Introduction

The history of screened potentials goes back nearly 75 years to Yukawa's [1] original meson theory for the interaction of nucleons. Over the decades, there has been an incredible amount of work on these potentials due to its widespread range of applications [2–6]. Although its original application was to nuclear physics, screened potentials now are found throughout a number of diverse fields including particle/nuclear physics, gravitational plasma physics, as well as atomic, solid state, and chemical physics. In solid-state and atomic physics, screened potentials are referred to as the Thomas–Fermi potential, while in plasma physics it is called the Debye–Hückel potential. It has also found in the calculation of the energy levels of impurity centers in doped semi-conductors [7]. As might be expected, there also exists an extensive list of calculational methods that have been applied to this potential. Among these are perturbative techniques [8–11] as well as a number of variational approaches [13, 14, 16, 17]. Direct numerical integration of the Schrödinger equation [18–20] has yielded very accurate results. A clever construction of bound-state solutions to the Schrodinger equation was utilized by Enflo [21] in which a momentum space representation of the integral equation was employed along with basic analytical features of the Hankel-transformed wave function. With so much work having been done on screened potentials, it is difficult to imagine that there is anything that may be added to the already exhaustive literature.

However, 20 years ago, a generalized variational method [22] was cleverly employed by Stubbins [23] to compute the energies of two variations of the screened potential: the Hulthén [24–29] and Yukawa potentials. The Hulthén potential has found a great applicability to a number of

diverse sub-fields such as atomic, nuclear, and solid-state physics.

In this brief report, we wish to review the generalized variational solutions of the Schrödinger equation for both the Hulthén and Yukawa potentials as proposed in Reference [21] and to show that it is, in fact, equivalent and a subset of a more systematic (and hence more useful) variational scheme [30]. The technique used in [23] is based on forming trial (independent) functions ψ_j according to:

$$\Psi = \sum_{k=1}^{N} c_k \psi_k. \tag{1}$$

One then solves the matrix eigenvalue equation

$$\mathcal{H}\Psi = \mathcal{E}\mathcal{F}\Psi, \tag{2}$$

where $\mathcal{H}$ is the Hamiltonian matrix of the system and $\mathcal{F}$ represents an overlap matrix. The eigenvectors of this $N \times N$ Hamiltonian matrix are the functions ϕ, while the N eigenvalues $\mathcal{E}$ represent an ordered set, according to the Hylleraas–Undheim theorem [31] as well as in Rayleigh–Ritz theory, which are upper bounds to the corresponding (exact) energies.

The Hulthén potential may be written in atomic units ($\hbar = m = e = 1$) as:

$$V(r) = -Z\lambda \frac{e^{-\lambda r}}{1 - e^{-\lambda r}}, \tag{3}$$

where Z is a constant (without loss of generality we will henceforth choose $Z = 1$) and λ is the screening parameter. After separation into angular and radial parts, the radial Schrödinger equation simplifies to:

$$\left[-\frac{1}{2r}\frac{d^2}{dr^2}r - \lambda \frac{e^{-\lambda r}}{1 - e^{-\lambda r}} + \frac{l(l+1)}{2r^2} \right] R(r) = E R(r). \tag{4}$$

After a brief discussion and with the insight that the denominator of the second term in Eq. (2) is troublesome, Stubbins then constructed a basis formed by the functions

$$\psi_k = A_k r^k e^{-\beta r} \left(1 - e^{\lambda r}\right), \tag{5}$$

where $k = -1, 0, 1, 2, \ldots$ for the s states and $k = l - 1, l, l + 1, \ldots$ for the $l \neq 0$ states. Here, β is a variational parameter determined by minimizing the energy for a given state and basis size, and the normalization "constant" may be shown to be dependent on the parameter β according to:

$$A_k = \frac{(2\beta + \lambda)^{k+j}}{\sqrt{(2k+2)!}}. \tag{6}$$

At this point, we wish to briefly describe a more systematic variational scheme [30] and show that the method employed by Stubbins [23] is a particular subset of it. Consider a trial variational function $\psi_0(\beta, x)$ chosen on the basis of the symmetries of the system and to have a non-zero overlap with the true ground state ϕ_0 such that $\langle \phi_0 | \psi_0 \rangle \neq 0$. Here, β is our variational parameter, while x is a generalized coordinate. An efficient and symmetric as well numerically stable scheme for generating a set of variational basis functions is then [30]:

$$\begin{aligned}
\psi_1(\beta, x) &= A_1(\beta) \frac{\partial}{\partial \beta} \psi_0(\beta, x), \\
\psi_2(\beta, x) &= A_2(\beta) \frac{\partial^2}{\partial \beta^2} \psi_0(\beta, x), \\
\psi_3(\beta, x) &= A_3(\beta) \frac{\partial^3}{\partial \beta^3} \psi_0(\beta, x), \\
&\vdots \\
\psi_N(\beta, x) &= A_N(\beta) \frac{\partial^N}{\partial \beta^N} \psi_0(\beta, x).
\end{aligned} \tag{7}$$

As was pointed out in [30], for the basis constructed in Eq. (7) , although not an orthogonal one (which is acceptable according to the Hylleraas–Undheim theorem), the overlap of any two functions $\langle \psi_i | \psi_j \rangle, i \neq j$ is nonzero. Thus, there is a little risk of encountering numerical instabilities.

Now, a comparison between the (systematic) scheme developed in Eq. (7) and the set of trial functions given by Eq. (5) shows that with the choice for the initial trial variational function:

$$\psi_0(\beta, r) = \frac{A_0}{r} e^{-\beta r} \left(1 - e^{-\lambda r}\right), \tag{8}$$

the equivalent basis of Stubbins may be generated according to the schema of Eq. (7)

$$\psi_k(\beta, r) = A_k(\beta) \frac{\partial^k}{\partial \beta^k} \psi_0(\beta, r). \tag{9}$$

In much the same spirit as the above discussion one may consider the Yukawa potential (in atomic units)

$$V(r) = -Z \frac{e^{-\lambda r}}{r}, \tag{10}$$

where once again Z is a constant and λ is the screening strength. The set of variational basis functions is chosen by Stubbins [23] to be:

$$\psi_k = B_k r^k e^{-(\beta/2)r}, \quad k = 0, 1, 2, \ldots \tag{11}$$

where the normalization constant is B_k is given by:

$$B_k = \left[\frac{\beta^{2k+3}}{(2k+2)!} \right]^{1/2}, \tag{12}$$

and β represents the variational parameter. Once again, we may follow the ansatz proposed in Eq. (7) in constructing a variational basis. With the choice

$$\psi_0(\beta, r) = B_0 e^{-(\beta/2)r}, \quad k = 0, 1, 2, \ldots \tag{13}$$

the basis of Eq. (11) may be generated straightforwardly

$$\psi_k(\beta, r) = B_k(\beta) \frac{\partial^k}{\partial \beta^k} \psi_0(\beta, r). \tag{14}$$

At this point, it is worth noting that numerical applications of the method proposed in this work have already been presented by two of the present authors nearly 15 years ago [32]. The reason for this is that at the time of our original work we were completely unaware of the paper by Stubbins [23] which became the motivation for our current work. This, however, does not in any way negate the conclusions of this work which is that the calculational schemes presented in both [22] and [23] are equivalent and indeed a subset of a systematic variational ansatz [30]. It should be noted that the results obtained with our variational scheme compared very well with those of a more standard variational approach [11] and those of a numerical integration scheme [33–35] for the Hulthén potential.

In conclusion, then we have shown that a very clever use of a generalized variational method to solve for the bound states of the Hulthén and Yukawa potentials is itself a subset of a more generalized and systematic variational scheme. Indeed, the range of applicability of this more generalized approach may be extended to a wide-range of differential equations having an asymptotic limit of the form $\psi_k \sim r^k e^{-\beta r}$.

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