Journal of Mathematical Chemistry Vol. 32, No. 4, November 2002 (© 2002)

Schrödinger equation solutions for the central field power potential energy II. $V(r) = -V_0(r/a_0)^{2\nu-2}$, $0 \leqslant \nu \leqslant 1$, the bound states

Paul Caylor McKinney

Department of Chemistry, Wabash College, P.O. Box 352, Crawfordsville, IN 47933-0352, USA

Received 12 August 2002

The bound states of the generalized Schrödinger equation system with radial potential energy $V(r) = -V_0(r/a_0)^{2\nu-2}$, $0 \leqslant \nu \leqslant 1$, are described. The solutions of the differential equation are related to the functions for the bound state problem with $\nu \geqslant 1$. The Green's function is constructed as well as its first iteration, the traces of both functions are calculated, and an upper and lower bound for the ground state is established. A WKB-like approximate solution for the eigenvalues and eigenfunctions is derived.

KEY WORDS: Schrödinger equation, eigenfunctions, eigenvalues, Green's function, WKB approximation, central field power potential

1. Introduction

The Schrödinger differential equation system for the bound states arising from the potential energy $V(r) = -V_0(r/a_0)^{2\nu-2}$, $0 \leqslant \nu \leqslant 1$, $r \in [0, \infty)$, is

$$\frac{\mathrm{d}^2}{\mathrm{d}y^2} T_\sigma^{q(\nu)}(\kappa; z) + \left[-\kappa^2 + z^{2\nu-2} - \frac{\sigma^2 - 1/4}{z^2}\right] T_\sigma^{(\nu)}(\kappa; z) = 0, \quad z \in [0, \infty),$$
$$T_\sigma^{(\nu)}(\kappa; 0) = 0 \quad \text{and} \quad T_\sigma^{(\nu)}(\kappa; \infty) = 0, \tag{1.1}$$

where $T(r) = rR(r)$, $z = \alpha r$, $(\alpha a_0)^{2\nu} = (2\mu a_0^2/\hbar^2)V_0$, and $\kappa^2 = (-\varepsilon/V_0)(\alpha a_0)^{2\nu-2}$. $R(r)$ is the central field radial function where r is the distance between the two particles, μ is the reduced mass of the two-particle system, ε is the energy of the stationary state and it is less than zero, V_0 is an arbitrary constant to set the potential energy scale, and a_0 may be taken as the Bohr radius or other appropriate distance for the problem under consideration. Although σ may take any value, $\sigma^2 \geqslant 1/4$ gives a pseudo-potential energy in equation (1.1) which guarantees the existence of quantized eigenvalues. When $\sigma = l + 1/2$, where l is the orbital angular momentum quantum number, the quantum problem with spherical symmetry is obtained; when $\sigma = m$, where m is the magnetic quantum number, equation (1.1) becomes the two-dimensional quantum problem with circular symmetry. (In this case, $T(z) = z^{1/2}R(z)$, $R(z)$ is the radial function.) Letting

$\sigma^2 = 1/4$ reduces equation (1.1) to the one-dimensional quantum problem, provided $z \in (-\infty, \infty)$ and the potential energy is expressed in terms of the absolute value of z.

Without regard for compatibility with the boundary conditions, equation (1.1) can be solved in terms of well-known functions for $\nu = 0$, $\nu = 1/2$, and $\nu = 1$:

(a) $\nu = 0$:

$$T_\sigma^{(0)}(\kappa; z) = z^{1/2} I_{\pm\sqrt{\sigma^2-1}}(\kappa z) \quad \text{or} \quad T_\sigma^{(0)}(\kappa; z) = z^{1/2} K_{\sqrt{\sigma^2-1}}(\kappa z).$$

The solutions are not quantized.

(b) $\nu = 1/2$:

$$T_\sigma^{(1/2)}(\kappa_n; z) = z^{\sigma+1/2}\,\mathrm{e}^{-\kappa_n z} L_n^{(2\sigma)}(2\kappa_n z),$$

where

$$\kappa_n = \frac{1}{2n + 2\sigma + 1}, \quad n \in \{0\} \cup \mathbb{N};$$

$L_n^{(2\sigma)}(x)$ are associated Laguerre polynomials and $T_\sigma^{(1/2)}(\kappa_n; z)$ are unnormalized eigenfunctions which satisfy the boundary conditions.

(c) $\nu = 1$:

(1) $\kappa^2 > 1$:

$$T_\sigma^{(1)}(\kappa; z) = z^{1/2} I_{\pm\sigma}\left(\sqrt{\kappa^2 - 1}z\right) \quad \text{or} \quad T_\sigma^{(1)}(\kappa; z) = z^{1/2} K_\sigma\left(\sqrt{\kappa^2 - 1}z\right),$$

(2) $\kappa^2 = 1$:

$$T_\sigma^{(1)}(\kappa; z) = z^{\pm\sigma+1/2},$$

(3) $\kappa^2 < 1$:

$$T_\sigma^{(1)}(\kappa; z) = z^{1/2} J_{\pm\sigma}\left(\sqrt{1 - \kappa^2}z\right).$$

The solutions are not quantized.

By letting $T(z) = z^{(1-\nu)/2}U(z)$ and then changing the variable so that $y = (\kappa z/\nu)^\nu$, a more useful differential equation

$$\frac{\mathrm{d}^2}{\mathrm{d}y^2} U_\sigma^{(\nu)}(\kappa; y) + \left\{ \frac{1}{\kappa^{2\nu}\nu^{2-2\nu}} - y^{2/\nu-2} - \left[\frac{(\sigma/\nu)^2 - 1/4}{y^2} \right] \right\} U_\sigma^{(\nu)}(\kappa; y) = 0 \qquad (1.2)$$

is obtained. Equation (1.2) has the same form as equation (1.1) in [1], hereafter referred to as paper I. The definitions and properties of mathematical functions in this paper are taken from the same reference texts which were used in paper I. The remarks made there apply to equation (1.2) once the parameters in paper I, equation (1.1), have been properly transformed as follows:

$$\lambda \to \frac{1}{\kappa^\nu \nu^{1-\nu}}, \quad \nu \to \frac{1}{\nu}, \quad \text{and} \quad \sigma \to \frac{\sigma}{\nu}. \qquad (1.3)$$

The general solutions of equation (1.1) can be written in terms of the solutions constructed in paper I (equation (3.5)), i.e.,

$$T_\sigma^{(\nu)}(\kappa; z) = C S_\sigma^{(\nu)}\bigl(\kappa\, \mathrm{e}^{(\nu/2)(1-1/\nu)\pi}; \mathrm{e}^{\mathrm{i}\pi/2\nu} z\bigr),$$

where C is a constant, chosen so that $T_\sigma^{(\nu)}(\kappa; z)$ is a real function. In paper I, equation (3.5), λy is replaced by $\mathrm{i}\kappa z$ and y^ν by $\mathrm{i}z^\nu$. The transformation is also valid for $S_{-\sigma}^{(\nu)}(\lambda; y)$. Similarly, for equation (1.2),

$$T_\sigma^{(\nu)}(\kappa; z) = D z^{(1-\nu)/2} S_{\sigma/\nu}^{(1/\nu)}\left(\frac{1}{\kappa\nu^{1-\nu}}; \left(\kappa\frac{z}{\nu}\right)^\nu\right).$$

Interestingly enough, $S(z)$ takes the second form of the solution discussed in paper I (equation (3.4)).

2. The Green's function

The Green's function can be constructed for equation (1.2) directly or by using the transformations of (1.3). It is

$$\begin{aligned} 0 \leqslant x \leqslant y < \infty: \quad & H(x, y) = \nu x^{1/2} I_\sigma\bigl(\nu x^{1/\nu}\bigr) y^{1/2} K_\sigma\bigl(\nu y^{1/\nu}\bigr), \\ 0 \leqslant y \leqslant x < \infty: \quad & H(x, y) = \nu x^{1/2} K_\sigma\bigl(\nu x^{1/\nu}\bigr) y^{1/2} I_\sigma\bigl(\nu y^{1/\nu}\bigr), \end{aligned} \tag{2.1}$$

where

$$U(x) = \frac{1}{\kappa^{2\nu}\nu^{2-2\nu}} \int_0^\infty H(x, y) U(y)\,\mathrm{d}y. \tag{2.2}$$

The trace of the Green's function is

$$\int_0^\infty H(y, y)\,\mathrm{d}y = \nu^{2-2\nu} \frac{1}{4\pi^{1/2}} \frac{\Gamma(\sigma+\nu)\Gamma(\nu)\Gamma(1/2-\nu)}{\Gamma(\sigma-\nu+1)}, \quad 0 < \nu < \frac{1}{2}. \tag{2.3}$$

In terms of the eigenvalues, the trace equals

$$\int_0^\infty H(y, y)\,\mathrm{d}y = \sum_{m=0}^\infty \kappa_m^{2\nu} \nu^{2-2\nu}, \tag{2.4}$$

and therefore,

$$T = \sum_{m=0}^\infty \kappa_m^{2\nu} = \frac{1}{4\pi^{1/2}} \frac{\Gamma(\sigma+\nu)\Gamma(\nu)\Gamma(1/2-\nu)}{\Gamma(\sigma-\nu+1)}. \tag{2.5}$$

It is possible to iterate the Green's function one time using Meijer's G-functions and, from it, one obtains

$$T_1 = \sum_{m=0}^{\infty} \kappa_m^{4\nu}$$
$$= A(\sigma,\nu)\sum_{m=0}^{\infty} \frac{(\sigma+1/2)_m(\sigma+\nu)_m(2\sigma+2\nu)_m(2\nu)_m(\sigma+2\nu)_m}{(1)_m(\sigma+1)_m(2\sigma+1)_m(\sigma+\nu+1)_m(\sigma+2\nu+1/2)_m}, \quad (2.6)$$

where

$$A(\sigma,\nu) = \frac{\Gamma(\sigma+1/2)\Gamma(\sigma+\nu)\Gamma(2\sigma+2\nu)\Gamma(2\nu)\Gamma(\sigma+2\nu)}{4\Gamma(\sigma+1)\Gamma(2\sigma+1)\Gamma(\sigma+\nu+1)\Gamma(\sigma+2\nu+1/2)}$$

and $0 < \nu < 3/4$. Because $\kappa_0 > \kappa_1 > \kappa_2 > \cdots > \kappa_\infty = 0$, T and T_1 provide upper and lower bounds for κ_0. Inspection of the infinite series defining T and T_1 gives the following inequalities:

$$\left(\frac{T_1}{T}\right)^{1/\nu} < \kappa_0^2 < T_1^{1/2\nu} < T^{1/\nu}. \quad (2.7)$$

When $\nu = 1/2$ in equation (2.6),

$$T_1 = \sum_{m=0}^{\infty} \kappa_m^2 = \sum_{m=0}^{\infty} \frac{1}{(2m+2\sigma+1)^2}, \quad (2.8)$$

which is just the sum of the squared eigenvalues.

3. The variation of $1/(\kappa^{2\nu}\nu^{2-2\nu})$ with respect to ν

Taking the partial derivative of equation (1.2) with respect to ν and integrating y over $[0,\infty)$ when $U(y)$ is an eigenfunction, gives the equation

$$\frac{\partial}{\partial\nu}\left(\frac{1}{\kappa^{2\nu}\nu^{2-2\nu}}\right) + \frac{2}{\nu^2}\int_0^\infty y^{2/\nu-2}\ln(y)\overline{U}^2(y)\,\mathrm{d}y + \frac{2\sigma^2}{\nu^3}\int_0^\infty \frac{\overline{U}^2(y)}{y^2}\,\mathrm{d}y = 0, \quad (3.1)$$

where $\overline{U}(y)$ is the normalized eigenfunction. Inspection of equation (3.1) shows that

$$\lim_{\nu\to 0}\frac{\partial}{\partial\nu}\left(\frac{1}{\kappa^{2\nu}\nu^{2-2\nu}}\right) = -\infty \quad \text{and} \quad \lim_{\nu\to 1}\frac{\partial}{\partial\nu}\left(\frac{1}{\kappa^{2\nu}\nu^{2-2\nu}}\right) = -\infty.$$

Furthermore, it follows from equation (3.1) that

$$-\frac{\partial}{\partial\nu}\left(\frac{1}{\kappa^{2\nu}\nu^{2-2\nu}}\right) - \frac{2}{\nu^2}\int_0^1 y^{2/\nu-2}\ln(y)\,\mathrm{d}y > 0$$

or

$$\frac{\partial}{\partial\nu}\left(-\frac{1}{\kappa^{2\nu}\nu^{2-2\nu}} + \frac{1}{2/\nu-1}\right) > 0, \quad (3.2)$$

therefore, the function inside the parenthesis is an increasing function of ν. Inspection of equation (3.2) indicates

$$\lim_{\nu\to 0}\frac{1}{\kappa^{2\nu}\nu^{2-2\nu}}=\infty \quad \text{and} \quad \lim_{\nu\to 1}\frac{1}{\kappa^{2\nu}\nu^{2-2\nu}}=1. \tag{3.3}$$

These results are valid for the eigenvalues κ_m, $m\in\{0\}\cup\mathbb{N}$.

4. The modified WKB approximation

The discussion of (1.2) takes the same form as the discussion in paper I. Again using the transformations (1.3), the appropriate equations for (1.2) are obtained. The most important result is the approximation for the eigenvalues:

$$\kappa(\nu,\sigma,n)=\left[\frac{\Gamma\left(\frac{1}{2/\nu-2}+1\right)\Gamma\left(\frac{3}{2}\right)}{\nu\Gamma\left(\frac{1}{2/\nu-2}+\frac{3}{2}\right)}\frac{1}{\left(n+\frac{\sigma}{2\nu}+\frac{1}{2}\right)\pi}\right]^{1-1/\nu}, \qquad n\in\{0\}\cup\mathbb{N}, \quad 0<\nu<1. \tag{4.1}$$

The approximation is good provided that

$$\frac{[(\sigma/\nu)^2-1/4]\kappa^{2\nu/(1-\nu)}\nu^2}{1/\nu-1}\ll 1. \tag{4.2}$$

When $\nu=1/2$, the approximation gives the correct value for the eigenvalue, i.e.

$$\kappa\left(\frac{1}{2},\sigma,n\right)=\frac{1}{2n+2\sigma+1}, \quad n\in\{0\}\cup\mathbb{N}, \tag{4.3}$$

which corresponds to the energy levels of the hydrogen-like atom.

5. Conclusions

This problem may be viewed as a special case of the problem discussed in paper I. All of the general properties and analytical methods of the first paper may be used in this paper once the proper transformations have been made. It is also possible to develop the power series solutions for the unbound states of the problem in this paper. If the general problems implied in the two papers are collected together in analogy to the Bessel functions with which they are so intimately related, it would be appropriate to choose the fundamental function definitions using paper I, equation (6.3). Then all other solutions can be developed as special cases of those oscillating functions. Once the new functions are better understood mathematically, a new set of quantum mechanical problems becomes easier to discuss. The more general problem opened here extends in interest beyond pertinent problems of quantum mechanics.

Acknowledgements

The solution of the problem presented in this paper came as an unexpected addition to the lengthy study presented in paper I. The author is grateful for the encouragement and financial support of the Wabash College Chemistry Department.

Reference

[1] P.C. McKinney, Schrödinger equation solutions for the central field power potential energy, I. $V(r) = V_0(r/a_0)^{2\nu-2}$, $\nu \geqslant 1$, J. Math. Chem. 32(4) (2002) 381–404 (this issue).