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ABSTRACT

The Schwinger variational method is used to compute Regge trajectories for the Schrödinger equation with Yukawa potentials.

1. INTRODUCTION

The Schwinger variational principle for systems obeying the Schrödinger equation is an efficient tool for determining both scattering phase shifts and bound-state energies.[1] This variational principle can also be used to calculate Regge trajectories in a manner similar to the Rayleigh-Ritz method used by Haymaker.[2] The advantage of the Schwinger method is faster convergence. The method works well even at threshold, where the method of Ref. 2 does not work, the asymptotic behavior of the wave function not being well approximated by the trial functions used. This note shows how the continuation proceeds in ℓ and gives the relevant matrix elements. Finally a few numerical examples are given and the generalization to combinations of Yukawa potentials is included.

2. EQUATIONS AND RESULTS

The partial-wave Schrödinger equation is

$$\psi_\ell(x) = \lambda \int_0^\infty G_\ell(x,x')\, V(x')\, \psi_\ell(x') x'^2\, dx' , \tag{2.1}$$

where[3]

$$G_\ell(x,x') = -i\,\frac{\pi}{2}\,(xx')^{-\frac{1}{2}}\, J_{\ell+\frac{1}{2}}(kx_<)\, H^{(1)}_{\ell+\frac{1}{2}}(kx_>) \tag{2.2}$$

$$= -2m \int_0^\infty \frac{q\,dq}{q^2 - 2mE - i\epsilon}\, J_{\ell+\frac{1}{2}}(qx) J_{\ell+\frac{1}{2}}(qx')(xx')^{-\frac{1}{2}}, \tag{2.3}$$

and $V(x)$ is taken to be $e^{-\mu x}/x$. Here μ is the exchange mass

and m is the reduced mass. Expressing (2.1) in terms of the function $u_\ell(x) = V(x)\,\psi_\ell(x)$ and multiplying the resulting expression by $u_\ell(x)$ gives, on integration,

$$\int_0^\infty u_\ell(x)\, V^{-1}(x)\, u_\ell(x)\, x^2\, dx = \lambda \int_0^\infty \int_0^\infty [x u_\ell(x)] G_\ell(x,x') \times [x' u_\ell(x')](x\, x')\, dx\, dx'. \tag{2.4}$$

This is the bound-state form of the Schwinger variational principle. At this point ℓ is allowed to become arbitrary, subject only to the condition that the integrals converge. This restriction will be removed later.

Now, following Schwartz,[1] the second integral of (2.4) is transformed. The Fourier transform is used in its partial-wave form, i.e., the Hankel transform:[4]

$$p\, \tilde{u}_\ell(p) = \int_0^\infty [x\, u_\ell(x)]\, J_\nu(px)(px)^{\frac{1}{2}}\, dx, \tag{2.5a}$$

$$x\, u_\ell(x) = \int_0^\infty [p\, \tilde{u}_\ell(p)]\, J_\nu(px)(px)^{\frac{1}{2}}\, dp, \tag{2.5b}$$

$$\nu = \ell + \frac{1}{2}.$$

The inversion "completeness" relation is

$$(y\, y')^{\frac{1}{2}} \int_0^\infty x\, J_\nu(x\, y')\, J_\nu(x\, y)\, dx = \delta(y - y'). \tag{2.6}$$

Applying this transform to (2.4) gives

$$\int_0^\infty u_\ell(x)\, V^{-1}(x)\, u_\ell(x)\, x^2\, dx = -2m\lambda \int_0^\infty \left(\frac{\tilde{u}_\ell(q)\, \tilde{u}_\ell(q)}{q^2 - 2mE - i\epsilon} \right) q^2\, dq. \tag{2.7}$$

The problem is reduced to one-dimensional integrals provided trial functions are chosen whose transforms are easily taken.

Each $\tilde{u}_\ell(p)$ is expanded in a sum of basic functions of the form

$$\tilde{u}_\ell^{\,\delta}(p) = \frac{p^\ell}{(p^2 + \alpha^2)^{\delta+1}}, \tag{2.8}$$

where $\delta = \delta_0 + M$ and $M = 0, 1, 2, \cdots$. We choose δ_0 to give the correct boundary condition in coordinate space as $x \to 0$. The adjustable parameter α has magnitude roughly $\sqrt{-E} + \mu$. Using (2.5b) and (2.8), one obtains

$$u_\ell^{\,\delta}(x) = A_{\ell,\delta}\, x^{\delta-\frac{1}{2}}\, K_{\ell+\frac{1}{2}-\delta}(\alpha\, x), \tag{2.9}$$

where $A_{\ell,\delta} = [\alpha^{\ell+\frac{1}{2}-\delta}/2^\delta\, \Gamma(\delta+1)]$ and $K_\lambda(z)$ is the modified Bessel function of order λ. If δ_0 equals ℓ, then $u_\ell^{\,\delta}(x) \underset{x \to 0}{\sim}$ const. $x^{\ell-1}$, as is desired. [Remember that $V(x) \underset{x\to 0}{\sim} x^{-1}$.] The coordinate space basis functions become[5]

$$u_\ell^{\,\ell+M}(x) = A_{\ell,\ell+M}\, x^{\ell+M-\frac{1}{2}}\, K_{\frac{1}{2}-M}(\alpha\, x). \tag{2.10}$$

In terms of this basis the potential matrix elements [i.e., the left side of (2.7)] are

$$(V^{-1})_{MM'} = A_{\ell,\ell+M}\, A_{\ell,\ell+M'}\ \frac{\pi}{2\alpha} \sum_{L=0}^{M-1} \sum_{L'=0}^{M'-1}$$

$$\times \frac{(M-\frac{1}{2},L)(M'-\frac{1}{2},L')(2\ell + M + M' - L - L' + 2)}{(2\alpha - \mu)^{2\ell+M+M'-L-L'+2}\ (2\alpha)^{L+L'}}\ , \tag{2.11}$$

where

$$(n,k) = \frac{\Gamma(\frac{1}{2} + n + k)}{k!\ \Gamma(\frac{1}{2} + n - k)} \qquad \text{if} \qquad n = \frac{1}{2},\ \frac{3}{2},\ \cdots\ .$$

Since $K_{-\frac{1}{2}}(z) = K_{\frac{1}{2}}(z)$, we define $(-\frac{1}{2},0) = (\frac{1}{2},0) = 1$. If M (or M') $= 0$, the sum contains only L (or L') $= 0$.

The right-hand side of (2.7) reduces to

$$(G)_{MM'} = -m\,\lambda \int_0^\infty \frac{w^{+\frac{1}{2}}\, dw}{(\alpha^2 + w)^{2\ell+M+M'+2}\ (w - 2mE - i\epsilon)}\ . \tag{2.12}$$

This can be expressed in terms of hypergeometric functions

$$(G)_{MM'} = \frac{\Gamma(\ell + \frac{3}{2})(\ell + \frac{3}{2} + N)}{\Gamma(2\ell + 3 + N)} \left(\frac{m\lambda}{\eta}\right)\left(\frac{1}{\alpha^2}\right)^{\ell+\frac{1}{2}+N} F[1,\ell+\tfrac{3}{2};\ 2\ell+3+N;(\eta - \alpha^2)/\eta], \tag{2.13}$$

where $\eta = -2mE - i\epsilon$ and $N = M + M'$. If $\ell = 0$ and $N = 0$, (2.13) collapses into a very simple closed form. From this and various recursion

formulas for the hypergeometric functions, matrix elements for all integer ℓ and N may be generated. For complex ℓ it is convenient to transform (2.13) into the form[6]

$$(G)_{MM'} = \frac{-m\lambda}{(\alpha^2)^{\ell+\frac{3}{2}+N}}\left[\frac{\Gamma(\ell+\frac{1}{2})\,\Gamma\left((\ell+\frac{1}{2})+N+1\right)}{\Gamma(2\ell+N+2)}\,F(1,\ell+\tfrac{3}{2}+N;\,\tfrac{1}{2}-\ell;\,\eta/\alpha^2)\right.$$

$$\left.+\left(\frac{\eta}{\alpha^2}\right)^{\ell+\frac{1}{2}}\left(\frac{1}{1-\frac{\eta}{\alpha^2}}\right)^{2\ell+2+N}\frac{\pi}{\sin\pi(\ell+\frac{3}{2})}\right] \tag{2.14}$$

$$\text{if}\quad \left|\arg\frac{\alpha}{\eta}\right| < \pi.$$

For reasonable values of α, the argument η/α^2 is within the circle of convergence of the power series representing F. For $E > 0$ on the scattering cut we choose the branch of $\eta^{\ell+\frac{1}{2}}$ by the $i\epsilon$ prescription. Equation (2.14) allows the continuation to all values of ℓ (even when the integral 2.12 diverges), since F is analytic in ℓ except for poles at $\ell = +\frac{1}{2}, +\frac{3}{2}, \cdots$.[7] Actually $(G)_{MM'}$ has poles only at $\ell = -\frac{1}{2}, -\frac{3}{2}, \cdots$. These come from the zeros of $\sin\pi(\ell+\frac{3}{2})$ and the poles of $\Gamma(\ell+\frac{3}{2}+N)\,\Gamma(\ell+\frac{1}{2})$. The apparent poles at $\ell = \frac{1}{2}, \frac{3}{2}, \cdots$ exactly cancel.[8] Also it may be worthwhile noting that the first term of (2.15) is analytic in η; the second term contains the standard threshold branch cut $(\eta)^{\ell+\frac{1}{2}}$. Finally, only the hypergeometric functions for $N = 0$ and $N = 1$ need be evaluated from the series expansion, since the recursion formula[9]

$$F(a,b+1;\ c;\ z) = \Big[(c - b)F(a,b-1;\ c;\ z) + [2b - c + (a-b)z]F(a,b;c;z)\Big]/b(1 - z) \tag{2.15}$$

gives all other N.

Numerical computations have been performed to test the rate of convergence of this method. The calculations were repeated for trial functions containing increasing numbers of basis functions, thus generating a sequence of successive approximations. That these sequences converge very rapidly can be seen from Tables I - IV. In all of these tables, m is 0.5 and λ is 1. "Dimension" denotes the number of basis functions per trial function. Table I shows that convergence is excellent even at threshold. Table II suggests that the value of the parameter α is not critical to the convergence rate. Tables III and IV contain random examples for $E \neq 0$. Except for the solution labelled by λ^* in Table III, all examples are for the leading trajectory. The data used in this article were found in about 20 seconds of computer time (CDC 6600).

3. SUM OF POTENTIALS

The primary new difficulties lie in the calculation of[10] $(V^{-1})_{ij} = \langle u_i | V^{-1} | u_j \rangle$. First, the integral may diverge if V has a node unless it is carefully built into the trial functions. Second, the integral may be very hard to do in a closed form (the closed form solution was most useful in doing the analytic continuation in ℓ).

One straightforward way[11] of overcoming this difficulty is to expand $\psi_\ell(x)$ instead of $u_\ell(x) = V(x)\ \psi_\ell(x)$. The expansion

$$\psi_\ell(x) = \sum_{M=0}^{\infty} c_M \, x^{M+\ell} \, e^{-\alpha x} = \sum_{M=0}^{\infty} d_M \, x^{(\ell+1)+M-\frac{1}{2}} \, K_{\frac{1}{2}-M}(\alpha x)$$

can be recast as

$$u_{\ell,i}(x) = V_i(x) \, \psi_\ell(x) = \sum_{M=0}^{\infty} c_M \, x^{M+\ell-1} \, e^{-(\alpha+\mu_i)x}$$

$$= \sum_{M=0}^{\infty} d_M \, x^{\ell+M-\frac{1}{2}} \, K_{\frac{1}{2}-M}\Big((\alpha + \mu_i)x\Big) \, ,$$

where d_M and c_M are simply related and $i(=1,2,\cdots N)$ labels the potentials. The Fourier transforms of these are of the form of Eq. (2.8).

Equation (2.7) then generalizes to

$$\int_0^\infty \psi_\ell(x) \sum_{i=1}^{N} V_i(x) \, \psi_\ell(x) \, x^2 \, dx =$$

$$= -2m\lambda \sum_{i=1}^{N} \sum_{j=1}^{N} \int_0^\infty \frac{\tilde{u}_{\ell,i}(q)\tilde{u}_{\ell,j}(q) \, q^2 \, dq}{q^2 - 2mE - i\epsilon} \, . \tag{3.1}$$

The V integrals are as easy to do as before. The integrals are now

$$\int_0^\infty \frac{q^{2\ell+2} \, dq}{\left[q^2 + (\alpha + \mu_i)^2\right]^{\ell+M_1} \left[q^2 + (\alpha + \mu_j)^2\right]^{\ell+M_2} (q^2 - 2mE - i\epsilon)} \, . \tag{3.2}$$

If $i = j$ this reduces to the hypergeometric form used earlier. Otherwise the integral is expressible as the Appell hypergeometric functions of two variables.[12] These functions have a convergent series expansion and satisfy transformation formulas analogous to Eq. (2.15). In particular, recursion formulas on the indices allow all values of M_1 and M_2 to be found once two explicit evaluations are done via, say, power series.

Since the several two-body channel integral equation is of the form

$$\sum_{k,j} \int_0^\infty \psi_k(x) V_{kj}(x) \psi_j(x) x^2 \, dx$$

$$= \sum_{k,j,i} \int_0^\infty \int_0^\infty dx \, dx' \, \psi_k(x) V_{ki}(x) G_i(x,x') V_{ij}(x') \psi_j(x'(xx')^2,$$

where k and j are channel indices, it is clear that the same tricks will work here.

Another way of attacking the problem of sums of potentials is to deal directly with approximations to the matrix (V^{-1}). Since (V) is easily calculated for a sum of Yukawa potentials,

$$V = \lambda[(e^{-\mu_1 x}/x) + \sigma(e^{-\mu_2 x}/x)] = V_1 + V_2 ,$$

where $\mu_1 < \mu_2$, one is led to try $(V)^{-1}$ as an approximation[13] to (V^{-1}).

In particular, we define[14]

$$(V)_{ij} = \langle \phi_i \, |V| \, \phi_j \rangle,$$

where

$$\phi_i = u_i/V_1 = (1 + V_2/V_1)\psi_i .$$

The inverse of (V) must be suitably modified to take into account that $\{\phi_i\}$ instead of $\{u_i\}$ is used as a basis set. If $\{u_i\}$ had been used as a basis set, $\langle u_i \, |V| \, u_j \rangle$ would have a pole at $\ell = 0$. The power of x in $1/V_1$ removes this.

We define $(M)_{ij} = \langle \phi_i \mid u_j \rangle$, the overlap matrix between the two bases. A generalized "completeness" relation can be written:

$$\sum_{n,n'} |\phi_n\rangle W_{nn'} \langle \phi_{n'}| = 1 . \tag{3.3}$$

To evaluate[15] (W) in terms of (M) we take matrix elements of (3.3), yielding

$$(M)^T = (M)^T (W) (M)^T$$

or

$$W = \left[(M)^T \right]^{-1} .$$

Next we take matrix elements of the operator identity $VV^{-1} = 1$; we use (3.3) and solve for (V^{-1}):

$$(V^{-1}) = (M)^T \, (V)^{-1} \, (M). \tag{3.4}$$

This equation is truncated to give <u>approximate</u> values for the matrix (V^{-1}) in terms of the easily calculated (M) and (V). Now notice that

$$(V)_{ij} = \langle \phi_i \,|V|\, \phi_j \rangle = \langle u_i \,|V_1^{-1}|\, u_j \rangle + \langle u_i \,|V_s^{-1}|\, u_j \rangle$$

and

$$(M)_{ij} = \langle \phi_i \,|\, u_j \rangle = \langle u_i \,|V_1^{-1}|\, u_j \rangle \,,$$

where

$$V_s = V_1^2/V_2 = \exp(-2\mu_1 + \mu_2)/x \,.$$

These matrix elements may be constructed directly from those given by Eq. (2.11). Using the same form for $u_i(x)$ as before leaves the Green's function matrix elements unchanged from Eq. (2.13). This form is probably not so realistic as that given by expanding $\psi(x)$ and forming $u(x) = V(x)\,\psi(x)$, but it has the advantage of not requiring the Apell hypergeometric functions mentioned earlier. It is also worth remarking that the two-body multichannel problem can also be solved in this manner and contains only integrals which are easily done.

Some examples of this method are included in Table V.

4. ACKNOWLEDGMENTS

I am very grateful to Professor C. Schwartz, Richard Haymaker, and Klaus Rothe for their helpful comments and interest. I would further like to thank Richard Haymaker for his help in the preparation of Table IV.

Table I. Convergence of the solution in ℓ at fixed λ and $E = 0$. Here α is arbitrarily set at 2.0. Dimension denotes the number of trial functions used.

Dimension	$\ell(\lambda = -3)$	$\ell(\lambda = -25)$
1	2.36435	1.88159
2	2.41630	2.03520
3	2.45496	2.11631
4	2.45770	2.15582
5	2.45874	2.17564
6	2.458862	2.18521
7	2.458900	2.18973
8	2.458905	2.19179

Table II. Fixed $\ell = 0$, $E = 0$. Note the relative insensitivity to choice of α.

Dimension	$\lambda(\alpha = 2.0)$	$\lambda(\alpha = 1.5)$	$\lambda(\alpha = 1.25)$
1	-1.77778	-1.687500	-1.73611
2	-1.70483	-1.687500	-1.69498
3	-1.70811	-1.679931	-1.68230
4	-1.68076	-1.679909	-1.68039
5	-1.68000	-1.679812	-1.67994
6	-1.67985	-1.679810	-1.67984
7	-1.67982	-1.679806	-1.67981

Table III. Some random examples of convergence of the method for $E < 0$. The notation is $\lambda(\ell,E)$, and $\lambda^*(\ell,E)$ denotes coupling strength to bind a first excited state with energy E and angular momentum ℓ.

Dimension	$\lambda(0.6,0)$	$\lambda(0.6,-5)$	$\lambda^*(0,-5)$	$\lambda(0.6,-15)$
1	-5.52365	-12.094	---	-17.37005
2	-5.51663	-12.075	-16.3605	-17.34987
3	-5.47468	-12.07410	-16.2104	-17.34785
4	-5.47454	-12.07402	-16.1847	-17.347818
5	-5.47349	-12.07401	-16.1832	-17.347816
6	-5.47349	-12.07401	-16.1830	-17.347816

Table IV. Some results for $Re(E) > 0$. $\lambda = -9$, $\mu = 1$, $m = 0.5$. This trajectory "turns over" at about $E = 2$.

Dimension	Re E	Im E	Re ℓ	Im ℓ
7	0.0250000	0.0226256	1.00544	0.01969
8			1.00544	0.01969
7	0.4965909	0.0148044	1.17553	0.22276
8			1.17553	0.22291
7	1.3261364	0.0175977	1.21240	0.54856
8			1.21434	0.54571
7	2.9965909	0.1432961	1.07886	0.96090
8			1.07254	0.98624

Table V. Combinations of potentials $V = \lambda(\ell,E,\sigma)(e^{-x}/x + \sigma\, e^{-2x}/x)$.

Dimension	$\lambda(0,0,-4)$	$\lambda(0,-5,-0.5)$	$\lambda(0.6,0,-0.5)$	$\lambda(0.6,0,-4)$
1	1.422222	-10.402	-6.897	9.31245
2	1.577477	-10.213	-6.90423	6.25718
3	1.497510	-10.21263	-6.90475	5.26559
4	1.496934	-10.2125623	-6.89998	4.93946
5	1.491888	-10.212561	-6.90020	4.79201
6	1.491640	-10.212561	-6.89995	4.72678
7	1.491232	-10.212560	-6.89964	4.69563

FOOTNOTES AND REFERENCES

* Work done under the auspices of the U. S. Atomic Energy Commission.

1. C. Schwartz, Phys. Rev. 141, 1468 (1966), whose basic method is followed. See also C. Schwartz and C. Zemach, ibid., 1454, for application to the Bethe-Salpeter equation.

2. R. Haymaker, Bulletin of the American Physical Society 12, 561 (1967). I have also used this method with the Bethe-Salpeter equation to calculate Regge trajectories for energies below elastic threshold (unpublished).

3. B. W. Lee, Determinantal Method for Complex Angular Momentum in Potential Scattering, in Theoretical Physics (Trieste Lectures), (IAEA Vienna, 1963), p. 339 and G. N. Watson, Theory of Bessel Functions (Cambridge University Press, 1922), p. 429.

4. Bateman Manuscript Project, Table of Integral Transforms, A. Erdelyi, Ed. (McGraw-Hill Co., Inc., New York, 1953).

5. The Bessel function $K_{\frac{1}{2}-M}(\alpha x)$ is of form $\Sigma_i c_i x^i e^{-\alpha x}$. See for example, Handbook of Mathematical Functions, Milton Abramowitz and Irene Stegun, Eds. (Dover Publications Inc., New York, 1965). p. 444.

6. Equations 15.3.8 and 6.1.17 of Reference 5.

7. The expression $F(a,b;c;z)/\Gamma(c)$ is an entire function of $a,b,$ and c if $|z| < 1$. The function $\Gamma(c)$ is meromorphic with poles at $c = 0, -1, -2, \cdots$. See Reference 5, Eqs. 15.1.1-2.

8. Richard Haymaker suggested that this should be true. It is.

9. See Ref. 5, Eq. 15.2.11.

10. The scalar product is

$$\langle \phi \mid \chi \rangle = \int_0^\infty \phi(x)\, \chi(x)\, x^2\, dx.$$

There is no complex conjugation. This aids in the analytic continuation. The functions are chosen real for integral ℓ. (A) stands for the matrix of the operator A.

11. I would like to thank Klaus Rothe for pointing this out.

12. W. N. Bailey, Generalized Hypergeometric Series (Cambridge Tract in Mathematics and Mathematical Physics No. 32, Cambridge University Press, 1935), p. 77.

13. C. Schwartz, Numerical Techniques in Matrix Mechanics, University of California, Berkeley, preprint.

14. Matrices (V^{-1}) and (V) will always be evaluated in the $\{u_i\}$ and $\{\phi_i\}$ bases respectively.

15. With these particular functions

$$(M)_{ij} = \langle \phi_i \mid u_j \rangle = \langle u_i \mid \phi_j \rangle = \langle \phi_j \mid u_i \rangle = (M)_{ji}$$

so

$$(M) = (M)^T .$$

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