Determination of the scattering matrix by use of the Sturmian representation of the wave function: Regular solution

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In a previous paper [Phys. Rev. A **35**, 3945 (1987)] the Sturmian expansion of the irregular solution of the Schrödinger equation was considered. Here I consider the expansion of the regular solution.

Recently Tang and I considered[1] the expansion of the irregular solution of the Schrödinger equation

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}+\frac{l(l+1)}{2r^2}-\frac{Z}{r}+W(r)-E\right]\psi(r)=0\ , \qquad (1)$$

where $rW(r)$ vanishes for $r\sim\infty$, in terms of the Sturmian functions

$$S_{nl}^{k}(r)=\frac{1}{(2l+1)!}\left[\frac{(n+l)!}{(n-l-1)!}\right]^{1/2} \times M_{n,l+1/2}(-2ikr)\ , \qquad (2)$$

where $M_{a,b}(z)$ is the regular Whittaker function and where $k=\sqrt{2E}$; I drew a branch cut along the positive real E axis and took the branch of k which is positive when E is on the upper edge of the cut. In this Brief Report I consider the expansion of the regular solution $\phi_{kl}(r)$ of Eq. (1). The regular solution, which for E on the upper edge of the cut contains an outgoing scattered wave, satisfies the integral equation

$$\phi_{kl}(r)=\phi_{kl}^{(0)}(r)+\int_0^\infty dr\, g_{kl}(r,r')W(r')\phi_{kl}(r')\ , \qquad (3)$$

where $\phi_{kl}^{(0)}(r)$ is the regular pure Coulomb wave solution, that is,

$$\phi_{kl}^{(0)}(r)=i^{l+1}\left[\frac{1}{2\pi k}\right]^{1/2}\frac{\Gamma(l+1-i\gamma)}{(2l+1)!} \times e^{\pi(\gamma/2)-i\eta_l(k)}M_{i\gamma,l+1/2}(-2ikr)\ , \qquad (4)$$

where $\gamma=Z/k$, $\eta_l(k)=\arg\Gamma(l+1-i\gamma)$, and where $g_{kl}(r,r')$ is the Coulomb Green's function, which can be expanded as[2]

$$g_{kl}(r,r')=\sum_{n=l+1}^{\infty}\frac{S_{nl}^{k}(r)S_{nl}^{k}(r')}{Z+ink}\ . \qquad (5)$$

I now assume that E is real and positive and lies on the upper edge of the cut. [Equations (7) in the following may be analytically continued to other E.] Since $\phi_{kl}^{(0)}(r)$ is a standing wave, and is therefore a superposition of both outgoing and ingoing waves, it cannot be expanded in terms of the $S_{nl}^{k}(r)$, which have outgoing-wave character.[3] However, the difference $\phi_{kl}(r)-\phi_{kl}^{(0)}(r)$ behaves as an outgoing wave, and furthermore it is regular at the origin. Consequently, $\phi_{kl}(r)$ can be expanded as

$$\phi_{kl}(r)=\phi_{kl}^{(0)}(r)+\sum_{n=l+1}^{\infty}a_nS_{nl}^{k}(r)\ , \qquad (6)$$

with coefficients a_n which should decrease rapidly (exponentially for a W of Yukawa form) as n increases. Inserting this expansion into both sides of Eq. (3), and using Eq. (5) and the linear independence of the $S_{nl}^{k}(r)$, immediately yields the following linear equations for the coefficients:

$$\sum_{m=l+1}^{\infty}F_{nm}a_m=b_n\ , \qquad (7a)$$

$$b_n=(S_{nl}^{k}\mid W\mid\phi_{kl}^{(0)})/(Z+ink)\ , \qquad (7b)$$

$$F_{nm}=\delta_{nm}-(S_{nl}^{k}\mid W\mid S_{ml}^{k})/(Z+ink)\ , \qquad (7c)$$

where the scalar product $(c\mid d)$ is defined as

$$(c\mid d)=\int_0^\infty dr\, c(r)d(r)\ .$$

We just used the Sturmian expansion (5) of the Coulomb Green's function without asking whether it

TABLE I. Diagonal $[N,N]$ Padé approximates to the $l=0$ and $l=1$ phase shifts for the potential $W(r)=4\exp(-2r)/r$, with $k=0.5$ and $Z=2$.

N	$\delta_0(k)$	$\delta_1(k)$
1	−0.37	−0.45
2	−0.37	−0.44
3	−0.40	−0.46
4	−0.29	−0.44
5	0.17	−0.55
6	0.95	−0.63
7	1.03	−0.572
8	1.39	−0.542
9	1.37	−0.541
10	1.34	−0.556
11	1.33	−0.555
12	1.35	−0.555
Exact	1.364	−0.5554

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converges. In fact, for E on the upper edge of the cut, it converges only when acting on a regular function which has outgoing wave character.[3] We must now pay the price for letting it act on $W(r)\phi_{kl}^{(0)}(r)$, a function which is regular but which contains a component having (damped) ingoing wave character since $\phi_{kl}^{(0)}(r)$ is a standing wave. The price we pay is that b_n grows (exponentially) as n increases, which calls into question the existence of Eqs. (7). However, since $W(r)\phi_{kl}^{(0)}(r)$ is a normalizable function, it could in principle be represented to arbitrary accuracy, over the significant range of r, by a finite sum of normalizable basis functions with (damped) outgoing wave character.[3] Using this device, we could modify Eq. (7b); the modified b_n would decrease (exponentially) as n increases beyond a sufficiently large value, and the coefficients a_n could be obtained by truncating the sum over m in Eq. (7a) and inverting a finite-dimensional matrix whose elements are F_{nm}. In practice, rather than modify b_n it is perhaps more convenient to use the Padé method. For example, suppose we wish to determine the non-Coulombic phase shift $\delta_l(k)$ defined by

$$\tan[\delta_l(k)] = A_{kl}/(1+iA_{kl}) , \tag{8a}$$

$$A_{kl} = -\pi(\phi_{kl}^{(0)} \mid W \mid \phi_{kl}) . \tag{8b}$$

We can express A_{kl} as $A_{kl}^{(0)} + \Delta A_{kl}$, where $A_{kl}^{(0)} = -\pi(\phi_{kl}^{(0)} \mid W \mid \phi_{kl}^{(0)})$ and

$$\Delta A_{kl} = -\pi \sum_{n=l+1}^{\infty} a_n(\phi_{kl}^{(0)} \mid W \mid S_{nl}^{k}) . \tag{9}$$

We now form a sequence of approximations $\{\Delta A_{kl}^{(M)}, M=1,2,\ldots\}$ where $\Delta A_{kl}^{(M)}$ is obtained by retaining only the first M terms in the sum of Eq. (7a), putting $a_n = 0 = b_n$ for $n > M+l$. We extrapolate the sequence by the Padé method. The phase shifts, obtained from the $[N,N]$ Padé approximates to ΔA_{kl} for the same potential $W(r) = 4\exp(-2r)/r$ considered previously,[1] are shown in Table I. The rate of convergence of $\delta_l(k)$ is comparable to that found from the Sturmian expansion of the irregular solution, but the present calculation was easier to implement.

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[1]R. Shakeshaft and X. Tang, Phys. Rev. A **35**, 3945 (1987).

[2]L. C. Hostler, J. Math. Phys. **11**, 2966 (1970); A. Maquet, Phys. Rev. A **15**, 1088 (1977).

[3]For further discusssion of this point see R. Shakeshaft, Phys. Rev. A **34**, 244 (1986); **34**, 5119 (1986).