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Renormalized method for multichannel inhomogeneous Schrödinger equations

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Abstract. A renormalized method is developed for the solution of multichannel inhomogeneous Schrödinger equations that appear frequently in atomic and molecular physics. The method is stable and accurate, its derivation is straightforward. Formulae are presented in both the Hartree and Numerov approximations. A numerical example is used to demonstrate the method.

In atomic and molecular physics, we frequently face the problem of solving the multichannel inhomogeneous Schrödinger equation of the form [1–3]

$$\left[I\frac{d^2}{dR^2} + Q(R)\right]\psi^+(R) = \Phi(R) \tag{1}$$

where I is the unit matrix of N by N, $\Phi(R)$ is an N-component vector inhomogeneous term, usually proportional to an interaction multiplied by a localized initial state wavefunction, $\psi^+(R)$ is the N-component vector solution which is required to vanish at the origin and to be outgoing asymptotically, $Q(R) = 2\mu[EI - V(R)]$ in which μ is the reduced mass, E is the energy, $V(R)$ is an N by N potential matrix including the asymptotic centrifugal repulsion term.

The solution of inhomogeneous Schrödinger equation is complicated by an instability problem and ordinary numerical integration schemes do not work. Presently there exist three methods proposed for the solution of (1): the invariant imbedding method [3,4]; the R-matrix propagation method [5]; and the log-derivative propagation method [6]. A common point of these methods is that they all propagate quantities related to the solution but cannot provide the solution explicitly. However the explicit solution is needed for many applications.

Our purpose here is to introduce a new renormalized method for the solution of (1). The new method is stable and accurate; its derivation is straightforward. Most important of all, the new method provides the solution explicitly. We will discuss formulae in both the Hartree and Numerov approximation and demonstrate the use of the method in a numerical example.

To be specific, let us assume in (1) the open channels are arranged with indices from 1 to N_0 and the closed channels with indices from $N_0 + 1$ to N. Channel i is open (closed) if $(E - V_{ii}(\infty))$ is positive (negative).

In Hartree's approximation, (1) is replaced by the following difference equations,

$$\psi^+(m+1) + \lambda(m)\psi^+(m) + \psi^+(m-1) = \chi(m) \qquad m = 1, \ldots, M \tag{2}$$

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where $\psi^+(m) \equiv \psi^+(R_m)$, $\chi(m) \equiv h^2\Phi(R_m)$, $\lambda(m) = h^2Q(R_m) - 2I$, and the grid points $R_m = R_0 + mh$, $m = 0, \ldots, M+1$, h being the step length.

Now we adopt and generalize a procedure used in the numerical solution of one-dimensional time-dependent Schrödinger equation [7] by assuming

$$\psi^+(m+1) = \alpha(m)\psi^+(m) + \beta(m) \tag{3}$$

where $\alpha(m)$ and $\beta(m)$ are respectively N by N matrices and N-component vectors. By substituting $\psi^+(m+1)$ in (3) into (2) and solving for $\psi^+(m)$, we obtain

$$\psi^+(m) = \left[\frac{1}{\alpha(m) + \lambda(m)}\right][-\psi^+(m-1) + \chi(m) - \beta(m)]. \tag{4}$$

Comparing (4) with (3) gives the backward recursion relations

$$\begin{aligned} \alpha(m-1) &= -[\alpha(m) + \lambda(m)]^{-1} \\ \beta(m-1) &= -\alpha(m-1)[\chi(m) - \beta(m)]. \end{aligned} \tag{5}$$

The corresponding forward recursion relations are

$$\begin{aligned} \alpha(m) &= -[\alpha(m-1)^{-1} + \lambda(m)] \\ \beta(m) &= \chi(m) + \alpha(m-1)^{-1}\beta(m-1). \end{aligned} \tag{6}$$

The starting condition for the above recursion relations can be obtained by writing (2) for $m = 1$ and noting the fact that $\psi^+(R_0) = 0$,

$$\psi^+(2) + \lambda(1)\psi^+(1) = \chi(1). \tag{7}$$

Equations (7) and (3) with $m = 1$ together specify

$$\alpha(1) = -\lambda(1) \qquad \beta(1) = \chi(1). \tag{8}$$

The initial condition in (8) and the forward recursion relation in (6) completely determine $\alpha(m)$ and $\beta(m)$ for all m, which in turn can be used to obtain any regular solution of the inhomogeneous Schrödinger equation.

For the outgoing solution, let us define a diagonal matrix B whose diagonal elements are $B_{ii} = \exp(ik_ih)$ $(i = 1, \ldots, N_0)$ and $B_{ii} = \exp(-\kappa_i h)$ $(i = N_0 + 1, \ldots, N)$ where $k_i = \sqrt{2\mu[E - V_{ii}(\infty)]}$ $(i = 1, \ldots, N_0)$ and $\kappa_i = \sqrt{2\mu[V_{ii}(\infty) - E]}$ $(i = N_0 + 1, \ldots, N)$. Assuming $R(M+1)$ is in the asymptotic region and the inhomogeneous term is negligibly small there then the outgoing boundary condition can be expressed as

$$\psi^+(M+1) = B\psi^+(M). \tag{9}$$

This equation may be combined with $\psi^+(M+1) = \alpha(M)\psi^+(M) + \beta(M)$ from (3) to yield

$$\psi^+(M) = \frac{1}{B - \alpha(M)}\beta(M). \tag{10}$$

If desired the outgoing wavefunction can now be determined from

$$\psi^+(m) = \alpha(m)^{-1}[\psi^+(m+1) - \beta(m)] \qquad m = M-1, \ldots, 1. \tag{11}$$

The above formulae obtained in the Hartree approximation produce a numerical solution having an error proportional to h^2. A more accurate approximation with an error proportional to h^4 is the renormalized Numerov method.

In the Numerov approximation, (1) is replaced instead by the following difference equations,

$$[I - T(m+1)]\psi^+(m+1) - [2I + 10T(m)]\psi^+(m) + [I - T(m-1)]\psi^+(m-1) = \frac{h^2}{12}[\Phi(m+1) + 10\Phi(m) + \Phi(m-1)] \tag{12}$$

where

$$T(m) = -\frac{h^2}{12}Q(m). \tag{13}$$

Equation (12) may be derived by combining the inhomogeneous Schrödinger equation (1) and the following identity

$$[y(m+1) - 2y(m) + y(m-1)] - \frac{h^2}{12}[y''(m+1) + 10y''(m) + y''(m-1)] = O(h^6) \tag{14}$$

which is valid for any smooth enough scalar or matrix function $y(R)$ as can be verified readily by Taylor expansions.

Now use the definitions

$$\begin{aligned} F(m) &= [I - T(m)]\psi^+(m) \\ \lambda(m) &= -\frac{[2I + 10T(m)]}{[I - T(m)]} \\ \chi(m) &= \frac{h^2}{12}[\Phi(m+1) + 10\Phi(m) + \Phi(m-1)]. \end{aligned} \tag{15}$$

Then (12) is written as

$$F(m+1) + \lambda(m)F(m) + F(m-1) = \chi(m) \tag{16}$$

which has the same structure as (2). Therefore by assuming

$$F(m+1) = \alpha(m)F(m) + \beta(m) \tag{17}$$

and following the steps in the Hartree approximation, we arrive at exactly the same recursion relations and starting condition as in equations (5), (6) and (8) except $\lambda(m)$ and $\chi(m)$ are defined differently.

To fix the outgoing boundary condition in the Numerov approximation we solve for $\psi^+(M)$ by using (9), the relation in (17) with index $m = M$ and the definition for $F(m)$, $m = M$, $M + 1$. The result is

$$\psi^+(M) = \frac{1}{[I - T(M+1)]B - \alpha(M)[I - T(M)]}\beta(M). \tag{18}$$

As in the Hartree approximation, once $\psi^+(M)$ is fixed, the solution at all the grid points can be obtained.

We now demonstrate the above renormalized formalism using a simple one-channel inhomogeneous equation of the form

$$\left[\frac{d^2}{dR^2}+2\right]\psi^+(R)=2\exp(-R). \tag{19}$$

Using Green's function method the exact outgoing solution for this example may be written as

$$\psi^+_{\text{exact}}(R)=-\sqrt{2}\int_0^\infty dR'\sin(\sqrt{2}R_<)\exp(i\sqrt{2}R_>)\exp(-R') \tag{20}$$

where $R_<(R_>)$ is the lesser (greater) of R and R'. The integral can be evaluated analytically and one finds that $\psi^+_{\text{exact}}(R)=-\frac{2}{3}[\exp(i\sqrt{2}R)-\exp(-R)]$.

We have used the renormalized method discussed above to calculate the outgoing solution of (20) and compared the numerical results with the exact one. Defining the position-dependent error function $\Delta(R)$ by

$$\Delta(R)=\frac{1}{R}\int_0^R dR'|\psi^+_{\text{approx}}(R')-\psi^+_{\text{exact}}(R')| \tag{21}$$

where $\psi^+_{\text{approx}}(R')$ depends upon the finite difference approximation and the step length in the calculation. We have performed the integration in (21) numerically using Simpson's rule. It is expected that $\Delta(R)/h^2$ in the Hartree approximation and $\Delta(R)/h^4$ in the Numerov approximation to be quite independent of the step length h. We have used three values for the step length and two values of R as the point to apply the outgoing boundary condition and at the same time to evaluate the error function. The results in table 1 confirm the expectations. We also found that the value of $\Delta(R)$ is a good order of magnitude estimate of the local error in the numerical solution at any R. We conclude that the approximate wavefunctions are very accurate.

Table 1. Comparing the calculated solutions and the exact one for the example in equation (19) with the error function $\Delta(R)$ defined in equation (21).

	h		
	0.005	0.01	0.02
$\Delta(R=30)/h^2$ (Hartree)	1.180	1.181	1.181
$\Delta(R=40)/h^2$ (Hartree)	1.572	1.572	1.571
$\Delta(R=30)/h^4$ (Numerov)	0.1167	0.1183	0.1183
$\Delta(R=40)/h^4$ (Numerov)	0.1553	0.1571	0.1570

Finally we note that one of the recursion formulae (the one for $\alpha(m)$) obtained here for the inhomogeneous equation is exactly the same as that obtained by Johnson [8] for the homogeneous equation. Therefore the present renormalized method can be regarded as a natural extension of the renormalized method of Johnson.

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