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Integration of the Schrödinger Equation in Imaginary Time[1]. I

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ABSTRACT

Numerical techniques for the integration of the Schrödinger equation in imaginary time are investigated. Because the spatial dependence of the solution in the limit of large imaginary time is that of the ground state of the Hamiltonian, the method can be applied to bound states of quantum-mechanical three-body systems. Knowledge of the analytic dependence of the asymptotic form of the wavefunction on the trial eigenvalue is not required. In this paper, the first of a series, we have confined our attention to the problems arising from the imaginary time integration and reserve for a later date a discussion of the problems that are due to a multidimensional spatial grid.

I. INTRODUCTION

In this paper we wish to discuss in detail the virtues and problems associated with the causal integration of the time-dependent Schrödinger equation in imaginary time. The reason for the interest in this technique is that the latest generation of computers has begun to make practical the exact solution of the ground state of a quantum mechanical three-body system with this method.

In recent years the three-body problem, i.e., three particles obeying the Schrödinger equation and interacting with each other via spatially varying potentials, has been the target of a massive assault by the weaponry of modern theoretical physics. Several quite elegant treatments of the general problem have appeared; the reduction of the Lippmann–Schwinger equation to nonsingular, semitractable

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form by Fadeev and his school [1], [2] and the application of nonlocal separable potentials by Mitra *et al.* [3]. In addition, there have been a number of monumental calculations, through variational methods, of the atomic-He ground-state energy [4] and the trinucleon [5] (^{3}H and ^{3}He) binding energies, the latter none too successful. All these studies have produced impressive new insights into the nature and difficulties of the problem. Their application to truly realistic problems, however, must await the conquest of a large number of formidable obstacles.

Another line of attack, i.e., the numerical imaginary time integration of the Schrödinger equation has as yet received only scant attention [6]. Although the procedure is quite straightforward and promises to generate three-body ground state energies and wave functions with *no* approximations, its use for even the relatively simpler atomic problems has become feasible only with the present generation of computers.

The three-body problem, when all trivial degrees of freedom, i.e., the center-of-mass coordinates and the Euler angles of rotation, have been removed [7], still contains three spatial variables. Since it is our intention in this paper to deal primarily with the problems arising from the time integration we shall focus our attention on the simpler two-body problem with only one variable, the coordinate in the reduced radial Schrodinger equation for two bodies interacting via a central potential, bearing in mind always the more complex problem, whose solution is the purpose of this effort.

II. Formal Considerations

The Schrödinger equation (with $\hbar = 1$) is

$$H\Psi(r, t) = i\partial\Psi(r, t)/\partial t \tag{1}$$

where r represents all the spatial coordinates. The time-independent Hamiltonian H possesses a complete set of orthonormal eigenfunction $\varphi_n(r)$ with corresponding eigenvalues ε_n, the lowest being ε_0. We assume that H has at least one well-defined bound state whose energy is $\varepsilon_0 < 0$ and which differs from the next-lowest energy ε_1 by a finite amount. [If φ_0 is a degenerate state due to a symmetry in some degree of freedom, one can extract that variable from the problem and consider Eq. (1) with the appropriate H in the reduced space.]

Let

$$\Psi(r, 0) = \sum_n a_n\varphi_n(r) \tag{2}$$

be the solution of Eq. (1) at time $t = 0$; then

$$\Psi(r, t) = \sum_n a_n \exp(-i\varepsilon_n t)\varphi_n(r) \tag{3}$$

satisfies this equation at any other time t. If we let

$$it = \tau,$$

Eq. (1) becomes

$$H\psi(r, t) = -\partial\psi(r, t)/\partial\tau \tag{4}$$

where $$\psi(r, \tau) = \Psi(r, -i\tau) = \Psi(r, t)$$

and

$$\psi(r, \tau) = \sum_n a_n \exp(-e_n\tau)\varphi_n(r). \tag{5}$$

Clearly for large positive values of τ, the series on the right-hand side is dominated by the $n = 0$ term. In fact,

$$\psi(r, \tau) \xrightarrow[\tau\to\infty]{} a_0 \exp(-\varepsilon_0\tau)\, \varphi_0(r)\, [1 + O(\exp - (\varepsilon_1 - \varepsilon_0)\tau)]. \tag{6}$$

Thus, provided $\psi(r, 0)$ is chosen such that $a_0 \neq 0$, this procedure generates a function with the spatial dependence of the ground-state wavefunction of H. Since the ground-state wavefunction has no nodes, one can be sure that the starting function $\psi(r, 0)$ will have a nonvanishing projection on the ground state by choosing it to be nodeless, for example.

The question of how to recognize when τ is sufficiently large so as to satisfy Eq. (6) is a delicate one. Clearly a sufficient condition is that

$$\psi(r, \tau + \delta\tau)/\psi(r, \tau) = \exp(-\varepsilon_0\, \delta\tau) \tag{7}$$

be independent of position. It is usually possible to satisfy this condition over an acceptable range of r and thereby end the calculation. We shall, however, have more to say on this point later.

The problem is then the integration of Eq. (4), starting with a conveniently chosen starting function $\psi(r, 0)$, and using equation (4) to generate $\psi(r, \tau)$ for τ sufficiently large that condition (7) obtain. The Hamiltonian is of the usual type

$$H = T + V,$$

with T the kinetic energy, containing second-order spatial derivatives, and V a local potential. Equation (4) differs from the diffusion equation by the presence

of the potential V. In addition, in this problem we are interested in the function $\psi(r, \tau)$ only in the limit of large τ; the τ-development *per se* is of no interest.

The integration proceeds in time steps $\delta\tau$, whereby an alternative form of Eq. (4) is

$$\psi(r, \tau + \delta\tau) = \exp(-\delta\tau H)\, \psi(r, \tau). \tag{8}$$

We shall discuss the methods of solution of (4) and (8) symbolically denoted by

explicit time integration: $\psi(r, \tau + \delta\tau) = [1 - \delta\tau H]\psi(r, \tau)$;

implicit time integration: $[1 + \delta\tau H]\psi(r, \tau + \delta\tau) = \psi(r, \tau)$;

Crank–Nicholson method: $[1 + (\frac{1}{2}\delta\tau)H]\psi(r, \tau + \delta\tau) = [1 - (\frac{1}{2}\delta\tau)H]\psi(r, \tau)$.

These methods answer all the important questions encountered in the *time* integration of Eq. (4), and we shall confine our discussion here to these methods.

III. Integration Methods

The imaginary time-dependent reduced radial Schrödinger equation for two particles of angular momentum l interacting through a Coulomb potential is, in atomic units,

$$\left[\frac{-\partial^2}{\partial x^2} - \frac{2}{x} + \frac{l(l+1)}{x^2}\right] \psi(x, \tau) = \frac{-\partial\psi(x, \tau)}{\partial\tau}, \quad 0 \leq x < \infty. \tag{9}$$

The boundary conditions require that

$$\psi(0, \tau) = 0 \tag{10}$$

and

$$\psi(x, \tau) \xrightarrow[x\to\infty]{} 0 \tag{11}$$

for bound states. The exact ground-state energy and wavefunction for fixed l are

$$\varepsilon_0 = -1/(l+1)^2,$$
$$\psi_0(X) = N_l x^{l+1} \exp[-x/(l+1)]$$

where N_l is the normalization constant. Since the infinite range of x makes it difficult to apply Condition (11), we shall solve this equation in the restricted space $0 \leq z < 1$ with

$$z = \beta x^s/(1 + \beta x^s), \quad \beta,\ s > 0. \tag{12}$$

By chosing a uniform mesh in z space and varying β and s we may vary the nature of the non-uniform mesh in x space thus exploring, in greater or lesser fine detail, the region of small x. The differential equation in z is then, for $s = 1$,

$$\left[-\beta^2(1-z)^4\frac{\partial^2}{\partial z^2}+2\beta^2(1-z)^3\frac{\partial}{\partial z}-\frac{2}{\beta}\frac{(1-z)}{z}+\frac{l(l+1)}{\beta^2}\left(\frac{1-z}{z}\right)^2\right]\psi(z),$$

$$=-\frac{\partial\psi(z,\tau)}{\partial\tau} \tag{13}$$

with

$$\psi(z=0,\tau)=\psi(z=1,\tau)=0. \tag{14}$$

Let the interval $0 \leq z < 1$ be subdivided into n equal intervals of length $\Delta z = 1/n$ and let

$$z_j = j\,\Delta z, \qquad j = 0, 1, \ldots n$$

and

$$\psi(z_j,\tau) \equiv \psi_j(\tau).$$

The spatial derivatives to second order in Δz are

$$\frac{\partial\psi(z_j,\tau)}{\partial z}=\frac{\psi_{j+1}(\tau)-\psi_{j-1}(\tau)}{2\Delta z}, \tag{15a}$$

$$\frac{\partial^2\psi(z_j\tau)}{\partial z^2}=\frac{\psi_{j+1}(\tau)-2\psi_j(\tau)+\psi_{j-1}(\tau)}{(\Delta z)^2}. \tag{15b}$$

Equation (15b) is replaced by the difference equations

$$\sum_k \tilde{H}_{jk}\psi_k(\tau)=\frac{-\partial\psi_j(\tau)}{\partial\tau}, \tag{16}$$

which is equivalent to

$$\psi_j(\tau+\delta\tau)=\sum_k\{\exp(-\delta\tau\tilde{H})\}_{jk}\,\psi_k(\tau) \tag{17}$$

where $\tilde{H}$ is the tridiagonal matrix

$$\tilde{H}_{jk}\equiv\frac{-\beta^2(1-z_j)^3}{(\Delta z)^2}[(1-z_{j+1})\delta_{j+1,k}+(1-z_{j-1})\delta_{j-1,k}]$$

$$+\left[\frac{2\beta^2(1-z_j)^4}{(\Delta z)^2}-\frac{2}{\beta}\left(\frac{1-z_j}{z_j}\right)+\frac{l(l+1)}{\beta^2}\left(\frac{1-z_j}{z_j}\right)^2\right]\delta_{jk}. \tag{18}$$

The specification of the differencing scheme remains incomplete until some prescription for evaluating the quantity $\partial\psi_j(\tau)/\delta\tau$ is offered. In fact, the choice of approximation for this time derivative is not to be made lightly since it will

strongly determine the character of the calculation, and, given the requirements of numerical stability, make the difference between a feasible and nonfeasible approach to any but the most trivial of problems.

Before specifying $\partial\psi_j(\tau)/\partial\tau$ and thereby determining which of several calculational methods will be employed, we should like to return briefly to the problem of identifying how large a value of τ is large enough, and the to associated problem of computing the energy.

The ground-state wavefunction is very small for large x due to the spatial exponential decay, and is relatively large for x small. Higher energy states, on the other hand, are relatively large at large x. Hence, one expects the time-developed function $\psi(x, \tau)$ to first begin to resemble the exact ground state at small distances and only much later at large distances. In the computations below we have computed the exponential growth rate in τ and thus the energy from Eq. (7) at the value of x for which $\psi(x, \tau)$ assumes its maximum value. This is quite sufficient since, when the energy calculated from successive values of $\psi(x, \tau)$ at this x is no longer changing, the spatial dependence of the wavefunction itself has also stabilized over the entire range.

Finally, we again emphasize that we are interested in the function $\psi(x, \tau)$ only for asymptotic values of τ. Hence, we want integration methods which allow the largest possible time steps $\delta\tau$ and the shortest possible computation time. We also wish to keep the number of spatial net points at the minimum required. Since the starting function is irrelevant, we have adopted the following procedure: the calculation is begun with a small number of net points n and with a convenient initial function $\psi(x, 0)$. When the energy ε_0 has stabilized, the number of net points is doubled and the calculation begun again, the new starting function being provided by the $\psi(x, \tau)$ just generated at the old mesh points and the values of $\psi(x, \tau)$ at the new points being calculated by interpolation from the eigenvalue equation,

$$\sum_k \tilde{H}_{jk}\psi_k(\tau) = \varepsilon_0\psi_j(\tau). \tag{19}$$

This is possible since $\tilde{H}$ is tridiagonal. The new starting function is already very close to the exact ground state; one then produces a much more accurate wavefunction very rapidly.

IV. Numerical Results

A. *Explicit Time Integration*

In Eq. (16) if $\partial\psi_j(\tau)/\partial\tau$ is replaced by $[\psi_j(\tau + \delta\tau) - \psi_j(\tau)]/\delta\tau$, we obtain

$$\psi_j(\tau + \delta\tau) = \sum_k [\delta_{jk} + \delta\tau \tilde{H}_{jk}]\psi_k(\tau). \tag{20}$$

The function at later time is given directly in terms of that at earlier time. This procedure is quite straightforward and immediately applicable to problems with more than one spatial variable. However, as is well known [8], numerical procedures for explicit integration are generally only conditionally stable. For an equation of the form we are using we may guarantee that the error introduced by using finite differences remains bounded if

$$2\delta\tau/(\Delta z)^2 < 1. \tag{21}$$

This is not a necessary condition in this problem, however, since in Eq. (13) the coefficient of the second derivative is not bounded away from zero [9]. In fact, we have obtained stable solutions of (1)3 using the explicit scheme of Eq. (20) for

$$2\delta\tau/(\Delta z)^2 > 2.$$

In particular, with 10 net points, $\Delta z = 0.1$, and a time step $\delta\tau = 0.013$, after 1000 time steps, beginning with a starting function

$$\psi(z, 0) = z(1 - z)^5, \tag{22}$$

Eq. (20) yields the results given in Column B of Table I for $l = 0$. The exact wavefunction is given in Column A. These results are surprisingly good. The energy as computed from successive time steps is

$$\varepsilon_0 = -1.00948,$$

correct to 1%. [Some appreciation of how the energy value, as calculated from (7), settles down as a function of the number of time steps is shown in Fig. 1. The behavior of the wavefunction is shown in Fig. 2.] The mesh width was then halved and the interpolated values of the wavefunction obtained from the eigenvalue equation. To maintain stability, a new $\delta\tau = .001$ was chosen. When the explicit integration was carried 1500 time steps further, an energy of

$$\varepsilon_0 = -1.00174$$

was obtained. The wavefunction that was generated is presented in Table I, Column C. It seems evident, therefore, that for one-dimensional problems explicit time integration is both feasible and gives quite satisfactory results. In order to satisfy the stability condition, however, we must use small time steps. This dif-

ficulty is aggravated even further with the introduction of a sufficiently fine spatial mesh to define the wavefunction well. The net result is an inordinately large number of calculations.

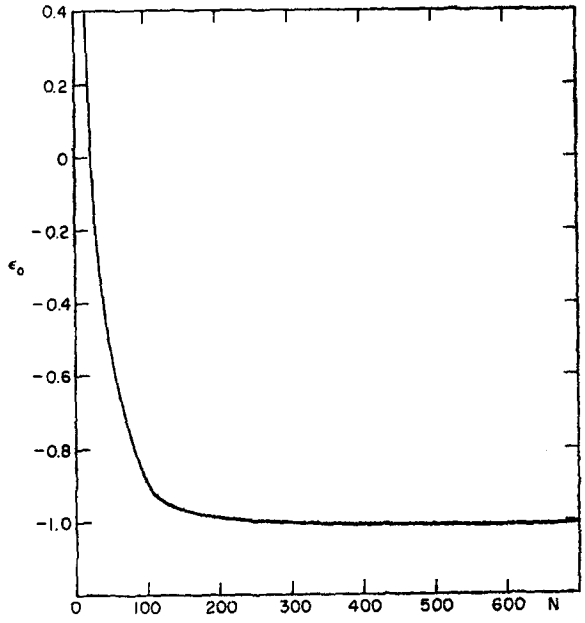

FIG. 1. The energy calculated from Eq. (7) as a function of the number of time steps for the explicit-integration method described.

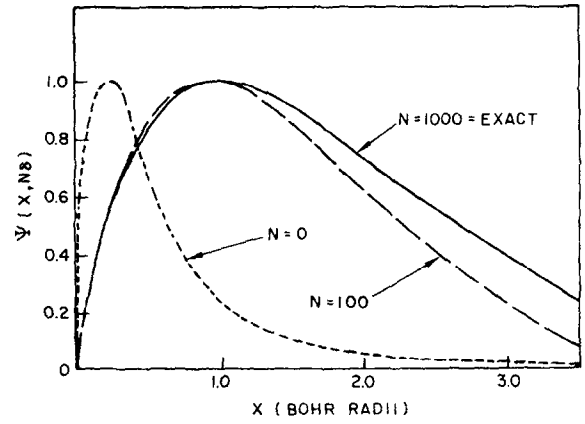

FIG. 2. The function $\psi(x, N\delta\tau)$ for several N using the explicit-integration method described.

TABLE 1

THE SPATIAL DEPENDENCE OF $\psi(x, \tau \to \infty)$ FOR A VARIETY OF NUMERICAL INTEGRATION METHODS[a]

X	A	B	C	D	E
0.0526	0.1357	—	0.1358	—	0.1357
0.1111	0.2703	0.2700	0.2703	0.2700	0.2702
0.1765	0.4021	—	0.4022	—	0.4020
0.2500	0.5293	0.5288	0.5294	0.5288	0.5291
0.3333	0.6493	—	0.6945	—	0.6492
0.4286	0.7590	0.7586	0.7592	0.7586	0.7588
0.5385	0.8543	—	0.8546	—	0.8542
0.6667	0.9304	0.9304	0.9307	0.9304	0.9304
0.8182	0.9813	—	0.9815	—	0.9813
1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
1.2222	0.9786	—	0.9782	—	0.9785
1.5000	0.9098	0.9076	0.9085	0.9076	0.9093
1.8571	0.7882	—	0.7853	—	0.7868
2.3333	0.6151	0.6037	0.6099	0.6037	0.6123
3.0000	0.4060	—	0.3980	—	0.4014
4.0000	0.1992	0.1737	0.1897	0.1737	0.1934
5.6667	0.5329×10^{-1}	—	0.4847×10^{-1}	—	0.4990×10^{-1}
9.0000	0.3043×10^{-2}	0.4265×10^{-2}	0.3629×10^{-2}	0.4268×10^{-2}	0.3474×10^{-2}
19.0000	0.2894×10^{-6}	—	0.7667×10^{-4}	—	0.1922×10^{-4}

[a] Column headings are as follows:
A — analytic solution;
B — explicit integration method;
C — interpolated explicit integration method;
D — implicit and Crank–Nicholson integration methods;
E — interpolated implicit and Crank–Nicholson integration methods.

B. *Implicit Time Integration*

In Eq. (16), $\partial\psi_j(\tau)/\partial\tau$ is taken to be $[\psi_j(\tau) - \psi_j(\tau - \delta\tau)]$, then we obtain

$$\sum_k [\delta_{jk} + \delta\tau H_{jk}]\psi_k(\tau) = \psi_j(\tau - \delta\tau). \tag{23}$$

This forms a set of linear algebraic equations which may be easily inverted, due to the tridiagonal nature of $\tilde{H}_{jk}$ to give $\psi_j(\tau)$ (See Appendix). This method is unconditionally stable and since we are interested in $\psi_j(\tau)$ only for large τ we may use much larger time steps, and consequently perform fewer calculations.

With 10 mesh points, this equation was integrated with $\delta\tau = 0.25$. The energy was constant to one part in 10^6 after 50 time steps. The energy obtained is given in Table II, and the wavefunction in Table I, Column D. It will be noted that, although the wavefunction is quite accurate, the energy is not. This is due to the large time step, and the consequent inaccuracy of determining the energy. The value of the energy can, however, be determined much more accurately by simply generating one more time step with a much smaller $\delta\tau$.

TABLE 2

ENERGY OF THE GROUND STATE OF THE $l = 0$ COULOMB HAMILTONIAN AS ARRIVED AT BY A VARIETY OF NUMERICAL INTEGRATION TECHNIQUES

Method	$\delta\tau$	n	N	ε_0
Explicit	0.013	10	1000	−1.00948
Explicit (interpolated)	0.001	20	1500	−1.00174
Implicit	0.25	10	50	−1.17231
Crank–Nicholson	0.25	10	50	−1.02166
Implicit (interpolated)	0.1	20	100	−1.05812
Crank–Nicholson (interpolated)	0.1	20	100	−1.00491

C. *Crank–Nicholson Method*

A considerably more accurate τ-integration can also be obtained by the Crank–Nicholson method, in which $\partial\psi_j/\partial\tau$ is written as $[\psi_j(\tau + \delta\tau) - \psi_j(\tau)]/\delta\tau$ and the left-hand side of Eq. (16) is taken as the arithmetic mean of its value at time $\tau + \delta\tau$ and τ. Equation (16) then becomes

$$\sum_k \left[\delta_{jk} + \frac{\delta\tau}{2} H_{jk}\right] \psi_k(\tau + \delta\tau) = \sum_k \left[\delta_{jk} - \frac{\delta\tau}{2} H_{jk}\right] \psi_k(\tau). \tag{24}$$

After evaluating the right-hand side, one then inverts these equations in the same manner employed in the fully implicit scheme above. This method is also unconditionally stable, allowing larger $\delta\tau$, but in this case the error is of order $(\delta\tau)^2$ rather than of order $\delta\tau$. For a 10-point grid and $\delta\tau = 0.25$, for example, the calculated wavefunction is identical with that determined above and tabulated in Table I, Column D. A considerably better value for the energy is obtained as is indicated in Table II.

To improve the wavefunction, the fully implicit and Crank–Nicholson calculations were then continued, after suitable interpolation on a mesh of 20 points, with a time step $\delta\tau = 0.1$. Again the wavefunctions were identical after 100 more time steps and are presented in Column E, Table I, with energies as indicated in Table II. Obviously, implicit time integration, especially in the Crank–Nicholson form, is a very powerful method of generating wavefunctions and energies, being both rapid and accurate, at least when applied to problems in one spatial dimension. As seen in the Appendix, however, its generalization to several dimensions is quite formidable.

Since all three methods discussed are in varying degree accurate, the choice of a particular method rests for the most part on its computational convenience. Table I indicates, in fact, that in all cases the wavefunction is given very well up to the region of its maximum, and then deteriorates badly for large x. This is, of course, due to the uniform mesh in the z-space producing a very crude mesh for large x. This may be improved simply by using more mesh points. However, as one uses more mesh points one must, for the explicit method, rapidly decrease the size of the time step. The implicit method does not suffer from this difficulty in one dimension. It is shown, however, in the Appendix that for three dimensions the computation time per time step is greatly increased. It would be preferable, it seems, to use this method to determine a good wavefunction at a small number of points, from them determine a good energy value, and use this information to then solve the time-independent Schrödinger equation for the wavefunction on a much more finely divided space.

V. Scattering States

If the Hamiltonian does not possess a bound state, one might then hope to extract information, for example, the scattering length, about the zero-energy scattering state via the above procedure. This, in fact, cannot be done, for two reasons. First, the zero-energy state is not isolated, but lies at the bottom of a continuum of eigenstates, so that the correction term in Eq. (6) is never negligible. Second, and more important, in any method of time integration one must know *a priori* the boundary values at $x = 0$ and $x \to \infty$. However, the latter is precisely what one wishes to calculate. If we prescribe a value for $x \to \infty$, we are then perforce dealing with some superposition of eigenstates whose only requirement is that it satisfy that boundary value. Thus, it appears that imaginary time integration is not a useful procedure for scattering problems.

VI. Discussion

The method of imaginary time integration is seen to be capable of generating ground-state wavefunctions in one-dimensional problems. Although we have presented for illustration only the results for a Coulomb potential, the method clearly presents no difficulty in the treatment of more complicated potentials, and, in fact, has successfully been applied to the Yukawa and Lennard-Jones potentials as well as to higher angular momentum values in the Coulomb potential. Its real application will be found, however, in three-body problems with three spatial variables. It is then possible to direct the three integration prescriptions described above to this system, and at present the explicit form is being programmed. In addition to the methods we have discussed there are other possible integration prescriptions which may be used. For example, we note that

$$\exp(-\delta\tau H) = \exp(-\delta\tau(T+V) = \exp(-\delta\tau T)\exp(-\delta\tau V) + \text{corrections}.$$

One could then apply the various methods to each factor. In problems of several dimensions a judicious choice of coordinates would allow one to use implicit integration while bypassing the storage difficulties noted in the Appendix. While these methods have not been discussed here, since it was our attention to concentrate on problems of the time development, it is clear that the spatial operator in three dimensions must be handled cleverly. A straightforward generalization of the one-dimensional implicit scheme is not practical. To indicate a possible solution, we shall simply observe that the form of the equations to be inverted in the three-dimensional case can be shown to be, in a suitable coordinate system,

$$[1 + \delta(T_j + T_k + T_l + V_{jkl})]\,\psi^{n+1}_{jkl} = \psi^n_{jkl},$$

where the T's involve spatial differential operators and the V is multiplicative. To first order in δ this is equivalent to

$$[1 + \delta T_j][1 + \delta T_k][1 + \delta T_l][1 + \delta V_{jkl}]\,\psi^{n+1}_{jkl} = \psi^n_{jkl}.$$

The three-body problem thus becomes a sequence of four one-dimensional problems. This then constitutes a vast simplification over the straightforward generalization of the methods presented here for the two-body problem, and to the best of our knowledge, over any existing calculational approach to the three-body problem. Approximations of this and similar types are still being studied.

One may also consider using these methods to construct the wavefunctions of excited bound states. If one has produced the ground state of the Hamiltonian,

one can then project it out of the initial function $\psi(r, 0)$ so that $a_0 = 0$. One then would in analogous fashion integrate equation (4), whose solution would tend in the limit of large τ, to the first excited state. There are difficulties associated with this procedure, however, since integration errors will introduce components of the ground state into the time-developed function. These can in turn build up and swamp the excited state being sought. This question is also under active investigation.

A third aspect of this general problem is that of scattering states. While it is not possible to use imaginary time integration here, one can apply these integration methods to the Schrödinger equation directly, in real time. Some success has been achieved and we shall report on these efforts in the near future.

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APPENDIX: SOLUTION OF IMPLICIT EQUATIONS FOR ONE- AND SEVERAL-VARIABLE PROBLEMS

The solution of the algebraic equations resulting from an implicit differencing scheme is well known [10], and is reproduced here for the sake of completeness. With one spatial variable, the equations are of the form

$$A_j\psi_{j-1} + B_j\psi_j + C_j\psi_{j+1} = D_j, \qquad j = 0,\ 1,\ 2,\ \ldots\ n, \tag{A1}$$

with

$$\psi_0 = \psi_n = 0.$$

The arrays A_j, B_j, C_j, and D_j are known, and $D_0 = D_n = 0$. In order to solve the set of equations (A1), we assume

$$C_j\psi_{j+1} = P_j(g_j - \psi_j). \tag{A2}$$

Substitution into Eq. (A1) then gives the recurrence relations

$$P_j = B_j - \frac{A_jC_{j-1}}{P_{j-1}}; \qquad g_j = \frac{D_j - A_jg_{j-1}}{P_j}. \tag{A3}$$

From (A2),

$$\psi_{n-1} = g_{n-1}; \quad \psi_j = g_j - C_j\psi_{j+1}/P_j. \tag{A4}$$

Since

$$\psi_0 = 0,$$

$$P_1 = B_1; \quad g_1 = D_1/P_1. \tag{A5}$$

Equations (A3)–(A5) constitute a solution to Eq. (A1). Notice that the array P_j is a constant throughout the time integration. One must then keep this array of $n-1$ numbers in addition to the g_j's, D_j's, and ψ_j's.

If threre are several spatial variables, e.g., two dimensions, the corresponding Eq. (A1′) is (we assume the differential equation to contain no mixed derivatives, although this is not necessary)

$$A_{ij}\psi_{i,j-1} + C_{ij}\psi_{i,j+1} + A'_{ij}\psi_{i-1,j} + C'_{ij}\psi_{i+1,j} + B_{ij}\psi_{ij} = D_{ij}$$
$$i = 0,\ 1,\ \ldots n_1; \qquad j = 0,\ 1,\ \ldots n_2 \tag{A1′}$$

with

$$\psi_{io} = \psi_{in_2} = \psi_{oj} = \psi_{n_1,j} = 0$$

If we now consider the arrays ψ_{ij}, and D_{ij} for given i to be the elements of column vectors,

$$\psi_i = \begin{bmatrix} \psi_{io} \\ \cdot \\ \cdot \\ \cdot \\ \psi_{in_2} \end{bmatrix}; \qquad D_i = \begin{bmatrix} D_{io} \\ \cdot \\ \cdot \\ \cdot \\ D_{in_2} \end{bmatrix}$$

and take the matrices

$$\mathscr{B}^i{}_{jk} = B_{ij}\delta_{jk} + A_{ij}\delta_{j-1,k} + C_{ij}\delta_{j+1,k},$$
$$\mathscr{A}^i{}_{jk} = A'_{ij}\delta_{jk}; \qquad \mathscr{G}^i{}_{jk} = C'_{ij}\delta_{ik},$$

then Eq. (A1′) becomes

$$\mathscr{A}^i\Psi_{i-1} + \mathscr{B}^i\Psi_i + \mathscr{G}^i\Psi_{i+1} = \mathscr{D}_i.$$

The solution is then given by (A3)–(A5) with g_i and P_i as matrices. In particular, only P_i^{-1} would have to be stored throughout the problem, but since there are $n-1$ matrices this would total $(n-1)^3$ would increase considerably, requiring the storage of an astronomical number of numbers.

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