JOURNAL OF COMPUTATIONAL PHYSICS 1, 448–453 (1967)

Integration of the Schrödinger Equation in Imaginary Time. II

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ABSTRACT

This paper, the second in a series, continues the investigation of numerical techniques for the integration of the time-dependent Schrödinger equation in imaginary time, with particular emphasis on those methods that can be generalized easily to several spacial variables.

I. INTRODUCTION

This report is a continuation of the program begun in [1]. In this previous work we indicated how numerical integration of the Schrödinger equation in imaginary time may be used to generate quantum-mechanical bound states, in particular, the ground state.[2] Various methods of performing the time integration were aplied to the S-wave Coulomb problem, quite successfully. The purposes of this program, however, lies in its potential application to the three-body problem with three spatial variables, and the generalization of these numerical methods to several dimensions presents some considerable difficulties. In this paper, we shall give several further prescriptions for the time integration—prescriptions designed for ease of generalization to several spatial variables.

In I we investigated the utility of several integration schemes, accurate to both

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[1] This work was performed under the auspices of the U.S. Atomic Energy Commission, under Contract No. W-7405-eng-48.

[2] We take this opportunity to correct a possible oversight in I. The idea of using imaginary time is hardly original and is traceable at least to 1942 (Feynman's dissertation). Since then the method has been mentioned many times.

first and second order in the time-step $\delta\tau$. While the particular approximations to the time-development operator worked admirably for the one-dimensional case, they are, with the exception of the explicit method, unsuitable for problems in more than one spatial dimension, with present-day high-speed computer memories. The explicit method is not feasible for three-body problems with realistic forces because, depending on the choice of coordinate system, the form of either the kinetic or potential energies aggravates the stability difficulties enormously. We therefore turn our attention to the construction of approximations to the time-development operator that can be generalized to several dimensions. Despite the fact that second-order schemes have been shown to converge much more rapidly to a stable energy, we shall look for both first- and second-order approximations that can be generalized. We do this because of the greater complexity of the computation at each time-step in the second-order schemes.

If we consider a Schrödinger equation in three suitably chosen variables x, y and z, the relevant operator can become

$$\exp(-\delta\tau H) = \exp\{-\delta\tau[T_x + T_y + T_z + V(xyz)]\}$$

with no cross-derivative terms in the kinetic energy [2]. By use of the approximation

$$\begin{aligned}\exp(-\delta\tau H) &\approx \exp\{-\delta\tau[T_x + T_y + T_z]\}\exp[-\delta\tau V(x, y, z)]\\ &= \exp(-\delta\tau T_x)\exp(-\delta\tau T_y)\exp(-\delta\tau T_z)\exp(-\delta\tau V),\end{aligned}$$

we could then apply the methods of I to each factor. While this would be a lengthy computation, it would lie well within the bounds of feasibility for available facilities. The objection to this procedure is, of course, that $V(xyz)$ and T_x (or T_y or T_z) do not necessarily commute with each other. We may, however, study the virtues and pitfalls of the factorization technique in the much simpler case of the one-dimensional S-wave radial problem, which also contains this all-important feature of noncommutatitivity.

II. THE FIRST-ORDER APPROXIMATION

We see from Eq. (I-8) that we are dealing with an operator of the form

$$\exp(-\delta\tau H) \equiv \exp\{-\delta\tau[T + V]\},$$

where T and V do not commute. Consider the approximation (expansions of this type are well-known [4].)

$$\exp\{-\delta\tau[T + V]\} \to \tfrac{1}{2}[\exp(-\delta\tau T)\exp(-\delta\tau V) + \exp(-\delta\tau V)\exp(-\delta\tau T)]. \quad (1)$$

This approximate form, as can be verified by expansion of the separate terms, is correct to second order in $\delta\tau$, the first correction term being proportional to $(\delta\tau)^3$ and involving the commutator T, V.[3] Expanding the separate exponentials, we obtain

$$\exp\{-\delta\tau[T + V]\} \to \frac{1}{2}\left[\frac{1}{1+\delta\tau T}\,\frac{1}{1+\delta\tau V} + \frac{1}{1+\delta\tau V}\,\frac{1}{1+\delta\tau T}\right].$$

Thus, Eq. (I 8) becomes

$$\begin{aligned}\psi(x, t + \delta\tau) &= \exp\{-\delta\tau[T + V]\}\,\psi(x, t)\\ &\approx \frac{1}{2}\left[\frac{1}{1+\delta\tau T}\,\frac{1}{1+\delta\tau V} + \frac{1}{1+\delta\tau V}\,\frac{1}{1+\delta\tau T}\right]\psi(x, t)\end{aligned}$$

or

$$\psi(x, t + \delta\tau) \approx \tfrac{1}{2}[X_1(x, t) + X_2(x, t)], \quad (2)$$

where

$$(1 + \delta\tau V)(1 + \delta\tau T)X_1(x, t) = \psi(x, t) \quad (2a)$$

and

$$(1 + \delta\tau T)(1 + \delta\tau V)X_2(x, t) = \psi(x, t). \quad (2b)$$

In the restricted z-space, $0 \leq z < 1$ (defined in I), and using the Hamiltonian appearing in (I-13) and the spatial differences of (I-15), these equations can be solved by the methods contained in the Appendix of I. It will be noted, however, that the choice of $\delta\tau$ is now restricted if V is anywhere attractive. In particular, if $V_{\min}$ is the largest negative value of the potential allowed by the spacial mesh, we require that

$$\delta\tau\,|\,V_{\min}\,| < 1. \quad (3)$$

The wavefunction resulting from the integration with a mesh of 10 points and

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[3] The reader will notice that since the exact Green's functions for the separate exponential operators are known, one could, in principle, propagate the solution by evaluating suitable integrals rather than making use of the differential equation. Since the leading correction term involves T, V, it is by no means clear that such a procedure would be preferable to the methods discussed below. A variation of the Green's function is being studied by H. Sahlin and J. L. Schwartz, using Monte Carlo techniques (private communication).

a time-step $\delta\tau = 0.01$ is presented in Column a of Table I. The calculated energy appears in Table II. It will be noted that neither the wavefunction nor the energy is remarkably good. In particular, in contrast to the results in I, the region near the origin is no longer described accurately. This is a direct result of the limitation on the time-step $\delta\tau$.

TABLE I

The 1*S*-Hydrogen Wavefunction Given by the Several Integration Methods[a]

x	Exact Wavefunct.	a	b	c	d
.0526	.1357	—	—	—	.1358
.1111	.2703	.3308	.2752	.2710	.2703
.1765	.4021	—	—	—	.4021
.2500	.5293	.5912	.5349	.5300	.5293
.3333	.6493	—	—	—	.6493
.4286	.7590	.8110	.7642	.7596	.7590
.5385	.8543	—	—	—	.8543
.6667	.9304	.9612	.9341	.9310	.9305
.8182	.9813	—	—	—	.9814
1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
1.2222	.9786	—	—	—	.9785
1.5000	.9098	.8749	.9021	.9070	.9092
1.8571	.7882	—	—	—	.7867
2.3333	.6151	.5539	.5918	.6026	.6122
3.0000	.4060	—	—	—	.4013
4.0000	.1992	.1471	.1619	.1729	.1933
5.667	.0532	—	—	—	.0498
9.0000	$.304 \times 10^{-2}$	$.333 \times 10^{-2}$	$.371 \times 10^{-2}$	$.210 \times 10^{-2}$	$.345 \times 10^{-2}$
19.0000	$.289 \times 10^{-6}$	—	—	—	9.39×10^{-6}

[a] Columns read as follows:

a — First order factorized method on a mesh of ten points;

b — Continuation of case a with decreased time-step;

c — Second-order factorized method on a mesh of ten points;

d — Continuation of Column c with smaller time-step on a mesh of 20 points, using the interpolation procedure.

The time step was then cut by a factor of 10 and the integration continued for another 1500 time-steps. The resulting wavefunction appears in Column b of Table I and the energy in Table II. The improvement is apparent.

TABLE II

ENERGY OF THE HYDROGEN 1*S*-STATES AS GENERATED BY THE METHODS OF TABLE I

Case[a]	Time-step	No. iterations	Energy
Exact	—	—	−19000
a	0901	1000	−19086
b	09001	1500	−19017
c	0903	280	−19017
d	0901	700	−19004

[a] Categories a–d the same as their respective columns in Table I.

While a function of this accuracy would be quite acceptable for a three-body system, the large number of time-steps required would make such a calculation prohibitively lengthy.

III. THE SECOND-ORDER APPROXIMATION

In light of these results, a second-order approximation might be desirable. There are many ways of generating such approximations. For example. Eq. (1) could be written as

$$\frac{1}{2}\left[\exp(-\delta\tau T)\exp(-\delta\tau V)+\exp(-\delta\tau V)\exp(-\delta\tau T)\right]$$
$$\approx\frac{1}{2}\left\{\frac{1-(\frac{1}{2}\delta\tau)T}{1+(\frac{1}{2}\delta\tau)T}\,\frac{1-(\frac{1}{2}\delta\tau)V}{1+(\frac{1}{2}\delta\tau)V}+\frac{1-(\frac{1}{2}\delta\tau)V}{1+(\frac{1}{2}\delta\tau)V}\,\frac{1-(\frac{1}{2}\delta\tau)T}{1+(\frac{1}{2}\delta\tau)T}\right\}. \tag{4}$$

This expression approximates $\exp(-\delta\tau H)$ correctly to second order in $\delta\tau$. The separate terms are correct only to order $\delta\tau$. The operator $\exp(-\delta\tau H)$ can also be written as

$$\begin{aligned}\exp(-\delta\tau H)&=\exp\{-\delta\tau[T+V\}\\&\approx\frac{1}{2}\left\{\frac{1}{1+(\frac{1}{2}\delta\tau)T}\,\frac{1}{1+(\frac{1}{2}\delta\tau)V}\,[1-(\tfrac{1}{2}\delta\tau)V][1-(\tfrac{1}{2}\delta\tau)T]\right.\\&\qquad\left.+\frac{1}{1+(\frac{1}{2}\delta\tau)V}\,\frac{1}{1+(\frac{1}{2}\delta\tau)T}\,[1-(\tfrac{1}{2}\delta\tau)T][1-(\tfrac{1}{2}\delta\tau)V]\right\}.\end{aligned} \tag{5}$$

Each term represents $\exp(-\delta\tau H)$ correctly to second order. Moreover, an expansion of each factor demonstrates that the leading correction to (5) is proportional to $(\delta\tau)^3[TV + VT]H$, whereas the leading correction to (4) contains $(\delta\tau)^3[TVT + VTV]$. Since in many problems of interest the operators V and T can become singular (for example, at the origin in the Coulomb problem), while their sum H remains bounded, the leading correction to (5) appears to be less singular. Hence Eq. (5) seemingly represents a more preferable expansion than does (4), and we shall confine ourselves to (5). Eq. (5) then represents a set of equations analogous to (2), (2a), and (2b) relating $\psi(x, t + \delta\tau)$ to $\psi(x, t)$ and which can be solved in like manner. Similarly, there is a limitation on the choice of $\delta\tau$ for attractive potentials.

Using the same Hamiltonian as above, and choosing $\delta\tau = 0.03$, Eq. (5) has been iterated over a mesh of 10 points. The resulting wavefunction and energy appears in Column c Table I and in Table II, respectively. To obtain a more detailed wavefunction, the time-independent Schrödinger equation was used as described in I to provide interpolated starting values on a mesh of 20 points. The integration was continued with $\delta\tau = 0.01$, with results in Table I, Column d, and in Table II. Since the amount of computation per time step is only twice that of the first-order approximation, the desirability of the second-order method is obvious.

It is obvious that, even with these crude spatial meshes, the method produces accurate wavefunctions and energies.

ACKNOWLEDGMENT

The authors are pleased to acknowledge the expert programming of Mr. Donald Freeman.

REFERENCES

1. A. GOLDBERG and L. J. SCHWARTZ, *J. Comp. Phys,* **1** 433–447 (1967) (preceding paper, this issue). Hereafter, this paper will be referred to as I. We shall adopt throughout this present paper the notation used in I. Moreover, equations of I will be labeled by their numbers there with the prefix I.
2. D. A. KIRZHNITZ, *Sov. Phys.* JEPT **5**, 64 (1957); or, for example, K. HUANG, "Statistical Mechanics," p. 217 ff. Wiley, New York (1963).
3. C. F. CURTISS, J. O. HIRSCHFELDER and F. T. ALDER, *J. Chem. Phys.* **18**, 1638–1642 (1950) for example.