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A Relaxation Method for Nonlocal and Non-Hermitian Operators

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We present a grid method to solve the time dependent Schrödinger equation (TDSE). It uses the Crank–Nicholson scheme to propagate the wavefunction forward in time and finite differences to approximate the derivative operators. The resulting sparse linear system is solved by the symmetric successive overrelaxation iterative technique. The method handles local and nonlocal interactions and Hamiltonians that correspond to either Hermitian or to non-Hermitian matrices with real eigenvalues. We test the method by solving the TDSE in the imaginary time domain, thus converting the time propagation to asymptotic relaxation. Benchmark problems solved are both in one and two dimensions, with local, nonlocal, Hermitian and non-Hermitian Hamiltonians.

1. INTRODUCTION

The evolution of quantum mechanical systems is governed by the time dependent Schrödinger equation (TDSE),

$$i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle, \tag{1}$$

where H is the Hamiltonian operator and $|\Psi(t)\rangle$ is the wave function describing the state of the system. In Eq. (1) the Hamiltonian is usually local and Hermitian. In general, however, it can be nonlocal and non-Hermitian. Such a case is encountered, for example, in the integro-differential equation obtained via the resonating group method (RGM) which contains a Hermitian, nonlocal, energy-dependent interaction [1, 2]. Other characteristic examples in this respect are the effective Hamiltonians for the Faddeev [3] and the integro-differential equation approach (IDEA) schemes [4] for few-body systems in configuration space, which are both nonlocal and non-Hermitian.

Various grid methods have been developed in the past to solve Eq. (1) directly. The mathematical formulation and description of various algorithms as well as an extensive literature can be found in the review articles by De Raedt [5] and Gerber *et al.* [6]. Alternatively, wave functions can be obtained by separating out the time dependence and then solving the resulting eigenproblem by expanding on some basis set. Examples of such techniques are the collocation and Galerkin methods implemented via piecewise polynomials such as the cubic [3] or quintic Hermite [7] splines, and the B-splines [4, 8]. These methods are nowadays extensively used in the field of few-body systems. Expansions in terms of general basis sets are also employed in the configuration interaction method [9], in the Hartree–Fock method [10], in variational methods [11], etc. The Monte-Carlo type methods [12] are also used. However, these belong to a different class since they are stochastic methods and not deterministic like the one presented in this paper. From the plethora of other numerical methods used to obtain bound state (and scattering) solutions, we mention here the pseudospectral methods (see Ref. [13], and references therein) the discrete variable representation (DVR) method [14], the Chebyshev–Lanzcos method of Ref. [15], the Kosloff and Tal-Ezer method [16], the filter-diagonalization method of Neuhauser [17], the Green function filter proposed by Wyatt [18], etc. More details, and references to similar methods can be found in the aforementioned references.

Most of these methods, although powerful enough and able to solve problems with many degrees of freedom, they have certain disadvantages. In the collocation method, for instance, one always faces the problem of the number and distribution of the grid points. An increase of the number of collocation points to obtain results of higher accuracy usually requires not only huge memory but also special techniques for handling large matrices. In the Galerkin method, where higher order Hermite- or B-splines are used, the results are more reliable and stable than those obtained by the collocation method, but one encounters, in addition, the question of implementing the boundary conditions besides the problem of large memory requirements. The expansion in terms of other basis sets is similarly handicapped from these problems. Moreover, one must use a lot of intuition in order to choose the proper set.

The method of the time evolution of a state via the TDSE, on the other hand, does not suffer from the afore-

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mentioned problems. One can obtain the desired ground state starting from an initial guess $\Psi(\mathbf{r}, t = 0)$ which is not crucial for the subsequent evolution. The memory requirements are comparatively small, and the implementation is quite simple. Furthermore, its extension to treat time-dependent Hamiltonians is rather straightforward. Schemes of this kind have been successfully used in atomic and molecular physics [19] to obtain bound state, as well as scattering, solutions.

In the present work we employ the relaxation technique; i.e., we solve the TDSE in imaginary time. This leads to the determination of the ground state of the system in a unique way. The method is, of course, applicable to the real time TSDE as well. We use a lattice representation of the Hamiltonian and the Crank–Nicolson (CN) algorithm [20–22] to propagate the wave function. In this, the evolution operator $e^{-\tau H}$, for small time step τ is approximated by $(1 + \tau/2H)^{-1}(1 - \tau/2H)$. Such a representation of the exponential has been employed by Golberg *et al.* [21] in the 1960s, where it was referred to as "Cayley form." It was emphasized there that this type of approximation to the exponential is simple, unitary, and has the desirable property of being exact to second order in τ. The biggest advantage of this approximation, however, is that in practical applications is unconditionally stable. Furthermore, it is flexible enough to handle nonlocal and non-Hermitian Hamiltonians. The major drawback, often cited (see, for example, Ref. [5]), of this method is the inversion of the matrix $(1 + \tau/2H)$. However, such an inversion, as we shall show, is not necessary and if, in addition, the sparsity of this matrix is exploited, the approach becomes a lot more economical and efficient. Moreover, since the CN method is unconditionally stable [22] and the procedure does not require an *a priori* deep understanding of the problem or any educated guess-work, it is suitable for practical applications.

In Section II, we describe the time-dependent scheme for the TDSE and the relaxation method for local, nonlocal, Hermitian, and non-Hermitian Hamiltonians. In Section III we describe in detail the implementation of the method. In Section IV we describe the problems solved and present our results, while in Section V we summarize our conclusions.

II. THE METHOD

The relaxation method proceeds by replacing t by $-it$ in Eq. (1). The TDSE then transforms into a diffusion-like equation ($\hbar = 1$),

$$\frac{\partial}{\partial t}|\Psi(t)\rangle = -H|\Psi(t)\rangle,$$

having the formal solution

$$|\Psi(t+\tau)\rangle = e^{-H\tau}|\Psi(t)\rangle.$$

For numerical work the latter is equivalently written

$$e^{H\tau/2}|\Psi(t+\tau)\rangle = e^{-H\tau/2}|\mathrm{C}(t)\rangle.$$

The CN scheme is obtained upon Taylor expanding the exponential and keeping only linear terms in τ,

$$\left(1 + \frac{\tau}{2}H\right)|\Psi(t+\tau)\rangle = \left(1 - \frac{\tau}{2}H\right)|\Psi(t)\rangle. \tag{2}$$

For a Hermitian Hamiltonian one can expand the wave function $|\Psi(t)\rangle$ in terms of its orthonormal eigenstates $|k\rangle$,

$$\begin{aligned}|\Psi(t)\rangle &= \sum_{k=0}^{\infty} a_k e^{-\mathscr{E}_k t}|k\rangle \\ &= e^{-\mathscr{E}_0 t}\left\{a_0|0\rangle + \sum_{k=1}^{\infty} a_k e^{-\Delta_k t}|k\rangle\right\},\end{aligned} \tag{3}$$

where $\mathscr{E}_0 < \mathscr{E}_1 \cdots$ are the eigenvalues of H and $\Delta_k \equiv \mathscr{E}_k - \mathscr{E}_0 > 0$. For large values of the time variable, only the first term survives, i.e.,

$$\lim_{t\to\infty}|\Psi(t)\rangle = a_0 e^{-\mathscr{E}_0 t}|0\rangle.$$

This is the principle on which the relaxation method is based. The expectation value estimator is defined by

$$E(t) \equiv \frac{\langle\Psi(t)|H|\Psi(t)\rangle}{\langle\Psi(t)|\Psi(t)\rangle}.$$

Using Eq.(3) we obtain

$$E(t) = \mathscr{E}_0 + \frac{\sum_{k=1}^{\infty}\Delta_k|a_k/a_0|^2\, e^{-2\Delta_k t}}{1 + \sum_{k=1}^{\infty}|a_k/a_0|^2\, e^{-2\Delta_k t}}$$

and, hence,

$$\lim_{t\to\infty} E(t) = \mathscr{E}_0.$$

Note that $E(t) \geq \mathscr{E}_0$ for $t > 0$. The asymptotic energy estimator is defined as

$$\begin{aligned}\mathscr{E}(t,\tau) &\equiv \frac{1}{2\tau}\ln\left[\frac{\langle\Psi(t)|\Psi(t)\rangle}{\langle\Psi(t+\tau)|\Psi(t+\tau)\rangle}\right] \\ &= \mathscr{E}_0 + \frac{1}{2\tau}\ln\left[\frac{1 + \sum_{k=1}^{\infty}|a_k/a_0|^2\, e^{-2\Delta_k t}}{1 + \sum_{k=1}^{\infty}|a_k/a_0|^2\, e^{-2\Delta_k t+\tau)}}\right].\end{aligned}$$

Again

$$\lim_{t\to\infty} \mathscr{E}(t,\tau) = \mathscr{E}_0,$$

and $\mathscr{E}(t,\tau) \geq \mathscr{E}_0$ for all $t > 0$. Furthermore, $\lim_{\tau\to 0} \mathscr{E}(t,\tau) = E(t)$.

For non-Hermitian Hamiltonians with real eigenvalues, such as those arising in the Faddeev decomposition of the interaction in pairwise components, the eigenstates are not orthogonal. Let us denote by $N_{mk} \equiv \langle m|k\rangle$ the overlap between the states $|m\rangle$ and $|k\rangle$. Then the expectation energy estimator in this case is written (we assume $\langle k|k\rangle = 1$)

$$E(t) = \mathscr{E}_0 + \frac{\displaystyle\sum_{k=1}^{\infty} \Delta_k \frac{a_k}{a_0} N_{0k} e^{-\Delta_k t} + \sum_{k=1}^{\infty}\sum_{l=1}^{\infty} \Delta_k \frac{a_k}{a_0}\frac{a_l^*}{a_0^*} N_{lk} e^{-(\Delta_k+\Delta_l)t}}{1 + \displaystyle\sum_{k=1}^{\infty} \frac{a_k}{a_0} N_{0k} e^{-\Delta_k t} + \sum_{k=1}^{\infty} \frac{a_k^*}{a_0^*} N_{k0} e^{-\Delta_k t} + \sum_{k=1}^{\infty}\sum_{l=1}^{\infty} \frac{a_k}{a_0}\frac{a_l^*}{a_0^*} N_{lk} e^{-(\Delta_k+\Delta_l)t}}.$$

The quantity on the right added to $\mathscr{E}_0$ is not necessarily positive for all t. Its form resembles that of a damped oscillation. This means that at times not long enough for the damping to dominate, we may have $E(t) < \mathscr{E}_0$, which is not the case for Hermitian Hamiltonians. In practice, this means that longer propagation times are necessary to ensure the dominance of the damping.

For the asymptotic energy estimator we similarly have

$$\mathscr{E}(t,\tau) = \mathscr{E}_0 + \frac{1}{2\tau}\ln\left[\frac{1 + \displaystyle\sum_{k=1}^{\infty} \frac{a_k}{a_0} N_{0k} e^{-\Delta_k t} + \sum_{k=1}^{\infty} \frac{a_k^*}{a_0^*} N_{k0} e^{-\Delta_k t} + \sum_{k=1}^{\infty}\sum_{l=1}^{\infty} \frac{a_k}{a_0}\frac{a_l^*}{a_0^*} N_{lk} e^{-(\Delta_k+\Delta_l)t}}{1 + \displaystyle\sum_{k=1}^{\infty} \left(\frac{a^k}{a_0} N_{0k} + \frac{a_k^*}{a_0^*} N_{k0}\right) e^{-\Delta_k(t+\tau)} + \sum_{k=1}^{\infty}\sum_{l=1}^{\infty} \frac{a_k}{a_0}\frac{a_l^*}{a_0^*} N_{lk} e^{-(\Delta_k+\Delta_l)(t+\tau)}}\right]$$

which displays similar limiting behaviour.

III. IMPLEMENTATION

A. Discretization

1. *One Dimensional*

Consider the one-dimensional n-point grid given by

$$r_i = r_1 + (i-1)h_r, \quad i = 1, 2, .., n.$$

Then we define $\Psi(r_i) \equiv \Psi_i \equiv \langle i|\Psi\rangle$. The matrix elements of the relevant operators in this representation are

$$\langle j|\hat{r}|i\rangle = r_i\langle j|i\rangle = r_i\delta_{i,j}.$$

Thus the $\hat{r}$ operator (and every function of it) corresponds to a diagonal matrix. Since we work on a discrete basis and derivatives are defined under continuity assumptions, it is necessary to assume some discrete approximation in order to calculate the matrix elements of the derivative operators. Using finite difference approximations, the first derivative can be expressed as

$$\left\langle i\left|\frac{\partial}{\partial r}\right|\Psi\right\rangle \equiv \frac{\partial}{\partial r}\Psi(r)|_{r=r_i} \approx \sum_j a_{ij}\Psi_j = \sum_j a_{ij}\langle j|\Psi\rangle;$$

hence $\langle i|\partial/\partial r|j\rangle \approx a_{ij}$ and $(\partial/\partial r)|i\rangle \approx \sum_k a_{ik}|k\rangle$. For the central difference approximation of order $O(h_r^2)$, one has

$$a_{ij} = \frac{1}{2h_r}[\delta_{i+1,j} - \delta_{i-1,j}]$$

and

$$\frac{\partial}{\partial r}|i\rangle = \frac{1}{2h_r}[|i-1\rangle - |i+1\rangle].$$

Similarly for the second-derivative operator,

$$\left\langle i\left|\frac{\partial^2}{\partial r^2}\right|\Psi\right\rangle \equiv \frac{\partial^2}{\partial r^2}\Psi(r)|_{r=r_i} \approx \sum_j b_{ij}\Psi_j = \sum_j b_{ij}\langle j|\Psi\rangle.$$

Hence $b_{ij} \approx \langle i|\partial^2/\partial r^2|j\rangle$ and $(\partial^2/\partial r^2)|i\rangle \approx \sum_k b_{ik}|k\rangle$.

Again if the central difference approximation of order $O(h_r^2)$ is used, we get

$$b_{ij} = \frac{1}{\Delta_r^2}[\delta_{i+1,j} - 2\delta_{i,j} + \delta_{i-1,j}]$$

and

$$\frac{\partial^2}{\partial r^2}|j\rangle = \frac{1}{h_r^2}[|j+1\rangle + |j-1\rangle - 2|j\rangle].$$

2. *Two Dimensional*

Suppose that the second direction is discretized as

$$z_j = z_1 + (j-1)h_z, \quad j = 1, 2, ..., m.$$

The representation now is given by $|i, j\rangle$, namely by a two index vector that specifies the point (r_i, z_j) on the two-dimensional grid. As in the one-dimensional case,

$$\langle i, j|\Psi\rangle \equiv \Psi_{ij}$$

and, again, for central difference approximations of order $O(h_r^2)$ and $O(h_z^2)$ we have

$$\left\langle k, l \left| \frac{\partial}{\partial r} \right| i, j \right\rangle = \frac{1}{2h_r}[\delta_{k,i-1} - \delta_{k,i+1}]\delta_{l,j}$$

and

$$\left\langle k, l \left| \frac{\partial}{\partial z} \right| i, j \right\rangle = \frac{1}{2h_z}[\delta_{l,j-1} - \delta_{l,j+1}]\delta_{k,i}.$$

Alternatively, each site (point on the two-dimensional mesh) with "coordinates" i, j can be labeled by a single index I that is given by

$$I = (j-1)n + i$$

and, hence, we may define the single index representation $|I\rangle \equiv |i, j\rangle$. Inversely i, j are given by

$$i = 1 + (I-1) \bmod n, \quad j = \frac{I-i}{n} + 1.$$

Letting $|K\rangle = |k, l\rangle$, we obtain for the derivative operator

$$\frac{\partial}{\partial r}|I\rangle = \frac{1}{2h_r}[|I-1\rangle - |I+1\rangle]$$

and, hence,

$$\left\langle K \left| \frac{\partial}{\partial r} \right| I \right\rangle = \frac{1}{2h_r}[\delta_{K,I-1} - \delta_{K,I+1}].$$

Similarly, for the derivative with respect to the z-variable we have

$$\frac{\partial}{\partial z}|I\rangle = \frac{1}{2h_z}[|I-n\rangle - |I+n\rangle]$$

and

$$\left\langle K \left| \frac{\partial}{\partial z} \right| I \right\rangle = \frac{1}{2h_z}[\delta_{K,I-n} - \delta_{K,I+n}].$$

In this approximation the derivative with respect to r is represented by a tridiagonal matrix (as in the one-dimensional case), while the derivative with respect to z is represented by a matrix with two paradiagonals, n elements above and below the main diagonal. Similar rules hold for the second derivatives. Formulae for matrix elements, when other difference approximations for the derivatives are employed, can easily be derived following the above formulation.

B. The Symmetric Successive Over-Relaxation Method

In general, the Hamiltonian is written

$$H = H_0 + H_{\mathrm{NL}},$$

where H_0 consists of local and derivative operators, and H_{NL} is the nonlocal part, consisting of integral operators. Then Eq. (2) is written

$$\left[1 + \frac{\tau}{2}(H_0 + H_{\mathrm{NL}})\right]|\Psi(t+\tau)\rangle = \left[1 - \frac{\tau}{2}(H_0 + H_{\mathrm{NL}})\right]|\Psi(t)\rangle.$$

The presence of the matrix H_{NL} usually destroys the sparsity of the representation. However we may recast it as

$$\left(1 + \frac{\tau}{2}H_0\right)|\Psi(t+\tau)\rangle = \left[1 - \frac{\tau}{2}(H_0 + H_{\mathrm{NL}})\right]|\Psi(t)\rangle - \frac{\tau}{2}H_{\mathrm{NL}}|\Psi(t+\tau)\rangle,$$

which lends itself to iteration. The latter equation is a linear system $B\Psi = C$, where B is sparse and thus it can be solved efficiently using iterative methods. For this, one splits the B-matrix as

$$B = D + L + U,$$

where D is the diagonal part while L and U are the lower and upper triangular parts. Thus, we may write

$$(D + L)\Psi = C - U\Psi$$

or

$$(D + U)\Psi = C - L\Psi,$$

suggesting the iterative procedure,

$$(D + L)\Psi^{(n+1/2)} = C - U\Psi^{(n)}$$
$$(D + U)\Psi^{(n+1)} = C - L\Psi^{(n+1/2)}.$$

These can be solved directly by forward and backward substitution, respectively. The scheme is known as the symmetric Gauss–Seidel method. However, another more

efficient scheme, namely, the symmetric successive over-relaxation (SSOR) method [22–25] can be used. In this, to accelerate convergence, an acceleration parameter $\omega \in [0, 2]$ is introduced to obtain the more efficient scheme,

$$(D + \omega L)\Psi^{(n+1/2)} = \omega(C - U\Psi^{(n)}) + (1 - \omega)D\Psi^{(n)}$$
$$(D + \omega U)\Psi^{(n+1)} = \omega(C - L\Psi^{(n+1/2)}) + (1 - \omega)D\Psi^{(n+1/2)},$$

which for $\omega = 1$ reduces to the symmetric Gauss–Seidel method. The advantages of this scheme, the choice of ω, and other technical details can be found in *Numerical Recipes* (Ref. [25]) and will not be repeated here.

IV. RESULTS

Various one- and two-dimensional Hamiltonians have been chosen to test our method. The results obtained are compared, where possible, with those of other methods. In general, the comparison shows that the results are indistinguishable for all practical purposes. However, to compare the efficiency among several methods, is a very difficult task, since CPU-times are either not given, or they correspond to different machines. Therefore we avoided to present such a comparison. Nevertheless, in what follows, we report our CPU-times to demonstrate that even though we did not spend time to optimize our code, the procedure we propose requires reasonable computer time on a small workstation. The agreement of our results with those obtained via other methods shows that our scheme is both convergent and accurate. We mention here that one can control the accuracy via the order of the approximations to the derivatives and the grid step size.

A. Local Hamiltonian

As a first example we consider the triplet state of the Malfliet-Tjon I + III nucleon–nucleon potential [26] which is widely used in bound state and scattering calculations in the field of few-nucleon physics. This potential is given by

$$V(r) = 1438.72 \exp(-3.11r)/r - 626.885 \exp(-1.55r)/r,$$

where the units are in the MeV-fm system.

The result obtained for the bound state, using 400 mesh points in the range (0, 28) fm with a time step $\tau = 0.001$, is -2.2305 MeV, in agreement with the result obtained by Payne [3] via the collocation method with Hermite splines. The initial wave function was taken to be $r^2 \exp(-r)$, and the required CPU-time was 43 s on an IBM RS6000-320H. All subsequently quoted CPU-times refer to this workstation. We note in passing that CPU-times depend strongly on the choice of the time step τ, the number of grid points, the required accuracy, and the SSOR acceleration parameter ω. In this work no effort was made for an optimal choice.

B. Nonlocal Hamiltonian

We consider here the resonating group method (RGM [1] nonlocality for the $n + \alpha$ system,

$$V_l(r, r') = V_D(r)\delta(r - r') + K_l(r, r'),$$

where $V_D(r)$ is the local or direct part of the interaction and $K_l(r, r')$ is the nonlocal part which, in general, is energy dependent. In the K-model of this method where the target-recoil effects and core-exchange contributions are omitted [27], the direct potential is given by

$$V_D(r) = -3V_0\gamma w \exp\left[-\frac{ak}{a + k}r^2\right],$$

and the nonlocal, for $l = 0$, by

$$K_0(r, r') = -3\pi\frac{V_0\beta w}{k}\exp[-(a/2 + k)(r^2 + r'^2)]$$
$$\{\exp[2krr'] - \exp[-2krr']\}$$

with $V_0 = 72.98$ MeV, $k = 0.46$ fm^{-2}, $w = 0.4075$, and $a = 0.685$ fm^{-2}. Further $\beta = (a/\pi)^{3/2}$ and $\gamma = (a/(a + k))^{3/2}$. This interaction is known to generate a deep bound state widely known as the Pauli forbidden state (PFS).

The Schrödinger equation is written

$$\left[\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + (E - V_D(r))\right]u_0(r) = \int_0^\infty K_0(r, r')u_0(r')\,dr'.$$

We solved this equation and obtained for the PFS, using 150 mesh points in the range (0, 20) fm, the value of $E = -24.07$ MeV in 40 CPU-seconds. The starting wave function was as in the local case.

C. Two-Dimensional, Local, Hermitian Hamiltonian

We consider here the Hénon–Heiles potential, which was treated by us using the Chebyshev–Lanczos method [15],

$$V(x, y) = \frac{1}{2}(x^2 + y^2) + \frac{1}{4\sqrt{5}}x\left(y^2 - \frac{1}{3}x^2\right).$$

We found for the ground state $\mathscr{E}_0 = 0.998592$, using a two-dimensional box $[-6, 6] \times [-6, 6]$ with 64 points taken in each direction. This compares favorably with the value of 0.9986 obtained in Ref. [16] and by us [15], $E = 0.998595$. The calculation required 80 CPU-seconds.

D. Two-Dimensional, Local, Non-Hermitian Hamiltonians

The test case chosen here is the ^{4}He atom system. The Hamiltonian, in the framework of the hyperspherical harmonics method and neglecting the e–e repulsion, is written [28]

$$H = -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{15}{8}\frac{1}{r^2} - \frac{2}{r^2}\left[(1-z^2)\frac{\partial^2}{\partial z^2} - 3z\frac{\partial}{\partial z}\right] - \frac{\sqrt{8}}{r}\left[\frac{1}{\sqrt{1+z}} + \frac{1}{\sqrt{1-z}}\right],$$

where the $r \in [0, \infty]$ and $z \in [-1, +1]$.

Using 86 points in the r-direction in $r \in (0, 22)$ and 126 points in the z-direction we obtained, after propagating the initial form $\Psi(r, t = 0) = r^4 e^{-3r\sqrt{1+z}}$, a value for the ground state energy $\mathscr{E}_0 = -3.9975$ a.u., in good agreement with the value of 3.9998 obtained by Fabre *et al.* [28].

The Hamiltonian that takes into account the e–e interaction is

$$H = -\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{15}{8}\frac{1}{r^2} - \frac{2}{r^2}\left[(1-z^2)\frac{\partial^2}{\partial z^2} - 3z\frac{\partial}{\partial z}\right] - \frac{\sqrt{8}}{r}\left[\frac{1}{\sqrt{1+z}} + \frac{1}{\sqrt{1+z}} - \frac{1}{2}\frac{1}{\sqrt{1+|z|}}\right].$$

Following the same procedure we get $\mathscr{E}_0 = -2.87875$ a.u. The extrapolated result of Ref. [28] is -2.879028 a.u. Each of these calculations requires approximately 30 CPU-minutes.

E. Two-Dimensional Nonlocal, Non-Hermitian Hamiltonian

We are concerned here with the solution of a two-dimensional integro-differential equation describing the bound state of an A-nucleon system known as IDEA [4, 29–33]. Since this is our main example, we will describe the equation solved and display its complexity in more detail. In this method, the A-body wave function of the Schrödinger equation is expanded as

$$\Psi(\mathbf{x}) = \sum_{i<j<A} \psi_{ij}(\mathbf{x}),$$

since the underlying interaction can be written as a sum of two-body forces $V(\mathbf{x}) = \sum_{i<j<A} V(r_{ij})$. The components $\psi_{ij}(\mathbf{x})$ obey the Faddeev-type equation

$$(T - E)\psi_{ij}(\mathbf{x}) = -V(r_{ij}) \sum_{i<j<A} \psi_{ij}(\mathbf{x}). \tag{4}$$

Here $\mathbf{x}$ represents all the coordinates and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $\mathbf{r}_i$ being the coordinate of the ith particle. The hyperradius of the system is given by $r^2 = 2/A \sum_{i<j<A} r_{ij}^2$. To bring Eq. (4) into a computationally manageable form, one applies the hyperspherical harmonics method [4], the description of which is beyond the scope of this article. For the A-boson system, one finally has to solve the IDEA equation

$$\left\{\frac{\hbar^2}{m^2}\left[-\frac{\partial^2}{\partial r^2} + \frac{\mathscr{L}_0(\mathscr{L}_0+1)}{r^2} - \frac{4}{r^2}\frac{1}{W_0(z)}\frac{\partial}{\partial r}(1-z^2)W_0(z)\frac{\partial}{\partial r}\right] + \frac{A(A-1)}{2}V_0(r) - E\right\}P(z,r) = -[V(r_{ij}) - V_0(r)]\Pi(z,r).$$

Here the nonlocal term enters via the function $\Pi(z, r)$ given by

$$\Pi(z,r) = P(z,r) + \int_{-1}^{+1} f_{(0)}(z,z')P(z',r)\,dz',$$

where

$$f_{(0)}(z,z') = W_0(z') \sum_{K=0}^{\infty} \frac{(f_K^2 - 1)}{h_K} \mathscr{P}_K^{\alpha,\beta}(z)\mathscr{P}_K^{\alpha,\beta}(z'),$$

$\mathscr{P}_K^{\alpha,\beta}(z)$ being the Jacobi polynomials while f_K^2, h_K, and $W_0(z)$ are given by

$$f_K^2 = 1 + \frac{\{2(A-2)\mathscr{P}_K^{\alpha,\beta}(-1/2) + [(A-2)(A-3)/2]\mathscr{P}_K^{\alpha,\beta}(-1)\}}{\mathscr{P}_K^{\alpha,\beta}(1)},$$

$$h_K = \int_{-1}^{+1} W_0(z)[\mathscr{P}_K^{\alpha,\beta}(z)]^2\,dz,$$

and

$$W_0(z) = (1-z)^\alpha(1+z)^\beta,$$

with $\alpha = (D-5)/2$, $\beta = 1/2$, and $D = 3(A-1)$. Further $\mathscr{L}_0 = (D-3)/2$ and $V_0(r)$ is the so-called hypercentral potential given by

$$V_0(r) = \frac{\Gamma(D/2)}{\sqrt{\pi}2^{D/2-2}\Gamma[(D-3)/2]}\int_{-1}^{+1} W_0(z)V(r\sqrt{(1+z)/2})\,dz.$$

TABLE I

Three-Boson Binding Energies (in MeV) Obtained with the Present Method and Compared with the Results of Other Methods

Potential	Present	HS	HHEM	ETBM	F	GFMC
MT-V [34]	7.72	7.73	7.783	7.778	—	—
MT-V [36]	8.19	8.19	—	—	8.253	8.26
S3 [38]	6.686	6.67	—	6.677	6.696	—

Note. Hermite splines (HS) [31], hyperspherical harmonic expansion method (HHEM) [34], equivalent two-body method (ETBM) [35], Faddeev (F) [37], and Green's function Monte Carlo (GFMC) [36] method.

In Table I we list our results for $A = 3$, along with the results obtained by different methods. The corresponding results for the four-boson case are given in Table II. In these calculations we used 86 points in the r-direction in the range (0–15) fm and 126 points in the z-direction. Using the same starting wave function as in the ^{4}He atom system, the required CPU-times are about 40 min. It is seen that our results are in excellent agreement with those obtained by other methods. The same excellent agreement was also found for other interactions as well as for the SIDE approximation [4], where the results practically coincide with those we obtained using Hermite splines of orders 5 and 7 and by B-splines of order 7 via the Galerkin method. It is noted that the component $P(r, z)$ obtained using the time-evolution method is identical to the one calculated via the Galerkin methods.

V. CONCLUSIONS

We presented a new method capable of solving the TDSE. We employed this method to solve one- and two-dimensional problems, with local and nonlocal Hermitian and non-Hermitian Hamiltonians having real eigenvalues. The non-Hermitian two-dimensional cases are by no means easy to solve, especially those corresponding to realistic three- and four-body systems. The successful application of the method in these cases demonstrates its robustness and reliability.

The advantages of the method are numerous, the most important being its simplicity. As shown, no guesswork or deep insight is required. The only guess is the initial wave function which is not crucial at all. In fact we experimented with various starting functions, all finally giving the same binding energy and wave function. The memory requirements are not severe as in other competing methods, since the matrices needed are sparse. Despite the fact that no attention was given, for the time being, to the efficiency of the method, it turns out that it is not prohibitively expensive in CPU time. Note that all our work has been performed on small workstations rated around 10 Mflops (Linpack 100DP [40].

TABLE II

As in Table I, but for the Four-Boson System

Potential	Present	HS	HHEM	ETBM
MT-V [34]	29.46	29.46	—	—
MT-V [36]	30.68	30.68	—	—
S3 [38]	27.11	27.09	26.0	26.47

As far as the performance in terms of CPU-time in three and higher dimensions is concerned, an estimate can be obtained as follows: Suppose we have a one-dimensional problem and a two-dimensional problem. To make a fair comparison of the CPU-times required for convergence in these two problems, let us assume that the gaps $E_i - E_0$ for the low lying energy levels E_i are identical in both problems. Then since convergence is achieved when the factors $e^{-(E_1-E_0)t}$, $e^{-(E_2-E_0)T}$, ... become small, both systems require the same time-of-propagation; i.e., both systems need the same number of time steps. Hence, the difference in the CPU-times will stem from the solution of the sparse linear system via the SSOR method. Since this system is sparse (a few diagonals) the number of operations is roughly proportional to the grid points. Therefore, one can state for the CPU-times the following approximate result:

$$\frac{\text{cpu}_{2-d}}{\text{cpu}_{1-d}} = \frac{N_1 N_2}{N_1} = N_2,$$

where N_1 and N_2 are the number of grid points in each of the directions. Similarly, for three-dimensional problems

$$\frac{\text{cpu}_{3-d}}{\text{cpu}_{2-d}} = \frac{N_1 N_2 N_3}{N_1 N_2} = N_3.$$

It is clear that the efficiency and the CPU-time concerned depends on the complexity and spectrum of the hamiltonians considered.

Since the method is under development there is plenty of room for improvements. Moreover, the use of faster computers will undoubtedly allow the solution of more complicated problems, coupled channels, and problems involving time-dependent Hamiltonians. The CN method may be generalized by using better approximants for the time-development operator, without destroying the sparse structure of the matrices. One such approximation may be obtained by expanding the exponential in terms of Chebyshev polynomials [6]. Another possible improvement is the use of nonuniform (or piecewise uniform) grids, so that fewer grid points will be necessary. This will result in a considerable decrease of the CPU-time, as well as the

memory requirements of the method. Such improvements are under way.

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