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Brief Reports

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Alternative algebraic method to solve the Schrödinger equation

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A new alternative local method to solve the Schrödinger equation is established, in which powers of the Hamiltonian are used to set up algebraic equations. The computation is integration-free and easy to carry out. The method is applied to the quartic anharmonic-oscillator problem.

The search for effective methods to solve the Schrödinger equation continues to be a topic of current research. A typical approach to the approximate solution usually employs a basis set to change the Schrödinger equation into corresponding algebraic equations. Commonly this procedure requires integration,[1] which makes it almost impossible to use certain basis sets. In the past decade several integration-free techniques have been shown to be useful in the solution of quantum-mechanical problems.[2-5] These integration-free techniques facilitate both computation and optimization of the basis set.

The purpose of the present paper is to present a new integration-free local method for solving the Schrödinger equation. Powers (or polynomials) of the Hamiltonian are used to transform the Schrödinger equation into algebraic equations. As a test case we solve the problem of the generalized anharmonic oscillator.

First we prove the following theorem: Given

$$H=-\tfrac{1}{2}\nabla_x^2+V(x)\ , \tag{1}$$

where $x\in\mathbb{R}^{3N}$, if

$$He^{-tH}\Psi=\mu(x)e^{-tH}\Psi \tag{2}$$

for any t, then $\mu(x)=\mu$ is a constant, and μ and Ψ are the eigenvalue and eigenfunction of H, respectively. The proof of this theorem goes as follows. Equation (2) holding true for any value of t implies that

$$H^{n+1}\Psi=\mu(x)H^n\Psi,\quad n=0,1,2,\ldots\ . \tag{3}$$

By induction we have

$$H^n\Psi=[\mu(x)]^n\Psi\ .$$

Hence

$$H^{n+1}\Psi=H\{[\mu(x)]^n\Psi\}$$
$$=[\mu(x)]^{n+1}\Psi\ .$$

This gives

$$-\tfrac{1}{2}\Psi\nabla_x^2[\mu(x)]^n-(\nabla_x\Psi)\{\nabla_x[\mu(x)]^n\}=0\ .$$

Since this equation holds for all n we get for $\mu(x)\neq0$ (or the theorem is trivial)

$$\Psi(\nabla_x\mu)^2=0\ ,$$

Excluding the irrelevant case $\Psi\equiv0$ we have $(\nabla_x\mu)^2=0$. Hence $\mu(x)=\text{constant}=\mu$. For $n=0$ in Eq. (3), $H\Psi=\mu\Psi$. This proves the theorem. The converse of the theorem is obviously true.

The operators He^{-tH} and e^{-tH} have recently been successfully used in solving quantum-mechanical problems.[6,7] The theorem above provides us with the basis for a new application of these operators. Expanding Ψ on a complete basis set which spans the domain of operator H we can get the full eigenspectrum of H by simply imposing Eq. (2) for arbitrary t, at any particular x_0. In practice we use Eq. (3) with a finite number of n's and a truncated basis set. Let $\{\phi_i\}$ be a complete basis set; we may expand Ψ as

$$\Psi=\sum_i c_i\phi_i(x)\ . \tag{4}$$

Coefficients c_i are determined such that Eq. (3) is satisfied for all n at an arbitrary space point x_0, with constant μ. We obtain

$$\sum_i c_iH^{n+1}\phi_i(x_0)=\mu\sum_i c_iH^n\phi_i(x_0),\quad n=0,1,\ldots\ . \tag{5}$$

This is the familiar secular equation. Now the truncated form of Eq. (5) reads

TABLE I. Ground-state and second-excited-state eigenvalues of the quartic anharmonic oscillator.

β	E_0 (Present)	E_0 (Exact[a])	E_2 (Present)	E_2 (Exact[a])
0.0001	1.000 074 986 880 20	1.000 074 986 880 20	5.000 974 615 938 39	5.000 974 615 938 39
0.01	1.007 373 672 081 38	1.007 373 672 081 38	5.093 939 132 742 31	5.093 939 132 742 31
1	1.392 351 641 530 27	1.392 351 641 530 29	8.655 049 957 815 93	8.655 049 957 959 31
100	4.999 417 545 138 17	4.999 417 545 137 59	34.873 984 263 586 5	34.873 984 261 994 8
10000	22.861 608 870 276 6	22.861 608 870 272 5	160.685 912 617 748	160.685 912 611 712

[a] Data from Ref. 9

$$\sum_{i=1}^{N} c_i H^{n+1}\phi_i(x_0)=\mu\sum_{i=1}^{N} c_i H^n\phi_i(x_0) \ , \quad n=0,1,\ldots,N-1 \qquad (6)$$

or

$$A\mathbf{C}=\mu B\mathbf{C} \qquad (7)$$

with

$$A=(a_{ij})=[H^{i+1}\phi_j(x_0)] \ , \qquad (8)$$

$$B=(b_{ij})=[H^i\phi_j(x_0)] \ , \qquad (9)$$

and

$$\mathbf{C}=(c_1,\ldots,c_N)^T \ , \qquad (10)$$

where T denotes transpose. Equations (7)–(10) usually define a generalized eigenvalue equation, with the elements of A and B obeying the important relation $a_{ij}=b_{i+1j}$.

We now apply this method to the quartic anharmonic problem, the eigenvalue equation of which is

$$H\Psi=E\Psi \ , \qquad (11)$$

with

$$H=-\frac{d^2}{dx^2}+x^2+\beta x^4, \quad \beta\geq 0 \ . \qquad (12)$$

To make the eigenvalue problem less sensitive to the β value we rescale the equation

$$\left[-\frac{d^2}{dx^2}+\nu^2x^2+(1-\nu^3)x^4\right]\Psi(x)=\nu E\Psi(x) \ , \qquad (13)$$

where

$$\nu=(1+\beta)^{-1/3}, \quad 1\geq\nu\geq 0 \ . \qquad (14)$$

We employ the following optimized basis set:[8]

$$\Psi(x)=\sum_i c_iP_i(\zeta-1)\exp(-\tfrac{1}{3}a_2\zeta^{-3}+a_1\zeta^{-1}+\ln\zeta) \ , \qquad (15)$$

where P_i is the Legendre polynomial and

$$\zeta=(1+\alpha x^2)^{-1/2} \ , \qquad (16)$$

$$\alpha=(1-\nu^3)/[1+(1-\nu^2)^{1/2}]^2 \ , \qquad (17)$$

$$a_1=(1-\nu^2)^{1/2}/\alpha \ , \qquad (18)$$

$$a_2=(1-\nu^3)^{1/2}/\alpha^{3/2} \ . \qquad (19)$$

This basis set can reproduce harmonic-oscillator basis set when β goes to zero.

TABLE II. Convergence rate of successive approximations as a function of the truncation order ($\beta=1$)

N	E_0	E_2
4	1.392 434 0	8.686 07
6	1.392 352 647	8.655 846 2
8	1.392 351 656 13	8.655 068 02
10	1.392 351 641 689 9	8.655 050 43
15	1.392 351 641 530 27	8.655 049 957 815 9
Exact[a]	1.392 351 641 530 29	8.655 049 957 759 31

[a] Data from Ref. 9

Now it is a routine to construct matrices A and B, and then solve Eq. (7). We take $x_0=0$ or $\zeta=1$. The calculated ground-state and second-excited-state eigenvalues along with exact solutions for different β values and $N=15$ are reported in Table I. In Table II the convergence rate of successive approximations as a function of truncation order N for $\beta=1$ is shown. We see from the tables that the convergence rate is very fast and that a large basis set is not needed for most practical purposes.

One can improve this method numerically by using polynomials of H, instead of pure powers of H, in Eqs. (7) and (8). The method can be used in combination with other local techniques.[2–5] One should note, however, that the fast convergence of the method depends on the chosen basis set being well tailored to the problem at hand. For example, if for the quartic oscillator one uses a truncated scaled oscillator basis set, one runs into difficulties both with complex eigenvalues and with extraneous eigenvalues. Note that with an arbitrary discrete basis, the eigenvalues of Eq. (7) are not necessarily real, and that the lowest eigenvalue does not necessarily approach E_0 from above as the number of basis functions is increased. Other local methods have the same problem.

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[1] See any quantum mechanics textbook for the conventional treatment of the eigenvalue problem.

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