JOURNAL OF COMPUTATIONAL PHYSICS 59, 493–498 (1985)

Note

Finite-Dimensional Approximation of the Differential Operator in Problems of Quantum Mechanics

Quantum-mechanical problems described by the Schrödinger equation or by the Faddeev equations in configurational space can be solved, with negligible exceptions, only numerically. In doing so the most difficult is the approximation of the differential operator that enters into the equations. Finite-difference approximations applied usually to solve differential equations lead to cumbersome calculations and do not involve available a priori information on the properties of the solution.

We shall construct such an approximation of the differential operator that will make an approximate operator $\tilde{T}$ to coincide with the exact one T on some finite set of functions $|\chi_i\rangle$. To this end we require the approximate operator $\tilde{T}$ to possess the following properties

$$\tilde{T}T^{-1}|\chi_i\rangle = |\chi_i\rangle \qquad i = 1,..., N, \tag{1}$$

and we will consider the Schrödinger equation

$$(T + V - E)|\psi\rangle = 0. \tag{2}$$

Here T is the exact kinetic-energy operator, V stands for the potential energy, and E the energy. It can be shown that with an appropriate choice of the set $|\chi_i\rangle$, i.e., if the solution to (2) $|\psi\rangle$ can be represented by

$$|\psi\rangle = (E - V)^{-1} \sum_{i=1}^{N} C_i |\chi_i\rangle \tag{3}$$

then $|\psi\rangle$ obeys also the approximate equation

$$(\tilde{T} + V - E)|\psi\rangle = 0. \tag{4}$$

Thus, each solution to (2) is a solution to (4), but the opposite is not true, and Eq. (4) can have extra solutions to be rejected.

The solution to (4) is given by (3) with coefficients satisfying the system of equations:

$$\sum_{i=1}^{N} C_i \langle \chi_j | T^{-1} - (E - V)^{-1} | \chi_i \rangle = 0 \tag{5}$$

obtained by projecting (4) onto the functions $T^{-1}|\chi_i\rangle$.

0021-9991/85 $3.00

Boundary conditions for the solution of (2) are introduced in the case of (4) with such a choice of the functions $|\chi_i\rangle$ that would provide a correct behaviour of $|\psi\rangle$. It may be easily achieved as $|\psi\rangle$ and $|\chi_i\rangle$ are related by (3).

From (3) it also follows that for any x_0 such that $E - V(x_0) = 0$ the condition $\sum_{i=1}^{N} C_i \chi_i(x_0) = 0$ should hold. This condition ensures the convergence of (5) at the point x_0. To what extent the above approximation is a success depends, as usual, on how appropriate is the set of the functions $|\chi_i\rangle$. Equation (3) relating $|\psi\rangle$ and $|\chi_i\rangle$ allows the choice of the set of $|\chi_i\rangle$ that ensures the known a priori properties of the solution $|\psi\rangle$ to hold. For instance, the wave function of an nth excited state should have n zeros, and it is therefore natural to choose the functions $|\chi_i\rangle$ having also n zeros.

In order that the choice of the set $|\chi_i\rangle$ be the best one, it is necessary to impose some condition on the approximate solution to be close to the exact one. Such a condition fixes not only the best choice of the set of $|\chi_i\rangle$ but also the single solution of (4) for that choice. The functionals the minimum of which provides the proximity of T and $\tilde{T}$ on the solution of (4) $|\psi\rangle$ are as follows:

$$F_n = |\langle\psi|(T-\tilde{T})^n|\psi\rangle| \tag{6}$$

$$\Phi_n = \sum_{i=1}^{N} |\langle\psi_i|(T-\tilde{T})^n|\psi\rangle|^2, \tag{7}$$

where $|\psi_i\rangle = (E-V)^{-1}|\chi_i\rangle$.

More delicate methods may be proposed, as well, for choosing a correct solution. For instance, in the case when a solution of (2) is found with a good accuracy for one value of the energy E the solution for another value E' can be singled out from the orthogonality condition

$$|\langle\psi_E|\psi_{E'}\rangle| = \min. \tag{8}$$

We shall further consider the 1-dimensional Schrödinger equation resulting from the separation of the angular dependence in the case of a spherical-symmetric potential $V(r)$: then

$$T_l = -\frac{d^2}{dx^2} + \frac{l(l+1)}{x^2}. \tag{9}$$

The kernel of the inverse operator T_l^{-1} is given by

$$g_l(x_1 x^1) = \frac{1}{2l+1} \cdot \frac{x_<^{l+1}}{x_>^l}. \tag{10}$$

When solving the eigenvalue problem it is not difficult to compute the integrals in (5) as the functions $|\chi_i\rangle$ should be exponentially damping at infinity.

Since in the scattering problem the asymptotic behaviour is as follows:

$\langle x|\psi\rangle \simeq \sin(kx+\delta_l)$, $k^2=E$, it is necessary to define the way of how integrals can be regularized at infinity. In the scattering theory this means the introduction of infinitesimal damping, that is, equated to zero only upon the calculation of all integrals.

As an ilustration we shall obtain an expression for the scattering phase δ_l at high energies $k^2 \gg V(x)$, when $\delta_l \ll 1$ and the Born approximation is valid. We shall restrict ourselves to one function $\langle x|\chi_l\rangle = xj_l(kx+\delta_l)$ that has a correct behaviour at zero and at infinity. We first rewrite (5) in the form

$$\langle \chi_l| T_l^{-1} - k^{-2}|\chi_l\rangle = k^{-2}\langle \chi_l| V(k^2-V)^{-1}|\chi_l\rangle \tag{11}$$

and calculate the integral

$$\begin{aligned}
&\int_0^\infty dy\, g_l(x,y)\, y j_l(y+\delta_l) \\
&\quad = (2l+1)^{-1}\left[x^{-l}\int_0^x dy\, y^{l+2} j_l(y+\delta_l) + x^{l+1}\int_x^\infty dy\, y^{1-l} j_l(y+\delta_l)\right] \\
&\quad = x j_l(x+\delta_l) - \frac{l+2}{x^l}\delta_l \int_0^x \frac{dy\, y^l}{(y+\delta_l)^2} j_l(y+\delta_l)[2ly+\delta_l(l+1)] \\
&\qquad - (l-1)\, x^{l+1}\delta_l \int_x^\infty dy\, j_l(y+\delta_l)\frac{2(l+1)\, y + l\,\delta_l}{y^{l+1}(y+\delta_l)^2}.
\end{aligned} \tag{12}$$

Here we made double use of the relations

$$\begin{aligned}
\frac{d}{dz}[z^{n+1} j_n(z)] &= z^{n+1} j_{n-1}(z) \\
\frac{d}{dz}[j_n(z)\, z^{-n}] &= -j_{n+1}(z)\, z^{-n}.
\end{aligned} \tag{13}$$

The integration by parts in (12) produces the quantity $\lim_{y\to\infty} y^{1-l} j_{l-1}(y+\delta_l)$. When $l=0$, this oscillating quantity is to be put zero in conformity with the notion of infinitesimal damping.

Inserting then (12) into (11) we get

$$\begin{aligned}
&\frac{\delta_l}{2l+1}\int_0^\infty dx\, x j_l(x+\delta_l)\left\{\frac{l+2}{x^l}\int_0^x \frac{dy\, y^l}{(y+\delta_l)^2} j_l(y+\delta_l)[2ly+\delta_l(l+1)]\right. \\
&\qquad \left. + (l-1)\, x^{l+1}\int_x^\infty dy\, j_l(y+\delta_l(y+\delta_l)\frac{2(l+1)\, y + l\,\delta_l}{y^{l+1}(y+\delta_l)^2}\right\} \\
&\quad = -k^3\int_0^\infty dx\cdot x^2 j_l(kx+\delta_l)\frac{V(x)}{k^2-V(x)}.
\end{aligned} \tag{14}$$

At small $\delta \sim V/k^2$, when $l \geqslant 1$, the expansion of the integrand of (14) into a series in δ_l gives:

$$\frac{2\delta_l}{2l+1}\int_0^\infty dx\, x j_l(x)\left[\frac{l(l+2)}{x^l}\int_0^x dy\, y^{l-1} j_l(y) + x^{l+1}(l^2-1)\int_x^\infty \frac{dy\, j_l(y)}{y^{l+2}}\right]$$

$$= -k\int_0^\infty dx (x j_l(kx))^2 V(x). \tag{15}$$

From (15) we obtain the Born approximation for the phase:

$$\delta_l = -k\int_0^\infty dx (x j_l(kx))^2 V(x). \tag{16}$$

When $l=0$, the phase is also given by (16), however the expansion in δ_l should be performed upon the integration of (14).

Now we shall present the results of calculation for the eigenvalue problem and for the scattering problem for the equation:

$$\left(\frac{d^2}{dx^2} + \frac{e^{-\mu x}}{x} + E\right)|\psi\rangle = 0. \tag{17}$$

In the limiting case $\mu = 0$ (the Coulomb potential), Eq. (17) is solved exactly. Choosing the functions $|\chi\rangle$ in the form:

$$\langle x|\chi\rangle = (1-\kappa^2 x)\, P(x)\, e^{-\kappa x}, \tag{18}$$

where $\kappa^2 = -E$, $P(x)$ is a polynomial, we obtain a set of solutions including the exact one. In particular, for $P(x) = 1$ we get two solutions with $\kappa = \frac{1}{2}$ and $\kappa = \frac{2}{3}$. The first of them is exact, and the functional F_1 on it vanishes, i.e., $\langle\psi|T-\tilde{T}|\psi\rangle = 0$. When $\mu \neq 0$, the numerical calculation was carried out for the set of functions $\langle x|\chi_i\rangle = (e^{-\mu x} - \kappa^2 x)\, e^{-\alpha_i x}$. Results are reported in Table I. Solutions were selected on the basis of the condition for the quantity

$$\Delta = \left(\frac{\langle\psi|(T-\tilde{T})|\psi\rangle}{\langle\psi|T|\psi\rangle}\right)^2$$

to be minimal.

From Table I it is seen that not very low values of the binding energy are obtained with high accuracy using two functions $|\chi_i\rangle$ only. An analogous situation occurs in the description of the energy of an excited state.

The magnitude of error of the approximation used Δ, in all cases except for those specially noted, does not exceed 10^{-6}. At such small Δ the energy value does not depend on the parameters of the functions $|\chi_i\rangle$.

In the scattering problem the set of $|\chi_i\rangle$ is added by the function $\langle x|\chi_1\rangle =$

$\sin(kx+\delta)$ that provides a correct asymptotic behaviour. Other functions are of the form:

$$\langle x|\chi_i\rangle = e^{-\alpha_i x} \qquad i=2,\ldots, N.$$

The calculations have been made for $\mu = 0.401696$ that corresponds to the potential describing the $^3S_1$ NN-scattering phase. The phases calculated with the use of four functions $|\chi_i\rangle$ are presented in Table II. For selection of the solution we used the functional Φ_1. The scattering length is found to be $a = 5.06$fm (The exact value quoted in [2] $a = 5.47$fm).

The results presented demonstrate that the proposed method may be more effective than the finite-difference scheme for solving some problems of quantum mechanics. The efficiency of the method is higher, the greater information is available on the solution properties. For multidimensional problems of quantum mechanics, i.e., a many-body problem, information available on the solution may reduce laborious work in calculations as compared with finite-difference methods, the complexity of which rapidly grows with increasing dimensionality.

The applicability of the presented method goes further than the examples described above. An approximation of this kind can be applied to more involved boundary-value problems with more complicated differential operators. The division of the complete operator into an approximated and nonapproximated part is arbitrary and rests merely on the will to do calculations as simple as possible.

TABLE I

μ	κ_{0R}^2	κ_0^2	κ_{1R}^2	κ_1^2
0.001	0.24900	0.24900	0.06150	0.06154
0.0025	0.24750	0.24751	0.060025	0.06006
0.005	0.245025	0.24503	0.05765	0.05767
0.007143	0.242925	0.24293	0.05565	0.05568
0.01	0.240225	0.24015	0.053075	0.05310
0.0125	0.237725	0.23773	0.05090	0.05088
0.01667	0.233750	0.23374	0.047375	0.04738
0.025	0.22590	0.22590	0.040875	0.04096
0.03333	0.218275	0.21827	0.0350	0.03501
0.05	0.203525	0.20353	0.024965	0.02496
0.071429	0.18560	0.18561	0.014985	0.01498
0.1	0.16340	0.16340	0.00605	0.00607**
0.125	0.145450	0.14546	0.001698	0.00171***
0.16667	0.118425	0.118440		
0.25	0.07405	0.07407*		
0.357143	0.033775	0.03377*		
0.5	0.005143	0.00515*		

Note. κ_{0R}^2 and κ_{1R}^2 are binding energies of the ground and an excited state obtained in [1]; κ_0^2 and κ_1^2 represent the present calculations; the index * stands for the result obtained with the use of a set of 4 functions $|\chi_i\rangle$; ** with 5 functions $|\chi_i\rangle$, $\Delta = 5\cdot 10^{-6}$; *** with 5 functions $|\chi_i\rangle$, $\Delta = 1\cdot 66\cdot 10^{-4}$.

TABLE II

E(MeV)	δ	$\delta^{(1)}$	$\delta^{(2)}$
176	0.7604	0.7289	0.7770
152	0.7928	0.7701	0.8080
104	0.8810	0.9064	0.9080
72	0.9725	1.0055	1.0104
48	1.0803	1.1191	1.1548
24	1.2818	1.2448	1.2432
12	1.5053	1.4872	1.4728

Note. δ is the scattering phase calculated in [2]; $\delta^{(1,2)}$-represent phases calculated in this work with different accuracy in the search of the minimum of the functional Φ_τ.

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RECEIVED: April 24, 1984; ACCEPTED: July 18, 1984

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