J. Austral. Math. Soc. Ser. B 32(1990), 115–132

SOLUTION OF A SCHRÖDINGER EQUATION BY ITERATIVE REFINEMENT

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(Received 6 October 1988)

Abstract

A simple eigenvalue and a corresponding wavefunction of a Schrödinger operator is initially approximated by the Galerkin method and by the iterated Galerkin method of Sloan. The initial approximation is iteratively refined by employing three schemes: the Rayleigh-Schrödinger scheme, the fixed point scheme and a modification of the fixed point scheme. Under suitable conditions, convergence of these schemes is established by considering error bounds. Numerical results indicate that the modified fixed point scheme along with Sloan's method performs better than the others.

1. Introduction

The purpose of this note is to illustrate the use of some recent iterative refinement schemes in computing solutions of the Schrödinger equation

$$[(-h^2/2m)\nabla^2 - E]\psi(r) = -V_s(r)\psi(r), \tag{1}$$

where $V_s(r)$ is a central attractive potential of the inverse power type:

$$V_s(r) = -g/r^{s+2}, \; -2 < s < 0,$$

$g > 0$ being the coupling constant.

Using the Fourier-Fock technique and the separation of variables, it is shown in [5] that the solution of the above Schrödinger equation can be

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reduced to an eigenvalue problem for an infinite matrix $\Lambda(s, l)$ depending upon the parameter s and the angular momentum l. The matrix $\Lambda(s, l)$ defines a compact positive operator on l^2, the space of all complex square-summable sequences.

Let $\lambda(s, l; q)$ denote the q-th eigenvalue of $\Lambda(s, l)$ and $E_q(s, l)$ denote the q-th energy level. Then $E_q(s, l) = -(K\lambda(s, l; q))^{-2/s}$, where K is a constant which can be predetermined by an appropriate choice of the units. A similar relationship holds between the corresponding eigenvectors of $\Lambda(s, l)$ and the wavefunctions.

In [5], the eigenvalues $\lambda(s, l; q)$ of the infinite matrix $\Lambda(s, l)$ were approximated by the eigenvalues $\lambda^{(n)}(s, l; q)$ of the matrix $\Lambda^{(n)}(s, l)$ of order n, obtained by selecting the first n rows and n columns of $\Lambda(s, l)$. It was observed there that the rate of convergence of $\lambda^{(n)}(s, l; q)$ to $\lambda(s, l; q)$ (as $n \to \infty$) is good in the interval $-2 < s < -0.5$, but is slow in the interval $-0.5 \leq s < 0$. Thus, in this latter range of s, eigenvalue problems for very large matrices $\Lambda^{(n)}(s, l)$ were required to be solved. The computer time needed for such a calculation increases exponentially with n, and often a solution can become infeasible due to excessive requirement of computer memory.

Eigenvalue problems for infinite or very large full matrices can be tackled economically by first solving an eigenvalue problem for a nearby matrix of moderate size to obtain a crude initial approximation of the eigenelements and then by employing iterative procedures to refine the initial approximation. In the present paper we shall consider three iteration schemes: the Rayleigh-Schrödinger scheme, a fixed point scheme and a modification of this fixed point scheme. The method of truncating an infinite or a very large matrix to its first n rows and n columns is known as the Galerkin method. An iterated Galerkin method is proposed by Sloan (see [7]) in which the matrix is truncated to its first n columns. We shall consider both these methods for finding the initial terms of the above iteration schemes. A comparison of large numerical data has prompted us to prefer the modified fixed point scheme along with Sloan's method to the remaining.

The iteration schemes provide sequences of iterates λ_j and φ_j converging to a simple eigenvalue λ and an eigenvector φ of the large matrix. At each stage, we compute the Rayleigh quotient $q(\varphi_j)$ based on φ_j. The Rayleigh quotient $q(\varphi_j)$ is a much better approximation of λ than φ_j is of φ. In [2, p. 360–361], some of our earlier numerical experiments have been reported for the case of the largest eigenvalue of $\Lambda(s, 0)$, with $s = -0.5$, -0.05, -0.01. These experiments were performed by using the Rayleigh-Schrödinger scheme with the Galerkin method. This was suggested to the authors by F. Chatelin, for which they are grateful.

2. Various iteration schemes

Let T denote a compact operator on l^2 and let T_0 denote a finite rank approximation of T. For example, if $\pi_n: l^2 \to l^2$ is the projection given by

$$\pi_n(x(1), x(2), \ldots) = (x(1), \ldots, x(n), 0, 0, \ldots),$$

then $T_0^G = \pi_n T \pi_n$ is the Galerkin approximation of T, while the Sloan approximation of T is $T_0^S = T\pi_n$.

Let λ_0 be a *simple* eigenvalue of T_0 with a corresponding eigenvector φ_0. Then $\bar{\lambda}_0$ is a simple eigenvalue of the adjoint operator $T_0^*: l^2 \to l^2$, and there is a unique eigenvector φ_0^* of T_0^* corresponding to $\bar{\lambda}_0$ such that $\langle \varphi_0, \varphi_0^* \rangle = 1$. The *spectral projection* P_0 *associated with* T_0 *and* λ_0 is given by

$$P_0 x = \langle x, \varphi_0^* \rangle \varphi_0, \qquad x \in l^2.$$

The *reduced resolvent* S_0 *associated with* T_0 *and* λ_0 is given by

$$S_0 = \lim_{z \to \lambda_0} (T_0 - zI)^{-1}(I - P_0).$$

Then it can be proved that (cf. [2], p. 107)

$$(T_0 - \lambda_0 I)S_0 = I - P_0 = S_0(T_0 - \lambda_0 I), \quad S_0 P_0 = 0 = P_0 S_0.$$

Let λ be a nonzero simple eigenvalue of T and let φ be an eigenvector of T such that $\langle \varphi, \varphi_0^* \rangle = 1$. If φ^* is the eigenvector of T^* corresponding to $\bar{\lambda}$ such that $\langle \varphi, \varphi^* \rangle = 1$, then the spectral projection P associated with T and λ is given by

$$Px = \langle x, \varphi^* \rangle \varphi, \; x \in X.$$

Rayleigh-Schrödinger Scheme

Since $T = T_0 + (T - T_0)$, one can consider the linear perturbation family

$$T(t) = T_0 + t(T - T_0), \quad t \in \mathbb{C},$$

so that $T(0) = T_0$ and $T(1) = T$. Let us assume that for $|t|$ sufficiently small, $T(t)$ has a simple eigenvalue $\lambda(t)$ and a corresponding eigenvector $\varphi(t)$ such that $\langle \varphi(t), \varphi_0^* \rangle = 1$, and that $\lambda(t)$ and $\varphi(t)$ are analytic at $t = 0$:

$$\lambda(t) = \lambda_0 + \sum_{k=1}^{\infty} \lambda_{(k)} t^k, \tag{2}$$

$$\varphi(t) = \varphi_0 + \sum_{k=1}^{\infty} \varphi_{(k)} t^k. \tag{3}$$

https://doi.org/10.1017/S0334270000008249 Published online by Cambridge University Press

By equating the coefficients of like powers of t in $T(t)\varphi(t) = \lambda(t)\varphi(t)$, we obtain

$$T_0\varphi_0 = \lambda_0\varphi_0,$$

(which is the initial eigenequation) and for $k = 1, 2, \ldots,$

$$\lambda_{(k)} = \langle (T - T_0)\varphi_{(k-1)}, \varphi_0^* \rangle,$$

$$\varphi_{(k)} = S_0\Big[-(T - T_0)\varphi_{(k-1)} + \sum_{i=1}^{k} \lambda_{(i)}\varphi_{(k-i)} \Big].$$

The series (2) and (3) are known as the *Rayleigh-Schrödinger series* with initial terms λ_0 and φ_0, respectively. At $t = 1$, consider the partial sums

$$\lambda_j = \lambda_0 + \sum_{k=1}^{j} \lambda_{(k)} \quad \text{and} \quad \varphi_j = \varphi_0 + \sum_{k=1}^{j} \varphi_{(k)}, \qquad j = 1, 2, \ldots.$$

It is then easy to see that for $j = 1, 2, \ldots,$

$$\lambda_j = \langle T\varphi_{j-1}, \varphi_0^* \rangle, \quad \text{and}$$

$$\varphi_j = \varphi_{j-1} + S_0\Big[-T\varphi_{j-1} + \lambda_1\varphi_{j-1} + \sum_{i=2}^{j} (\lambda_i - \lambda_{i-1})\varphi_{j-i} \Big]. \tag{4}$$

This yields the well-known *Rayleigh-Schrödinger iteration scheme.*

Schemes based on fixed point iterations

Since $T\varphi = \lambda\varphi$ and $\langle \varphi, \varphi_0^* \rangle = 1$, it follows that $\langle T\varphi, \varphi_0^* \rangle = \lambda$, and if $\lambda \neq 0$,

$$\varphi = T\varphi / \langle T\varphi, \varphi_0^* \rangle.$$

Thus, φ is a fixed point of the function $F(x) = Tx/\langle Tx, \varphi_0^* \rangle$ defined for all x which satisfy $\langle Tx, \varphi_0^* \rangle \neq 0$. Starting with some x_0 and x_0^* in l^2, we define *the power iteration scheme* by

$$x_j = Tx_{j-1} / \langle Tx_{j-1}, x_0^* \rangle, \qquad j = 1, 2, \ldots, \tag{5}$$

provided $\langle Tx_{j-1}, x_0^* \rangle \neq 0$. Let λ be the dominant (simple) eigenvalue of T. It can be proved that if $\langle x_0, \varphi_0^* \rangle \neq 0$ and $\langle \varphi, x_0^* \rangle \neq 0$, then the power iterates x_j converge to the eigenvector x of T which satisfies $\langle x, x_0^* \rangle = 1$, and $\lambda_j = \langle Tx_{j-1}, x_0^* \rangle$ converge to λ. (See, e.g., Theorem 11.12 of [6]). While we are at liberty to choose x_0 and x_0^* almost arbitrarily, the power iteration has the limitation that it can converge only to the dominant eigenvalue of T. This feature of the power iteration makes us seek other iteration schemes based on the fixed point principle for approximating intermediate eigenvalues of T.

We note that $\varphi \neq 0$ is an eigenvector of T corresponding to $\lambda = \langle T\varphi , \varphi_0^* \rangle$ if and only if

$$\langle T\varphi , \varphi_0^* \rangle \varphi - T\varphi = 0.$$

Now, for x in X, we observe that $x = 0$ if and only if $P_0 x = 0 = S_0 x$. If we let $x = \langle T\varphi , \varphi_0^* \rangle \varphi - T\varphi$, then $P_0 x = 0$. Thus, $\varphi \neq 0$ is an eigenvector of T if and only if

$$S_0(\langle T\varphi , \varphi_0^* \rangle \varphi - T\varphi) = 0,$$

or, in other words, if and only if $\varphi \neq 0$ is a fixed point of the function

$$Gx = x + S_0(\langle Tx , \varphi_0^* \rangle x - Tx).$$

This leads to a fixed point iteration scheme:

$$\begin{aligned} &\varphi_0 : \text{an eigenvector of } T_0, \text{ and for } j = 1, 2, \ldots, \\ &\lambda_j = \langle T\varphi_{j-1} , \varphi_0^* \rangle , \\ &\varphi_j = \varphi_{j-1} + S_0(\lambda_j \varphi_{j-1} - T\varphi_{j-1}). \end{aligned} \tag{6}$$

We refer to Theorem 11.5 of [6] for a proof of the convergence of this fixed point scheme as well as the Rayleigh-Schrödinger scheme under the conditions

$$\|(T - T_0)P_0\|, \|S_0\| < 1/4 \text{ and } \|(T - T_0)S_0\| < 1/4.$$

Another way of proving the convergence of the above fixed point scheme and of modifications of it is given in the following Propositions 2.1 and 2.2. The basic idea used here comes from Propositions 2 and 3 of [1]. In [3], convergence of several schemes based on the fixed point technique was similarly proved. This work is to appear in [4]. Refer also to Theorem 11.10 of [6].

PROPOSITION 2.1. *Let*

$$c_0 = \|S_0\|[1 + \|\varphi_0^*\|(\|\varphi\| + 2\|\varphi - \varphi_0\|)].$$

If $\|T - T_0\| < 1/c_0$, *then for* $j = 0, 1, 2, \ldots$.

$$\|\varphi - \varphi_j\| \leq \|\varphi - \varphi_0\|[c_0\|T - T_0\|]^j \to 0$$

and

$$|\lambda - \lambda_{j+1}| \leq \|P_0(T - T_0)\| \, \|\varphi_0^*\| \, \|\varphi - \varphi_0\|[c_0\|T - T_0\|]^j \to 0 \quad \text{as } j \to \infty.$$

PROOF. We first prove that if for some j

$$\|\varphi - \varphi_j\| \leq \|\varphi - \varphi_0\|,$$

then

$$\|\varphi - \varphi_{j+1}\| \leq c_0\|T - T_0\| \, \|\varphi - \varphi_0\|.$$

https://doi.org/10.1017/S0334270000008249 Published online by Cambridge University Press

Now, since $P_0\varphi = \varphi_0 = P_0\varphi_j$, we have

$$\begin{aligned}\varphi - \varphi_{j+1} &= \varphi - \varphi_j - S_0(\lambda_{j+1}\varphi_j - T\varphi_j)\\ &= S_0(T_0 - \lambda_0 I)(\varphi - \varphi_j) - S_0(\lambda_{j+1}\varphi_j - T\varphi_j)\\ &= S_0(T_0 - T)(\varphi - \varphi_j) + (\lambda - \lambda_{j+1})S_0(\varphi_j - \varphi + \varphi - \varphi_0)\\ &\quad + (\lambda - \lambda_0)S_0(\varphi - \varphi_j).\end{aligned}$$

Also,

$$|\lambda - \lambda_{j+1}| = |\langle (T - T_0)(\varphi - \varphi_j), \varphi_0^*\rangle| \le \|T - T_0\|\,\|\varphi_0^*\|\,\|\varphi_j - \varphi\|,$$

and

$$|\lambda - \lambda_0| = |\langle (T - T_0)\varphi, \varphi_0^*\rangle| \le \|T - T_0\|\,\|\varphi\|\,\|\varphi_0^*\|.$$

Hence

$$\begin{aligned}\|\varphi - \varphi_{j+1}\| &\le \|S_0\|\,\|T - T_0\|\,\|\varphi - \varphi_j\|\\ &\quad + 2\|T - T_0\|\,\|\varphi - \varphi_j\|\,\|\varphi_0^*\|\,\|S_0\|\,\|\varphi - \varphi_0\|\\ &\quad + \|T - T_0\|\,\|\varphi\|\,\|\varphi_0^*\|\,\|S_0\|\,\|\varphi - \varphi_j\|\\ &= c_0\|T - T_0\|\,\|\varphi - \varphi_j\|.\end{aligned}$$

We now establish the desired bound of $\|\varphi - \varphi_j\|$ by induction on j. The bound is obvious for $j = 0$. Assume that

$$\|\varphi - \varphi_j\| \le \|\varphi - \varphi_0\|[c_0\|T - T_0\|]^j.$$

Then $\|\varphi - \varphi_j\| \le \|\varphi - \varphi_0\|$, since $c_0\|T - T_0\| < 1$. Hence by what we have just proved,

$$\begin{aligned}\|\varphi - \varphi_{j+1}\| &\le c_0\|T - T_0\|\,\|\varphi - \varphi_j\|\\ &\le \|\varphi - \varphi_0\|[c_0\|T - T_0\|]^{j+1}.\end{aligned}$$

Thus, the induction is over. Finally, since $P_0^*\varphi_0^* = \varphi_0^*$, we have

$$\begin{aligned}|\lambda - \lambda_{j+1}| &= |\langle (T - T_0)(\varphi - \varphi_j), \varphi_0^*\rangle|\\ &= |\langle P_0(T - T_0)(\varphi - \varphi_j), \varphi_0^*\rangle|.\end{aligned}$$

The bound for $|\lambda - \lambda_{j+1}|$ given in the statement of the proposition now follows easily.

Finally, we consider a modification of the above fixed point scheme in which each iteration step consists of a power iteration followed by a fixed point iteration:

φ_0: an eigenvector of T_0, and for $j = 1, 2, \ldots,$

$$\begin{aligned}\psi_{j-1} &= T\varphi_{j-1}/\langle T\varphi_{j-1}, \varphi_0^*\rangle,\\ \nu_j &= \langle T\psi_{j-1}, \varphi_0^*\rangle\\ \varphi_j &= \psi_{j-1} + S_0(\nu_j\psi_{j-1} - T\psi_{j-1}).\end{aligned}$$

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Provided $\langle T\varphi_{j-1}, \varphi_0^*\rangle \neq 0$ it can be easily seen that for $j = 1, 2, \ldots,$

$$\varphi_j = [T\varphi_{j-1} + S_0 T(\mu_j \varphi_{j-1}/\lambda_j - T\varphi_{j-1})]/\lambda_j, \tag{8}$$

with $\lambda_j = \langle T\varphi_{j-1}, \varphi_0^*\rangle$ and $\mu_j = \langle T^2\varphi_{j-1}, \varphi_0^*\rangle$.

PROPOSITION 2.2. *Let c be a constant such that $\|\varphi - \varphi_0\| \leq c\|(T - T_0)T\|$. Let $d_0 = 2[\|S_0\| + c\|\varphi_0^*\|\,\|T\|]/|\lambda| + 2\|S_0\|\,\|\varphi_0^*\|\,\|T\|\,[\|\varphi\| + 8c\|T\|^2]/|\lambda|^2$. If $\|(T - T_0)T\| < 1/d_0$, then for $j = 0, 1, 2, \ldots,$*

$$\|\varphi - \varphi_j\| \leq \|\varphi - \varphi_0\|[d_0\|(T - T_0)T\|]^j \to 0$$

and

$$|\lambda - \lambda_{j+1}| \leq \|P_0(T - T_0)\|\,\|\varphi_0^*\|\,\|\varphi - \varphi_0\|[d_0\|(T - T_0)T\|]^j \to 0 \text{ as } j \to \infty.$$

PROOF. We first claim that if for some j

$$\|\varphi - \varphi_j\| \leq \|\varphi - \varphi_0\| \quad \text{and} \quad |\lambda_{j+1}| \geq |\lambda|/2,$$

then

$$\|\varphi - \varphi_{j+1}\| \leq d_0\|(T - T_0)T\|\,\|\varphi - \varphi_j\|.$$

This follows from the identity

$$\varphi - \varphi_{j+1} = \frac{1}{\lambda_{j+1}}\{S_0[(T_0 - T)T + (\lambda - \lambda_0)T](\varphi - \varphi_j) - (\lambda - \lambda_{j+1})\varphi\}$$

$$-\frac{1}{\lambda_{j+1}^2}\{\langle T^2(\varphi - \varphi_j), \varphi_0^*\rangle - \lambda(\lambda - \lambda_{j+1})]S_0[T(\varphi - \varphi_j) - \lambda(\varphi - \varphi_0)]\},$$

and the estimates

$$\begin{aligned} |\lambda - \lambda_0| &= |\langle (T - T_0)\varphi, \varphi_0^*\rangle| \\ &= |\langle (T - T_0)T\varphi, \varphi_0^*\rangle|/|\lambda| \\ &\leq \|(T - T_0)T\|\,\|\varphi\|\,\|\varphi_0^*\|/|\lambda|, \\ |\lambda - \lambda_{j+1}| &= |\langle T(\varphi - \varphi_j), \varphi_0^*\rangle| \\ &\leq \|T\|\,\|\varphi - \varphi_j\|\,\|\varphi_0^*\|, \quad j = 0, 1, 2, \ldots, \end{aligned}$$

$$\|\varphi - \varphi_0\| \leq c\|(T - T_0)T\|,$$
$$|\lambda| \leq \|T\|.$$

We now establish the desired bound of $\|\varphi - \varphi_j\|$ by induction on j. The bound is obvious for $j = 0$. Assume that

$$\|\varphi - \varphi_j\| \leq \|\varphi - \varphi_0\|[d_0\|(T - T_0)T\|]^j.$$

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Then $\|\varphi - \varphi_j\| \le \|\varphi - \varphi_0\|$, since $d_0\|(T - T_0)T\| < 1$. Also, since

$$2c\|T\|\,\|\varphi_0^*\|/|\lambda\| \le d_0,$$

we have

$$\begin{aligned}|\lambda - \lambda_{j+1}| &\le \|T\|\,\|\varphi - \varphi_j\|\,\|\varphi_0^*\| \\ &\le \|T\|\,\|\varphi - \varphi_0\|\,\|\varphi_0^*\| \\ &\le c\|T\|\,\|(T - T_0)T\|\,\|\varphi_0^*\| \\ &< |\lambda|/2.\end{aligned}$$

This implies $|\lambda_{j+1}| \ge |\lambda|/2$. Hence by the above claim,

$$\begin{aligned}\|\varphi - \varphi_{j+1}\| &\le d_0\|(T - T_0)T\|\,\|\varphi - \varphi_j\| \\ &\le \|\varphi - \varphi_0\|[d_0\|(T - T_0)T\|]^{j+1}.\end{aligned}$$

Thus, the induction is over. Finally, since $P_0^*\varphi_0^* = \varphi_0^*$, we have

$$|\lambda - \lambda_{j+1}| = |\langle P_0(T - T_0)(\varphi - \varphi_j),\, \varphi_0^*\rangle|.$$

The bound for $|\lambda - \lambda_{j+1}|$ given in the statement of the proposition now follows easily.

REMARK 2.3. Comparing Proposition 2.1 and Proposition 2.2, we observe that the iterates for the earlier fixed point scheme have geometrically decreasing error bounds with common ratio $c_0\|T - T_0\|$, while this ratio for the modified fixed point scheme is $d_0\|(T - T_0)T\|$. When T is a compact operator and (T_n) is a sequence of bounded operators which converges to T pointwise, we note that $\|T - T_n\|$ may *not* converge to zero, while $\|(T - T_n)T\|$ does converge to zero. This suggests that the modified fixed point scheme may have a wider application. Even when $\|T - T_n\|$ tends to zero, it is plausible that $\|(T - T_n)T\|$ will tend to zero much faster. For example, if $T_n = T\pi_n$, where π_n is a projection,

$$\begin{aligned}\|(T - T_n)T\| = \|T(I - \pi_n)T\| &= \|T(I - \pi_n)^2T\| \le \|T(I - \pi_n)\|\,\|(I - \pi_n)T\| \\ &= \|T - T_n\|\,\|(I - \pi_n)T\|.\end{aligned}$$

When T is compact and π_n converges to the identity operator pointwise, we note that $\|(I - \pi_n)T\|$ tends to zero, and as such $\|(T - T_n)T\|$ is much smaller than $\|T - T_n\|$. In cases T is self-adjoint and π_n is orthogonal, we see that $\|(I - \pi_n)T\| = \|T^*(I - \pi_n)^*\| = \|T(I - \pi_n)\|$. Hence in this case, we have

$$\|(T - T_n)T\| = \|(T - T_n)\|^2.$$

These observations will be illustrated by the actual computations reported in the last section. The better performance of the modified fixed point scheme is

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not surprising because each iteration of this scheme is composed of a power iteration and a fixed point iteration.

3. Residual and Rayleigh quotient

Let a nonzero vector ψ and a scalar μ be given. To what extent can the pair (ψ, μ) be thought of as an eigenpair of an operator T? A measure of this extent is given by the quantity $||T\psi - \mu\psi||_2/||\psi||_2$. For a fixed nonzero vector ψ, there is a scalar $q(\psi)$ which minimises this quantity. It is called the *Rayleigh quotient* of T at ψ:

$$q(\psi) = \langle T\psi, \psi\rangle/\langle\psi, \psi\rangle.$$

The minimal value is called the *residual* of T at ψ:

$$r(\psi) = ||T\psi - q(\psi)\psi||_2/||\psi||_2.$$

The iteration schemes considered in the previous section generate a sequence of approximate eigenvectors φ_j, $j = 1, 2, \ldots$. For a fixed φ_j, the pair $(\varphi_j, q(\varphi_j))$ represents the best approximate eigenpair. Hence a stopping criterion for the iteration process can be laid down as follows:

Stop if

$$(\text{RESID})_j = ||T\varphi_{j-1} - q(\varphi_{j-1})\varphi_{j-1}||_2/||\varphi_{j-1}||_2$$

is less than a predetermined small positive number, say 10^{-t}, $t > 0$.

Let T be a self-adjoint operator such as the infinite matrix $\Lambda(s, l)$ considered in Section 1. A result of Krylov and Weinstein (Theorem 8.5 of [6]) implies that if ψ is a nonzero vector, then there is a spectral value λ of T such that $|\lambda - q(\psi)| \leq r(\psi)$. Thus, if $r(\psi) < 10^{-t}$, then $q(\psi)$ equals a spectral value λ of T, correct up to t decimal places. If λ is a spectral value of T which is nearest to $q(\psi)$, then we have, in fact,

$$|\lambda - q(\psi)| \leq [r(\psi)]^2/\operatorname{dist}(q(\psi), \sigma(T)\backslash\{\lambda\}),$$

by the Kato-Temple inequality (Theorem 8.7 of [6]). Hence if $q(\psi)$ is sufficiently near λ, and if λ is well-separated from the rest of the spectrum of T, then $q(\psi)$ is an approximation of λ of order at least $[r(\psi)]^2$.

Let λ be a simple eigenvalue of T and let P denote the associated spectral projection. If $P\psi \neq 0$, and θ denotes the acute angle between ψ and the eigenvector $P\psi$ of T, then we have (cf. (8.25) of [6])

$$\sin\theta \leq ||r(\psi)||/\operatorname{dist}(q(\psi), \sigma(T)\backslash\{\lambda\}).$$

Thus, the smallness of the residual at ψ also implies the nearness of ψ to an eigenvector of T. These results are borne out by the numerical examples

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considered in the next section: When $(\text{RESID})_j$, is of order $10^{-t/2}$, the Rayleigh quotient $q(\varphi_j)$ is already an approximation of order 10^{-t} of the eigenvalue λ. (See Table 4.4.)

Further, if $T\varphi = \lambda\varphi$, then

$$q(\psi) - \lambda = \langle (T - \lambda I)(\varphi - \psi), \varphi - \psi \rangle / \langle \psi, \psi \rangle,$$

so that

$$|q(\psi) - \lambda| \leq ||T - \lambda I|| \, ||\varphi - \psi||^2 / ||\psi||^2.$$

Hence if $||T - \lambda I||/||\psi||^2$ is of moderate size and ψ is an approximation of an eigenvector φ of T of order $10^{-t/2}$, then $q(\psi)$ is an approximation of the eigenvalue λ of T of order 10^{-t}. These observations are also illustrated in the next section (Table 4.4).

4. Numerical experiments

In this section we report some computations we have carried out regarding the approximate solution of the Schrödinger equation described in the introduction. They are performed on CYBER SYSTEM 170/840 in single precision for which the floating-point arithmetic gives 14 reliable decimal digits.

The infinite matrix $\Lambda(s, l)$ mentioned in the introduction is given by the following: For $i, j = 1, 2, \ldots,$

$$\Lambda_{i,j}(s, l) = \Lambda_{j,i}(s, l),$$

and for $i \leq j$,

$$\Lambda_{i,j}(s, l) = \Gamma(2l + 1 - s)(-1)^{i+j} \left[\frac{(i-1)!}{(i+2l)!(i+l)}\right]^{1/2} \left[\frac{(j-1)!}{(j+2l)!(j+l)}\right]^{1/2} \times \sum_{k=1}^{i} \frac{(2l+1-s)_{k-1}}{(k-1)!} \frac{(s+1)_{i-k}}{(i-k)!} \frac{(s+1)_{j-k}}{(j-k)!},$$

where $(a)_n$ denotes the Pochhammer symbol: $(a)_n = \Gamma(a+n)/\Gamma(a)$.

As pointed out in Section 1, the use of iterative refinement is recommended when the convergence of $\lambda^{(n)}(s, l; q)$ to $\lambda(s, l; q)$ is slow as $n \to \infty$, i.e., in the range $-0.5 \leq s < 0$. For this reason, we have chosen -0.4 and -0.2 as the values of s for our experiments. We shall illustrate only the cases $l = 0$, and $q = 1, 2$ and 3 (i.e., the 3 largest eigenvalues). For the purpose of these computations we truncate T to its first m columns and m rows, i.e., we take $T = \Lambda^{(m)}(s, l)$. Let $T_0 = T_n^G$ (Galerkin method) or T_n^S (Sloan method), where n is much smaller than m. Thus, in effect, we initially solve

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an $n \times n$ matrix eigenvalue problem to find $\lambda^{(n)}(s, l; q) = \lambda_0$, and then use an iteration process to approximate $\lambda^{(m)}(s, l; q)$. We have chosen $m = 100$ and $n = 10$.

In each iteration we need to calculate $S_0 y$ for some y in X with $P_0 y = 0$. This computation can be reduced to a solution of a linear system of $(n+1)$ equations in n unknowns (Proposition 17.4 of [6]). This is done once in each iteration. Apart from this solution, the number of multiplications/divisions needed in the j-th iteration $(j = 1, 2, \ldots)$ is given in Table 4.1.

TABLE 4.1

Scheme	Method	Multiplications/Divisions
Rayleigh-Schrödinger	Galerkin	$m^2 + m(j+1) + n(n+j+1)$
	Sloan	$m^2 + m(n+j+1) + n(j+1)$
Fixed point	Galerkin	$m^2 + 2m + n(n=2)$
	Sloan	$m^2 + 2m + n(n+2)m^2 + m(n+2) + 2n$
Modified Fixed Point	Galerkin	$2m^2 + 3m + n(n+4)$
	Sloan	$2m^2 + 3m + n(n+4)2m^2 + m(n+3) + 4n$

For the basic computer program used in these computations, we refer to the Section 20 of [6].

The stopping criterion used is:

$$(\text{RESID})_j < 10^{-13}.$$

Table 4.2 shows the number of iterates needed to satisfy the stopping criterion for the three iteration schemes considered in Section 2, and the two choices T_0^G (Galerkin method) and T_0^S (Sloan method) for the initial approximation T_0 of T. A maximum of 125 iterates are calculated in each case; if the iteration does not stop at this stage, the current RESID is given at the end of the table.

It can be seen from Table 4.2 that the number of iterates for the cases corresponding to $s = -0.4$ is much less than those for the cases corresponding to $s = -0.2$. Also the number of iterates increases progressively as we move from the first to the second and then to the third eigenvalue.

Taking into account the relative effort needed for implementation, qualitatively (convergence or nonconvergence) and quantitatively (the number of iterates needed), the fixed point scheme seems to be superior to the Rayleigh-Schrödinger scheme.

Although the modified fixed point needs a larger number of multiplications than the fixed point scheme, it needs appreciably less number of iterations.

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TABLE 4.2

Scheme	Method	$q = 1$ $s = -0.4$	$q = 1$ $s = -0.2$	$q = 2$ $s = -0.4$	$q = 2$ $s = -0.2$	$q = 3$ $s = -0.4$	$q = 3$ $s = -0.2$
Rayleigh-Schrödinger	Galerkin	27	63	125(a)	X	X	X
	Sloan	21	36	60	X	X	X
Fixed Point	Galerkin	25	31	29	125(b)	95	X
	Sloan	21	27	33	92	60	X
Modified Fixed Point	Galerkin	14	17	26	59	125(c)	X
	Sloan	12	16	19	28	34	125(d)

(a): $(\text{RESID})_{125} = 2.4 \times 10^{-11}$
(b): $(\text{RESID})_{125} = 8.4 \times 10^{-13}$
(c): $(\text{RESID})_{125} = 3.9 \times 10^{-13}$
(d): $(\text{RESID})_{125} = 8.7 \times 10^{-12}$
X : No convergence

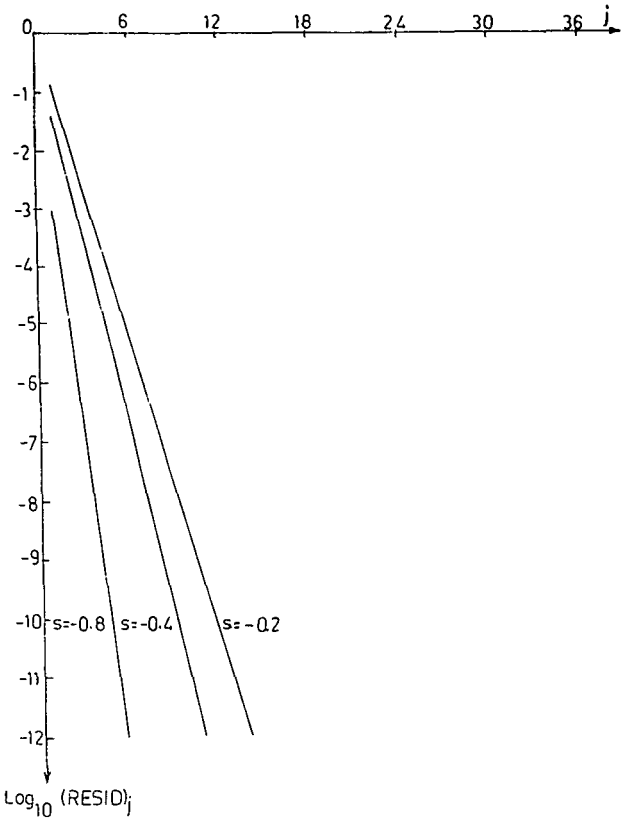

FIGURE 4.1. $q = 1$, the largest eigenvalue.

The amount of work for the Galerkin and the Sloan methods for each of the three schemes is comparable, whereas the Sloan method needs less number of iterates as compared to the Galerkin method in general.

It is for these reasons that we shall employ the modified fixed point scheme along with the Sloan method in the rest of the experiments. It is to be noted from Table 4.2 that for $s = -0.2$, $q = 3$, we have convergence only for the modified fixed point scheme with the Sloan method.

We next present some graphs which show how RESID decreases at each iteration for the cases $\lambda(s, l; q)$, $s = -0.8, -0.4, -0.2$; $l = 0$ and $q = 1, 2, 3$. The graphs for the five cases $\lambda(-0.8, 0; 1)$, $\lambda(-0.4, 0; 1)$, $\lambda(-0.2, 0; 1)$, $\lambda(-0.8, 0; 2)$ and $\lambda(-0.8, 0; 3)$ are straight lines indicating geometric convergence; the graph for $\lambda(-0.4, 0; 2)$ resembles a straight line. The graphs for $\lambda(-0.2, 0; 2)$ and $\lambda(-0.4, 0; 3)$ indicate semi-geometric or staggered convergence, while the graph for $\lambda(-0.2, 0; 3)$ is peculiar in the

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TABLE 4.4

j	$\lambda - \lambda_j$		$\lambda - q_j$		$\|\varphi - \varphi_j\|$		$(\text{RESID})_j$	
	−0.4	−0.2	−0.4	−0.2	−0.4	−0.2	−0.4	−0.2
0	2.0E − 2	1.3E − 1			5.1E − 2	1.8E − 1		
1	5.2E − 3	5.2E − 2	1.8E − 3	2.4E − 2	4.3E − 3	2.7E − 2	3.5E − 2	1.4E − 1
2	4.5E − 4	7.7E − 3	1.3E − 5	4.7E − 4	3.7E − 4	3.6E − 3	3.1E − 3	2.0E − 2
3	3.9E − 5	1.1E − 3	9.4E − 8	8.6E − 6	3.2E − 5	4.9E − 4	2.6E − 4	2.7E − 3
4	3.3E − 6	1.4E − 4	6.8E − 10	1.6E − 7	2.7E − 6	6.6E − 5	2.2E − 5	3.7E − 4
5	2.8E − 7	1.9E − 5	5.0E − 12	2.8E − 9	2.3E − 7	8.9E − 6	1.9E − 6	5.0E − 5
6	2.4E − 8	2.6E − 6	4.3E − 14	5.2E − 11	2.0E − 8	1.2E − 6	1.6E − 7	6.7E − 6
7	2.0E − 9	3.5E − 7	−7.1E − 15	8.5E − 13	1.7E − 9	1.6E − 7	1.4E − 8	9.1E − 7
8	1.7E − 10	4.7E − 8	−2.1E − 14	00	1.4E − 10	2.2E − 8	1.2E − 9	1.2E − 7
9	1.5E − 11	6.3E − 9	−7.1E − 15	−5.0E − 14	1.2E − 11	2.9E − 9	1.0E − 10	1.6E − 8
10	1.2E − 12	8.5E − 10	−2.8E − 14	−5.0E − 14	1.1E − 12	4.0E − 10	8.6E − 12	2.2E − 9
11	8.5E − 14	1.1E − 10	−5.0E − 14	−5.7E − 14	1.2E − 13	5.3E − 11	7.4E − 13	3.0E − 10
12	−7.1E − 15	1.5E − 11	−3.6E − 14	4.3E − 14	4.8E − 14	7.2E − 12	6.5E − 14	4.0E − 11
13	−−	2.0E − 12	−−	−8.5E − 14	−−	9.7E − 13	−−	5.4E − 12
14	−−	2.4E − 13	−−	−2.1E − 14	−−	1.6E − 13	−−	7.3E − 13
15	−−	−2.8E − 14	−−	−5.0E − 14	−−	5.4E − 14	−−	1.0E − 13
16	−−	−5.7E − 14	−−	−5.0E − 14	−−	4.9E − 14	−−	2.3E − 14

Notation: $E{-}t$ denotes 10^{-t}.

sense that it does not decrease steadily. Although we have plotted this last graph only for the first 36 iterations, the pattern continues to be the same for the next 89 iterations.

Since the main idea behind the use of the iteration schemes is to avoid solving large eigenvalue problems, we have not considered so far the actual accuracy attained by the iterates λ_j and φ_j. However, for an illustrative purpose, we give in Table 4.3 the actual values of $\lambda^{(100)}(s, l; q)$ and in Table 4.4 the actual values of $\lambda - \lambda_j$, $\lambda - q(\varphi_j)$, $||\varphi - \varphi_j||_2$ and $(\text{RESID})_j$ for the largest eigenvalue λ.

As commented in Section 2, it can be noticed from Table 4.4 that the Rayleigh quotients q_j satisfies $|\lambda - q_j| < 10^{-13}$ in about half the number of iterations needed to satisfy $||\varphi - \varphi_j||_2 < 10^{-13}$ or $(\text{RESID})_j < 10^{-13}$.

TABLE 4.3. Values of $\lambda^{(100)}(s, 0; q)$

$q \rightarrow$ s $\downarrow$	1	2	3
−0.8	0.953404	0.437882	0.274809
−0.4	1.142053	0.510090	0.297409
−0.2	1.551141	0.727840	0.384904

We remark that, if we solve a slightly larger initial eigenvalue problem, it is reasonable to expect that a smaller number of iterations will be needed to satisfy the stopping criterion. We give below the size n of the initial eigenvalue problem and the corresponding number of iterations needs to satisfy the stopping criterion for the case $s = -0.2$, $l = 0$, $q = 3$, using the modified fixed point scheme and the Sloan method:

n	*iterations*
10	125 (a)
15	60
20	51
25	42
30	35

(a): $(\text{RESID})_{125} = 8.7 \times 10^{-12}$

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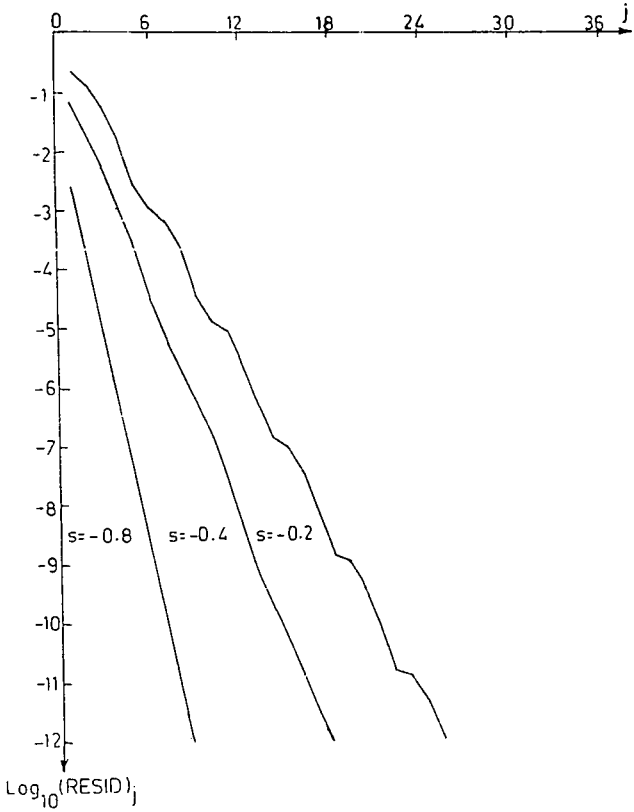

FIGURE 4.2. $q = 2$, the second largest eigenvalue.

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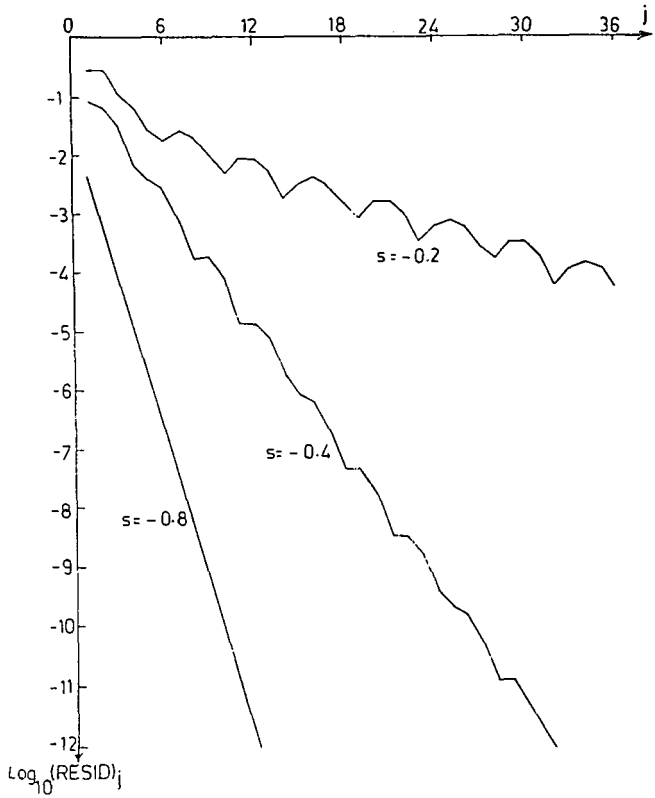

FIGURE 4.3. $q = 3$, the third largest eigenvalue.

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