Waxman’s algorithm for non-Hermitian Hamiltonian operators

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Abstract
An algorithm for finding the bound-state eigenvalues and eigenfunctions of a Hermitian Hamiltonian operator using Green’s method, developed by Waxman [1], has been extended to include non-Hermitian Hamiltonian operators.

Non-Hermitian Hamiltonian operators have played an important role in many fields of physics. In nuclear physics, optical model calculations as well as Gamow shell model calculations [2, 3] have long been of interest in describing states in the continuum. Of particular interest are the low lying resonant states of neutron-rich nuclei far from the region of stability. Recently, a Gamow shell model description of weakly bound systems in neutron-rich nuclei involving configuration mixing in a single particle Berggren basis [4] has been given [5, 6]. The Berggren basis contains bound single particle states as well as narrow resonances and a non-resonant continuum. In this basis the Hamiltonian to be diagonalized is large, non-Hermitian and not sparse. The Lanczos algorithm [7–9] has been used in this case to obtain the approximate eigenpairs.

In the present work we wish to explore an alternative method for dealing with this problem. For sparse non-Hermitian matrices, if one is primarily interested in good approximations to the lowest lying eigenvalues, inverse power iterative methods or preconditioned Rayleigh quotient methods [10–17] may be of interest. An alternative for Hermitian Hamiltonians is an algorithm developed by Waxmam [1] which iteratively solves Green’s equation for the lowest lying eigenstate. The algorithm has been successfully used to determine threshold bound states [18]. With this in mind, we have extended the algorithm to non-Hermitian Hamiltonian operators. We provide a proof of convergence as well as a few numerical examples.

The Waxman algorithm [1] is an iterative method based on Green’s method that allows one to determine eigenstates of a Hamiltonian operator without matrix diagonalization. Note Green’s method may be applied to Hermitian as well as non-Hermitian operators. In the Waxman algorithm approach, the coupling constant of the potential $\lambda$ is determined numerically as a function of the eigenvalue, $\varepsilon$. $\varepsilon$ is then varied until one obtains the value of $\lambda$ used in the Hamiltonian operator. For non-Hermitian Hamiltonian operators $\varepsilon$ may be a complex number and an iterative algorithm is required to determine the complex eigenvalue corresponding to the real value of $\lambda$ used in the Hamiltonian operator.

Consider the following eigenvalue problem

$$ (\hat{T} - \lambda \hat{V}) |u\rangle = \varepsilon |u\rangle, $$

where $\hat{T}$ is the kinetic energy operator, $\lambda$ is the real coupling constant, $\varepsilon$ is the energy eigenvalue, and $\hat{V}$ is the potential energy operator. For non-Hermitian potentials the energy eigenvalues will in general be complex. For bound states the solution of equation (1) via Green’s Method yields

$$ |u\rangle = \lambda \hat{G}_\varepsilon \hat{V} |u\rangle \tag{2} $$

where the Green’s operator, $\hat{G}_\varepsilon$, is defined as

$$ \hat{G}_\varepsilon = (\hat{T} - \varepsilon)^{-1} \tag{3} $$
and the vector $|u\rangle$ is normalized with a reference vector $\langle r |$ such that
\[
\langle r | u \rangle = 1
\]
(4)

With this, $\lambda$ can be written as
\[
\lambda = \langle r | \hat{G}_c \hat{V} | u \rangle^{-1}.
\]
(5)

Equation (5) can now be substituted into equation (2)
\[
|u\rangle = \hat{G}_c \hat{V} |u\rangle
\]
(6)

For a chosen value of $\varepsilon$, equation (6) can be iterated
\[
|u + 1\rangle = \frac{\hat{G}_c \hat{V} |u\rangle}{\langle r | \hat{G}_c \hat{V} |u\rangle}
\]
(7)

until a convergent solution is obtained, at which point $\lambda$ can be determined from equation (5).

Waxman has provided a proof of convergence to the ground state in the Hermitian case \cite{1} where it is shown that after $n$ iterations, the eigenvector of the Hamiltonian can be written in the form
\[
|u_n+1\rangle = \frac{|\phi_0\rangle}{\langle 0 | \phi_0\rangle} + \mathcal{O} \left( \left( \frac{\mu_0}{\mu_1} \right)^{n+1} \right)
\]
(8)

where $|\phi_0\rangle$ is the eigenvector associated with the ground state of the potential $-\mu_0 V$, $\mu_0$ is the smallest value for the strength of the potential leading to a bound state, and $\mu_1$ is the next smallest value corresponding to the first excited state of the potential $-\mu_1 V$. Therefore, there is convergence to $|\phi_0\rangle$, the ground state of the potential $-\mu_0 V$. Upon convergence, equation (5) gives $\lambda = \mu_0$. The proof of convergence for the non-Hermitian case is essentially the same, except now $\lambda$ is complex in general. In this case, convergence yields $|\lambda| = |\mu_0|$. For example, in the case of the $20 \times 20$ sample matrix studied below, the algorithm converges to the value $|\lambda| = 2$. Varying $\phi(\varepsilon)$ as described below amounts to moving along a circle of convergence of radius 2 in the complex plane. As long as one stays on this circle of convergence, one will eventually arrive at the correct real value of $\lambda$.

As already mentioned, if $\varepsilon$ is chosen to be complex, $\lambda$ determined from equation (5) will not necessarily be real. Using polar coordinates where $\lambda = |\lambda| e^{i\theta(\lambda)}$, $|\lambda| = \sqrt{\text{Re} \{\lambda\}^2 + \text{Im} \{\lambda\}^2}$, and $\phi(\lambda) = \arctan \left( \frac{\text{Im} \{\lambda\}}{\text{Re} \{\lambda\}} \right)$.

Waxman’s proof of convergence implies that there will be convergence of $|\lambda|$ to the magnitude of the chosen real value of $\lambda$, $\lambda_{\text{Re}}$, but convergence is not guaranteed to be a real solution. To converge to the real solution $\lambda_{\text{Re}}$, i.e. where $\phi(\lambda) = 0$, the following method was developed.

For a matrix whose ground state is complex, an arbitrary value of $\varepsilon = |\varepsilon| e^{i\theta(\varepsilon)}$ and a corresponding arbitrary eigenvector are chosen. $|\varepsilon|$ is then varied incrementally until $|\lambda|$ is within a small range close to the magnitude of the chosen real $\lambda_{\text{Re}}$. Figures 1 and 2 show $|\lambda|$ versus $|\varepsilon|$ for a sample $20 \times 20$ non-Hermitian Hamiltonian Matrix whose lowest lying eigenvalue is complex. One can see that $|\lambda|$ and $|\varepsilon|$ are related linearly and varying $\phi(\varepsilon)$ causes a vertical shift in $|\lambda|$.

At this point, $\phi(\varepsilon)$ can then be varied until either $|\lambda|$ is no longer within range of the magnitude of $\lambda_{\text{Re}}$, in which case the previous step is repeated, or until $\phi(\lambda) = 0$, in which case the equation has been solved. Figure 3
shows $\phi(\epsilon)$ versus $\phi(\lambda)$, which are also linearly related. When $\phi(\epsilon)$ is varied, this shifts $|\lambda|$ vertically, as seen in figure 2.

This alternating procedure must be done in order to ensure $|\lambda|$ is within a small range close to the magnitude $\lambda_{\text{ex}}$.

Next, consider the case where the lowest lying eigenvalue is real. The iterations, however, are in the complex plane and will not always converge to the proper value of $\lambda$. In order to correct for this, the potential, $\hat{V}$ is perturbed slightly by $\delta I \ast I$, where $\delta < 1$ and $I$ is the identity matrix, such that $\hat{V} + \delta I \ast I = \hat{V}'$. Replacing $\hat{V}$ with $\hat{V}'$ in the Hamiltonian will result in a ground state with a complex eigenvalue and the algorithm as described above can be applied. Figures 4 and 5 show the convergence for this case. It is also interesting to note that in physical applications, such as neutron-rich nuclei, bound states do not occur and the lowest lying states are sometimes simple scattering states which in the Berggren basis are states with small widths.

In the present work we have extended Waxman’s algorithm to include non-Hermitian Hamiltonian operators. A convergent iterative scheme is presented to find the lowest lying eigenstate of such operators. For Hamiltonians whose ground state eigenvalues are real a simple prescription is given to guarantee convergence. Excited states may be obtained from a new start vector in which the lower lying eigenstates are projected out of the original start vector.

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Figure 4. $|\lambda|$ versus $|\epsilon|$ for the $20 \times 20$ perturbed Hamilton matrix in which the original (unperturbed) ground state eigenvalue is real. Here $|\lambda| = 2 = \lambda_0$ with the corresponding value $|\epsilon| = 3.978$.

Figure 5. $\phi(\lambda)$ versus $\phi(\epsilon)$ for the shifted perturbed $20 \times 20$ Hamilton matrix. When $\phi(\lambda) = 0$, $\phi(\epsilon) = 0.05$. 