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Improving the convergence of an iterative algorithm proposed by Waxman

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Abstract

In an iterative algorithm recently proposed by Waxman for solving eigenvalue problems, we point out that the convergence rate may be improved. For many non-singular symmetric potentials which vanish asymptotically, a simple analytical relationship between the coupling constant of the potential and the ground state eigenvalue is obtained which can be used to make the algorithm more efficient.

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Recently, Waxman [1] has proposed a convergent iterative algorithm for obtaining solutions of the eigenvalue problem, which does not involve a matrix diagonalization. For operators which possess a continuum as well as a set of bound states this is most advantageous [2]. In the case of the ground state, for example, the eigenenergy, ϵ , is determined numerically as a function of the coupling constant of the potential, λ , and inverted to yield ϵ corresponding to the required value of λ . The convergence rate of the algorithm, therefore, depends on two factors: the number of iterations required to find an eigensolution for a particular choice of ϵ and the number of times this must be repeated in order to determine the value of ϵ which corresponds to the desired value of λ . In this regard, we wish to point out that for certain potentials a simple relationship between λ and ϵ exists which may be used to improve the convergence rate.

In the Waxman algorithm, eigenpairs are determined as functions of the strength of the potential in the following manner. For simplicity, consider a one-dimensional eigenvalue equation [1]

$$[-\partial_x^2 - \lambda V(x)]u(x) = -\epsilon u(x) \quad (1)$$

$$\lim_{|x| \rightarrow \infty} u(x) = 0 \quad (2)$$

where $\partial_x = \frac{\partial}{\partial x}$; $\lambda > 0$ is the strength parameter of the attractive potential ($\lambda V(x) > 0$ and $V(x) \rightarrow 0$ as $|x| \rightarrow \infty$) and the energy eigenvalue, $-\epsilon$ (with $\epsilon > 0$), is negative and

corresponds to a bound state. Using Green's method, a solution to equation (1) is given by

$$u(x) = \lambda \int_{-\infty}^{\infty} G_{\epsilon}(x - x')V(x')u(x') dx' \quad (3)$$

where the Green's function $G_{\epsilon}(x)$ satisfies

$$[-\partial_x^2 + \epsilon]G_{\epsilon}(x) = \delta(x) \quad (4)$$

$$\lim_{|x| \rightarrow \infty} G_{\epsilon}(x) = 0. \quad (5)$$

Normalizing $u(x)$ at an arbitrary x_{ref}

$$u(x_{\text{ref}}) = 1 \quad (6)$$

allows λ to be written as (see equation (3))

$$\lambda = \frac{1}{\int_{-\infty}^{\infty} G_{\epsilon}(x_{\text{ref}} - x')V(x')u(x') dx'} \quad (7)$$

which can then be used to eliminate λ from equation (3):

$$u(x) = \frac{\int_{-\infty}^{\infty} G_{\epsilon}(x - x')V(x')u(x') dx'}{\int_{-\infty}^{\infty} G_{\epsilon}(x_{\text{ref}} - x')V(x')u(x') dx'}. \quad (8)$$

Using equations (7) and (8), λ can be determined as a function of ϵ in the following manner. For a particular choice of ϵ , equation (8) can be iterated

$$u_{n+1}(x) = \frac{\int_{-\infty}^{\infty} G_{\epsilon}(x - x')V(x')u_n(x') dx'}{\int_{-\infty}^{\infty} G_{\epsilon}(x_{\text{ref}} - x')V(x')u_n(x') dx'} \quad (9)$$

until it converges and λ can then be determined from equation (7). Repeating for different values of ϵ yields a set of different values of the potential strength λ . When enough points have been determined, a simple interpolation procedure can be used to determine the dependence of ϵ on λ .

On the other hand, a simple relationship between λ and ϵ can be obtained for non-singular symmetric potentials which vanish asymptotically in the following manner. Note that the eigensolutions of such potentials have good parity. Taking the limit of equation (1) as $x \rightarrow x_{\text{ref}}$ yields

$$\lambda = \frac{\lim_{x \rightarrow x_{\text{ref}}} (-\partial_x^2 u(x)) + \epsilon}{V(x_{\text{ref}})} \quad (10)$$

since $u(x_{\text{ref}}) = 1$. If the potential is deep enough, the ground state eigenvalue, ϵ , is not small. In this case, it is reasonable to let

$$u(x) = f(x) e^{-\sqrt{a\epsilon}x} \quad x \geq 0 \quad (11)$$

where a is constant and $f(x)$ satisfies

$$u(x) \rightarrow 0 \quad \text{as } x \rightarrow \infty. \quad (12)$$

The only dependence of $u(x)$ on ϵ is in the exponential tail of the wavefunction and is neglected in $f(x)$ which generally has a polynomial structure. For larger values of ϵ , the exponential factor should account for the dominant dependence of $u(x)$ and its derivatives on ϵ . For small values of ϵ , the exponential factor is well approximated by the first few terms of a series expansion (in ϵ) which may no longer reflect the dominant dependence of $u(x)$ and its derivatives on ϵ . In this case, neglecting this dependence may not be possible in most

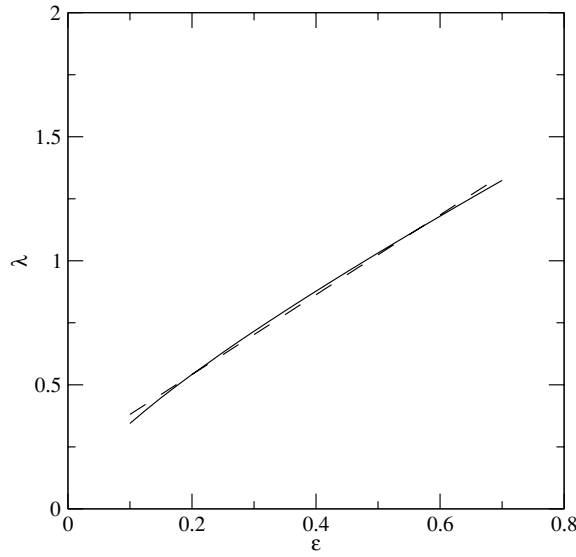


Figure 1. The coupling constant λ as a function of the ground state energy ϵ for the lowest lying even parity eigensolution of the inverted Gaussian potential (solid curve). The coupling constant for the potential is 1. The dashed curve is a fit to the data given by $\lambda = 0.21972 + 1.6087\epsilon$

cases unless additional information is available about the structure of the wavefunction and its dependence on ϵ .

From equation (11)

$$\lim_{x \rightarrow x_{\text{ref}}} (-\partial_x^2 u(x)) \rightarrow f''(x_{\text{ref}}) e^{-\sqrt{a\epsilon}x_{\text{ref}}} - 2\sqrt{a\epsilon} f'(x_{\text{ref}}) e^{-\sqrt{a\epsilon}x_{\text{ref}}} + a\epsilon \quad (13)$$

$$\rightarrow a_1 e^{-\sqrt{\epsilon}x_{\text{ref}}} + a_2 \sqrt{\epsilon} e^{-\sqrt{\epsilon}x_{\text{ref}}} + a_3 \epsilon \quad (14)$$

where $f' = \frac{df}{dx}$. Combining equations (10) and (14) yields

$$\lambda = a'_1 e^{-\sqrt{\epsilon}x_{\text{ref}}} + a'_2 \sqrt{\epsilon} e^{-\sqrt{\epsilon}x_{\text{ref}}} + a'_3 \epsilon. \quad (15)$$

Now for $x_{\text{ref}} = 0$ and potentials which are symmetric about 0, $u'(0) = 0$ ($\Rightarrow f'(0) = f(0)\sqrt{a\epsilon}$ for the even parity solutions). In this case, one obtains a simple linear dependence of λ on ϵ involving two unknown coefficients. In the more general case or for a different choice of x_{ref} , three values of λ must be calculated numerically for three different choices of ϵ to determine the three coefficients in equation (15) and the dependence of λ on ϵ . Care must be taken that eigensolutions used to determine λ are well converged. Numerical errors may lead to an incorrect dependence and require additional numerical determinations of λ .

In order to demonstrate the linear dependence of λ on ϵ , we have performed a calculation of lowest lying even parity eigensolution of the inverse Gaussian potential [2]:

$$V(x) = e^{-\frac{x^2}{2}}.$$

Note that $x_{\text{ref}} = 0$ and $\lambda = 1$. For each choice of ϵ , λ has been determined from equation (7) after the eigensolution, $u(x)$, has converged. In figure 1, the linear dependence is clearly demonstrated and confirms numerically the existence of a simple linear relationship between λ and ϵ as long as ϵ is not small. Note also that in the case of the $\text{sech}^2 x$ potential

[1] for larger values of ϵ a linear relation exists between λ and ϵ . However, for small values of ϵ the present approximation used for $u(x)$ (see equation (11)) is inadequate for the positive parity solution and will not yield the proper $\sqrt{\epsilon}$ dependence observed in the case of the $\sec^2 x$ potential [1] and also in the present case for $\epsilon < 0.1$. Clearly in this region more detailed information is required about the dependence of $u(x)$ and its derivatives on ϵ .

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