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Computing energy eigenvalues of anharmonic oscillators using the double exponential Sinc collocation method

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HIGHLIGHTS

- The method combined double exponential transformations with Sinc collocation method.
- The method efficiently computes energy eigenvalues of anharmonic oscillators.
- Theorematic results establish the convergence properties of DESCM.
- The new choice of mesh size results in substantial improvement of the method.
- The method solves the eigenvalues of both isolated and the multiple well potentials.

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ABSTRACT

A quantum anharmonic oscillator is defined by the Hamiltonian $\mathcal{H} = -\frac{d^2}{dx^2} + V(x)$, where the potential is given by $V(x) = \sum_{i=1}^{m} c_i x^{2i}$ with $c_m > 0$. Using the Sinc collocation method combined with the double exponential transformation, we develop a method to efficiently compute highly accurate approximations of energy eigenvalues for anharmonic oscillators. Convergence properties of the proposed method are presented. Using the principle of minimal sensitivity, we introduce an alternate expression for the mesh size for the Sinc collocation method which improves considerably the accuracy in computing eigenvalues for potentials with multiple wells.

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Sinc collocation method
Double exponential transformation

We apply our method to a number of potentials including potentials with multiple wells. The numerical results section clearly illustrates the high efficiency and accuracy of the proposed method. All our codes are written in Julia and are available upon request.

1. Introduction

The one dimensional anharmonic oscillator is of great interest to field theoreticians because it models complicated fields in one-dimensional space–time [1]. A complete overview of quantum anharmonic oscillators would lead to a better understanding of the realistic analytic structure of field theory. Moreover, outside the realm of field theory, the one dimensional anharmonic oscillator also provides an approximation to more complicated quantum potentials near a stable stationary point. The study of quantum anharmonic oscillators as potentials in the Schrödinger equation has been on the edge of thrilling and exciting research during the past three decades [2–32]. With advances in asymptotic analysis and symbolic computing algebra, the interest in developing more efficient methods was renewed recently [33–37]. The Hamiltonian in the time-independent Schrödinger equation is given by $\mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$ for some potential function $V(x)$. In the case of quantum anharmonic oscillators, the potential $V(x)$ is an even function of the form $V(x) = \sum_{i=1}^{m} c_i x^{2i}$ with $c_m > 0$. Several approaches have been used for the numerical evaluation of the differential eigenvalue problem $\mathcal{H}\psi = E\psi$. However, the existing numerical methods are mostly case specific and lack uniformity when faced with a general problem.

In [2–4], Rayleigh–Schrödinger perturbation series are used to evaluate the ground state energy for potentials $V(x) = x^2 + \beta x^{2m}$ for $\beta \in [0, \infty)$ and $m = 2, 3, 4$. These summations are strongly divergent for $\beta \neq 0$. To sum them efficiently, Padé approximants combined with nonlinear sequence transformations are used. In [5], Rayleigh–Schrödinger perturbation series are also used to evaluate energies of the ground state and the first excited state for potentials $V(x) = x^2 + \beta x^4$. In [6], Rayleigh–Schrödinger perturbation series are used to evaluate energies of the ground state and the first four excited states for the Hamiltonian $\mathcal{H} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}x^2 + \lambda x^4$ in the limits $\lambda \to 0^+$ and $\lambda \to \infty$. In [7], exact soluble models are used to construct Rayleigh–Schrödinger perturbation series for the eigenvalues of the anharmonic potentials $V(A, E) = \frac{1}{2}Ax^2 + Ex^4$. In [8–10], a study of Rayleigh–Schrödinger perturbation series is presented using the Wentzel–Kramers–Brillouin (WKB) method and a difference equation method. In [11], an averaging method is proposed to calculate energy eigenvalues for potentials $V(x) = \lambda x^{2m}$ for $m = 2, 3, \ldots$ with $\lambda > 0$, $V(x) = \mu x^2 + \lambda x^4 + \eta x^6$ with $\eta > 0$ and $V(x) = (ax^3 + bx)^2$ using a supersymmetric WKB approach. Their method yields appreciable accuracy for a variety of potentials and the accuracy increases as the energy level increases. In [12], the first four terms of the asymptotic expansion for the energy eigenvalues of the potential $V(x) = ax^2 + bx^4 + cx^6$ as $n \to \infty$ and in the large coupling limit $c \to \infty$ are found. Since no exact energy values were available at the time, comparisons with the values obtained via the Hill determinant method are shown. The values obtained using the asymptotic expansion agree with the values obtained using the Hill determinant method and increase in accuracy as the energy level increases. In [13], an asymptotic expansion is presented for the energy values of potentials of the form $V(x) = \sum_{i=}^{N} a_i x^i + \sum_{j=1}^{M} c_j x^{-j}$. This method allows for an easier way to obtain analytically the coefficients for the leading terms in the WKB expansion, which normally would require computation of a considerably large number of complicated contour integrals. As an example of application, the first seven coefficients of the WKB expansion for the energy eigenvalues of the potentials $V(x) = x^4 + bx^2$ and $V(x) = x^6$ are presented. In [14], the WKB method and the Lanczos algorithm are used to calculate energy eigenvalues of the potential $V(x) = \frac{1}{2}x^2 + \lambda x^{2m}$ with $m = 2, 3, \ldots, 6$ to a high accuracy. Using a starting energy value from a JWKB analysis, their shifted Lanczos algorithm is able to achieve 33 correct digits in three iterations or less for all energy states. In [15], the variational principle is used