Annals of Physics 337 (2013) 261–277

Contents lists available at ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

An asymptotic expansion for energy eigenvalues of anharmonic oscillators

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HIGHLIGHTS

- We derived the asymptotic expansion for energy eigenvalues of anharmonic oscillators.
- A highly efficient recursive algorithm for computing $S_k'(z)$ for WKB.
- We contributed to series reversion theory by reverting a new form of asymptotic series.
- Our numerical algorithm achieves high accuracy for higher energy levels.

ARTICLE INFO

Article history:
Received 15 February 2013
Accepted 2 July 2013
Available online 10 July 2013

Keywords:
Quantum anharmonic oscillator
Asymptotic expansion
WKB theory

ABSTRACT

In the present contribution, we derive an asymptotic expansion for the energy eigenvalues of anharmonic oscillators for potentials of the form $V(x) = \kappa x^{2q} + \omega x^2, q = 2, 3, \ldots$ as the energy level n approaches infinity. The asymptotic expansion is obtained using the WKB theory and series reversion. Furthermore, we construct an algorithm for computing the coefficients of the asymptotic expansion for quartic anharmonic oscillators, leading to an efficient and accurate computation of the energy values for $n \geq 6$.

1. Introduction

The quantum anharmonic oscillator energy eigenvalues have been studied extensively during the last three decades [1–15]. For a quantum anharmonic oscillator, the Hamiltonian in the time-independent Schrödinger equation is $\mathcal{H} = -\frac{d^2}{dx^2} + V(x)$, where the potential $V(x) = \omega x^2 + \kappa x^{2q}$ with $\omega \in \mathbb{R}$, $\kappa \in \mathbb{R}^+$ and $q \in \mathbb{N} \setminus \{1\}$. The quartic anharmonic oscillator corresponds to $q = 2$, the sextic anharmonic oscillator corresponds to $q = 3$, and the challenging octic anharmonic oscillator corresponds to $q = 4$.

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0003-4916/$ – see front matter
http://dx.doi.org/10.1016/j.aop.2013.07.001

In [16–18], a study of Rayleigh–Schrödinger perturbation series is presented using techniques from the Wentzel–Kramers–Brillouin (WKB) method as well as a difference equation method. The WKB method proved very useful in the calculation of higher-order energy states as the convergence is quite rapid. We refer the interested readers to [1] for an introduction of the WKB method as well as several examples for potentials of the form $V(x) = \lambda x^{2m}$ for $m = 2, 3, \ldots$ with $\lambda > 0$. In [19], an averaging method is proposed to calculate energy eigenvalues for potentials of the form $V(x) = \lambda x^{2m}$ for $m = 2, 3, \ldots$ with $\lambda > 0$, $V(x) = \mu x^2 + \lambda x^4 + \eta x^6$ with $\eta > 0$ and $V(x) = (a x^3 + b x)^2$ using a supersymmetric WKB approach.

In [7], an asymptotic energy expansion is presented for potentials $V(x) = \sum_{i=1}^{N} a_i x^i + \sum_{j=1}^{M} c_j x^{-j}$. This method allows for an easier way to obtain the symbolic coefficients for WKB expansions. As examples of application, in [7] Nanayakkara derived explicit analytic expressions for the first seven coefficients of the WKB expansion for the energy eigenvalues for the potentials $V(x) = x^4 + \omega x^2$ and $V(x) = x^6$. Although this method is very efficient for obtaining symbolic coefficients for WKB expansions, it is cumbersome to obtain several terms in these expansions due to the complexity of the integrals involved in the calculation. A considerably large number of terms are in fact needed if one desires to obtain high accuracy particularly for low energy levels.

In the present work, we derive an asymptotic expansion for the energy eigenvalues of anharmonic oscillators for potentials of the form $V(x) = \kappa x^{2q} + \omega x^2$ for $q = 2, 3, \ldots$ using the WKB approach. This leads to an asymptotic series relating the energy levels to their corresponding energy values. This form is quite cumbersome from a numerical point of view as it would require the use of a root finding method to compute the energy values. Therefore, using series reversion theory, we revert this series to obtain an analytic expression for the energy values in terms of their corresponding energy levels. This is significantly more efficient as it requires only the summation of a series for different values of n eliminating the need for a root-finding method. The difficulty in evaluating the coefficients of the asymptotic expansion numerically increases significantly as q increases. Nevertheless, we construct an algorithm capable of obtaining a large number of coefficients for quartic anharmonic oscillators (see Table 2). The numerical results obtained using the proposed method are in a complete agreement with those obtained using explicit analytic expressions obtained in [7] and leads to a highly accurate computation of the energy values for $n \geq 6$.

2. WKB for anharmonic oscillators

When a differential equation demonstrates dissipative or dispersive phenomena characterized by (complex) exponential behavior, one can seek an approximation of the solution of the form:

$$\psi(x) \sim A(x) \exp\left(\frac{S(x)}{\delta}\right) \quad \text{as } \delta \to 0^+, \tag{1}$$

where the solution has a boundary layer of thickness δ.

For the approximation $\psi(x)$ in (1), which is known as the WKB approximation, to be valid we assume that the phase $S(x)$ is non constant and slowly varying in the breakdown region.

The form given by Eq. (1) is not ideal for deriving asymptotic approximations since both the amplitude and the phase functions $A(x)$ and $S(x)$ depend implicitly on δ. To simplify this matter, it is best to expand $A(x)$ and $S(x)$ as series in powers of δ and combine them into a single exponential power series of the form:

$$\psi(x) \sim \exp\left(\frac{1}{\delta}\sum_{n=0}^{\infty} \delta^n S_n(x)\right) \quad \text{as } \delta \to 0^+. \tag{2}$$

WKB approximations for the solution of second order differential equations are derived from Eq. (2).

Now, let us consider the time-independent Schrödinger equation which is defined by the following equation:

$$\mathcal{H}\,\psi(x) = E\,\psi(x) \quad \text{with } \mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x), \tag{3}$$