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Ground state energies from converging and diverging power series expansions

C. Lisowski, S. Norris, R. Pelphrey, E. Stefanovich *, Q. Su, R. Grobe

Intense Laser Physics Theory Unit and Department of Physics, Illinois State University, Normal, IL 61790-4560, USA

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It is often assumed that bound states of quantum mechanical systems are intrinsically non-perturbative in nature and therefore any power series expansion methods should be inapplicable to predict the energies for attractive potentials. However, if the spatial domain of the Schrödinger Hamiltonian for attractive one-dimensional potentials is confined to a finite length L, the usual Rayleigh–Schrödinger perturbation theory can converge rapidly and is perfectly accurate in the weak-binding region where the ground state's spatial extension is comparable to L. Once the binding strength is so strong that the ground state's extension is less than L, the power expansion becomes divergent, consistent with the expectation that bound states are non-perturbative. However, we propose a new truncated Borel-like summation technique that can recover the bound state energy from the diverging sum. We also show that perturbation theory becomes divergent in the vicinity of an avoided-level crossing. Here the same numerical summation technique can be applied to reproduce the energies from the diverging perturbative sums.

1. Introduction

Perturbation theory was developed to analyze otherwise intractable problems in nearly all areas of science [1]. This method assumes that the full solution to a problem can be expressed as a power

* Corresponding author.
E-mail address: eugene-stefanovich@usa.net (E. Stefanovich).

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series expansion in terms of a (usually small) dimensionless parameter, which measures the strength of the interaction with the unperturbed system [2]. It is generally believed to be applicable when the solution is adiabatically connected to the unperturbed solution, i.e., it evolves smoothly from an unperturbed state. It is also assumed to fail for those scenarios where the perturbation transitions the system to a different phase with qualitatively different properties. In many important situations the dimensionless parameter is larger than the actual radius of convergence of the power series expansion and as a result the value of the series can no longer be computed by simply approximating the infinite series by its partial sums. However, numerous summation techniques [3] have been developed that permit us to accurately determine the (usually finite) value of these diverging sums.

In this work we examine the applicability of perturbation theory to predict the occurrence of quantum mechanical bound states in attractive short-range potentials in one spatial dimension. Here the dimensionless parameter is directly proportional to the strength of the interaction energy denoted by V_0. It is argued that the transition of a non-Hilbert state [with a wave function proportional to $\exp(ikx)$ for vanishing momentum k] to a normalizable discrete bound state (as V_0 is increased from $V_0 = 0$) is intrinsically non-perturbative. However, if a bound energy eigenstate is obtained numerically by diagonalizing the fully coupled Hamiltonian matrix in a finite basis set there is no ab initio reason why this transition from the quasi-continuum states to bound states should not be perturbative. This study was motivated by the well-known computational and also conceptual difficulty to obtain bound state energies from quantum field theoretical descriptions that often rely on perturbative approaches. In this work we also examine the applicability of perturbation theory to describe the quantum mechanical energies close to an avoided crossing [4–6]. This rather universal phenomenon occurs when two energetically neighboring energy states approach each other as the perturbation strength V_0 is increased. In the general case when there is no underlying symmetry (associated with a conserved quantity) the two levels repel each other and therefore avoid any degeneracy. As the character of the two involved state changes drastically after this passage through an avoided crossing, one might also wonder whether this "phase changing" transition can be computed based on perturbation theory.

While there exists obviously a large amount of literature in mathematics and physics about various summation techniques for diverging sums and their respective regions of applicability, almost all of these works assume that (a) the series have infinitely many terms and (b) that the precise form of each individual coefficient in the power series expansion is known analytically. In the opposite and purely numerical situation, where each coefficient has to be constructed computationally and therefore only a finite number of terms is accessible, much less is known. For example, we believe that the current work describes two important aspects for quantum mechanical bound states that have not been discussed before. First, we show that under a spatial confinement the perturbative method can actually be applied to predict reliable bound state energies. Second, in the corresponding diverging domain we propose a approach that permits us to obtain the correct energies even if only a limited number of perturbative power series terms are available.

The article is structured as follows. In Section 2 we examine the regime where the perturbation V_0 is sufficiently weak such that the spatial extension of the lowest energetic state is comparable to the finite size L of our numerical box. Here perturbation theory of arbitrarily high order is in fact convergent and highly accurate. We then show that for larger V_0 the power expansion becomes divergent but this is not a problem as a proposed Borel-type summation technique [7,8] can recover the bound state energies. In Section 3 we examine the energies before and after an avoided crossing. Before the avoided crossing the series is convergent and therefore can be summed up using the finite partial sums whereas after the avoided crossing the perturbative expansion becomes divergent. However, we show that also here the finite value of this divergent series can be obtained by the Borel summation technique and its prediction matches perfectly the exact one. We propose a numerical truncated Borel-based technique that permits us to estimate the diverging sums from only a finite number of perturbative terms. We finish this article with an outlook to future challenges.

2. Converging and diverging perturbation theory for bound states

While our main study focuses on the Schrödinger Hamiltonian $H(V_0) = p^2/(2m) + V(x)$, where we use the short range one dimensional Yukawa potential $V(x) = -V_0 \exp(-b|x|)$, we have also