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New ways to solve the Schroedinger equation☆

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Abstract

We discuss a new approach to solve the low lying states of the Schroedinger equation. For a fairly large class of problems, this new approach leads to convergent iterative solutions, in contrast to perturbative series expansions. These convergent solutions include the long standing difficult problem of a quartic potential with either symmetric or asymmetric minima.

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1. Introduction

Quantum physics is largely governed by the Schroedinger equation. Yet, exact solutions of the equation are relatively few. Besides lattice and other numerical calculations, we rely mostly on perturbative expansions. Such expansion quite often leads to a divergent series with zero radius of convergence, as in quantum electrodynamics, quantum chromodynamics, and problems involving tunneling and

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instantons. In a series of previous papers [1–4] we have presented a new approach to solve the low lying states of the Schroedinger equation. In the special case of one-dimensional problems, this new approach leads to explicit convergent iterative solutions, in contrast to perturbative series expansions. These convergent solutions include the long standing difficult problem [5–14] of a quartic potential with symmetric minima.

In this paper, we discuss some additional results bearing on the new method. In the one-dimensional case, we show that by changing the boundary condition to be applied at each iteration, we can obtain a convergent alternating sequence for the ground state energy and wave function instead of the monotonic sequence found before [4]. This result will be spelled out later in this section and proved in Section 3. We also find that the asymmetric quartic double-well potential can be treated by an extension of the procedure used previously for the symmetric case. This extension is treated in Section 4.

In addition, we have begun the exploration of higher dimensional problems along the same line. Although the same kind of iterative procedure can be set up, the linear inhomogeneous equation to be solved at each step cannot now be reduced to simple quadratures, as was done for one dimension. However, it is of interest that this equation is identical in form to an electrostatic analog problem with a given position-dependent dielectric constant media; at each nth iteration, there is an external electrostatic charge distribution determined by the $(n-1)$th iterated solution, as we shall discuss in this section.

Consider the Schroedinger equation

$$H\psi = E\psi, \tag{1.1}$$

where H is the Hamiltonian operator, ψ the wave function, and E its energy. For different physics problems, H assumes different forms. For example, for a system of n non-relativistic particles in three dimensions, H may be written as

$$H = \sum_{i,j} C_{ij} p_i p_j + V(x), \tag{1.2}$$

where x stands for $x_1, x_2, \ldots, x_{3n}$ the coordinate components of these n particles, $V(x)$ is the potential function, C_{ij} are constants, and $p_1, p_2, \ldots, p_{3n}$ are the momentum operators satisfying the commutation relation

$$[p_i, x_j] = -\mathrm{i}\delta_{ij}. \tag{1.3}$$

(Throughout the paper, we set Planck's constant $\hbar = 1$.) For a relativistic field theory, the Hamiltonian usually takes on a different form. Let $\Phi(\mathbf{r})$ be a scalar boson field at a three-dimensional position vector $\mathbf{r}$, and $\Pi(\mathbf{r})$ be the corresponding conjugate momentum operator. In this case we may write

$$H = \int \mathrm{d}^3 r [\Pi^2(\mathbf{r}) + V(\Phi(\mathbf{r}))] \tag{1.4}$$

with $\Pi(\mathbf{r})$ and $\Phi(\mathbf{r}')$ satisfying the commutation relation

$$[\Pi(\mathbf{r}), \Phi(\mathbf{r}')] = -\mathrm{i}\delta^3(\mathbf{r}-\mathbf{r}'). \tag{1.5}$$