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LETTER TO THE EDITOR

A new efficient method for calculating perturbation energies using functions which are not quadratically integrable

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Abstract. A new approach to calculating perturbation energies of bound states based on the use of functions which are not quadratically integrable is suggested. The key to the method is one simple property of the perturbation equations which, to our knowledge, has not been noticed until know. The use of the resolvent in this method is avoided and the energy spectrum of the unperturbed Hamiltonian is not needed in the calculation. The resulting method is very simple and straightforward and gives very accurate eigenvalues and wavefunctions.

In this letter, we are interested in the perturbation theory for the Schrödinger equation

$$H\psi(x) = E\psi(x). \qquad (1)$$

Despite the well known formulations which can be found in any textbook on quantum mechanics [1] there is one property of the perturbation equations which has not, to our knowledge, been noticed until now. The aim of this letter is to show how this property can be used for very efficient calculation of the bound-states perturbation energies and wavefunctions. In this letter, we discuss the one-dimensional Schrödinger equation.

As usual in the perturbation theory, we assume the Hamiltonian, wavefunction and energy of the form

$$H = H_0 + \lambda H_1 \qquad (2)$$

$$\psi = \psi_0 + \lambda\psi_1 + \lambda^2\psi_2 + \cdots \qquad (3)$$

and

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots \qquad (4)$$

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where λ is the perturbation parameter. Using these assumptions in the Schrödinger equation (1) we get the well known equations for E_n and ψ_n

$$H_0\psi_0 = E_0\psi_0 \tag{5}$$

and

$$H_0\psi_n + H_1\psi_{n-1} = \sum_{i=0}^{n} E_i\psi_{n-i} \qquad n = 1, 2, \ldots. \tag{6}$$

To calculate the zero-order energy E_0 the Schrödinger equation (5) can be solved by standard methods or by the Taylor series expansion method [2]. The usual numerical approach is based on choosing some value of the energy E_0 and assuming a small value of the wavefunction at one point representing one boundary condition. From the first boundary condition, the wavefunction $\psi_0(x)$ is calculated by means of the Schrödinger equation (5) until another point x_0 at which the second boundary condition is to be taken. The energy E_0 is found from the second boundary condition. For the sake of simplicity, we assume now that the potential in H_0 goes to infinity for $x \to \pm\infty$. In such a case the wavefunction $\psi_0(x)$ goes to zero for $x \to \pm\infty$ and the boundary conditions are usually taken at points which are sufficiently far from the minimum of the potential. We assume in this letter that the second approximate boundary condition applied to ψ_0 has the form

$$\psi_0(x_0) = 0 \tag{7}$$

where x_0 is a sufficiently large number.

Equations (6) are usually solved in a way similar to that described above with the boundary conditions of the form

$$\psi_n(x_0) = 0 \qquad n = 1, 2, 3, \ldots. \tag{8}$$

There is, however, a much more advantageous approach described below.

Let us assume that the wavefunctions ψ_i and perturbation corrections E_i are already calculated for $i = 0, \ldots, n - 1$. It follows from (6) that the wavefunction ψ_n depends on the perturbation energy E_n and the coordinate x

$$\psi_n = \psi_n(E_n, x). \tag{9}$$

Here, the perturbation energy E_n is taken as a variable in the wavefunction $\psi_n(E_n, x)$. Calculating the derivative of $\psi_n(E_n, x)$ with respect to the energy E_n we get from (6)

$$(H_0 - E_0)\frac{\partial\psi_n(E_n, x)}{\partial E_n} = \psi_0(x) \qquad n = 1, 2, \ldots. \tag{10}$$

This equation shows that the derivative

$$\frac{\partial\psi_n(E_n, x)}{\partial E_n} = F(x) \tag{11}$$

is a function $F(x)$ independent of E_n and n. Integrating this equation we see that the function $\psi_n(E_n, x)$ is a *linear* function of E_n

$$\psi_n(E_n, x) - \psi_n(0, x) = E_n F(x). \tag{12}$$

This is very interesting property since it makes possible to calculate the perturbation energy E_n from the equation

$$E_n = \frac{\psi_n(E_n, x) - \psi_n(0, x)}{F(x)}. \tag{13}$$

Now we assume that the perturbation energy E_n has the value for which the boundary condition $\psi_n(E_n, x_0) = 0$ is obeyed. Taking $x = x_0$ in (13) the resulting remarkably simple equation for the perturbation energy E_n reads

$$E_n = -\frac{\psi_n(0, x_0)}{F(x_0)} \,. \tag{14}$$

The value of $F(x_0)$ can be most easily calculated from the equation

$$F(x_0) = \frac{\psi_n(E_n, x_0) - \psi_n(E_n', x_0)}{E_n - E_n'} \tag{15}$$

following from (12). Due to the independence of $F(x)$ on E_n and n, E_n and E_n' in this equation can be *arbitrary* numbers. The most simple result is obtained for $E_n = 1$, $E_n' = 0$ and $n = 1$ when the final expression for $F(x_0)$ equals

$$F(x_0) = \psi_1(1, x_0) - \psi_1(0, x_0) \,. \tag{16}$$

The meaning of the function $F(x)$ can be clarified in the following way. Assuming that $\psi_0 = \psi_0(E_0, x)$ and calculating the derivative of (5) with respect to E_0 we get

$$(H_0 - E_0)\frac{\partial \psi_0(E_0, x)}{\partial E_0} = \psi_0(E_0, x) \,. \tag{17}$$

We see therefore that

$$F(x) = \frac{\partial \psi_0(E_0, x)}{\partial E_0} \tag{18}$$

where the derivative is taken at point E_0 for which the boundary condition $\psi_0(E_0, x_0) = 0$ is satisfied.

This method is a very interesting example of the use of solutions which do not satisfy the boundary conditions (8) and are not therefore quadratically integrable. Equation (14) shows that to calculate E_n it is not necessary to solve the differential equation (6) and search for the solution satisfying the boundary conditions (8). To calculate E_n it is sufficient to evaluate the function $-\psi_n(0, x_0)$ and divide it by $F(x_0)$. The functions $\psi_n(0, x)$, $\psi_1(1, x)$ and $\psi_1(0, x)$ do not, in general, satisfy the boundary conditions (8) and are not quadratically integrable [3, 4] (see figure 1). Therefore, depending on the value of x_0, values of $\psi_n(0, x_0)$ and $F(x_0)$ may be large. However, the resulting value of E_n as given by (14) may be small. Due to the simplicity of (14), the calculation of the perturbation energy E_n is very fast and straightforward. If the perturbation energy E_n is known the wavefunction ψ_n can easily be calculated from (6). We note that the use of the resolvent is avoided in this method and the energy spectrum of the zero-order Hamiltonian H_0 is not needed in the calculation.

The method described in this letter has many advantages both from the methodological and numerical point of view as verified for one-dimensional anharmonic oscillators and double-well potential problems [2]. In these cases, it was possible to get perturbation energies and wavefunctions with 50 digits or even higher accuracy and calculate perturbation corrections to a very high order ($n = 200$). It appears that this approach is complementary to techniques for the transformation of the divergent weak coupling perturbation theory to the convergent strong coupling one [5–8]. From this point of view, the above described method has an impact on the quantum field theory, namely, in the renormalized version [9–11]. A detailed report will be given elsewhere [2].

The modification of the perturbation theory presented in this paper is very promising and we believe that this method can also be used successfully for other potentials and boundary conditions. However, the most interesting application of this method seems to be to the perturbation theory of many-dimensional systems.
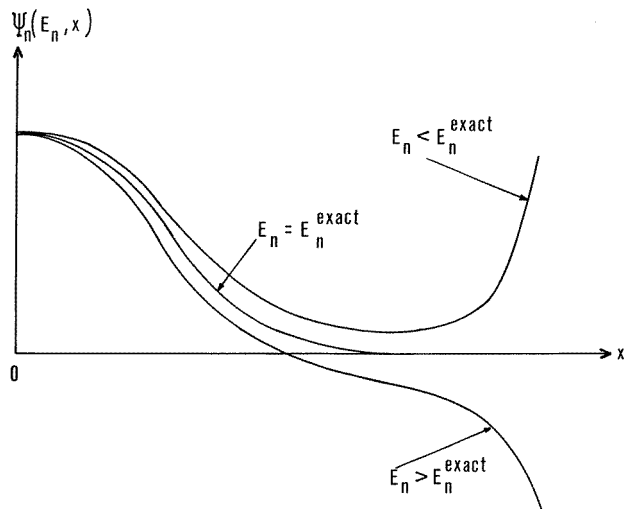
Figure 1. Character of the wavefunction $\psi_n(E_n, x)$ for different values of E_n. Here, E_n^{exact} denotes the exact value of E_n for which the boundary condition $\psi_n(E_n, x) \to 0$ for $x \to \infty$ is obeyed. For $E_n \neq E_n^{\text{exact}}$, the function is not quadratically integrable.

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