Efficient method for calculating perturbation energies for two-dimensional systems

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Abstract. Recently, a new method for calculating perturbation energies in one-dimensional systems has been suggested. In this paper, we show that this method can successfully be used also for two-dimensional systems. Combining this method with a standart numerical technique a simple and straightforward method yielding perturbation eigenvalues and eigenfunctions is obtained.

Introduction

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

$$H\psi(x) = E\psi(x). \tag{1}$$

Despite of the well-known formulations which can be found in any textbook on quantum mechanics [*Schiff*, 1955], there is one property of the perturbation equations which has been noticed only recently [*Skála et al.*, 1996]. Till now, this method has been applied to one-dimensional systems only. The aim of this paper is to show that this method can be used also for two-dimensional systems.

As usual in the perturbation theory, we assume the hamiltonian, wave function and energy in the form

$$H = H_0 + \lambda H_1, \tag{2}$$

$$\psi = \psi_0 + \lambda\psi_1 + \lambda^2\psi_2 + \cdots \tag{3}$$

and

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots, \tag{4}$$

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

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

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

$$\psi_n = \psi_n(E_n, x). \tag{7}$$

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

$$(H_0 - E_0)\frac{\partial\psi_n(E_n, x)}{\partial E_n} = \psi_0(x),\ n = 1, 2, \ldots. \tag{8}$$

This equation shows that the derivative

$$\frac{\partial\psi_n(E_n, x)}{\partial E_n} = F(x) \tag{9}$$

is a function $F(x)$ independent of E_n. A general solution of eq. (8) is a *linear* function of E_n

$$\psi_n(E_n, x) = E_n F(x) + \alpha\psi_0(x) + \beta, \tag{10}$$

where α and β are arbitrary constants. However, it follows from eq. (6) that

$$\beta = 0. \tag{11}$$

Equation (10) is very interesting result since it yields the equation for the perturbation energies

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

valid for arbitrary x.

Now we assume that instead of the usual orthonormality condition $\langle\psi_0|\psi_n\rangle = \delta_{0,n}$, the perturbation function ψ_n obeys the condition

$$\psi_n(E_n, x_0) = 0. \tag{13}$$

It is seen from eqs. (10) and (11) that this condition corresponds to

$$\alpha = -\frac{E_n F(x)}{\psi_0(x)}. \tag{14}$$

This condition can be used in an arbitrary point x_0, for which $\psi_0(x_0) \neq 0$. Taking $x = x_0$ in eq. (12) we see that the perturbation energy E_n can be calculated from the equation

$$E_n = -\frac{\psi_n(0, x_0)}{F(x_0)}. \tag{15}$$

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

$$F(x_0) = \frac{\psi_n(E_n, x_0) - \psi_n(E_n', x_0)}{E_n - E_n'} \tag{16}$$

following from eq. (10). Due to independence of $F(x)$ on E_n, energies 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

$$F(x_0) = \psi_1(1, x_0) - \psi_1(0, x_0). \tag{17}$$

This method is a very interesting example of the use of solutions which are not quadratically integrable. Equation (15) shows that to calculate E_n it is not necessary to solve the differential equation (6) and search for the solution satisfying the condition (13). 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 condition (13) and are not quadratically integrable. 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 eq. (15) may be small. Due to the simplicity of eq. (15), the calculation of the perturbation energy E_n is very fast and straightforward. If the perturbation energy E_n is known the wave function ψ_n can easily be calculated from eq. (6). We note that the energy spectrum of the zero order hamiltonian H_0 is not needed in the calculation.

It is seen that the method described in this section can be used for one-dimensional as well as multi-dimensional problems.

In this paper, we show that this method can be successfully applied also to two-dimensional systems.

Difference equations

In this section, we describe a numerical method for solving the perturbation equations suitable for one-dimensional as well two-dimensional systems. In two dimensions, the Schrödinger equation has the form

$$\left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + U(x, y)\right)\psi = E\psi. \tag{18}$$

The partial derivatives in this equation can be replaced by finite differences

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\psi_{i-1,j} - 2\psi_{i,j} + \psi_{i+1,j}}{a^2}, \tag{19}$$

$$\frac{\partial^2\psi}{\partial y^2} = \frac{\psi_{i,j-1} - 2\psi_{i,j} + \psi_{i,j+1}}{a^2}, \tag{20}$$

where a is a step of the grid. Using the last equations in (18) we obtain a system of equations

$$-\psi_{i-1,j-1} - \psi_{i-1,j+1} - \psi_{i+1,j-1} - \psi_{i+1,j+1} + [2 + a^2(U_{i,j} - E)]\psi_{i,j} = 0 \tag{21}$$

We assume that the boundary conditions for all orders of the perturbation theory have the form

$$\psi(x_b) = 0, \tag{22}$$

where x_b are points on the rectangular border sufficiently far from the minimum of the potential $U(x, y)$.

The system of equations (21) is a system of $(n-1)^2$ equations with $(n-1)^2$ unknowns, where the grid of $(n+1) \times (n+1)$ points in the rectangle is considered. Here, the points $i = 0$ and $i = n$ are located on the rectangular border.

Solution of equations

First we solve the zero-order eigenvalue problem

$$(H_0 - E_0)\psi_0 = 0. \tag{23}$$

First we calculate E_0. Then we put $b = (10^{-18}, 10^{-18}, \ldots, 10^{-18})$ and get

$$\psi_0 = (H_0 - E_0)^{-1} b. \tag{24}$$

Then we solve the problem

$$H_0\psi_1 + H_1\psi_0 = E_0\psi_1 + E_1\psi_0 \tag{25}$$

yielding

$$\psi_1 = (H_0 - E_0)^{-1}(-H_1 + E_1)\psi_0. \tag{26}$$

From this equation we obtain the wavefunction ψ_1 for $E_1 = 0$ and $E_1 = 1$ and get

$$F(x_0) = \psi_1(1, x_0) - \psi_1(0, x_0). \tag{27}$$

The energy E_1 follows from the equations

$$E_1 = -\frac{\psi_1(0, x_0)}{F(x_0)}. \tag{28}$$

Then we solve the equation

$$\psi_1 = (H_0 - E_0)^{-1}(-H_1 + E_1)\psi_0 \tag{29}$$

with the energy given by eq. (28) and obtain the wavefunction ψ_1 corresponding to E_1.

For general n, we solve the equations

$$H_0\psi_n + H_1\psi_{n-1} = \sum_{i=1}^{n} E_i\psi_{n-i}. \tag{30}$$

For $E_n = 0$, these equations lead to

$$\psi_n = (H_0 - E_0)^{-1}\left[(-H_1 + E_1)\psi_{n-1} + \sum_{i=2}^{n-1} E_i\psi_{n-1}\right]. \tag{31}$$

The perturbation energy E_n is obtained from the equation

$$E_n = -\frac{\psi_n(0, x_0)}{F(x_0)}. \tag{32}$$

The wavefunction ψ_n corresponding to eq. (32) equals

$$\psi_n = (H_0 - E_0)^{-1}\left[(-H_1 + E_1)\psi_{n-1} + \sum_{i=2}^{n} E_i\psi_{n-1}\right]. \tag{33}$$

Numerical results

As an example of using this method we calculated the perturbation energies for the well-known hamiltonian

$$H_0 = p_x^2 + p_y^2 + x^2 + y^2, \tag{34}$$

$$H_1 = x^2 y^2 - x^2 - y^2. \tag{35}$$

The perturbation energies can be obtained exactly and compared with those obtained by our method. Using to the algorithm described in the preceding section we calculated ten perturbation energies at points $x_0 = [0,0]$ and $x_0 = [1,1]$ for grids of $40 \times 40, 42 \times 42, \ldots, 60 \times 60$ points. The values given in the table were obtained by means of the Richardson extrapolation.

n	E_n numerically for $x_0 = [0,0]$	E_n numerically for $x_0 = [1,1]$	exact E_n
1	-0.750000×10^{0}	-0.750000×10^{0}	-0.750000×10^{0}
2	-0.9375×10^{-1}	-0.9374×10^{-1}	-0.937500×10^{-1}
3	-0.2344×10^{-1}	-0.2343×10^{-1}	-0.234375×10^{-1}
4	-0.1331×10^{-1}	-0.1330×10^{-1}	-0.133057×10^{-1}
5	-0.321×10^{-3}	-0.335×10^{-3}	-0.315348×10^{-3}
6	-0.1329×10^{-1}	-0.1307×10^{-1}	-0.132794×10^{-1}
7	0.239×10^{-1}	0.233×10^{-1}	0.240443×10^{-1}
8	-0.73×10^{-1}	-0.71×10^{-1}	-0.743030×10^{-1}
9	0.23×10^{0}	0.22×10^{0}	0.234920×10^{0}
10	-0.8×10^{0}	-0.8×10^{0}	-0.845542×10^{0}

Conclusions

We have shown that the method of calculating the perturbation energies based on the fact that $\psi_n(E_n, x_0)$ is for fixed x_0 a linear function of E_n combined with a simple method of the solution of the differential equations for the perturbation functions can be extended to two dimensions. The main advantage of this method is that the knowledge of the complete systems of the energies and wave functions for the zero-order problem $(H_0 - E_0)\psi_0 = 0$ is not needed here. The numerical results for a model hamiltonian agree well with the exact ones. The numerical tests confirm that, within numerical errors, the results are independent on the choise of the point x_0.

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