# A new approach to the solution of the Schrödinger equation: the anharmonic oscillator

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A new technique for solving the Schrödinger equation based on an approach similar to perturbation theory applied to degenerate states is proposed. The method, however, is not limited to the case of small perturbations. In the initial stage of the calculation, the unperturbed wave function of the state under consideration and those wave functions which are connected with the initial function by the perturbation are selected. As a result, a system of algebraic equations replaces the Schrödinger equation. The technique has been tested by calculating energy levels of an anharmonic oscillator. Its energies in the ground and two excited states have been determined. The calculations are in a good agreement with exact values when the anharmonicity parameter is less than or of order unity. © *1996 American Institute of Physics.* [S1063-7761(96)00305-8]

1. It is known that the Schrödinger equation can be solved exactly only for a limited set of problems, therefore various approximate techniques are commonly used in calculations. The Rayleigh–Schrödinger perturbation theory is used most often, but this technique is applicable only when a perturbation is relatively small. Moreover, in some problems, such as an oscillator with a fourth-power anharmonicity,[1] the perturbation series for the energy levels is divergent even when the perturbation is small. For this reason, the search for perturbation techniques for the Schrödinger equation with no limitations on the perturbation amplitude is, undoubtedly, an important problem.

In recent years, several researchers[2–8] have proposed some versions of rapidly convergent perturbation techniques. An important point is that the application domain of these methods is not limited to small perturbations. Another advantage of these methods over the Rayleigh-Schrödinger perturbation theory is that, in contrast to the latter, they do not demand knowledge of the entire spectrum of unperturbed states.

The paper is devoted to one approach to the Schrödinger equation which, in our opinion, may yield satisfactory results even if the problem does not have a small parameter in the traditional sense. The technique has been tested by calculating energy levels of an anharmonic oscillator. The concept of this approach is quite simple.

2. Let us outline the general idea of the method. The Schrödinger equation is written in general form as

$$\mathscr{H}\Psi = E\Psi, \quad \mathscr{H} = \mathscr{H}_0 + V, \tag{1}$$

where $\mathscr{H}_0$ is the Hamiltonian of the unperturbed system and $V$ is the perturbation. Given eigenfunctions of the Hamiltonian $\mathscr{H}_0$, we can write the desired wave function $\Psi$ using these functions as a basis:

$$\Psi = \sum_n c_n |n\rangle, \tag{2}$$

where $c_n$ are the expansion coefficients and the ket-vector $|n\rangle$ denotes the functions of the basis. Suppose that we are seeking a solution of Eq. (1) which reduces to $|n\rangle$ when $V=0$. Then we only select the basis functions which are admixed to $|n\rangle$ by the perturbation operator $V$, i.e., the matrix element of $V$ connecting these functions is nonzero. In accordance with the method proposed previously,[9] the admixed functions are treated, in a sense, on equal footing with $|n\rangle$. This approach is quite similar to that of the perturbation technique applied to degenerate states, although the functions are not degenerate in our case. It is obvious that the state $|n\rangle$ can be coupled to other states of the basis only when higher orders of the perturbation $V$ are taken into account.

Let us assume for definiteness that the state $|n\rangle$ is coupled only to the two states, $|m\rangle$ and $|t\rangle$. Then, using the results of the previous publication,[9] which contains various equivalent "matrix forms" of the Schrödinger equation, we obtain the following equation system for the expansion coefficients $c_n$, $c_m$, and $c_t$:

$$\begin{aligned}
&-(E-\mathscr{H}_{nn})c_n + V_{nm}c_m + V_{nt}c_t = 0,\\
&V_{mn}c_n - (E-\mathscr{H}_{mm}-F_{mm})c_m + (V_{mt}+F_{mt})c_t = 0,\\
&V_{tn}c_n + (V_{tm}+F_{tm})c_m - (E-\mathscr{H}_{tt}-F_{tt})c_t = 0,
\end{aligned} \tag{3}$$

where $V_{\alpha\beta}$ is the matrix element of the perturbation between the states $|\alpha\rangle$ and $|\beta\rangle$, and

$$\begin{aligned}
&F_{\alpha\beta} = F^{(1)}_{\alpha\beta} + F^{(2)}_{\alpha\beta} + F^{(3)}_{\alpha\beta} + \ldots,\\
&F^{(1)}_{\alpha\beta} = \sum_{k(\neq\alpha,\beta,n,m,t)} \frac{V_{\alpha k}V_{k\beta}}{E-\mathscr{H}_{kk}},\\
&F^{(2)}_{\alpha\beta} = \sum_{\substack{kp(\neq\alpha,\beta,n,m,t)\\(k\neq p)}} \frac{V_{\alpha k}V_{kp}V_{p\beta}}{(E-\mathscr{H}_{kk})(E-\mathscr{H})_{pp}}, \ldots
\end{aligned} \tag{4}$$

It directly follows from this definition that $F_{nn}=F_{nm}=F_{nt}=F_{mn}=F_{tn}=0$. This property was taken into account in writing the system (3).

The condition for the existence of nontrivial solutions of Eq. (3) is that the determinant of the system of equations

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TABLE I. Energies of the ground ($N=0$) and excited ($N=2,4$) states of an anharmonic oscillator.

| $g$ | | Approximation | | | |
|---|---|---|---|---|---|
| | | $F_{\alpha\beta}=0$ | $F_{\alpha\beta}=F^{(1)}_{\alpha\beta}$ | $F_{\alpha\beta}=F^{(1)}_{\alpha\beta}+F^{(2)}_{\alpha\beta}$ | Exact solution [1] |
| 0.1 | $N=0$ | 0.559385 | 0.559163 | 0.559182 | 0.559146 |
| 0.5 | | 0.697535 | 0.697209 | 0.697017 | 0.696176 |
| 1 | | 0.808228 | 0.802928 | 0.806833 | 0.803771 |
| 10 | | 2.16495 | 1.53492 | 2.01549 | 1.50497 |
| 0.1 | $N=2$ | 3.15477 | 3.13402 | 3.14300 | 3.13862 |
| 0.5 | | 5.05196 | 4.35647 | 4.72047 | 4.32752 |
| 1 | | 7.38282 | 5.58723 | 6.55510 | 5.17929 |
| 10 | | 49.6846 | 27.5621 | 39.7056 | 10.3471 |
| 0.1 | $N=4$ | 7.91083 | 6.42299 | 6.76970 | 6.22030 |
| 0.5 | | 22.3755 | 13.6214 | 15.9898 | 9.02878 |
| 1 | | 40.5589 | 22.8727 | 27.7035 | 10.9636 |

should be zero, from which an equation for the energy levels can be derived. For the parameter $\Delta=E-\mathscr{H}_{nn}$ we have the equation

$$\Delta^3+\Delta^2(2\mathscr{H}_{nn}-\mathscr{H}_{mm}-\mathscr{H}_{tt}-F_{mm}-F_{tt})+\Delta[(\mathscr{H}_{nn}-\mathscr{H}_{mm}-F_{mm})(\mathscr{H}_{nn}-\mathscr{H}_{tt}-F_{tt})-(V_{mt}+F_{mt})(V_{tm}+F_{tm})-V_{nm}V_{mn}-V_{nt}V_{tn}]-V_{nm}V_{mn}(\mathscr{H}_{nn}-\mathscr{H}_{tt}-F_{tt})-V_{nt}V_{tn}(\mathscr{H}_{nn}-\mathscr{H}_{mm}-F_{mm})-V_{mn}V_{nt}(V_{tm}+F_{tm})-V_{tn}V_{nm}(V_{mt}+F_{mt})=0. \quad (5)$$

From the formal viewpoint, this equation is exact and equivalent to the Schrödinger equation because it has been obtained without any approximations. But in fact it cannot be treated as an algebraic equation of a finite degree with respect to $E$ because the latter is contained in the infinite series which define $F_{\alpha\beta}$ in Eq. (4). In this sense, the proposed technique can be treated as a new version of the Brillouin-Wigner perturbation theory. There are many ways of solving the problem using this theory.[10]

In order to transform Eq. (5) to an ordinary algebraic equation, we propose the following. Let us assume in the first stage of the calculation that $F_{\alpha\beta}=F^{(1)}_{\alpha\beta}$. Then we can derive $E$ from Eq. (5). Then let us include the next term in the series of $F_{\alpha\beta}$ in Eq. (4) and again derive $E$ from Eq. (5). When the two values of $E$ coincide to within a specified accuracy for a given perturbation potential $V$, we assume that we have obtained the final result. If the discrepancy is too large, we must include in our calculation the next term for $F_{\alpha\beta}$ in Eq. (4) and once again derive $E$ from Eq. (5). The comparison of intermediate results allows us to determine for what amplitudes of the perturbation $V$ the procedure must be continued. The terms $F^{(1)}_{\alpha\beta}, F^{(2)}_{\alpha\beta}, \ldots$ may be considered in a sense as small parameters in the proposed approach to the Schrödinger equation. In this discussion we assume that the calculation is convergent.

3. In order to test the efficiency of this technique, let us consider an anharmonic oscillator described by the Hamiltonian

$$\mathscr{H}=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2+gx^4. \quad (6)$$

Here $p$ and $x$ are operators of the momentum and coordinate, $m$ is the mass of the particle, $\omega$ is its oscillation frequency in the harmonic approximation, and $g$ is the constant of the anharmonic perturbation. This problem is very important because the model is used in various fields of physics. Numerical solutions of this problem can be found in the review by Hioe *et al.*[11] We recall that the problem cannot be solved using the conventional perturbation theory. Several authors[1,12–15] investigated series of the perturbation calculations for this problem in detail and found out that energy corrections increased in proportion to the factorial of the order. Interesting results concerning the problem were reported by Dolgov and Popov,[3] who developed a version of perturbation theory based on the deviation from the asymptotic limit, which allowed them to solve the problem for arbitrary $g$.

Let us consider a solution of the Schrödinger equation with the Hamiltonian $\mathscr{H}$ given in Eq. (6) for the ground state. This is the state which goes over to the state $|0\rangle$ with zero excitation quanta when $g=0$. One can easily determine that the state $|0\rangle$ is coupled by the perturbation $V=gx^4$ to the states $|2\rangle$ and $|4\rangle$ with two and four excitation quanta, respectively. In the above equations, we take $|n\rangle=|0\rangle$, $|m\rangle=|2\rangle$, and $|t\rangle=|4\rangle$. Then the ground-state energy is determined by Eq. (5), in which the explicit form of $F_{\alpha\beta}$ should be derived from Eq. (4). Note that calculation of matrix elements of the perturbation operator in the basis of eigenstates $|N\rangle$ of the unperturbed Hamiltonian is quite easy.

Table I lists calculations of the ground state energy of the anharmonic oscillator using Eq. (5) at several values of $g$ in three cases: when the parameters $F_{\alpha\beta}$ equal zero, $F^{(1)}_{\alpha\beta}$, and $F^{(1)}_{\alpha\beta}+F^{(2)}_{\alpha\beta}$. Recall that we are only interested in the solutions of Eq. (5) which correspond to $E=1/2$ ($\Delta=0$) at $g=0$. Table I also lists exact energies[11] calculated by numerically solving the Schrödinger equation (we take $m=\omega=\hbar=1$).

Table I demonstrates that the best results were obtained in the approximation with $F_{\alpha\beta}=F^{(1)}_{\alpha\beta}$, whereas the approximation with $F_{\alpha\beta}=F^{(1)}_{\alpha\beta}+F^{(2)}_{\alpha\beta}$ yields values deviating further from the exact solution for large perturbation amplitude, $g\gg 1$. In this case the calculation error increases with $g$. This may be caused by the divergence of the sum at these values of $g$ when higher-order corrections are taken into account. It

seems, however, that the issue of convergence of this calculation is rather complicated.

This calculation leads us to the conclusion that the approximation accuracy is quite good in the range $g \lesssim 1$. Note that Graffi and Grecchi[16] numerically solved the Schrödinger equation using the standard Rayleigh–Ritz method (references to publications about the problem solution using other approximations are given in their paper). The calculation for $g=0.05$ and $g=0.5$ with a $28\times 28$ matrix yields the exact values of energy given in Table I. The distinctive feature of our approach is its simplicity, in fact the calculation can be performed without a computer.

4. In addition to the ground state, on which our attention has been focused, Eq. (5) yields two other solutions corresponding to $E=5/2$ and $E=9/2$ at $V=0$. In other words, for $g\neq 0$ Eq. (5) yields two branches which tend to the states $|2\rangle$ and $|4\rangle$ at $g\to 0$. Strictly speaking, the calculation of these levels should also consider the states $|6\rangle$ and $|6\rangle$, $|8\rangle$ from the start. Nonetheless, it is interesting to observe how the calculations of these energies listed in Table I change with $g$. The apparent tendency is similar to the case of the ground state, but the calculation errors of higher levels are notably larger.


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