A superconvergent perturbation theory in quantum mechanics

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We build a perturbation theory that can be considered a quantum analog of a classical superconvergent perturbation theory. The theory is recursive in form and can easily be implemented numerically. Its efficacy is demonstrated using the example of an anharmonic oscillator with nonlinearities of the form x^2 and x^8. © *1995 American Institute of Physics.*

1. INTRODUCTION

The exact solutions of a quantum problem provide exhaustive information about the quantum system. Such solutions, however, can be found only in exceptional cases. At the same time there exists a broad class of problems in which the Hamiltonian operator H differs little in a certain sense from an operator H^0 corresponding to an exactly integrable problem. This fact makes it possible to obtain an approximate solution of the initial equation, which is the essence of perturbation theory. In this paper we consider the problem of building a perturbation theory in its classical formulation.

Suppose that we wish to find the set of eigenfunctions $\{\psi_i\}$ belonging to the Hilbert space L_2 and the corresponding spectrum of the problem

$$H\psi_i \equiv (H^0+\varepsilon H^1)\psi_i = E_i\psi_i, \quad \psi_i \in L_2. \tag{1}$$

Here ε is a small parameter and H^1 is a self-adjoint operator. We assume that we already know the solution of the unperturbed problem

$$H^0\varphi_i = E_i^0\varphi_i, \quad \varphi_i \in L_2. \tag{2}$$

For the sake of simplicity, we assume below that all of the eigenvalues E_i and E_i^0 of problems (1) and (2) belong to the discrete spectrum.

For a perturbation theory to be formulated properly, certain conditions must be met. One is that the family of operators $H=H(\varepsilon)$ of the problem (1) must be analytic. Here we do not give the exact definitions, referring the reader to the literature,[1–3] and we assume that all conditions of analyticity of $H(\varepsilon)$ are met. The validity of this assumption has been established for all of the examples considered below.[3]

As is well known, conventional perturbation theory, which expands the eigenfunctions

$$\psi_i = \sum_{k=0}^{\infty} \psi_i^{(k)}\varepsilon^k$$

and eigenvalues

$$E_i = E_i^0 + \sum_{k=1}^{\infty} \varepsilon^k E_i^{(k)}, \tag{3}$$

in powers of a small parameter ε, is often inapplicable because the appropriate asymptotic series prove to be divergent. For instance, the series (3) for the Schrödinger equation with an anharmonic-oscillator potential,

$$H = H^0 + \varepsilon x^4, \quad H^0 = -\partial_x^2 + x^2 \tag{4}$$

has a vanishing radius of convergence in ε (see Ref. 4). Hence there has been sustained interest in the idea of building various perturbation-theory variants that might give "reasonable" answers to the questions posed here. Nowadays there are many such variants (see, e.g., Ref. 5), which have usually been adapted to the solution of specific problems. Among all of the perturbation theories, two of the most general methods of solving the problem (1) approximately can be singled out:

1. Borel summation of divergent series of the type (3). Here it is assumed that all of the coefficients $E_i^{(k)}$ for a given level number i are known.

2. The Padé approximant method, in which a finite number of terms of a divergent asymptotic power series in ε are used to build a convergent sequence of rational functions in ε.

Note that in addition to being extremely complicated in practical terms, these two perturbation-theory methods have one more important drawback: they do not make it possible to obtain the wave functions of the problem (1), which also play an important role in studying physical systems. Also, despite their broad applicability, the methods are not universal. For instance, it has been established that the Padé approximant method does not work when the perturbation of the harmonic oscillator Hamiltonian H^0 is $H^1=x^8$.

The goal of the present investigation is to build a perturbation theory that, on the one hand, is as universal and simple to apply as conventional perturbation theory and, on the other, enables one to considerably broaden the class of perturbing potentials. We display the merits of our perturbation theory by using the example of $H^1=x^4$ and $H^1=x^8$, where H^1 is the perturbation to the harmonic oscillator Hamiltonian.

2. PERTURBATION THEORY IN CLASSICAL MECHANICS AND THE AVERAGING PROCEDURE

We consider a $2s$-dimensional Hamiltonian system

$$\dot{z} = \{H,z\}, \quad z=(x,p) \in R^{2s} \tag{5}$$

with a Hamiltonian H, which is the sum of an unperturbed Hamiltonian H^0 corresponding to an exactly integrable probHlem and a perturbing small addition εH^1. Here and in what follows we assume that H describes the finite motion of the Hamiltonian system.

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In the simplest case we can try to construct a solution of the system (5) as a power series in the small parameter ε, i.e., $x(t)=\Sigma_{n=0}x^{(n)}(t)\varepsilon^n$, where $x^{(0)}(t)$ is the trajectory of the unperturbed Hamiltonian system, $x^{(1)}(t)$ is the solution of the linearized system in the neighborhood of $x^{(0)}(t)$, etc. It is well known that such a solution becomes invalid by times t of order ε^{-1} because of the presence in $x^{(n)}$ $(n>0)$ of secular terms $x^{(n)}\propto t^k$ $(k\geqslant 1)$.[6] In particular, $x^{(1)}\propto t$ for the anharmonic oscillator. It can be shown that in the quantum case, the expansion (3) of the energy spectrum in powers of the small parameter ε diverges.

The usual approach in classical mechanics to eliminating secular terms is to employ various versions of the averaging method, which entails finding equations for "slow" variables that provide a correct description of the behavior of systems over long time intervals.[6] In the canonical formalism, the phases act as the "fast" variables. The averaging method consists in replacing variables so that the phase dependence of the Hamiltonian in the new variables is retained only by the leading terms in the small parameters.

Nevertheless, such procedures do not generally make it possible to find, or prove the existence of, solutions of the original problem. One way to accelerate the convergence of perturbation expansions is to employ a method that consists in redefining at each iteration the "unperturbed" (i.e., dependent only on the action variables) Hamiltonian, incorporating the corrections found in the preceding iterations. This variant of perturbation theory has been used to prove the Kolmogorov–Arnol'd–Moser (KAM) theorem, and is often called the KAM perturbation theory. Following Ref. 7, we now provide a brief overview.

We denote the action–angle variables for the unperturbed Hamiltonian $H^0\equiv H^0(I)$ by (I,φ). Then

$$H=H^0(I)+\varepsilon H^1(I,\varphi,\varepsilon).$$

The next step is to carry out a change of variables that is symplectically close to the identity, $(I,\varphi)\to(J,\psi)$, so that in the new variables the terms in the Hamiltonian of order ε are phase-independent. Such a change of variables is specified by the generating function

$$F=J\varphi+\varepsilon S(J,\varphi),\quad I=J+\varepsilon\frac{\partial S}{\partial\varphi},\quad \psi=\varphi+\varepsilon\frac{\partial S}{\partial J},$$

where $S(J,\varphi)$ is a 2π-periodic function of the variable φ and a solution of the equation

$$-\sum_{i=1}^{s}\frac{\partial H^0(J)}{\partial J_i}\frac{\partial S(J,\varphi)}{\partial\varphi_i}=H^1(J,\varphi,\varepsilon)-\langle H^1\rangle(J,\varepsilon). \quad (6)$$

Here $\langle H^1\rangle$ is the average over the period:

$$\langle H^1\rangle(J,\varepsilon)=\frac{1}{(2\pi)^s}\int_0^{2\pi}\cdots\int_0^{2\pi}H^1(J,\varphi,\varepsilon)\,d\varphi_1\ldots d\varphi_s. \quad (7)$$

Taking Eq. (6) into account, we can write the Hamiltonian H in terms of the new variables:

$$H=H^0\left(J+\varepsilon\frac{\partial S}{\partial\varphi}\right)+\varepsilon H^1\left(J+\varepsilon\frac{\partial S}{\partial\varphi},\varphi,\varepsilon\right)$$
$$=H^0(J)+\varepsilon\langle H^1\rangle(J,\varepsilon)$$
$$+\left[H^0\left(J+\varepsilon\frac{\partial S}{\partial\varphi}\right)-H^0(J)-\varepsilon\frac{\partial H^0(J)}{\partial J}\frac{\partial S(J,\varphi)}{\partial\varphi}\right.$$
$$\left.+\varepsilon H^1\left(J+\varepsilon\frac{\partial S}{\partial\varphi},\varphi,\varepsilon\right)-\varepsilon H^1(J,\varphi,\varepsilon)\right].$$

The expression in square brackets is phase-dependent and quadratic in small quantities. Hence, in terms of the variables (J,ψ), the Hamiltonian H has the form:

$$H=\tilde H^0(J,\varepsilon)+\varepsilon^2\tilde H^1(J,\psi,\varepsilon),$$

$$\tilde H^0(J,\varepsilon)=H^0(J)+\varepsilon\langle H^1\rangle(J,\varepsilon),$$

$$\varepsilon^2\tilde H^1(J,\psi,\varepsilon)=\left[H^0\left(J+\varepsilon\frac{\partial S}{\partial\varphi}\right)-H^0(J)\right.$$
$$\left.-\varepsilon\frac{\partial H^0(J)}{\partial J}\frac{\partial S(J,\varphi)}{\partial J}\right]$$
$$+\varepsilon\left[H^1\left(J+\varepsilon\frac{\partial S}{\partial\varphi},\varphi,\varepsilon\right)-H^1(J,\varphi,\varepsilon)\right].$$

On the right-hand side of the last equation we must express φ in terms of ψ and J using the formulas for changing variables.

In terms of the new variables, the Hamiltonian H has the same appearance as in terms of the old, but now the phases are present in the terms of order ε^2. After N such changes of variable, the phase dependence remains solely in terms of order ε^{2^N}. This phenomenon is also known as superconvergence.

An important fact is worth noting. The canonical transformation described above exists if there exists a periodic solution of Eq. (6), which is equivalent to the absence of resonances, i.e., for fixed values of the variable J and for all integers $(k_1,\ldots,k_s)$,

$$\sum_i k_i\omega_i(J)\neq 0,\quad \omega_i(J)=\frac{\partial H^0(J)}{\partial J_i}. \quad (8)$$

In what follows we assume that no resonances are present.

Actually, even in the absence of resonances, due to the effect of small denominators (with the function S assumuing exceptionally high values), the rate of convergence of the KAM perturbation theory may be somewhat lower.

As we have shown above, the KAM perturbation theory consists in constructing a canonical transformation in which the term that depends on the new phases is of higher order in the small parameters. Here the "regular" (phase-independent) part of the Hamiltonian is the average of the Hamiltonian over the "old" phases. The important feature of the KAM perturbation theory is that the Hamiltonian is represented by the sum of the "regular" part and a small phase-dependent term.

The basic problem of transferring the methods of classical mechanics to quantum theory is the lack of an algorithm for setting up the quantum "action–angle" variables explicitly. Shapovalov and Shirokov[8] have attempted to resolve

this problem by applying approximate symmetries. However, the method they suggest is only applicable to a fairly narrow class of perturbing potentials.

Let us attempt to reformulate the perturbation theory algorithm discussed above in such a way as to make it possible to transfer this superconvergent perturbation theory to the quantum case. For this we recall the well-known theorem of averages.

Suppose that g is a function of the coordinates of a $2s$-dimensional Hamiltonian system. The time average of g is

$$\bar{g}=\lim_{T\to\infty}\frac{1}{T}\int_0^T g(\varphi(t),I)\,dt, \tag{9}$$

where I is a constant and $\varphi(t)$ is the solution of the Hamiltonian system. The phase average is defined by Eq. (7). The theorem of averages states that if the function g is reasonably "well-behaved" and that motion takes place on a nondegenerate torus, i.e., conditions (8) are met, then the phase and time averages will be equal: $\bar{g}=\langle g\rangle$.

Schematically the algorithm of a superconvergent perturbation theory can be represented as follows. Suppose that at a certain step the Hamiltonian H has the form $H=\bar{H}+\varepsilon V$, where $\bar{H}$ is the Hamiltonian averaged over time (or phase), and V is the remainder ($\bar{V}=0$). We carry out a special canonical transformation. We average H over time, where the dynamics is determined by the part of the Hamiltonian $\bar{H}$ obtained at the previous step. The result is $\bar{\bar{H}}$. If the canonical transformation is chosen properly, the remainder will be second-order in ε^2, i.e., $H=\bar{\bar{H}}+\varepsilon^2\bar{\bar{V}}(\bar{\bar{V}}=0)$.

In this approach, we make use of canonical transformation and time averaging. Both ideas exist in the quantum theory. For instance, the analog of a canonical transformation in quantum theory is the transformation from one basis of the Hilbert space to another: $\{\varphi_i\}\to\{\psi_i\}$. In the process the matrix H_{ij} of the operator H in the basis $\{\varphi_i\}$ is transformed into the matrix $\tilde{H}_{ij}$ of the operator H in the basis $\{\psi_i\}$. Clearly, in the absence of degeneracy, the time averaging procedure in quantum mechanics corresponds to specifying the diagonal part of the operator in the basis of the Hamiltonian's eigenfunctions.

Indeed, let X be an operator corresponding to a certain observable of a quantum system described by the time-independent Schrödinger equation (2), and let $X(t)$ be its representation in the Heisenberg picture. The evolution of the operator $X(t)$ is determined by the Heisenberg equation

$$i\hbar\frac{\partial X(t)}{\partial t}=[H^0,X(t)],\quad X(t)|_{t=0}=X. \tag{10}$$

By analogy with Eq. (9) we introduce the time average of the operator X:

$$\bar{X}=\lim_{T\to\infty}\frac{1}{T}\int_0^T X(t)\,dt. \tag{11}$$

The condition (8) for the absence of resonances transforms in the quantum case into the condition that the spectrum E_i^0 of the operator H^0 be nondegenerate. In the basis $\{\varphi_i\}$ of the eigenfunctions of H^0, the solution to problem (10) has the form

$$X_{kn}(t)=\exp\left\{-\frac{i}{\hbar}(E_k^0-E_n^0)t\right\}X_{kn}.$$

Using the fact that the spectrum is nondegenerate, we find from Eq. (11) that $\bar{X}_{kn}=\delta_{kn}X_{nn}$. The operator $\bar{X}$ is an integral operator that commutes with H^0.

3. THE QUANTUM ANALOG OF A CLASSICAL SUPERCONVERGENT PERTURBATION THEORY

Consider the quantum eigenvalue problem (1). In the basis $\{\varphi_i\}$ of the eigenfunctions of the unperturbed Hamiltonian H^0, the operator H is

$$H_{ij}=\delta_{ij}E_i^0+\varepsilon H_{ij}^1.$$

Here $H_{ij}\equiv(\varphi_i,H\varphi_j)$ and $(\varphi_i,\varphi_j)=\delta_{ij}$, with $(\cdot,\cdot)$ being the scalar product in the space L_2.

Following the ideas of a superconvergent perturbation theory in classical mechanics, we write H_{ij} in the form of an averaged term (which, according to Sec. 2, is the analog of the phase-averaged classical Hamiltonian) plus a residual term:

$$H_{ij}=\delta_{ij}E_i+\varepsilon V_{ij}, \tag{12}$$

$$V_{ij}=\begin{cases}H_{ij}^1 & \text{if } i\neq j,\\ 0 & \text{if } i=j,\end{cases}$$

$$V_{ij}^*=V_{ji},\quad E_i=E_i^0+\varepsilon H_{ii}^1.$$

We now carry out the canonical transformation, i.e., go to the basis $\{\psi_n\}$:

$$\psi_n=\sum_j S_{nj}\varphi_j. \tag{13}$$

We call S the transformation matrix and select it in such a way that the residual term in the expansion (12) for $\tilde{H}_{nm}\equiv(\psi_n,H\psi_m)$ is of order ε^2. At the Nth step, the residual is then obviously of order ε^{2^N}. Setting up such a recursive procedure in which the basis $\{\psi_n\}$ is orthonormalized at each step is impossible. Clearly, the requirement that the basis be orthonormalized is superfluous, and it is sufficient to require the normalization condition $(\psi_n^{(N)},\psi_n^{(N)})=1$ (here $\{\psi_n^{(N)}\}$ is the basis in the space L_2 obtained after the Nth iteration), and that

$$\lim_{N\to\infty}(\psi_n^{(N)},\psi_m^{(N)})=\delta_{nm}.$$

With these two conditions met, the constructed sets of functions $\{\psi_n^{(N)}\}$ tend, as $N\to\infty$, to a complete orthonormalized system of eigenfunctions of the operator H.

Thus, suppose that in a basis $\{\varphi_i\}$ of the space L_2 the operator H has matrix elements like those in (12) and

$$(\varphi_i,\varphi_j)\equiv\Delta_{ij}=\delta_{ij}+\varepsilon\sigma_{ij},$$

$\sigma_{ij}^*=\sigma_{ji}$ and $\sigma_{ii}=0$.

We introduce matrices α and β and the vector μ as follows:

$$\beta_{nj}=\frac{V_{jn}-E_n\sigma_{jn}}{E_n-E_j},$$

$$\alpha_{nj}=\delta_{nj}+\varepsilon\beta_{nj},\quad \mu_n=\frac{1}{\sqrt{\sum_{ij}\alpha^*_{ni}\alpha_{nj}\Delta_{ij}}}. \tag{14}$$

We specify the matrix S of the transformation to the new basis as follows:

$$S_{nj}=\mu_n\alpha_{nj}. \tag{15}$$

We then have

Theorem 1. In the basis $\{\psi_n\}$ defined via Eqs. (13)–(15), the operator H has the form

$$(\psi_n,H\psi_m)\equiv\tilde{H}_{nm}=\delta_{nm}\tilde{E}_n+\varepsilon^2\tilde{V}_{nm}, \tag{16}$$

$$\tilde{V}_{nn}=0,\quad \tilde{V}^*_{nm}=\tilde{V}_{mn},$$

and

$$(\psi_n,\psi_m)\equiv\tilde{\Delta}_{nm}=\delta_{nm}+\varepsilon^2\tilde{\sigma}_{nm}, \tag{17}$$

$$\tilde{\sigma}_{nn}=0,\quad \tilde{\sigma}^*_{nm}=\tilde{\sigma}_{mn}.$$

Proof. By definition,

$$\tilde{\Delta}_{nn}=\sum_{ij}S^*_{ni}S_{nj}\Delta_{ij}=\mu_n^2\sum_{ij}\alpha^*_{ni}\alpha_{nj}\Delta_{ij}=1.$$

For the off-diagonal elements we obtain

$$\tilde{\Delta}_{nm}=\sum_{ij}S^*_{ni}S_{mj}\Delta_{ij}$$

$$=\mu_n\mu_m\sum_{ij}(\delta_{ni}+\varepsilon\beta^*_{ni})(\delta_{mj}+\varepsilon\beta_{mj})(\delta_{ij}+\varepsilon\sigma_{ij})$$

$$=\varepsilon\mu_n\mu_m(\sigma_{nm}+\beta^*_{nm}+\beta_{mn})+O(\varepsilon^2).$$

Since the matrices V_{ij} and σ_{ij} are Hermitian, Eqs. (14) imply that $\tilde{\Delta}_{nm}=O(\varepsilon^2)$ for $n\neq m$. The hermiticity of $\tilde{\Delta}_{nm}$ follows from the definition of $\tilde{\Delta}_{nm}$. Thus we have proved the validity of Eq. (17). For the matrix $\tilde{H}_{nm}$ we have

$$\tilde{H}_{nm}=\sum_{ij}S^*_{ni}S_{mj}H_{ij}$$

$$=\mu_n\mu_m\sum_{ij}(\delta_{ni}+\varepsilon\beta^*_{ni})(\delta_{mj}+\varepsilon\beta_{mj})(\delta_{ij}E_j+\varepsilon V_{ij})$$

$$=\delta_{nm}\mu_n^2E_n$$

$$+\varepsilon\mu_n\mu_m(\beta^*_{nm}E_m+\beta_{mn}E_n+V_{nm})+O(\varepsilon^2).$$

Equations (14) imply that the second term in this expression vanishes and hence Eqs. (16) are valid. This completes the proof.

Thus, Theorem 1 provides a recipe for constructing a recursive perturbation theory for the eigenvalue problem (1). As in classical perturbation theory, here at each step the Hamiltonian matrix is the sum of a diagonal matrix, which corresponds to specifying the average Hamiltonian $\bar{H}$ in a certain basis, and a small residual term. This representation is used to construct a canonical transformation as a result of which the new Hamiltonian matrix $\tilde{H}_{nm}$ and the nonorthogonality matrix $\tilde{\Delta}_{nm}$ have the same form as before, but the small parameter ε is replaced by ε^2.

After N iterations we have

$$\psi_n^{(0)}=\varphi_n,\quad \psi_n^{(1)}=\sum_j S_{nj}^{(1)}\varphi_j,\ldots,\psi_n^{(N)}=\sum_j S_{nj}^{(N)}\psi_j^{(N-1)},$$

$$\tilde{H}_{nm}^{(N)}=\delta_{nm}\tilde{E}_n^{(N)}+\varepsilon^{2^N}\tilde{V}_{nm}^{(N)},\quad \tilde{E}_n^{(N)}=(\psi_n^{(N)},H\psi_n^{(N)}),$$

$$(\psi_n^{(N)},\psi_m^{(N)})\equiv\Delta_{nm}^{(N)}=\delta_{nm}+\varepsilon^{2^N}\tilde{\sigma}_{nm}^{(N)}.$$

The functions $\psi_n^{(N)}$, which are the eigenfunctions of the operator H with the eigenvalues $E_n^{(N)}$ can now be easily expressed, to within ε^{2^N}, in terms of the wave functions of the unperturbed Hamiltonian:

$$\psi_n^{(N)}=\sum_j\left(\prod_{m=1}^{N}S^{(M)}\right)_{nj}\varphi_j. \tag{18}$$

We have been unable to prove any theorem on convergence requirements for the above perturbation theory. The usefulness of the perturbation theory developed in this paper, we believe, lies in its practical application. All cases in which the perturbation theory has been applied have yielded good results. The given perturbation theory is recursive in form, and can easily be implemented numerically.

4. DISTINCTIVE FEATURES IN APPLYING THE PERTURBATION THEORY. EXAMPLES

The main drawback of a matrix perturbation theory is that no calculations with infinite matrices are allowed. The only infinite-dimensional space L_2 with its finite-dimensional subspace V with the basis $\{\varphi_i|i=0,\ldots,M-1\}$ and limit all operators to V. This transforms the spectral problem (1) into an M-dimensional linear system. But how is the spectrum $\{E_i\}$ of the operator H in L_2 related to the eigenvalues of the corresponding finite-dimensional linear system? The answer is given by

Theorem 2 (the Rayleigh–Ritz technique[3]). Let H be a semibounded self-adjoint operator. Let V be an n-dimensional subspace, $V\subset D(H)$ [$D(H)$ is the domain of H], and let P be the orthogonal projection operator onto V. Let $H_V=PHP$. Let λ_{M-1} be the eigenvalues of $H_V\upharpoonright V$. If H has eigenvalues (counting multiplicity) $E_0,\ldots,E_k$ at the bottom of the spectrum with $E_0\leqslant\cdots\leqslant E_k$, then $E_m\leqslant\lambda_m$, $m=0,\ldots,\min(k,M-1)$.

We restrict the operators H, H^0, and H^1 to the M-dimensional subspace, i.e., we assume that the indices in Eqs. (12)–(18) run through the values 0 to $M-1$. After a fairly large number N ($N\to\infty$) of convergent iterations, the infinite-dimensional matrix H_{ij} will assume the form

$$\|H_{ij}\| = \begin{pmatrix} \lambda_0 & 0 & \vdots & * \\ 0 & \ddots & \lambda_{M-1} & \\ \dots & & \dots & \\ & & * & * \end{pmatrix}.$$

If we are interested in the ground state, then according to Theorem 2 the number λ_0 is an upper bound on the value E_0 and, as can be shown, $\lambda_0 \to E_0$ as $M \to \infty$. Two problems emerge when the dimensionality M of space V is large. The first is that even with a simple computational algorithm one is forced to operate with high-dimensional matrices, and the computer may lack the necessary resources. The second problem is more fundamental: there sometimes exists a critical value M_{cr} of the dimensionality of space V above which the perturbation theory begins to diverge. We demonstrate this phenomenon below.

We start with the simplest nontrivial case, the spectral problem (1) with a one-dimensional time-independent Schrödinger operator

$$H^0 = -\partial_x^2 + U(x), \quad H^1 = W(x),$$

where $x \in R^1$, and H belongs to a family of operators analytic in the neighborhood of $\varepsilon = 0$. Since we assume that the operator H has only a discrete spectrum, the potential $U(x)$ is an increasing function at $x = \pm\infty$. If the function $W(x)$ increases at infinity more slowly than $U(x)$, then obviously the matrix elements H^1_{ij} decrease with increasing i and j, and perturbation theory presents no problems. The dimensionality of space may be arbitrary ($M_{cr} = \infty$).

A more important and complicated case is that in which the perturbing potential $W(x)$ rises more rapidly than the unperturbed potential $U(x)$. A characteristic example is the Schrödinger equation with the anharmonic potential

$$U(x) = x^2, \quad W(x) = x^{2m}, \quad m > 1.$$

Simon[9] proves that the family of operators H with an anharmonic oscillator potential is analytic on the real semiaxis $\varepsilon > 0$.

Let us examine the problem (1) with an anharmonic oscillator potential: $U(x) = x^2$ and $W(x) = x^4$ at $\varepsilon = 0.2$. Here the conventional perturbation-theory expansion diverges rapidly. Loeffel *et al.*[10] use the Padé approximant method to calculate the ground-state energy, and demonstrate the convergence of the method in this case:

$$E[1,1] = 1.111\ 111, \quad E[2,2] = 1.117\ 541,$$
$$E[3,3] = 1.118\ 183, \quad E[4,4] = 1.118\ 272,$$
$$E[5,5] = 1.118\ 288, \quad E[6,6] = 1.118\ 292,$$
$$E[7,7] = 1.118\ 292.$$

Here $E[N,N]$ is the ground-state energy calculated via $[N,N]$ Padé approximants. These are found using $2N$ Rayleigh–Schrödinger coefficients $a_1, \dots, a_{2N}$:

$$a_k = \frac{(-1)^{k+1}}{2\pi i} \oint_{|E-E_0|=\delta} (\varphi_0, [W(H^0 - E)^{-1}]^{k+1} \varphi_0)\, dE.$$

TABLE I.

M	$E_0^{(9)}$	Remark
9	1.118 293 304 285 56	$E_0^{(5)} = \dots = E_0^{(9)}$
11	1.118 293 214 376 55	$E_0^{(6)} = \dots = E_0^{(9)}$
13	1.118 292 799 233 28	$E_0^{(6)} = \dots = E_0^{(9)}$
15	1.118 292 664 885 40	$E_0^{(7)} = \dots = E_0^{(9)}$
17	1.118 292 654 794 33	$E_0^{(7)} = \dots = E_0^{(9)}$
19	1.118 292 654 792 53	
20	1.118 292 654 792 53	

Note that calculating the coefficients $a_1, \dots, a_{2N}$ is an extremely involved process, and furthermore the Padé approximant method does not enable one to obtain the corresponding eigenfunctions.

Below we give the results of applying the suggested perturbation theory to this example. Table I shows how the value of the ninth iteration for the ground-state energy $E_0^{(9)}$ varies depending on the dimensionality $M = \dim V$ in a finite-dimensional approximation. All further iterations introduce no changes: $E_0^{(N)} = E_0^{(9)}$, $N \geqslant 9$.

For the sake of comparison we give the value $E_0 = 1.118\,292\,654\,367\,05$ obtained by the method of steepest descent[11] as the smallest eigenvalue of a 41-by-41 matrix H_{ij}.

The results of iterations for $M = 20$ are listed in Table II ($E_0^{(0)} = E_0^0 + \varepsilon W_{00}$).

If we take $M = 21$ or higher, the perturbation theory begins to diverge. Apparently this is a general situation with rapidly increasing potentials. Hence the best approximation can be obtained by varying M until the perturbation theory diverges.

The divergence of the perturbation theory for a certain value of M greater than M_{cr} does not mean that the given theory can never be employed. Since the theory converges for $M \leqslant M_{cr}$, it yields least upper bounds. As Table I demonstrates, every increase in M in our example yields a more accurate estimate. Theorem 2 implies that such behavior of $E_i^{(N)}$ as a function of M is observed in the general case as well.

As a still more complicated example, consider the potential $W(x) = x^8$ at $\varepsilon = 0.2$. The Padé approximant method fails in this case.[10] An interesting aspect of this example is that the

TABLE II.

N	$E_0^{(N)}$
0	1.150 000 000 000 00
1	1.121 050 464 002 62
2	1.119 272 008 266 84
3	1.118 939 822 526 86
4	1.118 570 779 507 57
5	1.118 388 407 356 24
6	1.118 298 319 443 38
7	1.118 292 668 798 68
8	1.118 292 654 793 07
9	1.118 292 654 792 53
10	1.118 292 654 792 53

TABLE III.

N	$E_0^{(N)}$
0	2.3125
1	2.382 698 887 561 65
2	2.210 478 119 515 02
3	1.721 229 454 088 97
4	2.313 116 105 933 44
5	4.236 629 512 348 85
6	5.876 082 675 117 20
7	3.949 467 434 430 25
8	2.872 466 803 285 56
9	1.382 212 389 933 93
10	1.251 205 758 012 46
11	1.247 454 188 608 12
12	1.247 454 136 311 76
13	1.247 454 136 311 76

method of steepest descent applied to a 41-by-41 matrix H_{ij} yielded, with an error $\delta=5\times10^{-5}$, an incorrect result, $E_0=2.069\,11$, while for a 21-by-21 matrix $E_0=1.4727$. The shooting method gives $E_0=1.241$. Below we give the results of calculations by the perturbation theory method.

The perturbation theory converges for $M\leqslant 12$. The result of calculating E_0 at $M=12$ is listed in Table III.

If we assume that the shooting method yields an accurate value of E_0, the error introduced by the perturbation theory calculations in this case is 0.52%. The complexity of this example obviously results from the fact that εW is too "large," and in particular, the first correction in conventional perturbation theory, $E_0^{(0)}=E_0^0+\varepsilon W_{00}$ (which is equal to $E_0^{(0)}$ in our perturbation theory), is almost twice the accurate value.

In conclusion, we note once more that the perturbation theory developed in this paper in extremely simple to apply, and enables one to calculate, in addition to the ground-state energy E_0, the higher energy levels (albeit with a large error) and their corresponding wave functions, which are often inaccessible via other perturbation theory approaches. The regularity of the perturbation theory considered here has yet to be proved, but since this perturbation theory is a conceptual offshoot of the one used in proving the KAM theorem, we hope that it will find broad application.

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