AVERAGING METHOD FOR SELF-ADJOINT OPERATORS*

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Using the method of averaging we construct two perturbation algorithms anologous to the classical constructions. One of them reproduces the known Rayleigh-Schrödinger perturbation theory (PT) in quantum mechanics but with new closed form expressions. The other (Kolmogorov's PT) yields a new PT where the resulting expansion is in terms of functions of the perturbation parameter.

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1. Introduction

The use of *Hamiltonian* or *symplectic methods* has been very fruitful in dynamical systems in general and in classical mechanics in particular. It has produced deep structural insights (*e.g.* KAM-Theorem) as well as techniques (*e.g.* reduction of systems with symmetries) and algorithms (*e.g.* canonical perturbation theories).

Quantum mechanics on the other hand has mostly been treated using the tools of *functional analysis* although it is fairly well known that the Schrödinger equation may be written as an infinite-dimensional Hamiltonian system [1]. What seems to prevent the transfer of Hamiltonian methods known in classical mechanics to quantum mechanics is the fact that classical mechanics lives on a finite-dimensional symplectic manifold whereas quantum mechanics on an infinite-dimensional Hilbert space. This, however, is only an obstacle if the classical information is formulated in a coordinate dependent manner. At least formally most geometric concepts of classical

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Hamiltonian systems can be transferred to quantum mechanics. Loosely speaking, the *main philosophy* behind this is:

a) formulate the classical theory in as *purely geometric* a fashion as possible

b) formulate the Schrödinger equation as an *infinite-dimensional Hamiltonian system*

c) repeat the geometric construcions of a) for the system in b).

This way many formal expressions in the quantum version arise which may reproduce known concepts or yield new ones and which in most cases will require *functional analytic concepts* to make them mathematically well defined.

In the light of this "philosophy" the work presented here concerns perturbation algorithms for self-adjoint operators using the method of averaging. This method has been well known in classical mechanics and is used there to construct perturbation theories (PTs) free of so called secular terms. It is only quite recently, however, that I have extended the method of averaging to self-adjoint operators and with the help of that method have constructed analogues of the classical Poincaré-von Zeipel [2] as well as of Kolmogorov's so called superconvergent PT [3]. In the case of the Poincaré-von Zeipel perturbation algorithm the analogue construction for self-adjoint operators yields a new way of constructing the well known Rayleigh-Schrödinger PT [2]. The analogue of Kolmogorov's algorithm for self-adjoint operators, however, leads to a *new perturbation theory* for the spectra and eigenvectors of of self-adjoint operators [3].

The extension of the method of averaging to self-adjoint operators thus permits to investigate Rayleigh-Schrödinger PT from a new point of view and it allows the construction of a KAM-like theory for self-adjoint operators in general and quantum mechanics in particular. Using these constructions it is not only possible to elucidate the relation between quantum PT and the PT of the corresponding classical system but the new Kolmogorov-type algorithm may yield better convergence properties than the known PTs.

These perturbation algorithms for self-adjoint operators so far have been constructed purely on a formal level by formulating the classical theory in a geometric fashion using the language of symplectic geometry and exploiting the fact that the time dependent Schrödinger equation built with the self-adjoint operator can also be viewed as an infinite-dimensional symplectic system. Construction on a formal level means that one can write down operator equations and their solutions at each step in formulae and also evaluate these expressions in some examples. But so far only few results about the convergence of the resulting series or the rate thereof are available.

2. Poincaré-von Zeipel PT

The perturbation algorithm for self-adjoint operators along the lines of the classical Poincaré-von Zeipel PT has been developed in [2]. Let H_0 be the unperturbed Hamiltonian operator which is assumed to be diagonal in some basis and let

$$H(\varepsilon) := \sum_{p=0}^{\infty} \frac{\varepsilon^p}{p!} H_p \tag{1}$$

be the perturbed Hamiltonian with ε as the perturbation parameter and $H_p, p \geq 1$ the perturbations. In order to diagonalize this Hamiltonian we seek a unitary transformation operator $\Phi(\varepsilon)$ such that

$$\Phi(\varepsilon)^{-1} H(\varepsilon) \Phi(\varepsilon) =: K(\varepsilon) = \sum_{p=0}^{\infty} \frac{\varepsilon^p}{p!} K_p \tag{2}$$

commutes with the unperturbed operator H_0 in which case we could diagonalize $K(\varepsilon)$ in the given basis. According to (2) $K(\varepsilon)$ is unitarily related to $H(\varepsilon)$ hence the diagonalization of $K(\varepsilon)$ amounts to solving the spectral problem for the perturbed operator $H(\varepsilon)$.

We try to achieve the commutativity of H_0 and $K(\varepsilon)$ successively by requiring for each coefficient operator K_p of ε in (2)

$$[H_0, K_p] = 0\,, \tag{3}$$

and in order to achieve this we seek a self adjoint operator

$$W(\varepsilon) := \sum_{p=0}^{\infty} \frac{\varepsilon^p}{p!} W_{p+1} \tag{4}$$

such that $-W(\varepsilon)$ generates the unitary operator $\Phi(\varepsilon)^{-1}$. The transformation $\Phi(\varepsilon)$ has an expansion

$$\Phi(\varepsilon) = \sum_{p=0}^{\infty} \frac{\varepsilon^p}{p!} \Phi_p\,, \tag{5}$$

where the following recursive relation for the Φ_p can be derived:

$$\Phi_{p+1} = -\frac{i}{\hbar} \sum_{l=0}^{p} \binom{p}{l} \Phi_{p-l} W_{l+1} \qquad \text{and } \Phi_0 = \mathbf{1}\,. \tag{6}$$

From (2) one finds

$$K_0 = H_0 \quad \text{and} \quad K_p = \frac{i}{\hbar}[W_p, H_0] + F_p \quad \text{for } p \geq 1\,, \tag{7}$$

where the first few F_p are

$$\begin{aligned} F_0 &= 0\,, \\ F_1 &= H_1\,, \\ F_2 &= H_2 + \frac{i}{\hbar}[W_1, K_1 + H_1]\,, \end{aligned} \tag{8}$$

and in general

$$F_p = F_p(H_0, \ldots, H_p, K_1, \ldots, K_{p-1}, W_1, \ldots, W_{p-1})\,. \tag{9}$$

The idea is now to construct the W_p and the K_p successively such that (3) and (7) hold. This means that one has to find an operator W_p such that

$$[H_0, \frac{i}{\hbar}[W_p, H_0] + F_p] = 0\,. \tag{10}$$

This problem can be solved using the averaging method for operators [2]. Let G be a self-adjoint operator, define

$$\Phi_{H_0}(t) := \exp(-\frac{i}{\hbar}tH_0) \qquad \Phi_{H_0}(t)^* G := \Phi_{H_0}(t)^\dagger G \Phi_{H_0}(t) \tag{11}$$

and suppose that

$$\lim_{T\to\infty} \frac{\Phi^*_{H_0}(-T)\, G - G}{T} = 0\,, \tag{12}$$

and

$$\overline{G}^{(H_0)} := \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, \Phi_{H_0}(-t)^* G\,, \tag{13}$$

$$S^{(H_0)}(G) := \lim_{T\to\infty} \frac{1}{T} \int_0^T dt \int_0^t ds \left(\Phi_{H_0}(-s)^* G - \overline{G}^{(H_0)}\right) \tag{14}$$

exist. Then it follows that [2]

$$\left[H_0, \frac{i}{\hbar}[S^{(H_0)}(G), H_0] + G\right] = 0\,, \tag{15}$$

and

$$\overline{G}^{(H_0)} = \frac{i}{\hbar}[S^{(H_0)}(G), H_0] + G\,. \tag{16}$$

Eqs. (12)–(14) henceforth will be referred to as averaging equations along H_0.

Thus we can solve (10) by choosing $W_p = S^{(H_0)}(F_p)$ and consequently

$$K_p = \overline{F_p}^{(H_0)} = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, \Phi_{H_0}(-t)^*\, F_p\,. \tag{17}$$

Let us see how we can use these constructions to obtain approximative solutions to the original eigenvalue problem

$$H(\varepsilon)|j\rangle(\varepsilon) = E_j(\varepsilon)|j\rangle(\varepsilon) \tag{18}$$

for the perturbed operator $H(\varepsilon)$. Define the finite sums

$$K^N(\varepsilon) = \sum_{p=0}^{N} \frac{\varepsilon^p}{p!} \overline{F_p}\,, \tag{19}$$

$$\Phi^N(\varepsilon) = \sum_{p=0}^{N} \frac{\varepsilon^p}{p!} \Phi_p\,, \tag{20}$$

which give

$$K^N(\varepsilon) = (\Phi^N(\varepsilon))^{-1}\, H(\varepsilon)\, \Phi^N(\varepsilon) + O(\varepsilon^{N+1})\,. \tag{21}$$

Let $E_j^N(\varepsilon)$ and $|j\rangle^N(\varepsilon)$ be eigenvalues and eigenvectors of the finite sum $K^N(\varepsilon)$

$$K^N(\varepsilon)|j\rangle^N(\varepsilon) = E_j^N(\varepsilon)|j\rangle^N(\varepsilon)\,. \tag{22}$$

$K^N(\varepsilon)$ can be diagonalized in the original basis in which H_0 is diagonal, since by construction $[H_0, K^N(\varepsilon)] = 0$. Evidently

$$H(\varepsilon)\Phi^N(\varepsilon)|j\rangle^N(\varepsilon) = E_j^N(\varepsilon)\Phi^N(\varepsilon)|j\rangle^N(\varepsilon) + O(\varepsilon^{N+1})\,, \tag{23}$$

and the eigenvalues $E_j(\varepsilon)$ and eigenvectors $|j\rangle(\varepsilon)$ of the perturbed Hamiltonian $H(\varepsilon)$ are approximated as follows

$$E_j(\varepsilon) = E_j^N(\varepsilon) + O(\varepsilon^{N+1})\,, \tag{24}$$

$$|j\rangle(\varepsilon) = \Phi^N(\varepsilon)|j\rangle^N(\varepsilon) + O(\varepsilon^{N+1})\,. \tag{25}$$

For example if we are dealing with a perturbed operator

$$H(\varepsilon) = H_0 + \varepsilon H_1 \tag{26}$$

whose unperturbed part H_0 has purely discrete and non-degenerate spectrum:

$$H_0 = \sum_j |j\rangle E_j^0 \langle j| \tag{27}$$

then one finds

$$K_0 = \sum_j |j\rangle E_j^0 \langle j|\,, \tag{28}$$

$$K_1 = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, \Phi_{H_0}(-t)^* H_1 = \sum_j |j\rangle\langle j|H_1|j\rangle\langle j|\,, \tag{29}$$

$$\begin{aligned} K_2 &= \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, \Phi_{H_0}(-t)^* \left(\frac{2i}{\hbar}[W_1, H_1]\right) \\ &= 2\sum_j |j\rangle \left(\sum_{j\neq k} \frac{|\langle j|H_1|k\rangle|^2}{E_j^0 - E_k^0}\right) \langle j|\,, \end{aligned} \tag{30}$$

such that the diagonalization of $K^2(\varepsilon) = K_0 + \varepsilon K_1 + \frac{\varepsilon^2}{2} K_2$ yields exactly the same second order results as the usual Ralyeig-Schrödinger PT. Indeed, it can be shown that the PT so constructed coincides with the well known Rayleigh-Schrödinger PT in the complete expansion for eigenvalues and eigenvectors in general [2], *i.e.* including the degenerate case. However, this way of looking at Rayleigh-Schrödinger PT yields closed form expressions such as the one for K_p in (17). These may be difficult to evaluate and they can be shown to be equivalent to the usual sums over intermediate states (see *e.g.* (30) but they are conceptually close to the classical analogue and (17) permits a semiclassical analysis of the Rayleigh-Schrödinger PT and a term by term comparison between classical and quantum PT at each order of the perturbation.

In addition this way of constructing the standard PT may be more useful to find out when a perturbative result is exact because under certain conditions one can show inductively that all K_p beyond a certain order vanish, a result which is difficult to establish in the usual construction. This will be illustrated with a simple example at the beginning of Sect. 4.1.

3. Kolmogorov's PT

Kolmogorov's PT [4–6] is an improved version of Poincaré-von Zeipel PT using instead of one transformation $\Phi(\varepsilon)$ an infinite sequence of $\Phi^n(\varepsilon)$ leading at each step to a new transformed operator [3] $K^n(\varepsilon)$

$$\Phi^n(\varepsilon)^{-1} H^{n-1}(\varepsilon)\Phi^n(\varepsilon) =: K^n(\varepsilon) = \sum_{p=0}^{\infty} \frac{\varepsilon^p}{p!} K_p^n \,. \tag{31}$$

for which one repeats the procedure of Sect. 2 but each time with a modified "unperturbed Hamiltonian" H_0^n and a modified choice of the generators W_p^n.

Let H_0^0 be the unperturbed Hamiltonian and let

$$H^0(\mathrm{e}) := H_0^0 + \sum_{p=1}^{\infty} \frac{\mathrm{e}^p}{p!} H_p^0 \tag{32}$$

be the perturbed Hamiltonian which we transform with $\Phi^1(\mathrm{e})$ to $K^1(\mathrm{e})$:

$$K^1(\mathrm{e}) := \Phi^1(\mathrm{e})^* H^0(\mathrm{e}) \tag{3}$$

$$= \sum_{p=0}^{\infty} \frac{\mathrm{e}^p}{p!} K_p^1 \,, \tag{34}$$

where one has

$$K_0^1 = H_0^0 \,, \tag{35}$$

$$K_{p+1}^1 = \sum_{l=0}^{p} \binom{p}{l} \left(\frac{i}{\hbar} \left[W_{l+1}^1, K_{p-l}^1 \right] + T_{p-l}^1 (H_{l+1}^0) \right) . \tag{36}$$

In particular, one has for K_1^1

$$K_1^1 = \frac{i}{\hbar} \left[W_1^1, H_0^0 \right] + H_1^0 \,, \tag{37}$$

such that the choice

$$W_1^1 = S^{(H_0^0)}(H_1^0) \,, \tag{38}$$

$$W_p^1 = 0 \qquad \forall p \geq 2 \tag{39}$$

leads to

$$K_1^1 = \overline{H_1^0}^{(H_0^0)} \,, \tag{40}$$

$$K_{p+1}^1 = F_{p+1}^1 \qquad \forall p \geq 1 \,, \tag{41}$$

and thus

$$K^1(\mathrm{e}) = H_0^0 + \mathrm{e}\overline{H_1^0}^{(H_0^0)} + \sum_{p=2}^{\infty} \frac{\mathrm{e}^p}{p!} K_p^1 \,, \tag{42}$$

where $\overline{H_1^0}^{(H_0^0)}$ commutes with H_0^0. For the second step we treat the "commuting" part of $K^1(\mathrm{e})$ as the unperturbed Hamiltonian and the higher order terms as perturbations, *i.e.* we set

$$H^1(\mathrm{e}) := K^1(\mathrm{e}) = \underbrace{H_0^0 + \mathrm{e}\overline{H_1^0}^{(H_0^0)}} + \sum_{p=2}^{\infty} \frac{\mathrm{e}^p}{p!} K_p^1 \tag{43}$$

$$= H_0^1 + \sum_{p=2}^{\infty} \frac{\mathrm{e}^p}{p!} H_p^1 \,, \tag{44}$$

such that

$$H_0^1 = H_0^0 + \mathrm{e}\overline{H_1^0}^{(H_0^0)}, \quad H_1^1 = 0, \quad H_p^1 = K_p^1, \quad \forall p \geq 2 \,, \tag{45}$$

and $H^1(\mathrm{e})$ has no perturbation of first order in e. The algorithm may be summarized as follows. Suppose now that after $n-1$ transformations we have the following Hamiltonian

$$H^{n-1}(\mathrm{e}) = H_0^{n-1} + \sum_{p=2^{n-1}}^{\infty} \frac{\mathrm{e}^p}{p!} H_p^{n-1} \tag{46}$$

such that

$$H_p^{n-1} = 0, \quad \forall 1 \leq p < 2^{n-1} \,. \tag{47}$$

To this Hamiltonian we apply the transformation $\Phi^n(\mathrm{e})$ to obtain

$$K^n(\mathrm{e}) = \Phi^n(\mathrm{e})^* H^{n-1}(\mathrm{e}) \tag{48}$$

$$= \sum_{p=0}^{\infty} \frac{\mathrm{e}^p}{p!} K_p^n \,, \tag{49}$$

where the W_p^n are now chosen as

$$W_p^n = \begin{cases} 0 & \text{if} \quad p < 2^{n-1} \\ S^{(H_0^{n-1})}(H_p^{n-1}) & \text{if} \quad 2^{n-1} \leq p < 2^n \\ 0 & \text{if} \quad 2^n \leq p \,. \end{cases} \tag{50}$$

This choice leads to the following expansion for $K^n(\mathrm{e})$

$$K_p^n = \begin{cases} H_0^{n-1} & \text{if} \quad p = 0 \\ 0 & \text{if} \quad 1 \le p < 2^{n-1} \\ \overline{H_p^{n-1}}^{(H_0^{n-1})} & \text{if} \quad 2^{n-1} \le p < 2^n \\ \frac{i}{\hbar}\left[W_p^n, K_0^n\right] + F_p^n & \text{if} \quad 2^n \le p\,. \end{cases} \tag{51}$$

Thus we have

$$H^n(\mathrm{e}) = H_0^n + \sum_{p=2^n}^{\infty} \frac{\mathrm{e}^p}{p!} H_p^n\,, \tag{52}$$

where

$$H_0^n = H_0^{n-1} + \underbrace{\sum_{p=2^{n-1}}^{2^n-1} \frac{\mathrm{e}^p}{p!} \overline{H_p^{n-1}}^{(H_0^{n-1})}}_{\text{commutes with } H_0^{n-1}} \tag{53}$$

$$H_p^n = K_p^n, \qquad \forall p \ge 2^n\,. \tag{54}$$

Eq. (53) permits us to write down H_0^n explicitly:

$$H_0^n = H_0^0 + \sum_{l=1}^{n} \left(\sum_{p=2^{l-1}}^{2^l-1} \frac{\mathrm{e}^p}{p!} \overline{H_p^{l-1}}^{(H_0^{l-1})} \right)\,. \tag{55}$$

How does one use this algorithm to obtain approximations for spectrum and eigenvectors? Let the unperturbed Hamiltonian be diagonal in some basis

$$\mathcal{B} := \{|j\rangle\,\alpha 0 \mid \alpha \in D_j\}_{j=1}^{\infty}\,, \tag{56}$$

where j denotes the level, α is the degeneracy-index, $D_j := \{1, \ldots, d_j\}$, and d_j is the degeneracy of the j-th eigenvalue E_j^0 of H_0^0:

$$H_0^0 = \sum_{j=1}^{\infty} \sum_{\alpha \in D_j} |j\rangle\,\alpha 0\, E_j^0\, \langle j|\,\alpha 0\,. \tag{57}$$

By construction (see (53)) $\overline{H_1^0}^{(H_0^0)}$ commutes with H_0^0, hence

$$H_0^1 = H_0^0 + \mathrm{e}\overline{H_1^0}^{(H_0^0)} \tag{58}$$

can be diagonalized in the same basis $\mathcal{B}$. Having done this we note that again by construction $\overline{H_2^1}^{(H_0^1)}$ and $\overline{H_3^1}^{(H_0^1)}$ commute with H_0^1, hence

$$H_0^2 = H_0^1 + \frac{\mathrm{e}^2}{2}\overline{H_2^1}^{(H_0^1)} + \frac{\mathrm{e}^3}{3!}\overline{H_3^1}^{(H_0^1)} \tag{59}$$

can be diagonalized in the same basis $\mathcal{B}$. Suppose now that H_0^{n-1} is diagonal in $\mathcal{B}$. By construction (see again (53)) all $\overline{H_p^{n-1}}^{(H_0^{n-1})}$ with $2^{n-1} \leq p \leq 2^n - 1$ commute with H_0^{n-1} and thus

$$H_0^n = H_0^{n-1} + \sum_{p=2^{n-1}}^{2^n-1} \frac{\mathrm{e}^p}{p!}\overline{H_p^{n-1}}^{(H_0^{n-1})} \tag{60}$$

can be diagonalized in $\mathcal{B}$.

Note that

$$\begin{aligned} H^n(\mathrm{e}) &= \Phi^n(\mathrm{e})^* \circ \cdots \circ \Phi^1(\mathrm{e})^* H^0(\mathrm{e}) \\ &= \Phi^n(\mathrm{e})^\dagger \cdots \Phi^1(\mathrm{e})^\dagger H^0(\mathrm{e}) \Phi^1(\mathrm{e}) \cdots \Phi^n(\mathrm{e}) \end{aligned} \tag{61}$$

implies that $H^n(\mathrm{e})$ and our original perturbed Hamiltonian $H(\mathrm{e}) = H^0(\mathrm{e})$ are unitarily equivalent:

$$H^n(\mathrm{e}) = U^n(\mathrm{e})^\dagger H^0(\mathrm{e}) U^n(\mathrm{e})\,, \tag{62}$$

where $U^n(\mathrm{e})$ is the unitary transformation

$$U^n(\mathrm{e}) := \Phi^1(\mathrm{e}) \cdots \Phi^n(\mathrm{e})\,. \tag{63}$$

Moreover, one has

$$H^n(\mathrm{e}) = H_0^n + O(\mathrm{e}^{2^n}) \tag{64}$$

which implies that H_0^n unitarily approximates the original perturbed Hamiltonian:

$$H(\mathrm{e}) = H^0(\mathrm{e}) = U^n(\mathrm{e}) H_0^n U^n(\mathrm{e})^\dagger + O(\mathrm{e}^{2^n})\,. \tag{65}$$

Consequently, since H_0^n can be diagonalized in $\mathcal{B}$ as shown above, we can read off its eigenvalues which coincide with those of our original perturbed Hamiltonian $H(\mathrm{e})$ up to $O(\mathrm{e}^{2^n})$. In formulae:

- Let $E_{j,\alpha}^n(\mathrm{e})$ be an eigenvalue of H_0^n with eigenvector $|j\rangle\,\alpha n(\mathrm{e})$:

$$H_0^n(\mathrm{e})\,|j\rangle\,\alpha n(\mathrm{e}) = E_{j,\alpha}^n(\mathrm{e})\,|j\rangle\,\alpha n(\mathrm{e})\,, \tag{66}$$

- and let $E_{j,\alpha}(\mathrm{e})$ be an eigenvalue of $H^0(\mathrm{e}) = H(\mathrm{e})$ with eigenvector $|j\rangle\,\alpha(\mathrm{e})$:

$$H(\mathrm{e})\,|j\rangle\,\alpha(\mathrm{e}) = E_{j,\alpha}(\mathrm{e})\,|j\rangle\,\alpha(\mathrm{e}) \tag{67}$$

then

$$E_{j,\alpha}(\mathrm{e}) = E^n_{j,\alpha}(\mathrm{e}) + O(\mathrm{e}^{2^n})\,, \tag{68}$$

$$|j\rangle\,\alpha(\mathrm{e}) = U^n(\mathrm{e})\,|j\rangle\,\alpha n(\mathrm{e}) + O(\mathrm{e}^{2^n})\,. \tag{69}$$

Eq. (68) gives the desired approximation of the eigenvalues of $H(\mathrm{e})$ and for the approximation of its eigenvectors one can determine $U^n(\mathrm{e})$ up to $O(\mathrm{e}^{2^n})$ in terms of the W^n_p from (5), (6), and (63).

The quantum PT resulting from Kolmogorov's construction is new and yields expansions in powers of ε where the expansion coefficients are functions of ε as well. The difference to the usual Rayleigh-Schrödinger PT, however, shows up only in fourth and higher orders. *E.g.* for the non-degenerate system considered in Eqs. (26), (27) one finds with Kolmogorov's algorithm for the fourth order coefficient [3]

$$\begin{aligned}
E^{(4)}_j &= 24 \sum_{j\neq l} \frac{|V_{lj}|^2 (V_{ll} - V_{jj})^2}{(E^0_j - E^0_l)^2 (E^1_j - E^1_l)} \\
&6 \sum_{j\neq l\neq k\neq j\neq m\neq k} \frac{V_{jl} V_{lk} V_{km} V_{mj}}{E^1_j - E^1_k} \\
&\times \left(\frac{1}{E^0_j - E^0_l} - \frac{1}{E^0_l - E^0_k}\right)\left(\frac{1}{E^0_k - E^0_m} - \frac{1}{E^0_m - E^0_j}\right) \\
&+ 12 \sum_{j\neq l\neq k\neq j} V_{jl} V_{lk} V_{kj} \left\{ \frac{V_{ll} - V_{kk}}{(E^0_j - E^0_l)(E^0_l - E^0_k)(E^0_k - E^0_j)} \right. \\
&+ \frac{V_{ll} - V_{jj}}{(E^0_j - E^0_l)(E^1_j - E^1_l)} \left(\frac{1}{E^0_l - E^0_k} - \frac{1}{E^0_k - E^0_j}\right) \\
&\left. + \frac{V_{kk} - V_{jj}}{(E^0_j - E^0_k)(E^1_j - E^1_k)} \left(\frac{1}{E^0_j - E^0_l} - \frac{1}{E^0_l - E^0_k}\right) \right\} \\
&+ \sum_{k\neq l\neq j\neq m\neq k} V_{jl} V_{lk} V_{km} V_{mj} \left\{ \frac{9}{(E^0_m - E^0_j)(E^0_j - E^0_l)} \left(\frac{1}{E^0_k - E^0_m} - \frac{1}{E^0_l - E^0_k}\right) \right. \\
&\left. + \frac{3}{(E^0_l - E^0_k)(E^0_k - E^0_m)} \left(\frac{1}{E^0_j - E^0_l} - \frac{1}{E^0_m - E^0_j}\right) \right\}
\end{aligned}$$

which contains denominators of the form $E_j^1 - E_k^1 = E_j^0 - E_k^0 + \varepsilon(V_{jj} - V_{kk})$ which are functions of ε.

For the quantum version of Kolmogorov's method the same statements about semiclassical limits as for the Poincaré-von Zeipel apply.

4. Example: anharmonic oscillator

4.1. Poincaré–von Zeipel

We shall illustrate the method in the example of the harmonic oscillator $H_0 = -\frac{d^2}{dx^2} + x^2$. First we illustrate how the new way of construction by itself tells when a result is exact. For this we consider a perturbation $H_1 = x$, $H_p = 0$, $p \geq 2$ where the exact solution $E_j(\varepsilon) = 2j + 1 - \frac{\varepsilon^4}{4}$ is easy to find. All calculations are straightforward if we use the operators

$$a := \frac{1}{\sqrt{2}}\left(\frac{d}{dx} + x\right) \qquad a^\dagger := \frac{1}{\sqrt{2}}\left(-\frac{d}{dx} + x\right) \tag{70}$$

for which one finds

$$\Phi_{H_0}(-t)^* a = e^{2it} a \qquad \Phi_{H_0}(-t)^* a^\dagger = e^{-2it} a^\dagger \tag{71}$$

such that

$$\begin{aligned}
&H_1 = \frac{1}{\sqrt{2}}\left(a^\dagger + a\right) && \Phi_{H_0}(-t)^* H_1 = \frac{1}{\sqrt{2}}\left(e^{-2it} a^\dagger + e^{2it} a\right) \\
&W_1 = \frac{1}{2i\sqrt{2}}\left(a^\dagger - a\right) && K_1 = 0 \\
&K_2 = i[W_1, H_1] = -\tfrac{1}{2}\mathbb{1} && W_p = 0 \quad \forall p \geq 2 \\
&K_p = 0 \qquad \forall p \geq 3 && K(\varepsilon) = a^\dagger a + \left(1 - \frac{\varepsilon^2}{4}\right)\mathbb{1}
\end{aligned} \tag{72}$$

which reproduces the exact result but because of the last line also immediately shows that this perturbative result *is exact.*

As a second example we consider the perturbation $H_1 = x^4$, $H_p = 0$, $p \geq 2$ (anharmonic oscillator with $\hbar = 1$) where the quantum Poincaré–von Zeipel method will permit us to compute the sums over intermediate

states and the corrections up to $O(\varepsilon^2)$ without much effort. Now we have

$$\begin{aligned}
\Phi_{H_0}(-t)^* H_1 &= \frac{1}{4}\left(e^{8it}a^4 + e^{-8it}(a^\dagger)^4 + 2e^{4it}aH_0a + 2e^{-4it}a^\dagger H_0 a^\dagger\right) \\
&\quad + \frac{3}{8}\left((H_0)^2 + \mathbb{1}\right), \\
\overline{H_1} &= \frac{3}{8}\left((H_0)^2 + \mathbb{1}\right), \\
W_1 &= \frac{1}{32i}\left((a^\dagger)^4 - a^4 + 4a^\dagger H_0 a^\dagger - 4aH_0a\right), \\
\Phi_{H_0}(-t)^* W_1 &= \frac{1}{32i}\left(e^{-8it}(a^\dagger)^4 - e^{8it}a^4 + 4e^{-4it}a^\dagger H_0 a^\dagger - 4e^{4it}aH_0a\right), \\
K_2 &= \frac{1}{64}\left([(a^\dagger)^4, a^4] + 8[a^\dagger H_0 a^\dagger, aH_0a]\right), \\
E_j^2(\varepsilon) &= 2j+1+\varepsilon\left(\frac{3}{2}j^2+\frac{3}{2}j+\frac{3}{4}\right)-\varepsilon^2\left(\frac{34}{16}j^3+\frac{51}{16}j^2+\frac{59}{16}j+\frac{21}{16}\right).
\end{aligned}$$

Calculating up to fourth order one finds *e.g.*for the ground state energy

$$E_0^{N=4}(\mathrm{e})_{RS} = 1 + \frac{3}{4}\mathrm{e} - \frac{21}{16}\mathrm{e}^2 + \frac{333}{64}\mathrm{e}^3 - \frac{30885}{1024}\mathrm{e}^4 . \tag{73}$$

As already pointed out this is identical to the standard the standard Rayleigh-Schrödinger result, hence the subscript *RS*.

4.2. Kolmogorov's PT

The superconvergent method gives for the ground state of the anharmonic oscillator considered in Sect. 4.1

$$\begin{aligned}
E_0^{n=2}(\mathrm{e})_{KO} &= 1 + \frac{3}{4}\mathrm{e} - \frac{21}{16}\mathrm{e}^2 + \frac{333}{64}\mathrm{e}^3 \qquad (74)\\
&\quad - \frac{3(1317760 + 12935472\mathrm{e} + 36433368\mathrm{e}^2 + 25183305\mathrm{e}^3)}{2048(4+9\mathrm{e})(4+15\mathrm{e})(4+21\mathrm{e})}\,\mathrm{e}^4 \\
&= 1 + \frac{3}{4}\mathrm{e} - \frac{21}{16}\mathrm{e}^2 + \frac{333}{64}\mathrm{e}^3 - \frac{30885}{1024}\mathrm{e}^4 + \frac{354249}{8192}\mathrm{e}^5 + \ldots . \qquad (75)
\end{aligned}$$

This is the result after two iterations $n = 2$, which approximates to order $O(\mathrm{e}^{2^2} = \mathrm{e}^4)$ but does contain all powers of e in its expansion. As it should be, the two perturbation methods do however give the same *asymptotic expansions* (73) and (75) when expanded in *pure powers* of ε. Hence Kolmogorov's method may be viewed as a resummation of the divergent Rayleigh-Schrödinger PT. Comparison with numerically calculated eigenvalues shows that Kolmogorov's method does indeed improve on the usual

Rayleigh-Schrödinger PT. This is expected to be even more pronounced in higher orders since the first different term is of order four. Convergence of the new series has not been established yet but it is known from classical mechanics that Kolmogorov's method does lead to convergent expansions even if the usual Poincaré-von Zeipel PT is divergent.

5. Conclusion

The method of averaging has allowed us to construct quantum analogues of the PTs used in classical mechanics. These PTs are either reproductions of a known PT (*i.e.* Poincaré-von Zeipel yields Rayleigh-Schrödinger) or new a new PT where the expansion comes in terms of functions of the perturbation parameter.

It should be noted that the constructions presented here are (at least formally) applicable to any self-adjoint operator and give approximations to the spectrum and the eigenvectors for all type of spectra (degenerate, continuous).

The averaging constructions are at the heart of the algorithms and the conditions on the operators under which rigorous validity of the averaging equations (12)–(14) can be established are thus of great importance to the theory. Work on this is in progress.

Moreover, it is also possible to construct time-dependent PTs with the averaging method [7]. In this case it turns out that already the quantum analogue of Poincaré-von Zeipel yields a PT different from the standard Dyson expansion. As in any theory using averaging the new time-dependent PT is free of secular terms.

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