Hamiltonian Point of View of Quantum Perturbation Theory

A.D Bermúdez Manjarres

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1Universidad Distrital Francisco José de Caldas, Cra 7 No. 40B-53, Bogotúa, Colombia. Email: ad.bermudez168@uniandes.edu.co

Abstract

We explore the relation of Van Vleck-Primas perturbation theory of quantum mechanics with the Lie-series based perturbation theory of Hamiltonian systems in classical mechanics. In contrast to previous works on the relation of quantum and classical perturbation theories, our approach is not based on the conceptual similarities between the two methods. Instead, we show that for quantum systems with a finite-dimensional Hilbert space, the Van Vleck-Primas procedure can be recast exactly into a classical perturbation problem.

1 Introduction

Concepts from classical mechanics played an important role in the early days of quantum theory. For example, in the influential paper of Born, Heisenberg, and Jordan [1], an adaptation of the concept of canonical transformation is used to discuss approximations of a given problem using a perturbation procedure. In the words of Heisenberg “the analogy with the classical Hamilton–Jacobi technique was the beginning of all efforts; what we did first was just to try to imitate the old methods as closely as we could” [2].

Nowadays, the formalism of quantum mechanics is well established and plenty of research is done without taking into consideration classical ideas. However, there are still cases where developments in quantum mechanics originate in adaptations of concepts and techniques from classical mechanics. In the context of perturbation theory we can find: averaging theory to avoid secular terms [3][4], normal forms [5][6], analogues to canonical perturbation theory and the KAM theorem [7], and time-dependent methods [8][9][10][11]. On the other hand, results from quantum mechanics have also inspired investigation in classical perturbation theory, like Kato expansion applied to the Liouville operator [12][13] and the use of Feynman diagrams in classical mechanics [14][15].
This work focuses on the relation between quantum and classical perturbation theories. The central question of time-independent quantum perturbation theory we address in this work can be stated as follows: let $\hat{H}_0$ be a Hamiltonian operator with discrete and non-degenerate spectrum. Assume the eigenvalues $\{E_n\}$ and eigenvectors $\{|n\rangle\}$ of $\hat{H}_0$ are known. If $\hat{V}$ is a small perturbation, what are the eigenvalues $\{E_n'\}$ and eigenvectors $\{|n'\rangle\}$ of $\hat{H} = \hat{H}_0 + \hat{V}$? There are several approaches to deal with the quantum perturbation problem like Rayleigh-Schrödinger [16] or Brillouin-Wigner [17, 18]. In this work we only consider the perturbation procedure known as the Van Vleck-Primas theory (VPP) [19, 20, 21, 22].

The equivalent perturbation problem of classical mechanics is the following: Let $H_0$ be a Hamiltonian function with a set of action-angle variables $(I, \theta)$ such that $H_0 = H_0(I)$. If $V(I, \theta)$ is a small perturbative function, what are the action-angle variables $(I', \theta')$ of the Hamiltonian function $H = H_0(I) + V(I, \theta)$ such that $H = H(I')$? Mainly developed to deal with problems in celestial mechanics, the main methods in classical perturbation theory are the Von Zeipel-Poincare [23], and the ones based on Lie series like Hori’s [24] and Lie-Deprit [25, 26] (see [27] for a complete exposition of the mentioned methods). While all the classical perturbation theories mentioned give the same result at all orders, they differ in their approach and usefulness for a given problem.

In this work we investigate the relation between VVP and the classical perturbation theory based on Lie series. The formal similarities between the quantum and classical procedures are well known, see for example [4, 10]. Instead of comparing the two theories as analogues, we will show that VVP procedure can be recast exactly into a classical perturbation theory. We will show that a direct translation of VVP gives Hori’s classical procedure.

The bridge between quantum and classical perturbation theory will be given using the Hamiltonian version of quantum mechanics [28, 29]. The idea is to put quantum dynamics in the same language of classical Hamiltonian mechanics. Using this version of quantum mechanics we will show that, in a quantum system with finite Hilbert space, the quantum perturbation problem can be restated and solved as a problem in classical perturbation theory.

This work has the following organization: In section 2 we present the necessary aspects of the Hamiltonian version of quantum mechanics. We explain the relation between the Schrödinger equation and the Hamilton equations, the commutator and the Poisson bracket, and unitary and canonical transformations. Section 3 deals with the Van Vleck-Primas perturbation theory. Our presentation of the theory will follow the one found in [21]. The purpose of the section is to present the theory in a way that will allow a quick recast into

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1While Van Vleck-Primas perturbation theory can be used in more general cases, in this work we only consider the restricted case of Hamiltonian operators with non-degenerate spectrum.
the classical Lie series formalism. In section 4 we will rewrite the quantum
perturbation problem in the mathematical language of classical mechanics.

Through this paper we set \( \hbar = 1 \).

2 Hamiltonian Version of Quantum Mechanics

In this section our presentation follows [28, 29], we refer to those work for the
proof of the statements presented here.

Consider a quantum system with a Hamiltonian \( \hat{H} \) with finite spectrum. The evolution of an arbitrary vector \( |\psi\rangle \) is given by the Schrödinger equation

\[
\frac{i}{\hbar} \frac{d}{dt} |\psi\rangle = \hat{H} |\psi\rangle.
\]

We can write (1) in classical Hamiltonian form as follows: Let \( \{|\phi_k\rangle\} \) be a basis of orthonormal vectors of the Hilbert space. The vector \( |\psi\rangle \) can be expanded as

\[
|\psi\rangle = \sum_k \lambda_k |\phi_k\rangle,
\]

where the expansion coefficients \( \lambda_k \) are complex numbers. The coefficients can be written in terms of their real and imaginary part as

\[
\lambda_k = \frac{q_k + ip_k}{\sqrt{2}}.
\]

Inserting Eq.(2) into Eq.(1) and taking the scalar product with \( |\psi\rangle \) gives the following set of Hamiltonian equations for the real and imaginary part of \( \lambda_k \)

\[
\frac{dq_k}{dt} = \frac{\partial H}{\partial p_k},
\]

\[
\frac{dp_k}{dt} = -\frac{\partial H}{\partial q_k},
\]

where the (real-valued) Hamiltonian function is given by

\[
H(q, p) = \langle \psi | \hat{H} |\psi\rangle.
\]

The coordinates \((q, p)\) define a phase space \( \mathcal{P} \) of twice the dimension of the Hilbert space. \( \mathcal{P} \) is endowed with a natural bracket operation defined by

\[
\{f, g\} = \sum_k \left( \frac{\partial f}{\partial q_k} \frac{\partial g}{\partial p_k} - \frac{\partial f}{\partial p_k} \frac{\partial g}{\partial q_k} \right),
\]

where \( f \) and \( g \) are real-valued functions of \((q, p)\). It can be shown that Eq.(6) has all the defining properties of the Poisson bracket of classical Hamiltonian mechanics. Clearly, the coordinates \((q, p)\) obey

\[
\{q_k, p_l\} = \delta_{kl},
\]

\[
\{q_k, q_l\} = \{p_k, p_l\} = 0.
\]
Just as it was done for the Hamiltonian in (5), we can define a real valued function \( g = g(q,p) \) for any self-adjoint operators \( \hat{g} \) by

\[
g = \langle \psi | \hat{g} | \psi \rangle = \sum_{k,l} \frac{g_{kl}}{2} \left[ \left( q_k q_l + p_k p_l \right) + i \left( q_k p_l - p_k q_l \right) \right],
\]

(8)

where \( g_{kl} = \langle \phi_k | \hat{g} | \phi_l \rangle \). An important result links the commutator of operators with the Poisson brackets. Namely, the following holds true for any two arbitrary self-adjoint operators \( \hat{f} \) and \( \hat{g} \):

\[
\{ f, g \} = -i \langle \psi | [\hat{f}, \hat{g}] | \psi \rangle.
\]

(9)

Eq. (9) will be used repeatedly in section 4 to link VVP perturbation theory with the classical Lie series method.

There exist transformations on \( \mathcal{P} \) that are canonical in the sense that they let the bracket \( \{ f, g \} \) invariant. Among the set of all canonical transformations on \( \mathcal{P} \), the subset induced by an unitary transformation on the Hilbert space is of special interest. Let \( U \) be a unitary transformation with an associated unitary operator \( \hat{U} \). Let us write the action of \( \hat{U} \) on the basis vectors \( \{ | \phi_k \rangle \} \) as

\[
\hat{U} | \phi_k \rangle = | \phi'_k \rangle.
\]

(10)

The vector \( | \psi \rangle \) can be expanded in terms of the new basis \( \{ | \phi'_k \rangle \} \) as

\[
| \psi \rangle = \sum_k \frac{1}{\sqrt{2}} \left( q'_k + ip'_k \right) | \phi'_k \rangle,
\]

(11)

hence, \( U \) defines a change of coordinates in \( \mathcal{P} \)

\[
U : (q,p) \rightarrow (q',p').
\]

(12)

The transformation given by (12) is canonical. It has the property that

\[
U \{ f, g \} = \{ U(f), U(g) \},
\]

(13)

or writing (13) in terms of the coordinates

\[
\{ f, g \}_{(q,p)} = \{ f, g \}_{(q',p')}.
\]

(14)

The VVP perturbation theory deals with unitary transformation \( U \) that are close to the identity. Considering only the first order expansion of \( \hat{U} \), we can write

\[
\hat{U} = 1 + i \epsilon \hat{W},
\]

(15)

where \( \hat{W} \) is an Hermitean operator. The action of \( U \) on a given self adjoint operator \( \hat{g} \) is
\[ U : \hat{g} \rightarrow \hat{U} \hat{g} \hat{U}^\dagger = \hat{g}' = \hat{g} + i\varepsilon \left[ \hat{W}, \hat{g} \right]. \quad (16) \]

The canonical transformation induced by (16) on the function \( g \) is

\[ U : g \rightarrow g' = g + \varepsilon \{ g, W \}, \quad (17) \]

where the generator function of the canonical transformation is \( W = \langle \psi | \hat{W} | \psi \rangle \).

Finally, we are interested in the basis of eigenvectors of the Hamiltonian \( \{|n\}\)\)

\[ \hat{H} |n\rangle = E_n |n\rangle. \quad (18) \]

We can write \(|\psi\rangle\) in terms of \(\{|n\}\) as

\[ |\psi\rangle = \sum_n \frac{1}{\sqrt{2}} (q_n + ip_n) |n\rangle, \]

\[ = \sum_n \sqrt{I_n} e^{-i\theta_n} |n\rangle, \quad (19) \]

where the variables \((\theta, I)\) are defined by

\[ q_n = \sqrt{2I_n} \cos \theta_n, \]

\[ p_n = -\sqrt{2I_n} \sin \theta_n. \quad (20) \]

In terms of variables (20), the Hamiltonian function reads

\[ H = \sum_n E_n \frac{q_n^2 + p_n^2}{2} \]

\[ = \sum_n E_n I_n. \quad (21) \]

The coordinates \((\theta, I)\) are a set of action-angle variables for \( H \). They are canonical variables

\[ \{\theta_k, I_l\} = \delta_{kl}, \]

\[ \{\theta_k, \theta_l\} = \{I_k, I_l\} = 0, \quad (22) \]

and they obey the Hamilton equations

\[ \frac{d\theta_k}{dt} = \frac{\partial H}{\partial I_k} = E_k, \]

\[ \frac{dI_k}{dt} = -\frac{\partial H}{\partial \theta_k} = 0. \quad (23) \]
In terms of the action-angle variables, the expectation value of any operator $\hat{A}$ can be written as

$$A(\theta, I) = \sum_{n,n'} \sqrt{I_n I_{n'}} A_{n'n} e^{i(\theta_{n'} - \theta_n)}$$  \hspace{1cm} (24)

where the matrix elements of $\hat{A}$ are given by $A_{n'n} = \langle n' | \hat{A} | n \rangle$.

These are all the results we need from the Hamiltonian version of quantum mechanics. We now proceed to introduce the VVP perturbation theory.

3 Van Vleck - Primas perturbation theory

Following [21][22], let us consider a quantum system described by a N-dimensional Hilbert space and a Hamiltonian operator given by

$$\hat{H} = \hat{H}_0 + \sum_{n=1}^{\infty} \varepsilon^n \hat{V}_n,$$  \hspace{1cm} (25)

where $\varepsilon$ is a small parameter. We assume that we know exactly the set of eigenvalues $\{E^0_n\}$ and eigenvectors $\{|n_0\rangle\}$ of $\hat{H}_0$

$$\hat{H}_0 |n_0\rangle = E^0_n |n_0\rangle.$$  \hspace{1cm} (26)

We also assume the spectrum of $\hat{H}_0$ and $\hat{H}$ to be non-degenerated for all the values of interest of $\varepsilon$.

The Van Vleck-Primas method consists in looking for a unitary operator

$$\hat{U} = \exp \left( i \hat{W} \right),$$  \hspace{1cm} (27)

such that

$$\hat{\tilde{H}} = \hat{U} \hat{H} \hat{U}^\dagger = \hat{H}_0 + \hat{K},$$  \hspace{1cm} (28)

$$[\hat{H}_0, \hat{K}] = [\hat{\tilde{H}}, \hat{K}] = 0.$$  \hspace{1cm} (29)

The operator $\hat{K}$ is called the shift operator because, as we will see, it has the effect of shifting the energy levels. If the unitary operator $\hat{U}$ exist and can be found, then the eigenvalues and eigenvectors of $\hat{H}$ are given by

$$E_n = E^0_n + \langle n | \hat{K} | n \rangle,$$

$$|n\rangle = \hat{U} |n_0\rangle.$$  \hspace{1cm} (30)-(31)

We are going to show a formal way to obtain $\hat{U}$ to all orders in $\varepsilon$. For now we are not going to worry about the convergence of the procedure. Let us start by noting that Eq.(28) can be expanded using the Baker-Campbell-Haussdorf lemma as follows
\[ \hat{H} = \hat{U} \hat{H} \hat{U}^\dagger = \hat{H}_0 + i \left[ \hat{W}, \hat{H} \right] - \frac{1}{2!} \left[ \hat{W}, \left[ \hat{W}, \hat{H} \right] \right] \]
\[ - \frac{i}{3!} \left[ \hat{W}, \left[ \hat{W}, \left[ \hat{W}, \hat{H} \right] \right] \right] \ldots \]
\[ = \sum_{n=0}^{\infty} \frac{i^n}{n!} D^n_{\hat{W}} (\hat{H}) , \quad (32) \]
where the superoperator \( D_{\hat{W}} \) is defined by
\[ D_{\hat{W}} = \left[ \hat{W}, \cdot \right] . \quad (33) \]
Moreover, we assume we can expand \( \hat{K} \) and \( \hat{W} \) in a power series as
\[ \hat{W} = \epsilon \hat{W}_1 + \epsilon^2 \hat{W}_2 + \epsilon^3 \hat{W}_3 + \ldots , \]
\[ \hat{K} = \epsilon \hat{K}_1 + \epsilon^2 \hat{K}_2 + \epsilon^3 \hat{K}_3 + \ldots . \quad (34) \]
Inserting Eqs. (32) and (34) in Eq. (28), the following equation is obtained
\[ \hat{H}_0 + \sum_{n=1}^{\infty} \epsilon^n \hat{K}_n = \sum_{k=0}^{\infty} \frac{i^n}{n!} D^n_{\hat{W}} \left( \hat{H}_0 + \sum_{n=1}^{\infty} \epsilon^n \hat{V}_n \right) . \quad (35) \]
Equating terms of the same order in \( \epsilon \) in Eq. (35), it is possible to write the following equations
\[ i \left[ \hat{H}_0, \hat{W}_n \right] = \hat{\Psi}_n - \hat{K}_n , \quad (36) \]
where the first three \( \hat{\Psi} \) are given by
\[ \hat{\Psi}_1 = \hat{V}_1 \]
\[ \hat{\Psi}_2 = \hat{V}_2 - \frac{1}{2} \left[ \hat{W}_1, \left[ \hat{W}_1, \hat{H}_0 \right] \right] + i \left[ \hat{W}_1, \hat{V}_1 \right] \]
\[ \hat{\Psi}_3 = \hat{V}_3 - \frac{1}{2} \left[ \hat{W}_2, \left[ \hat{W}_1, \hat{H}_0 \right] \right] - \frac{1}{2} \left[ \hat{W}_1, \left[ \hat{W}_2, \hat{H}_0 \right] \right] \]
\[ - \frac{i}{6} \left[ \hat{W}_1, \left[ \hat{W}_1, \left[ \hat{W}_1, \hat{H}_0 \right] \right] \right] + i \left[ \hat{W}_2, \hat{V}_1 \right] \]
\[ - \frac{1}{2} \left[ \hat{W}_1, \hat{V}_1 \right] + i \left[ \hat{W}_2, \hat{V}_2 \right] . \quad (37) \]
The Eqs. (36) can be simplified further. Let the parallel-projection linear superoperator \( \pi \) be defined by giving its action on an arbitrary \( \hat{X} \) as
\[ \pi(\hat{X}) = \sum_{n=1}^{N} \langle n_0 | \hat{X} | n_0 \rangle | n_0 \rangle \langle n_0 | . \quad (38) \]
Any arbitrary operator \( \hat{X} \) will commute with \( \hat{H}_0 \) if and only if \( \pi(\hat{X}) = \hat{X} \). Moreover, the following identity can be shown to always hold true for any \( \hat{X} \),

\[
\pi \left( \left[ \hat{H}_0, \hat{X} \right] \right) = 0. \tag{39}
\]

Since the shift operator is defined by Eq. (29) to commute with \( \hat{H}_0 \), we can use the linearity of \( \pi \) and the identity (39) to take the parallel-projection of Eq. (36) and obtain the following

\[
\pi \left( \hat{K}_n \right) = \hat{K}_n = \pi \left( \hat{\Psi}_n \right). \tag{40}
\]

Hence, Eq (40) reduces to

\[
i \left[ \hat{H}_0, \hat{W}_n \right] = \hat{\Psi}_n - \pi \left( \hat{\Psi}_n \right). \tag{41}
\]

Notice that it is necessary to solve Eqs. (41) in ascending order. To find \( \hat{W}_n \), all the \( \hat{W}_i \) from \( \hat{W}_1 \) to \( \hat{W}_{n-1} \) have first to be known.

To end this section, we point out that the operation \( \pi \left( \hat{\Psi}_n \right) \) can be written as a time average in the following way [30]

\[
\pi \left( \hat{\Psi}_n \right) = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\infty dt \, e^{-i\hat{H}_0 t} \hat{\Psi}_n e^{i\hat{H}_0 t}. \tag{42}
\]

\[
\hat{W}_n = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\infty dt \int_0^t ds \, e^{-i\hat{H}_0 s} \left( \hat{\Psi}_n - \pi \left( \hat{\Psi}_n \right) \right) e^{i\hat{H}_0 s}
\]

\[
= -i \sum_{k \neq k'} \frac{\langle k_0 | \hat{\Psi}_n | k'_0 \rangle}{E_{k}^{0} - E_{k'}^{0}} | k_0 \rangle \langle k_0 |. \tag{43}
\]

4 Quantum perturbation as a classical theory

We define a “classical” function of the Hamiltonian operator (25) by taking its expectation value according to the rule given by Eq. (8). We can take the expectation value \( H = \langle \psi | \hat{H} | \psi \rangle \) using \( | \psi \rangle = \sum_n \sqrt{I_{n}^{(0)}} e^{-i\theta_{k}^{(0)}} | n_{0} \rangle \). The expectation value of \( \hat{H} \) reads

\[
H(I, \theta) = H_0 + \sum_{n=1}^{\infty} \varepsilon^n \langle \psi | \hat{V}_n | \psi \rangle
\]

\[
= \sum_{k=1}^{N} E_{n}^{0} \left( \frac{(q_{k}^{0})^2 + (p_{k}^{0})^2}{2} \right) + \sum_{n=1}^{\infty} \varepsilon^n V_n(q^0, p^0)
\]

\[
= \sum_{k=1}^{N} E_{n}^{0} I_{n}^{(0)} + \sum_{n=1}^{\infty} \varepsilon^n V_n(I^{(0)}, \theta^{(0)}). \tag{44}
\]
A classical system described by a Hamiltonian of the form of Eq. (44) is said to be quasiharmonic. The energies $E_0^n$ play the role of frequencies of the unperturbed oscillators. There is no problem if the energies (frequencies) are negative numbers. However, in what follows we cannot allow any $E_0^n$ to vanish. This does not present a problem since, without changing the quantum dynamics, we can always redefine $\hat{H}_0$ by adding to it a constant multiple of the identity so that no energy is equal to zero.

The goal of classical Hamiltonian perturbation theory is to find a time-independent canonical transformation into a new set of action-angle variables

$$T: (\theta^{(0)}, I^{(0)}) \rightarrow (\theta, I),$$  \hspace{1cm} (45)$$

such that the perturbed Hamiltonian becomes a function only of the new actions\footnote{Here we use the conservation of the Hamiltonian under time-independent canonical transformation.} $H^* (I) = H (\theta, I)$. \hspace{1cm} (46)

Here and hereafter, the $^*$ will remind us that the function involved have to be considered as a function of the new action-angle variables i.e., $f^* (\theta, I, I^{(0)}) (\theta, I, I^{(0)})$. Now, If such transformation can be found, the Hamilton equations of motion become

$$\frac{d\theta_i}{dt} = \frac{\partial H^*}{\partial I_i} = E_i,$$

$$\frac{dI_i}{dt} = -\frac{\partial H^*}{\partial \theta_i} = 0.$$  \hspace{1cm} (47)

Staying within the classical formalism, the canonical transformation that allows a solution\footnote{By a solution we mean a formal solution. Classical perturbation theory is famous for its problem with small denominators that can cause terms in perturbation expansion to diverge.} of the perturbed Hamiltonian can be investigated using Lie series. However, we already know the unitary transformation that solves the quantum problem, at least formally. The associated canonical transformation of the unitary operator (27) is the solution to the classical problem (46), as we shall see. The vector $|\psi\rangle$ can be written in the basis given by Eq.(31) as

$$|\psi\rangle = \sum_n \sqrt{I_n} e^{-i\theta_n} |n\rangle = \sum_n \sqrt{I_n} e^{-i\theta_n} (\hat{U} |n_0\rangle).$$

Hence, Taking the expectation value of $\hat{H}$ in this basis would give

$$H^* = \sum_{n=1}^{N} E_n \left( \frac{q_k^2 + p_k^2}{2} \right) = \sum_{n=1}^{N} E_n I_n,$$  \hspace{1cm} (48)$$

where the perturbed energies $E_n$ are given by Eq. (30). The Eq. (48) correspond to the desired Hamiltonian function (46). The Eq. (48) is said to be the Birkhoff normal form of $H^*$. As $\hat{H}$ should always be diagonalizable, there should always
exist variables \((\theta, I)\) such that \(H^*\) can be put in normal form. This is, \(\hat{H}\) is always integrable in the Liouville-Arnold sense.

The concept of resonance in the frequencies is of fundamental importance in classical perturbation theories. The non-degeneracy of the quantum Hamiltonian means that \(E_n^0 \neq E_m^0\). In the classical jargon it is said that there is no trivial degeneracy in the energies (frequencies). The energies are called to be non-resonant if for all integers \(k_n\) (not all equal to zero) we have that

\[
k \cdot E^0 = \sum_{n=1}^{N} k_n E_n^0 \neq 0.
\]  

On the other hand, a resonance is called of order \(l\) when there exist a vector of integers \(k\) such that

\[
k \cdot E^0 = 0, \\
\sum_{n=1}^{N} |k_n| = l.
\]

If the system does not have any resonance of order \(l\) or lower, the Birkhoff normalization theorem guarantees that we can put \(H\) in a normal form up to remaining terms of order \(l + 1\)

\[
H^* = \sum_{n=1}^{N} E_n I_n + \sum_{n=1}^{l} H^*_n(I) + \mathcal{O}(l + 1).
\]

In the case considered in this work, i.e., the case of a Hamiltonian function that comes from the expectation value of an operator, we will see that there is no need to pay attention to possible resonances in the energies due to the restricted form of the perturbation potentials.

We will now translate the Van Vleck-Primas quantum algorithm into the classical Hamiltonian formalism. Let us note that the expectation value of Eq.(32) can be written as

\[
H^* = \sum_{n=0}^{\infty} \frac{1}{n!} \mathcal{D}_W^n (H),
\]

where \(H^* = \langle \psi | \hat{H} | \psi \rangle\), \(\mathcal{D}_W = \{ , W^* \}\), and the generator of the canonical transformation is \(W^* = \langle \psi | \hat{W} | \psi \rangle\). Both sides of Eq.(51) can be expanded in power series to get a perturbation procedure. Alternatively, we can just take the expectation value of Eqs.(30) to get the set of equations

\[
\{ W_n^*, H_0 \} = \Psi_n - \langle \Psi_n \rangle,
\]
where
\[
\Psi_n = \langle \psi | \hat{\Psi}_n | \psi \rangle, \quad (53)
\]
\[
\langle \Psi_n \rangle = \langle \psi | \pi \left( \hat{\Psi}_n \right) | \psi \rangle. \quad (54)
\]

The Eqs. (52) are known in the classical context as the homological equations [27]. The functions \( \Psi_k \) obtained as expectation values coincide with the ones found using Hori’s classical procedure [24, 27]. The first three \( \Psi \) functions are
\[
\Psi_1 = V_1, \\
\Psi_2 = V_2 + \{ V_1, W_1^* \} + \frac{1}{2} \{ \{ H_0, W_1^* \}, W_1^* \}, \\
\Psi_3 = V_3 + \{ V_2, W_1^* \} + \{ V_1, W_2^* \} + \frac{1}{2} \{ \{ V_1, W_1^* \}, W_1^* \} \\
+ \frac{1}{2} \{ \{ H_0, W_1^* \}, W_2^* \} + \frac{1}{2} \{ \{ H_0, W_2^* \}, W_1^* \} \\
+ \frac{1}{6} \{ \{ H_0, W_1^* \}, W_1^* \}, W_1^* \}. \quad (55)
\]

We point out that in Eqs. (52) and (55) the functions \( H_0 \) and \( V_n \) are to be read as functions of \((\theta, I)\) in the same way as they originally depended on \((\theta^{(0)}, I^{(0)})\).

Let us note that, using Eq. (24), the functions \( \Psi_n \) can be written as
\[
\Psi_n(\theta, I) = \sum_{n,n'} \sqrt{I_n I_{n'}} \langle n' | \hat{\Psi}_n | n \rangle e^{i(\theta_{n'} - \theta_n)}. \quad (56)
\]

It remains for us to find an expression for \( \langle \Psi_n \rangle \). Using the definition (42), we can write
\[
\langle \Psi_n \rangle = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau \langle \psi | e^{-iH_0 t} \hat{\Psi}_n e^{iH_0 t} | \psi \rangle dt \\
= \sum_{n,n'} \sqrt{I_n I_{n'}} \langle n' | \hat{\Psi}_n | n \rangle. \quad (57)
\]

The time average (57) can be transformed from a time average into a space average over a torus without changing the value of \( \langle \Psi_n \rangle \), though generally a non-resonance condition is needed to guarantee the equality of the time average and the space average (page 286 of [23]). As a space average, \( \langle \Psi_n \rangle \) reads
\[
\langle \Psi_n \rangle = \frac{1}{(2\pi)^N} \int_0^{2\pi} \cdots \int_0^{2\pi} \Psi_n(\theta, I) d\theta_1 \cdots d\theta_N. \quad (58)
\]
Now, let us note that, as a function of the new variables \((\theta, I)\), the unperturbed Hamiltonian reads \(H_0 = \sum_{n=1}^{N} E_n I_n\). This means that Eq. (52) can be simplified to be

\[
\sum_{n=1}^{N} E_n \frac{\partial W_n^*}{\partial \theta_{\mu}} = \Psi_n - \langle \Psi_n \rangle .
\] (59)

The Eq. (59) can be solved by taking the Fourier expansion of \(\Psi_n - \langle \Psi_n \rangle = \sum_k A_{n,k} e^{i k \cdot \vec{\theta}}\). The solution is

\[
W_n^* = - \sum_k \frac{A_{n,k} e^{i k \cdot \vec{\theta}}}{k \cdot E^0} .
\] (60)

We can see that Eq. (60) has a small divisor problem if the energies are resonant for some \(k\) unless \(A_{n,k}\) vanishes for such \(k\). There will be no diverging terms in Eq. (60) in the non-degenerate case at hand. Indeed, we can see from Eqs. (56) and (57) that

\[
W_n^* = - \sum_{n \neq n'} \sqrt{T_n T_{n'}} \langle n' | \hat{\Psi}_n | n \rangle \frac{\Psi_n}{E_n^0 - E_{n'}^0} e^{i(\theta_{n'} - \theta_n)}. \] (61)

The Eq. (61) completes our recasting of VVP perturbation theory into a classical formalism. As there is a one-to-one correspondence between an Hermitian operator and the real-valued function defined by Eq. (53), the quantum problem will be solved if the classical generators functions are known. Given \(W_n^*\), the matrix elements of \(\hat{W}_n\) can be read using the relation (24).

To finish, let us say that if the energies do not have a resonance of any order, the integrability of Hamiltonian (44) implies the convergence of classical perturbation series (and therefore, the original quantum one) [31].

5 Conclusions

We have shown that the Van Vleck-Primas quantum perturbation theory can be recast into the formalism of classical Lie-series. The requirement for our procedure was that the Hamiltonian operator has a finite, discrete, and non-degenerate spectrum. On the other hand, complete non-resonance in the energies guarantees the convergence of the classical (and therefore, the quantum) perturbation series.

\*Notice that the effect of \(\langle \Psi_n \rangle\) is to eliminate the secular terms from \(\Psi_n\).
It is not a priori evident what advantages would bring to give a classical perturbation treatment to a given quantum problem. Though, this might be due to our neglect of degeneracy and resonance. The classical perturbation theory has a rich history of dealing with these issues, mainly due to the particularities of the gravitational interaction in celestial mechanics. For example, there are the Von Zeipel-Brouwer and Bohlin theories (see [27] for an exposition of both theories and a large list of references). We can also mention the convergence theorems of the Birkhoff normalization even for resonant cases [32, 33, 34]. We hope that new procedures to deal with resonances in quantum systems can be developed by taking into consideration the classical techniques.

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