Beyond the Quantum Adiabatic Approximation: Adiabatic Perturbation Theory

Gustavo Rigolin,[1,*] Gerardo Ortiz,[1,†] and Víctor Hugo Ponce[2]

[1] *Department of Physics, Indiana University, Bloomington, IN 47405, USA*
[2] *Centro Atómico Bariloche and Instituto Balseiro, Com. Nac. de Energía Atómica and Univ. Nac. de Cuyo, 8400 Bariloche, Argentina*

(Dated: November 19, 2009)

We introduce a perturbative approach to solving the time dependent Schrödinger equation, named adiabatic perturbation theory (APT), whose zeroth order term is the quantum adiabatic approximation. The small parameter in the power series expansion of the time-dependent wave function is the inverse of the time it takes to drive the system's Hamiltonian from the initial to its final form. We review other standard perturbative and non-perturbative ways of going beyond the adiabatic approximation, extending and finding exact relations among them, and also compare the efficiency of those methods against the APT. Most importantly, we determine APT corrections to the Berry phase by use of the Aharonov-Anandan geometric phase. We then solve several time dependent problems allowing us to illustrate that the APT is the only perturbative method that gives the right corrections to the adiabatic approximation. Finally, we propose an experiment to measure the APT corrections to the Berry phase and show, for a particular spin-1/2 problem, that to first order in APT the geometric phase should be two and a half times the (adiabatic) Berry phase.

PACS numbers: 31.15.xp, 03.65.Vf
Keywords: Perturbation theory; Phases: geometric; dynamic or topological

I. INTRODUCTION

Aside from interpretation, Quantum Mechanics (QM) is undoubtedly one of the most successful and useful theories of modern Physics. Its practical importance is evidenced at microscopic and nano scales where Schrödinger's Equation (SE) dictates the evolution of the system's state, i.e., its wave function, from which all the properties of the system can be calculated and confronted against experimental data. However, SE can only be exactly solved for a few problems. Indeed, there are many reasons that make the solution of such a differential equation a difficult task, such as the large number of degrees of freedom associated with the system one wants to study. Another reason, the one we want to address in this paper, is related to an important property of the system's Hamiltonian: its time dependence.

For time independent Hamiltonians the solution to SE can be cast as an eigenvalue/eigenvector problem. This allows us to solve SE in many cases exactly, in particular when we deal with systems described by finite dimensional Hilbert spaces. For time dependent Hamiltonians, on the other hand, things are more mathematically involved. Even for a two-level system (a qubit) we do not, in general, obtain a closed-form solution given an arbitrary time dependent Hamiltonian, although a general statement can be made for slowly varying Hamiltonians. If a system's Hamiltonian $\mathbf{H}$ changes slowly during the course of time, say from $t = 0$ to $t = T$, and the system is prepared in an eigenstate of $\mathbf{H}$ at $t = 0$, it will remain in the instantaneous (snapshot) eigenstate of $\mathbf{H}(t)$ during the interval $t \in [0, T]$. This is the content of the well-known adiabatic theorem [1].

But what happens if $\mathbf{H}(t)$ is not slowly enough varied? For how long can we still consider the system to be in a snapshot eigenstate of $\mathbf{H}(t)$, i.e., for how long the adiabatic approximation is reliable? What are the corrections to the adiabatic approximation? One of our goals in this manuscript is to provide practical and useful answers to these questions. We introduce a perturbative expansion about the adiabatic approximation, named adiabatic perturbation theory (APT), using the quantity $v = 1/T$ as our small parameter. This power series expansion in v is subsequently used to calculate corrections to the adiabatic approximation for several time dependent two-level systems. It is worth noting that answers to previous questions can also be seen, under certain provisos, as a way of solving perturbatively any time dependent problem. We should stress that the APT is not related to the time-ordered Dyson series method since the latter is not a perturbative expansion about the adiabatic approximation, in terms of the small parameter v. Rather, it is an iterative way of getting the unitary operator governing the evolution of a system, in terms of a small perturbative potential in the Hamiltonian.

Another goal is to present an exhaustive comparison of all the approximation methods developed so far to solving SE. In particular, we show the exact equivalence between Garrison's multi-variable expansion method [2] (which solves an extended set of partial differential equations) and APT. However, it is important to stress that the APT, being an algebraic method, is straightforward to use while Garrison's approach is very hard to extend beyond first order. We also provide an extension to Berry's iterative method [3] where, contrary to the original ap-

*Electronic address: rigoling@indiana.edu
†Electronic address: ortizg@indiana.edu

proach, we keep all terms of the new Hamiltonian obtained after each iteration. We then discuss the possibility to choose other types of iteration (unitary transformations) to potentially do better than Berry's prescription.

Furthermore, it is known that if the conditions of the adiabatic theorem are satisfied and $\mathbf{H}(T) = \mathbf{H}(0)$, it follows that the state $|\Psi(T)\rangle$ describing the system at $t = T$ is given by $|\Psi(T)\rangle = \mathrm{e}^{\mathrm{i}\phi(T)}|\Psi(0)\rangle$, where $|\Psi(0)\rangle$ is the initial state and $\phi(T)$ is a phase that can be split into dynamical and geometrical parts [4]. This raises another question we address here and which is not independent from the ones above: what are the corrections to the Berry phase [4] as the system deviates from the adiabatic approximation? To provide an answer we make use of the Aharonov-Anandan (AA) geometric phase [5], which is a natural extension of the Berry phase having a geometric meaning whenever the initial state returns to itself, even for a non-adiabatic evolution. We thus compute the AA phase for the corrections to the adiabatic approximation which, therefore, possess the geometrical and gauge invariance properties of any AA phase. We then show, for a particular spin-1/2 example, that whenever $\mathbf{H}(T) = \mathbf{H}(0)$ and the evolving state corrected up to first order returns to itself (up to a phase) at $t = T$, we obtain a geometric phase that is two and a half Berry's phase value.

In order to provide a clear and complete analysis of the questions raised above we structure our paper as follows. (See Fig. 1 for a structural flowchart of the paper.) In

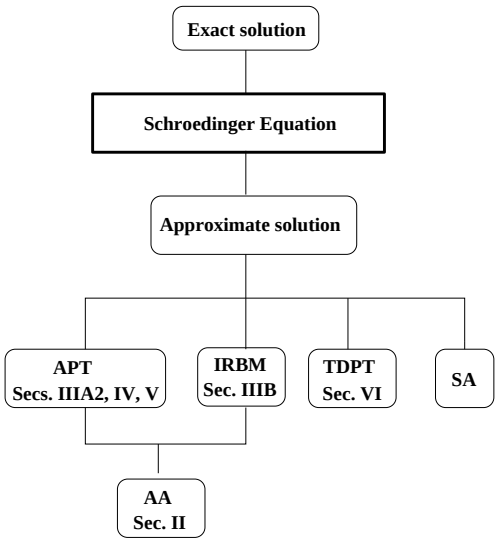

FIG. 1: Different approximation methods to solving the time-dependent Schödinger equation. APT: Adiabatic perturbation theory (Garrison, Ponce, this paper); IRBM: Iterative rotating-basis method (Kato, Garrido, Nenciu, Berry); TDPT: Time-dependent perturbation theory (Dirac); SA: Sudden approximation (Messiah); AA: Adiabatic approximation (Born and Fock).

Sec. II we review the adiabatic approximation, highlighting the conditions that the snapshot eigenvectors and eigenvalues of $\mathbf{H}(t)$ must satisfy for this approximation to be valid. In Sec. III we review many strategies that may be employed to find corrections to the adiabatic approximation as well as to the Berry phase. As shown later, those methods are unsatisfactory since either they do not furnish all the terms that correct the geometrical phase and the adiabatic approximation or they cannot be seen as a perturbation in terms of the small parameter $v = 1/T$. In Sec. IV we present our perturbation method, i.e. APT, in its full generality and provide explicit corrections to the adiabatic approximation up to second order. In Sec. V we deal with corrections to the geometric phase using the previous method, presenting its first order correction. In Sec. VI we compare all other methods with the APT, emphasizing the main differences among them. In Sec. VII we review the exact and analytical solution of a time dependent problem and expand it in terms of the small parameter v. Then we show that our perturbative method is the only one that gives all the terms obtained from the expansion of the exact solution. We also propose an experiment where APT corrections to the Berry can be measured. In Sec. VIII we solve numerically three other time dependent problems and compare them with our perturbative method. Finally, in Sec. IX we provide our concluding remarks.

II. THE ADIABATIC APPROXIMATION

Let us start rewriting the time dependent SE in terms of the rescaled time $s = v\,t$, where $T = 1/v$ is the relevant time scale of our Hamiltonian $\mathbf{H}(t)$. We then formally solve the SE, emphasizing the assumptions imposed on the spectrum of $\mathbf{H}(t)$, and show the conditions the instantaneous (snapshot) eigenvectors of $\mathbf{H}(t)$ must satisfy for the adiabatic approximation to be valid.

The time dependent SE is written as

$$\mathrm{i}\,\hbar\,\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = \mathbf{H}(t)|\Psi(t)\rangle, \tag{1}$$

where $|\Psi(t)\rangle$ is the state describing our system at time t. Since we want to work with the rescaled time s and $\frac{\mathrm{d}}{\mathrm{d}t} = v\,\frac{\mathrm{d}}{\mathrm{d}s}$ it results

$$\mathrm{i}\,\hbar\,v\,\frac{\mathrm{d}}{\mathrm{d}s}|\Psi(s)\rangle = \mathbf{H}(s)|\Psi(s)\rangle. \tag{2}$$

Building on the knowledge that the adiabatic phase can be split into a geometrical (γ) and a dynamical (ω) part [4] we may write down the solution $|\Psi(s)\rangle$ as

$$|\Psi(s)\rangle = \sum_{n=0} \mathrm{e}^{\mathrm{i}\gamma_n(s)}\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)}b_n(s)|n(s)\rangle, \tag{3}$$

in which $b_n(s)$ are time dependent coefficients to be determined later on. The sum over n includes all snapshot eigenvectors of $\mathbf{H}(s)$,

$$\mathbf{H}(s)|n(s)\rangle = E_n(s)|n(s)\rangle, \tag{4}$$

with eigenvalue $E_n(s)$ ($n=0$ represents its ground state (GS)). The Berry phase associated to the eigenvector $|n(s)\rangle$ is

$$\gamma_n(s) = \mathrm{i}\int_0^s \langle n(s')|\frac{\mathrm{d}}{\mathrm{d}s'}n(s')\rangle \mathrm{d}s' = \mathrm{i}\int_0^s M_{nn}(s')\mathrm{d}s', \quad (5)$$

while

$$\omega_n(s) = \frac{1}{\hbar}\int_0^s E_n(s')\mathrm{d}s' = v\,\omega_n(t) \quad (6)$$

defines its dynamical phase. Let us start assuming that $\mathbf{H}(s)$ has a non-degenerate spectrum during the whole evolution. Note that the initial ($s=0$) conditions on $|\Psi(s)\rangle$ are encoded in $b_n(0)$. Therefore, if the initial state is $|0(0)\rangle$ we will have $b_n(0)=\delta_{n0}$, where δ_{ij} is the Kronecker delta. In this case, as we will see below, the spectrum needs to satisfy the less restrictive condition $E_0(s)\neq E_n(s)$, $\forall s\in[0,T]$, $n\neq 0$, for our perturbation method to work. In other words, our method will work whenever one starts the evolution at the GS and there is no level crossing between $E_0(s)$ and any other $E_n(s)$ (even though the excited state part of the spectrum may display level crossings). Similar type of conditions can be shown to apply to states living in subspaces spectrally separated from the rest.

Replacing Eq. (3) into (2) using Eq. (4) and left multiplying it by $\langle m(s)|$ leads to

$$\dot{b}_n(s) + \sum_{\substack{m=0\\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}(s)}\mathrm{e}^{\mathrm{i}\gamma_{mn}(s)}M_{nm}(s)b_m(s) = 0, \quad (7)$$

where the dot means $\frac{\mathrm{d}}{\mathrm{d}s}$ and the indices $m\leftrightarrow n$ were exchanged. Here $\omega_{mn}(s)=\omega_m(s)-\omega_n(s)$, $\gamma_{mn}(s)=\gamma_m(s)-\gamma_n(s)$, and

$$M_{nm}(s) = \langle n(s)|\dot{m}(s)\rangle. \quad (8)$$

So far no approximation was invoked and in principle the time dependence can be found by solving the system of coupled differential equations given in (7). General numerical methods to solve such equations will face the computational difficulty of integrating highly oscillatory terms such as $\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}(s)}\mathrm{e}^{\mathrm{i}\gamma_{mn}(s)}$, making the approach numerically unstable. Later on we show that our perturbative method gets rid of this problem.

The adiabatic approximation consists in neglecting the coupling terms (7), i.e., setting $M_{nm}(s)=0$,

$$b_n(s) = b_n(0) \longrightarrow \textsf{adiabatic approximation}. \quad (9)$$

Replacing Eq. (9) into (3) we obtain,

$$|\Psi^{(0)}(s)\rangle = \sum_{n=0}\mathrm{e}^{\mathrm{i}\gamma_n(s)}\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)}b_n(0)|n(s)\rangle, \quad (10)$$

where we used $|\Psi^{(0)}(s)\rangle$ instead of $|\Psi(s)\rangle$ since the adiabatic approximation will be the zeroth order term in the perturbative method developed later. In the case the system starts at the GS,

$$|\Psi^{(0)}(s)\rangle = \mathrm{e}^{\mathrm{i}\gamma_0(s)}\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_0(s)}|0(s)\rangle. \quad (11)$$

For the sake of completeness, let us analyze some general properties of $M_{nm}(s)$. Since the eigenvectors of $\mathbf{H}(s)$ are orthonormal we have $\langle n(s)|m(s)\rangle=\delta_{nm}$. Taking the derivative with respect to s we get $M_{nm}(s)+M^*_{mn}(s)=0$, which implies that $M_{nn}(s)$ is a purely imaginary number, as it should be since $\gamma_n(s)$ is real. When $n\neq m$, by taking the derivative of Eq. (4) with respect to s and left multiplying by $\langle m(s)|$ one gets

$$M_{nm}(s) = \langle n(s)|\dot{\mathbf{H}}(s)|m(s)\rangle/\Delta_{mn}(s), \quad (12)$$

where $\Delta_{mn}(s)=E_m(s)-E_n(s)$. This last expression indicates that the adiabaticity condition is related to the existence of a gap. A spectrum of discussions on the validity of the adiabatic approximation can be found in Refs. [6, 7, 8, 9, 10].

III. CORRECTIONS TO THE ADIABATIC APPROXIMATION

We can classify all the strategies to find corrections to the adiabatic approximation into two groups. The first one includes those methods that perform a series expansion of the wave function in terms of the small parameter $v=1/T\ll 1$, with T representing the time scale for adiabaticity. In this group we include the pioneering approach of Garrison [2] and the seminal work of Ponce *et al.* [11]. The second group includes those methods that intend to approximate the solution to the time dependent SE without relying on a formal series expansion of the wave function [3, 12, 13, 14] but using the adiabatic approximation as their zeroth-order step. In this section we review two methods belonging to the first group and one to the second, called *adiabatic iteration* by Berry [3]. We then comment on a possible extension of the latter.

A. Examples of the first group

We first show how to manipulate Eq. (7) in order to get a series expansion in terms of the small parameter v, which we call the *standard* (textbook) approach. We then discuss the *multi-variable expansion method* of Garrison [2], who also dubbed it APT.

1. The standard approach

One can formally integrate Eq. (7) to obtain

$$b_n(s) = b_n(0) - \sum_{\substack{m=0\\ m\neq n}}\int_0^s \mathrm{d}s'\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}(s')}B_{mn}(s'), \quad (13)$$

where

$$B_{mn}(s) = \mathrm{e}^{\mathrm{i}\gamma_{mn}(s)} M_{nm}(s) b_m(s). \tag{14}$$

The integral inside the sum in Eq. (13) can be written as

$$I = \int_0^s \mathrm{d}s' B_{mn}(s') \mathrm{e}^{\frac{1}{v}\int_0^{s'} \mathrm{d}s'' C_{mn}(s'')}, \tag{15}$$

in which $C_{mn}(s) = -\mathrm{i}\Delta_{mn}(s)/\hbar$. Our goal here is to expand I in powers of v. This can be done by using the mathematical identity

$$B_{mn}(s)\mathrm{e}^{\frac{1}{v}\int_0^s \mathrm{d}s' C_{mn}(s')} = \frac{\mathrm{d}}{\mathrm{d}s}\left(v\frac{B_{mn}(s)}{C_{mn}(s)}\mathrm{e}^{\frac{1}{v}\int_0^s \mathrm{d}s' C_{mn}(s')}\right) - v\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{B_{mn}(s)}{C_{mn}(s)}\right)\mathrm{e}^{\frac{1}{v}\int_0^s \mathrm{d}s' C_{mn}(s')}. \tag{16}$$

Replacing Eq. (16) into (15) we arrive at

$$I = v\left(\frac{B_{mn}(s)}{C_{mn}(s)}\mathrm{e}^{\frac{1}{v}\int_0^s \mathrm{d}s' C_{mn}(s')} - \frac{B_{mn}(0)}{C_{mn}(0)}\right) - v\int_0^s \mathrm{d}s' \frac{\mathrm{d}}{\mathrm{d}s'}\left(\frac{B_{mn}(s')}{C_{mn}(s')}\right)\mathrm{e}^{\frac{1}{v}\int_0^{s'} \mathrm{d}s'' C_{mn}(s'')}. \tag{17}$$

One can apply the identity (16) again to the integrand of the last term by substituting $B_{mn}(s)$ for $v\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{B_{mn}(s)}{C_{mn}(s)}\right)$,

$$I = v\left(\frac{B_{mn}(s)}{C_{mn}(s)}\mathrm{e}^{\frac{1}{v}\int_0^s \mathrm{d}s' C_{mn}(s')} - \frac{B_{mn}(0)}{C_{mn}(0)}\right) - v^2\left(\frac{1}{C_{mn}(s)}\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{B_{mn}(s)}{C_{mn}(s)}\right)\mathrm{e}^{\frac{1}{v}\int_0^s \mathrm{d}s' C_{mn}(s')}\right)\Bigg|_0^s + \mathcal{O}(v^3), \tag{18}$$

with the symbol $\mathcal{O}(v^3)$ standing for the term

$$v^2\int_0^s \mathrm{d}s' \frac{\mathrm{d}}{\mathrm{d}s'}\left(\frac{-1}{C_{mn}(s')}\frac{\mathrm{d}}{\mathrm{d}s'}\left(\frac{B_{mn}(s')}{C_{mn}(s')}\right)\right)\mathrm{e}^{\frac{1}{v}\int_0^{s'} \mathrm{d}s'' C_{mn}(s'')}.$$

One can similarly continue the iteration to obtain higher order terms but the first two are already enough for our purposes. We should note that, strictly speaking, the procedure just described is not a genuine power series expansion in terms of the small parameter v. This is because to all *orders* we have a phase contribution ($C_{mn}(s)$ is purely imaginary) of the form $\mathrm{e}^{\frac{1}{v}\int_0^{s'} \mathrm{d}s'' C_{mn}(s'')}$. This term is related to the dynamical phase of our system and together with the Berry phase will play an important role in the APT developed in Sec. IV.

Using Eq. (18) in (13) and keeping terms up to first order in v we obtain after substituting the values of $B_{mn}(s)$ and $C_{mn}(s)$

$$\begin{aligned} b_n(s) &= b_n(0) - \mathrm{i}\hbar v \\ &\times \sum_{\substack{m=0 \\ m\neq n}} \left(\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}(s)}\mathrm{e}^{\mathrm{i}\gamma_{mn}(s)}\frac{M_{nm}(s)}{\Delta_{mn}(s)} b_m(s)\right)\Bigg|_0^s. \end{aligned} \tag{19}$$

Note that we have to solve this equation iteratively keeping terms up to first order in v. This is equivalent to replacing $b_m(s) \to b_m(0)$ at the right-hand side of (19),

$$\begin{aligned} b_n(s) &= b_n(0) - \mathrm{i}\hbar v \\ &\times \sum_{\substack{m=0 \\ m\neq n}} \left(\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}(s)}\mathrm{e}^{\mathrm{i}\gamma_{mn}(s)}\frac{M_{nm}(s)}{\Delta_{mn}(s)} b_m(0)\right)\Bigg|_0^s. \end{aligned} \tag{20}$$

Finally, substituting Eq. (20) into (3) we get the (unnormalized; normalization introduces higher order corrections in v) state that corrects the adiabatic approximation up to first order via the standard approach,

$$|\Psi(s)\rangle = |\Psi^{(0)}(s)\rangle + v|\Psi^{(1)}(s)\rangle + \mathcal{O}(v^2), \tag{21}$$

where $|\Psi^{(0)}(s)\rangle$ is given by Eq. (10) and

$$\begin{aligned} |\Psi^{(1)}(s)\rangle &= \mathrm{i}\hbar \sum_{\substack{n,m=0 \\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m(s)}\mathrm{e}^{\mathrm{i}\gamma_m(s)}\frac{M_{nm}(s)}{\Delta_{nm}(s)} b_m(0)|n(s)\rangle \\ &- \mathrm{i}\hbar \sum_{\substack{n,m=0 \\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)}\mathrm{e}^{\mathrm{i}\gamma_n(s)}\frac{M_{nm}(0)}{\Delta_{nm}(0)} b_m(0)|n(s)\rangle, \end{aligned} \tag{22}$$

with $\Delta_{mn}(s) = -\Delta_{nm}(s)$. If the system is at the GS at $s = 0$, $b_n(0) = \delta_{n0}$, and Eq. (22) reduces to

$$\begin{aligned} |\Psi^{(1)}(s)\rangle &= \mathrm{i}\hbar \sum_{n=1} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_0(s)}\mathrm{e}^{\mathrm{i}\gamma_0(s)}\frac{M_{n0}(s)}{\Delta_{n0}(s)}|n(s)\rangle \\ &- \mathrm{i}\hbar \sum_{n=1} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)}\mathrm{e}^{\mathrm{i}\gamma_n(s)}\frac{M_{n0}(0)}{\Delta_{n0}(0)}|n(s)\rangle, \end{aligned} \tag{23}$$

which displays no linear in v correction to the $|0(s)\rangle$ component (the sum starts at $n = 1$). As shown in Sec. IV, there is a missing term correcting the coefficient multiplying the GS that naturally appears in the APT. Also, $|\Psi^{(1)}(0)\rangle = 0$, as we would expect since we must recover the initial state $|\Psi^{(0)}(0)\rangle$ at $s = 0$.

2. *Multi-variable expansion method*

To obtain a time dependent multi-variable SE we consider the quantities $\omega_n(s)$ as independent variables, i.e. $\omega_n(s) \to \omega_n$ [2]. They are called *fast variables* in contrast to the rescaled time s, which is the *slow variable*. In this language the differential operator $v\frac{\mathrm{d}}{\mathrm{d}s}$ is replaced by $v\partial_s + D_w$, where

$$D_w = \sum_{n=0} \frac{E_n}{\hbar} v\ \partial_{w_n},$$

and the modified SE is written as,

$$\mathrm{i}\,\hbar\,(v\partial_s + D_w)\,|\Psi(s)\rangle = \mathbf{H}(s)|\Psi(s)\rangle. \tag{24}$$

To solve Eq. (24) we write the wave function as follows

$$|\Psi(s)\rangle = \sum_{n=0} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n} c_n(\omega, s)|n(s)\rangle, \tag{25}$$

where ω represents all the variables ω_n and

$$c_n(\omega, s) = \sum_{p=0}^{\infty} v^p c_n^{(p)}(\omega, s). \tag{26}$$

Note that $c_n(\omega, s)$ is written as a power series in v and our goal is to obtain $c_n^{(p)}(w, s)$ to all orders. Using Eq. (26) we can rewrite (25) as

$$|\Psi(s)\rangle = \sum_{n=0}\sum_{p=0}^{\infty} v^p \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n} c_n^{(p)}(\omega, s)|n(s)\rangle. \tag{27}$$

Substituting Eq. (27) in the modified SE (Eq. (24)), carrying out the derivatives, and taking the scalar product with $\langle m(s)|$ we get

$$\sum_{p=0}^{\infty} v^{p+1}\left(\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m}\partial_s c_m^{(p)}(\omega, s) + \sum_{n=0} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n} M_{mn}(s) c_n^{(p)}(\omega, s)\right) + \sum_{p=0}^{\infty} v^p \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m} D_\omega c_m^{(p)}(\omega, s) = 0. \tag{28}$$

Noting that the last term of the previous equality can be written as

$$\sum_{p=0}^{\infty} v^p \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m} D_\omega c_m^{(p)}(\omega, s) = \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m} D_\omega c_m^{(0)}(\omega, s) + \textstyle\sum_{p=0}^{\infty} v^{p+1} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m} D_\omega c_m^{(p+1)}(\omega, s),$$

we can rewrite Eq. (28) in the following form

$$\sum_{p=0}^{\infty} v^{p+1} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n}\left(D_\omega c_n^{(p+1)}(\omega, s) + \partial_s c_n^{(p)}(\omega, s) + \sum_{m=0} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} M_{nm}(s) c_m^{(p)}(\omega, s)\right) + \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n} D_\omega c_n^{(0)}(\omega, s) = 0, \tag{29}$$

where we have exchanged $n \leftrightarrow m$. A sufficient condition for the validity of Eq. (29) is obtained when we set

$$D_\omega c_n^{(0)}(\omega, s) = 0, \tag{30}$$

and

$$D_\omega c_n^{(p+1)}(\omega, s) + \partial_s c_n^{(p)}(\omega, s) + \sum_{m=0} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} M_{nm}(s) c_m^{(p)}(\omega, s) = 0. \tag{31}$$

Hence, we can calculate the coefficients $c_n^{(p)}(\omega, s)$ by solving the partial differential Eqs. (30) and (31). Note that to seek for the solution of order p we need to have the previous, $p-1$, order solution. Furthermore, as we increase the order, the partial differential equations become more cumbersome constituting a practical limitation of this method. The APT developed in Sec. IV, on the other hand, does not rely on any differential equations whatsoever. All corrections to the adiabatic approximation of order p are obtained via algebraic recursive relations that involve coefficients of order $p-1$. This will allow us to derive in a relative straightforward manner explicit expressions up to second order in the small parameter v.

In what follows we derive explicit expressions for $c_n^{(0)}(\omega, s)$ and $c_n^{(1)}(\omega, s)$. To zeroth-order Eq. (30) tells us that $c_n^{(0)}(\omega, s)$ does not depend on the variables ω, i.e., $c_n^{(0)}(\omega, s) = c_n^{(0)}(s)$. Moreover, since at $s = 0$ we have the initial condition $|\Psi(0)\rangle = \sum_{n=0} b_n(0)|n(0)\rangle$ then it immediately follows that $c_n^{(0)}(0) = b_n(0)$ and

$$c_n^{(p)}(0, 0) = 0, \qquad p \neq 0. \tag{32}$$

To have the adiabatic approximation as the zeroth order term in the power series solution we must have (cf.

Eq. (3) with (27))

$$c_n^{(0)}(s) = \mathrm{e}^{\mathrm{i}\gamma_n(s)} b_n(0), \tag{33}$$

which according to Eq. (31) leads to

$$D_\omega c_n^{(1)}(\omega,s) + \partial_s c_n^{(0)}(s) + M_{nn}(s) c_n^{(0)}(s) + \sum_{\substack{m=0 \\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} M_{nm}(s) c_m^{(0)}(s) = 0. \tag{34}$$

But Eq. (33) together with (5) imply that $\partial_s c_n^{(0)}(s) + M_{nn}(s) c_n^{(0)}(s) = 0$. Thus, Eq. (34) becomes

$$D_\omega c_n^{(1)}(\omega,s) + \sum_{\substack{m=0 \\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} \mathrm{e}^{\mathrm{i}\gamma_m(s)} M_{nm}(s) b_m(0) = 0, \tag{35}$$

and we now want to solve this equation.

Following Garrison [2] we write

$$c_n^{(p)}(\omega,s) = \bar{c}_n^{(p)}(s) + d_n^{(p)}(\omega,s), \tag{36}$$

with the assumption that (average over ω)

$$\langle d_n^{(p)}(\omega,s)\rangle_\omega = \langle D_\omega d_n^{(p)}(\omega,s)\rangle_\omega = 0. \tag{37}$$

In other words, we have separated out the ω and s dependence of $c_n^{(p)}$ into two contributions; the first depends only on s, and is called the average term; the second one depends on both ω and s, but with the additional condition that its average over the fast variables ω is zero. Thus, $\langle \bar{c}_n^{(p)}(s)\rangle_\omega = \bar{c}_n^{(p)}(s)$. Substituting Eq. (36) into (35) we get

$$D_\omega d_n^{(1)}(\omega,s) + \sum_{\substack{m=0 \\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} \mathrm{e}^{\mathrm{i}\gamma_m(s)} M_{nm}(s) b_m(0) = 0, \tag{38}$$

and solving for $d_n^{(1)}$ we obtain

$$d_n^{(1)}(\omega,s) = \mathrm{i}\hbar \sum_{\substack{m=0 \\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} \mathrm{e}^{\mathrm{i}\gamma_m(s)} \frac{M_{nm}(s)}{\Delta_{nm}(s)} b_m(0). \tag{39}$$

Note that $d_n^{(1)}(\omega,s) + \alpha(s)$, with $\alpha(s)$ independent of the variables ω, is also a solution of Eq. (38). However, since we imposed that $\langle d_n^{(p)}(\omega,s)\rangle_\omega = 0$, the only possible value for $\alpha(s)$ is zero.

If the initial state is $|0(0)\rangle$ ($b_n(0) = \delta_{n0}$) one gets

$$d_n^{(1)}(\omega,s) = \mathrm{i}\hbar \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{0n}} \mathrm{e}^{\mathrm{i}\gamma_0(s)} \frac{M_{n0}(s)}{\Delta_{n0}(s)} (1-\delta_{n0}), \tag{40}$$

and since $\langle d_n^{(p)}(\omega,s)\rangle_\omega = 0$ and the only dependence on ω in Eq. (39) is in $\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}}$ we get

$$\langle \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}}\rangle_\omega = \delta_{nm}. \tag{41}$$

We are now able to determine the average term $\bar{c}_n^{(1)}(s)$. Inserting Eq. (36) into (31) we get for $p=1$,

$$D_\omega d_n^{(2)}(\omega,s) + \partial_s d_n^{(1)}(\omega,s) + \partial_s \bar{c}_n^{(1)}(s) + M_{nn}(s) d_n^{(1)}(\omega,s) + M_{nn}(s)\bar{c}_n^{(1)}(s) + \sum_{\substack{m=0 \\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} M_{nm}(s) d_m^{(1)}(\omega,s) + \sum_{\substack{m=0 \\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} M_{nm}(s)\bar{c}_m^{(1)}(s) = 0,$$

where we have used that $D_\omega c_n^{(2)}(s) = 0$. Averaging over ω, and noticing that $\langle D_\omega d_n^{(2)}(w,s)\rangle_\omega = \langle d_n^{(1)}(\omega,s)\rangle_\omega = 0$, $\langle \partial_s d_n^{(1)}(\omega,s)\rangle_\omega = \partial_s \langle d_n^{(1)}(\omega,s)\rangle_\omega = 0$, and using Eq. (41) we obtain

$$\partial_s \bar{c}_n^{(1)}(s) + M_{nn}(s)\bar{c}_n^{(1)}(s) + \sum_{\substack{m=0 \\ m\neq n}} M_{nm}(s) \langle \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} d_m^{(1)}(\omega,s)\rangle_\omega = 0. \tag{42}$$

We can recast the average (using Eq. (39)) as

$$\langle \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} d_m^{(1)}(\omega,s)\rangle_\omega = \mathrm{i}\hbar \sum_{\substack{k=0 \\ k\neq m}} \frac{M_{mk}(s)}{\Delta_{mk}(s)} \mathrm{e}^{\mathrm{i}\gamma_k(s)} \langle \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{kn}}\rangle_\omega b_k(0) = \mathrm{i}\hbar \frac{M_{mn}(s)}{\Delta_{mn}(s)} \mathrm{e}^{\mathrm{i}\gamma_n(s)} b_n(0), \tag{43}$$

in which we have used that $\omega_{mn} + \omega_{km} = \omega_{kn}$. Equation (43) plus $M_{nm}(s) = -M_{mn}^*(s)$ imply that Eq. (42) can be written as

$$\frac{\mathrm{d}\bar{c}_n^{(1)}(s)}{\mathrm{d}s} + p(s)\bar{c}_n^{(1)}(s) = q(s), \tag{44}$$

where

$$p(s) = M_{nn}(s), \tag{45}$$

$$q(s) = \mathrm{i}\hbar \sum_{\substack{m=0 \\ m\neq n}} \frac{|M_{mn}(s)|^2}{\Delta_{mn}(s)} \mathrm{e}^{\mathrm{i}\gamma_n(s)} b_n(0), \tag{46}$$

and whose well known general solution is

$$\bar{c}_n^{(1)}(s) = \frac{1}{\mu(s)} \left(\int_0^s \mu(s') q(s') \mathrm{d}s' + \bar{c}_n^{(1)}(0) \right), \tag{47}$$

$$\mu(s) = \mathrm{e}^{\int_0^s p(s')\mathrm{d}s'} = \mathrm{e}^{-\mathrm{i}\gamma_n(s)}.$$

It is interesting to note that the integrating factor $\mu(s)$ is related to the Berry phase $\gamma_n(s)$. Inserting Eqs. (45) and (46) into (48) we get

$$\bar{c}_n^{(1)}(s) = \mathrm{i}\hbar \mathrm{e}^{\mathrm{i}\gamma_n(s)} \int_0^s \mathrm{d}s' \sum_{\substack{m=0 \\ m\neq n}} \frac{|M_{mn}(s')|^2}{\Delta_{mn}(s')} b_n(0) + \mathrm{e}^{\mathrm{i}\gamma_n(s)} \bar{c}_n^{(1)}(0). \tag{48}$$

We can now write down the expression for $c_n^{(1)}$ given $d_n^{(1)}$ (Eq. (39)) and $\bar{c}_n^{(1)}$ (Eq. (48)),

$$\begin{aligned} c_n^{(1)}(\omega,s) &= \mathrm{i}\hbar \sum_{\substack{m=0\\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} \mathrm{e}^{\mathrm{i}\gamma_m(s)} \frac{M_{nm}(s)}{\Delta_{nm}(s)} b_m(0) \\ &\quad + \mathrm{i}\hbar \mathrm{e}^{\mathrm{i}\gamma_n(s)} \int_0^s \mathrm{d}s' \sum_{\substack{m=0\\ m\neq n}} \frac{|M_{mn}(s')|^2}{\Delta_{mn}(s')} b_n(0) \\ &\quad + \mathrm{e}^{\mathrm{i}\gamma_n(s)} \bar{c}_n^{(1)}(0). \end{aligned} \tag{49}$$

To determine $\bar{c}_n^{(1)}(0)$ we use Eq. (32), which guarantees that the adiabatic approximation is obtained as zeroth order,

$$\bar{c}_n^{(1)}(0) = -\mathrm{i}\hbar \sum_{\substack{m=0\\ m\neq n}} \frac{M_{nm}(0)}{\Delta_{nm}(0)} b_m(0). \tag{50}$$

Finally, expressing $|\Psi(s)\rangle$ as given in Eq. (21) and using Eqs. (27), (49), and (50) we get for the first order correction to the adiabatic approximation,

$$\begin{aligned} |\Psi^{(1)}(s)\rangle &= \mathrm{i}\hbar \sum_{\substack{n,m=0\\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)} \mathrm{e}^{\mathrm{i}\gamma_n(s)} J_{mn}(s) b_n(0) |n(s)\rangle \\ &+ \mathrm{i}\hbar \sum_{\substack{n,m=0\\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m(s)} \mathrm{e}^{\mathrm{i}\gamma_m(s)} \frac{M_{nm}(s)}{\Delta_{nm}(s)} b_m(0) |n(s)\rangle \\ &- \mathrm{i}\hbar \sum_{\substack{n,m=0\\ m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)} \mathrm{e}^{\mathrm{i}\gamma_n(s)} \frac{M_{nm}(0)}{\Delta_{nm}(0)} b_m(0) |n(s)\rangle, \end{aligned} \tag{51}$$

in which

$$J_{mn}(s) = \int_0^s \mathrm{d}s' \frac{|M_{mn}(s')|^2}{\Delta_{mn}(s')}. \tag{52}$$

Note that now we are writing again explicitly the dependence of ω_n on time, i.e., $\omega_n \to \omega_n(s)$. For completeness, we write down the first order correction when we start at the GS ($b_n(0) = \delta_{n0}$)

$$\begin{aligned} |\Psi^{(1)}(s)\rangle &= \mathrm{i}\hbar \sum_{n=1} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_0(s)} \mathrm{e}^{\mathrm{i}\gamma_0(s)} J_{n0}(s) |0(s)\rangle \\ &+ \mathrm{i}\hbar \sum_{n=1} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_0(s)} \mathrm{e}^{\mathrm{i}\gamma_0(s)} \frac{M_{n0}(s)}{\Delta_{n0}(s)} |n(s)\rangle \\ &- \mathrm{i}\hbar \sum_{n=1} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)} \mathrm{e}^{\mathrm{i}\gamma_n(s)} \frac{M_{n0}(0)}{\Delta_{n0}(0)} |n(s)\rangle, \end{aligned} \tag{53}$$

where we have replaced $m \to n$ in the first sum.

Comparing Eqs. (51) and (53) with Eqs. (22) and (23) we immediately see that now we have a new extra term for the first order correction, the one proportional to $J_{mn}(s)$. We would like to remark, though, that in Garrison's original work [2] he only obtained the first line in Eq. (53), and thus our presentation constitutes an elaboration on his general idea. Going beyond first order in v within Garrison's approach is an extraordinary *tour de force*. Fortunately, we will see in Sec. IV that not only the extra term appears in our APT but, moreover, it is quite easy to obtain higher order corrections. Indeed, we will prove the mathematical equivalence between the two methods.

B. Example of the second group

The iterative method proposed by Berry [3] consists of successive unitary operations that hopefully *rotate* the original basis or axes (the eigenvectors of the original Hamiltonian) closer and closer to the evolving state. In the most optimistic scenario a finite number of rotations would bring us to a moving frame in which the Hamiltonian, as seen from this new frame, becomes time independent (this is the case in the simple single spin problem of Ref. [21]). Then we can solve the transformed Hamiltonian using well developed time independent techniques and, by reversing the transformations, we would have the answer to the original problem.

Berry [3] was *only* interested in corrections to the geometric phase that can be obtained by such a procedure. He showed that this strategy leads to successive corrections to the Berry phase although only in an asymptotic sense, i.e., after, let us say, the k-th rotation, the next following terms cannot improve the result achieved up to this iteration; rather, they spoil any possible useful correction. In Ref. [3] it was also shown, and we will review it here, that this iterative process is not an expansion in the small parameter v since every iteration contains v to infinite orders. We should also note that, as stated in Ref. [14], Berry's iterative method is equivalent to the ones of Refs. [12, 13, 14].

In what follows we will extend Berry's approach to include corrections to the wave functions. For the ease of notation, and since we will be dealing with successive iterations, we will denote the original Hamiltonian, its eigenvalues, and eigenvectors as $\mathbf{H}^{(0)}(s)$, $E_n^{(0)}(s)$, and $|n^{(0)}(s)\rangle$, respectively; after j iterations we will have $\mathbf{H}^{(j)}(s)$, $E_n^{(j)}(s)$, and $|n^{(j)}(s)\rangle$. Also, as in previous sections, the initial state is written as $|\Psi^{(0)}(0)\rangle$.

The main idea behind Berry's approach lies in the realization that the unitary operator $\mathbf{U}_0(s)$ ($\mathbf{U}_0(s)\mathbf{U}_0^\dagger(s) = \mathbf{U}_0^\dagger(s)\mathbf{U}_0(s) = \mathbf{1}$) that gives the snapshot eigenvector of $\mathbf{H}^{(0)}(s)$, i.e.,

$$|n^{(0)}(s)\rangle = \mathbf{U}_0(s)|n^{(0)}(0)\rangle, \tag{54}$$

can be used to construct the state

$$|\Psi^{(1)}(s)\rangle = \mathbf{U}_0^\dagger(s)|\Psi^{(0)}(s)\rangle, \tag{55}$$

whose time evolution is determined to be

$$\mathrm{i}\hbar v|\dot{\Psi}^{(1)}(s)\rangle = \mathbf{H}^{(1)}(s)|\Psi^{(1)}(s)\rangle, \tag{56}$$

with

$$\mathbf{H}^{(1)}(s) = \mathbf{U}_0^\dagger(s)\mathbf{H}^{(0)}(s)\mathbf{U}_0(s) - \mathrm{i}\hbar v\mathbf{U}_0^\dagger(s)\dot{\mathbf{U}}_0(s). \tag{57}$$

Repeating the previous argument with a new unitary operator $\mathbf{U}_1(s)$, which gives the snapshot eigenvectors of $\mathbf{H}^{(1)}(s)$,

$$|n^{(1)}(s)\rangle = \mathbf{U}_1(s)|n^{(0)}(0)\rangle, \tag{58}$$

allows us to generate a new state $|\Psi^{(2)}(s)\rangle$, and by iterating this procedure j times we obtain

$$\begin{aligned}|\Psi^{(j)}(s)\rangle &= \mathbf{U}_{j-1}^\dagger(s)|\Psi^{(j-1)}(s)\rangle \\ &= \mathbf{U}_{j-1}^\dagger(s)\mathbf{U}_{j-2}^\dagger(s)\cdots\mathbf{U}_1^\dagger(s)\mathbf{U}_0^\dagger(s)|\Psi^{(0)}(s)\rangle,\end{aligned}$$

that satisfies the SE

$$\mathrm{i}\hbar v|\dot{\Psi}^{(j)}(s)\rangle = \mathbf{H}^{(j)}(s)|\Psi^{(j)}(s)\rangle, \tag{59}$$

with $|n^{(j)}(s)\rangle = \mathbf{U}_j(s)|n^{(0)}(0)\rangle$ and

$$\begin{aligned}\mathbf{H}^{(j)}(s) &= \mathbf{U}_{j-1}^\dagger(s)\mathbf{H}^{(j-1)}(s)\mathbf{U}_{j-1}(s) \\ &\quad -\mathrm{i}\hbar v\mathbf{U}_{j-1}^\dagger(s)\dot{\mathbf{U}}_{j-1}(s).\end{aligned} \tag{60}$$

Using that $M_{mn}^{(j-1)}(s) = \langle m^{(j-1)}(s)|\dot{n}^{(j-1)}(s)\rangle$, the matrix elements of $\mathbf{H}^{(j)}(s)$ are

$$\langle m^{(0)}(0)|\mathbf{H}^{(j)}(s)|n^{(0)}(0)\rangle = E_n^{(j-1)}(s)\delta_{nm} - \mathrm{i}\hbar v M_{mn}^{(j-1)}(s). \tag{61}$$

Loosely speaking, $|\Psi^{(j)}(s)\rangle$ can be seen as the state obtained after *cancelling* or *freezing* ($\mathbf{U}_{j-1}^\dagger(s)$) the time evolution of the snapshot eigenvectors of $\mathbf{H}^{(j-1)}(s)$, i.e., we are always trying to suppress the time dependence of the new Hamiltonian $\mathbf{H}^{(j)}(s)$. Before we move on we should remark that $\mathbf{U}_j(s)$ is not the usual unitary operator $\mathcal{U}_j(s)$ that evolves an arbitrary state $|\Psi^{(j)}(0)\rangle$ into the state $|\Psi^{(j)}(s)\rangle$, i.e., $|\Psi^{(j)}(s)\rangle = \mathcal{U}_j(s)|\Psi^{(j)}(0)\rangle$.

Let us now explicitly show how to determine the state $|\Psi^{(j)}(s)\rangle$ [15]. For this purpose we write it as

$$|\Psi^{(j)}(s)\rangle = \sum_{n=0} \mathrm{e}^{\mathrm{i}\gamma_n^{(j-1)}(s)}\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n^{(j-1)}(s)}b_n^{(j)}(s)|n^{(0)}(0)\rangle, \tag{62}$$

in which $\gamma_n^{(j-1)}(s) = \mathrm{i}\int_0^s M_{nn}^{(j-1)}(s')\mathrm{d}s'$ is Berry's phase for the snapshot eigenvector $|n^{(j-1)}(s)\rangle$, with dynamical phase $\omega_n^{(j-1)}(s) = \frac{1}{\hbar}\int_0^s E_n^{(j-1)}(s')\mathrm{d}s'$. Note that as opposed to Eq. (3), the eigenbasis used in (62) is not changing over time, i.e., instead of the snapshot eigenvectors $|n^{(0)}(s)\rangle$ we now have $|n^{(0)}(0)\rangle$. But as before, our goal is to find the equations satisfied by $b_n^{(j)}(s)$ which are obtained after inserting Eq. (62) into (59):

$$\dot{b}_n^{(j)}(s) + \sum_{\substack{m=0\\m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}^{(j-1)}(s)}\mathrm{e}^{\mathrm{i}\gamma_{mn}^{(j-1)}(s)}M_{nm}^{(j-1)}(s)b_m^{(j)}(s) = 0, \tag{63}$$

where $\omega_{mn}^{(j-1)}(s) = \omega_m^{(j-1)}(s) - \omega_n^{(j-1)}(s)$ and $\gamma_{mn}^{(j-1)}(s) = \gamma_m^{(j-1)}(s) - \gamma_n^{(j-1)}(s)$. We see that Eq. (63) is formally identical to Eq. (7), which means that any technique developed to solve (7) can be employed to solve (63); in particular the APT of Sec. IV. Moreover, this formal similarity between these two equations evidences that Berry's iterative procedure is not a perturbative expansion about the small parameter v. Actually, as already anticipated, after each iteration we still have (in general) terms involving v to all orders.

In closing, let us indicate a way to, in principle, extend Berry's iterative approach. One can easily check that unitary iterations not constrained by the relations $|n^{(j)}(s)\rangle = \mathbf{U}_j(s)|n^{(0)}(0)\rangle$ lead to the same formal set of equations previously derived. Nonetheless, for a given number of iterations, the optimal choice of unitaries approximating the real time evolution is a difficult problem related to the complexity of efficiently approximating an arbitrary unitary operator in a quantum circuit.

IV. ADIABATIC PERTURBATION THEORY

The reasons for introducing an APT are three fold. First, APT is a method that allows straightforward evaluation of corrections to the geometrical phase (Berry phase). Such corrections are presented as a power series in terms of the small parameter $v = 1/T$, where T is the relevant time scale of the problem (see Sec. I). Secondly, it is an algebraic procedure that does not involve correction terms determined as solutions of differential equations (such as Garrison's approach). Finally, we want a useful and practical method, one that allows us to do actual calculations; we want to be able to check the first and second order corrections formally deduced here against the exact solutions of many time dependent problems.

To accomplish the expectations above, we need to come up with the *right ansatz* for the state $|\Psi(s)\rangle$. An ideal ansatz should *factor out* the dependence of $|\Psi(s)\rangle$ on all the terms of order $\mathcal{O}(v^0)$, $\mathcal{O}(v^{-1})$, and below. The terms of order $\mathcal{O}(v^{-1})$ and below are related to $\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)}$ (See Eq. (3)) and they are extremely oscillatory when $v \to 0$, while the zeroth order term is connected to Berry's phase $\mathrm{e}^{\mathrm{i}\gamma_n(s)}$. If this factorization could be done, we would have control over the divergent terms in v and immediately have information about the Berry phase.

Inspired by Ponce *et al.* [11] we write down the following ansatz for the state $|\Psi(s)\rangle$

$$|\Psi(s)\rangle = \sum_{p=0}^{\infty} v^p|\Psi^{(p)}(s)\rangle, \tag{64}$$

where

$$|\Psi^{(p)}(s)\rangle = \sum_{n=0} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)}\mathrm{e}^{\mathrm{i}\gamma_n(s)}b_n^{(p)}(s)|n(s)\rangle \tag{65}$$

and

$$b_n^{(p)}(s) = \sum_{m=0} \mathrm{e}^{\frac{\mathrm{i}}{v}\omega_{nm}(s)} \mathrm{e}^{-\mathrm{i}\gamma_{nm}(s)} b_{nm}^{(p)}(s), \qquad (66)$$

with all quantities defined in Sec. II. We should note that the *geometrical* terms $\mathrm{e}^{\mathrm{i}\gamma_n(s)}$ and $\mathrm{e}^{\mathrm{i}\gamma_{nm}(s)}$ were absent in the original ansatz given in Ref. [11]. Inserting Eqs. (65) and (66) into (64) we get

$$|\Psi(s)\rangle = \sum_{n,m=0} \sum_{p=0}^{\infty} v^p \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m(s)} \mathrm{e}^{\mathrm{i}\gamma_m(s)} b_{nm}^{(p)}(s) |n(s)\rangle. \quad (67)$$

Since the initial condition is $|\Psi(0)\rangle = |\Psi^{(0)}(0)\rangle = \sum_{n=0} b_n(0)|n(0)\rangle$ it follows that $b_n^{(0)}(0) = b_n(0)$ and

$$|\Psi^{(p)}(0)\rangle = 0 \Longrightarrow b_n^{(p)}(0) = \sum_{m=0} b_{nm}^{(p)}(0) = 0, \qquad p \geq 1. \quad (68)$$

Also, imposing that the adiabatic approximation be the zeroth order term in the power series expansion implies

$$b_n^{(0)}(s) = b_n^{(0)}(0) \Longrightarrow b_{nm}^{(0)}(s) = b_{nm}^{(0)}(0) = b_n(0)\delta_{nm}. \quad (69)$$

Inserting Eq. (67) into the SE, Eq. (2), and left multiplying by $\langle k(s)|$ one gets

$$\sum_{m=0} \sum_{p=0}^{\infty} v^p \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m(s)} \mathrm{e}^{\mathrm{i}\gamma_m(s)} \left(\frac{\mathrm{i}}{v\hbar} \Delta_{km}(s) b_{km}^{(p)}(s) + \dot{b}_{km}^{(p)}(s) + \mathrm{i}\dot{\gamma}_m(s) b_{km}^{(p)}(s) + \sum_{n=0} M_{kn}(s) b_{nm}^{(p)}(s) \right) = 0. \qquad (70)$$

Noting that $\dot{\gamma}_m(s) = \mathrm{i}M_{mm}(s)$ and

$$\sum_{p=0}^{\infty} v^p \frac{\mathrm{i}}{v\hbar} b_{km}^{(p)}(s) = \frac{\mathrm{i}}{v\hbar} b_{km}^{(0)}(s) + \sum_{p=0}^{\infty} v^p \frac{\mathrm{i}}{\hbar} b_{km}^{(p+1)}(s), \quad (71)$$

one can rewrite Eq. (70) in the following form

$$\sum_{m=0} \sum_{p=0}^{\infty} v^p \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m(s)} \mathrm{e}^{\mathrm{i}\gamma_m(s)} \left(\frac{\mathrm{i}}{\hbar} \Delta_{nm}(s) b_{nm}^{(p+1)}(s) + \dot{b}_{nm}^{(p)}(s) - M_{mm}(s) b_{nm}^{(p)}(s) + \sum_{k=0} M_{nk}(s) b_{km}^{(p)}(s) \right)$$
$$+ \sum_{m=0} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m(s)} \mathrm{e}^{\mathrm{i}\gamma_m(s)} \frac{\mathrm{i}}{v\hbar} \Delta_{nm}(s) b_{nm}^{(0)}(s) = 0, \qquad (72)$$

where we have exchanged $n \leftrightarrow k$. The last term in Eq. (72) seems to diverge when $v \to 0$. However, it does not because for $n = m$ we have $\Delta_{nm}(s) = 0$ while for $n \neq m$ the following holds, $b_{nm}^{(0)}(s) = 0$ (initial conditions given by Eq. (69)).

A sufficient condition to satisfy Eq. (72) (since its last term vanishes) is

$$\frac{\mathrm{i}}{\hbar} \Delta_{nm}(s) b_{nm}^{(p+1)}(s) + \dot{b}_{nm}^{(p)}(s) + W_{nm}(s) b_{nm}^{(p)}(s) + \sum_{\substack{k=0 \\ k\neq n}} M_{nk}(s) b_{km}^{(p)}(s) = 0, \quad (73)$$

with

$$W_{nm}(s) = M_{nn}(s) - M_{mm}(s). \qquad (74)$$

Equation (73) is a main result of this paper. With the aid of the initial conditions given by Eqs. (69) and (68) one can build corrections to the adiabatic approximation recursively. The coefficients $b_{nm}^{(p+1)}(s)$ are readily calculated with the knowledge of $b_{nm}^{(p)}(s)$, without the need to solve any partial differential equation as in the multivariable expansion method presented in Sec. III A 2. As we will show next, this fact allows us to calculate the second order correcting terms in a straightforward manner. Moreover, we have removed the highly oscillatory terms $\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m(s)}$ from the expression for the coefficients $b_{nm}^{(p)}(s)$, allowing a better control over any numerical algorithm designed to solve Eq. (73), i.e., it is numerically *stable*.

We now proceed to calculate explicitly the first and second order correction terms $|\Psi^{(1)}(s)\rangle$ and $|\Psi^{(2)}(s)\rangle$. The zeroth order term $|\Psi^{(0)}(s)\rangle$ is given by Eq. (10), the adiabatic approximation.

A. Determination of $|\Psi^{(1)}(s)\rangle$

When $p=0$ Eq. (73) becomes

$$\frac{\mathrm{i}}{\hbar}\Delta_{nm}(s)b^{(1)}_{nm}(s)+\dot{b}^{(0)}_{nm}(s)+W_{nm}(s)b^{(0)}_{nm}(s) + \sum_{\substack{k=0\\k\neq n}} M_{nk}(s)b^{(0)}_{km}(s)=0. \qquad (75)$$

Using Eq. (69) we see that $\dot{b}^{(0)}_{nm}(s)=0$ and that $W_{nm}(s)b^{(0)}_{nm}(s)=W_{nm}(s)b_n(0)\delta_{nm}=0$, since $W_{nn}(s)=0$. For $n\neq m$ the sum in Eq. (75) is simply $M_{nm}(s)b_m(0)$ and we get

$$b^{(1)}_{nm}(s)=\mathrm{i}\hbar\frac{M_{nm}(s)}{\Delta_{nm}(s)}b_m(0), \qquad n\neq m. \qquad (76)$$

When $n=m$ Eq. (75) is an identity and we need to work with the higher order expression. Setting $p=1$ and $n=m$ in Eq. (73) we have

$$\dot{b}^{(1)}_{nn}(s)+\sum_{\substack{k=0\\k\neq n}} M_{nk}(s)b^{(1)}_{kn}(s)=0. \qquad (77)$$

Integrating Eq. (77) using (76) and changing $k\to m$ we obtain after using $M_{nm}(s)=-M^*_{mn}(s)$,

$$\begin{aligned} b^{(1)}_{nn}(s) &= \mathrm{i}\hbar\sum_{\substack{m=0\\m\neq n}}\int_0^s \mathrm{d}s'\frac{|M_{mn}(s')|^2}{\Delta_{mn}(s')}b_n(0)+b^{(1)}_{nn}(0)\\ &= \mathrm{i}\hbar\sum_{\substack{m=0\\m\neq n}} J_{mn}(s)b_n(0)+b^{(1)}_{nn}(0), \end{aligned} \qquad (78)$$

where Eq. (52) was employed to arrive at the last expression. The constant $b^{(1)}_{nn}(0)$ is determined using Eq. (68),

$$\begin{aligned} b^{(1)}_{nn}(0) &= -\sum_{\substack{m=0\\m\neq n}} b^{(1)}_{nm}(0)\\ &= -\mathrm{i}\hbar\sum_{\substack{m=0\\m\neq n}}\frac{M_{nm}(0)}{\Delta_{nm}(0)}b_m(0). \end{aligned} \qquad (79)$$

Since we now have $b^{(1)}_{nm}(s)$, for any n,m, we can insert Eqs. (78), (76), and (66) into (65) to get

$$\begin{aligned} |\Psi^{(1)}(s)\rangle &= \mathrm{i}\hbar\sum_{\substack{n,m=0\\m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)}\mathrm{e}^{\mathrm{i}\gamma_n(s)}J_{mn}(s)b_n(0)|n(s)\rangle\\ &+ \mathrm{i}\hbar\sum_{\substack{n,m=0\\m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m(s)}\mathrm{e}^{\mathrm{i}\gamma_m(s)}\frac{M_{nm}(s)}{\Delta_{nm}(s)}b_m(0)|n(s)\rangle\\ &- \mathrm{i}\hbar\sum_{\substack{n,m=0\\m\neq n}} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)}\mathrm{e}^{\mathrm{i}\gamma_n(s)}\frac{M_{nm}(0)}{\Delta_{nm}(0)}b_m(0)|n(s)\rangle. \end{aligned} \qquad (80)$$

Had we started at the GS ($b_n(0)=\delta_{n0}$) we would get

$$\begin{aligned} |\Psi^{(1)}(s)\rangle &= \mathrm{i}\hbar\sum_{n=1} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_0(s)}\mathrm{e}^{\mathrm{i}\gamma_0(s)}J_{n0}(s)|0(s)\rangle\\ &+ \mathrm{i}\hbar\sum_{n=1} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_0(s)}\mathrm{e}^{\mathrm{i}\gamma_0(s)}\frac{M_{n0}(s)}{\Delta_{n0}(s)}|n(s)\rangle\\ &- \mathrm{i}\hbar\sum_{n=1} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)}\mathrm{e}^{\mathrm{i}\gamma_n(s)}\frac{M_{n0}(0)}{\Delta_{n0}(0)}|n(s)\rangle, \end{aligned} \qquad (81)$$

where $m\to n$ in the first sum.

By looking at Eqs. (80) and (81) we see that they are identical to the ones obtained via the multi-variable expansion method, Eqs. (51) and (53), respectively. Also, we have a new additional term for the first order correction, the one proportional to $J_{mn}(s)$, as compared to the results of the standard approach, Eqs. (22) and (23).

Using Eq. (81) we can also give the conditions for the validity of the adiabatic approximation that comes from the APT by imposing that $|\Psi^{(1)}(s)\rangle$ be negligible,

$$\left|v\hbar\sum_{n=1}J_{n0}(s)\right|\ll 1,$$
$$\left|v\hbar\sum_{n=1}\left(\frac{M_{n0}(s)}{\Delta_{n0}(s)}-\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{n0}(s)}\mathrm{e}^{\mathrm{i}\gamma_{n0}(s)}\frac{M_{n0}(0)}{\Delta_{n0}(0)}\right)\right|\ll 1.$$

B. Determination of $|\Psi^{(2)}(s)\rangle$

We can proceed as before and write Eq. (73) for $p=1$ and $n\neq m$ as

$$\begin{aligned} b^{(2)}_{nm}(s) &= \frac{\mathrm{i}\hbar}{\Delta_{nm}(s)}\Big(\dot{b}^{(1)}_{nm}(s)+W_{nm}(s)b^{(1)}_{nm}(s)\\ &+\sum_{\substack{k=0\\k\neq n}} M_{nk}(s)b^{(1)}_{km}(s)\Big), \qquad n\neq m. \end{aligned} \qquad (82)$$

Using Eq. (76) to replace $\dot{b}^{(1)}_{nm}(s)$ above and separating out from the sum the term where $k=m$ we get

$$\begin{aligned} b^{(2)}_{nm}(s)=\frac{\mathrm{i}\hbar}{\Delta_{nm}(s)}\Big(\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{M_{nm}(s)}{\Delta_{nm}(s)}\right)b_m(0)+W_{nm}(s)b^{(1)}_{nm}(s)\\ +M_{nm}(s)b^{(1)}_{mm}(s)+\sum_{\substack{k=0\\k\neq n,m}} M_{nk}(s)b^{(1)}_{km}(s)\Big). \end{aligned} \qquad (83)$$

We can now employ Eqs. (76) and (78) to replace $b^{(1)}_{nm}(s)$, $n\neq m$, and $b^{(1)}_{nn}(s)$ in (83) to finally obtain

$$b_{nm}^{(2)}(s)=\frac{(\mathrm{i}\hbar)^2}{\Delta_{nm}(s)}\left\{\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{M_{nm}(s)}{\Delta_{nm}(s)}\right)+\frac{W_{nm}(s)M_{nm}(s)}{\Delta_{nm}(s)}+M_{nm}(s)\sum_{\substack{k=0\\k\neq m}}J_{km}(s)+\sum_{\substack{k=0\\k\neq n,m}}\frac{M_{nk}(s)M_{km}(s)}{\Delta_{km}(s)}\right\}b_m(0)$$
$$-\frac{(\mathrm{i}\hbar)^2}{\Delta_{nm}(s)}M_{nm}(s)\sum_{\substack{k=0\\k\neq m}}\frac{M_{mk}(0)}{\Delta_{mk}(0)}b_k(0),\qquad n\neq m. \tag{84}$$

To calculate $b_{nn}^{(2)}(s)$ we set $p=2$ and $n=m$ in Eq. (73), which gives

$$b_{nn}^{(2)}(s)=-\sum_{\substack{m=0\\m\neq n}}\int_0^s \mathrm{d}s' M_{nm}(s')b_{mn}^{(2)}(s')+b_{nn}^{(2)}(0), \tag{85}$$

where $b_{mn}^{(2)}(s')$ is given by Eq. (84) and the constant term $b_{nn}^{(2)}(0)$ is determined by the initial condition in Eq. (68),

$$b_{nn}^{(2)}(0) \;=\; -\sum_{\substack{m=0\\m\neq n}} b_{nm}^{(2)}(0), \tag{86}$$

with $b_{nm}^{(2)}(0)$ obtained from Eq. (84) setting $s=0$. Finally, the second order correction to the state $|\Psi(s)\rangle$ is

$$|\Psi^{(2)}(s)\rangle=\sum_{n,m=0}\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m(s)}\mathrm{e}^{\mathrm{i}\gamma_m(s)}b_{nm}^{(2)}(s)|n(s)\rangle. \tag{87}$$

We should point out that, as can be seen from Eqs. (84) and (85), the second order correction can be calculated with just the knowledge of the snapshot eigenvalues $E_n(s)$ and eigenvectors $|n(s)\rangle$ of the Hamiltonian $\mathbf{H}(s)$. This also holds true for the first order correction and all higher order terms. In other words, the APT can be seen as a way of converting the time dependent SE into an eigenvalue problem and a series expansion in the small parameter v.

1. *Two-level system*

We now want to apply the results obtained in Eqs. (84) and (85) to the case of a qubit. The sum in Eq. (87) runs from $n,m=0$ to $n,m=1$, and the Hamiltonian $\mathbf{H}(s)$ is assumed to be non-degenerate. Thus, the second order correction is

$$\begin{aligned}|\Psi^{(2)}(s)\rangle \;=\;& \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_0(s)}\mathrm{e}^{\mathrm{i}\gamma_0(s)}b_{00}^{(2)}(s)|0(s)\rangle\\ &+\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_1(s)}\mathrm{e}^{\mathrm{i}\gamma_1(s)}b_{01}^{(2)}(s)|0(s)\rangle\\ &+\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_0(s)}\mathrm{e}^{\mathrm{i}\gamma_0(s)}b_{10}^{(2)}(s)|1(s)\rangle\\ &+\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_1(s)}\mathrm{e}^{\mathrm{i}\gamma_1(s)}b_{11}^{(2)}(s)|1(s)\rangle.\end{aligned} \tag{88}$$

Since we assume that the qubit starts at the GS $|0(0)\rangle$ of $\mathbf{H}(0)$, i.e., $b_n(0)=\delta_{n0}$, Eq. (84) gives,

$$b_{01}^{(2)}(s)=-(\mathrm{i}\hbar)^2\frac{M_{01}(s)M_{10}(0)}{\Delta_{01}(s)\Delta_{10}(0)} \tag{89}$$

and

$$\begin{aligned}b_{10}^{(2)}(s) \;=\;& \frac{(\mathrm{i}\hbar)^2}{\Delta_{10}(s)}\left\{\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{M_{10}(s)}{\Delta_{10}(s)}\right)+\frac{W_{10}(s)M_{10}(s)}{\Delta_{10}(s)}\right.\\ &\left.+M_{10}(s)J_{10}(s)\right\}.\end{aligned} \tag{90}$$

For a two-level system Eq. (86) is reduced to

$$b_{00}^{(2)}(0)=-b_{01}^{(2)}(0)\;\text{ and }\;b_{11}^{(2)}(0)=-b_{10}^{(2)}(0).$$

Inserting the previous result into (85) and using Eqs. (89) and (90) we get,

$$\begin{aligned}b_{00}^{(2)}(s) \;=\;& (\mathrm{i}\hbar)^2\int_0^s \mathrm{d}s'\left\{\frac{M_{01}(s')}{\Delta_{01}(s')}\frac{\mathrm{d}}{\mathrm{d}s'}\left(\frac{M_{10}(s')}{\Delta_{10}(s')}\right)\right.\\ &\left.+\frac{W_{10}(s')|M_{10}(s')|^2}{\Delta_{10}^2(s')}+\frac{|M_{10}(s')|^2}{\Delta_{10}(s')}J_{10}(s')\right\}\\ &+(\mathrm{i}\hbar)^2\frac{|M_{10}(0)|^2}{\Delta_{10}^2(0)}\end{aligned} \tag{91}$$

and

$$\begin{aligned}b_{11}^{(2)}(s) \;=\;& \frac{(\mathrm{i}\hbar)^2}{\Delta_{10}(0)}\left\{M_{10}(0)J_{10}(s)-\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{M_{10}(s)}{\Delta_{10}(s)}\right)\Big|_{s=0}\right.\\ &\left.-\frac{W_{10}(0)M_{10}(0)}{\Delta_{10}(0)}\right\}.\end{aligned} \tag{92}$$

In the examples of Secs. VII and VIII Eqs. (88)-(92) will be extensively used.

V. CORRECTIONS TO THE GEOMETRIC PHASE

Let us consider a system in which its time dependent Hamiltonian $\mathbf{H}(s)$ returns to itself at the rescaled time τ_s, i.e., $\mathbf{H}(\tau_s)=\mathbf{H}(0)$. As is well know [4], if the system is initially prepared in one of the eigenvectors of $\mathbf{H}(0)$, i.e, $|\Psi^{(0)}(0)\rangle=|n(0)\rangle$, and the adiabatic approximation is valid, then the state of the system at τ_s is $|\Psi^{(0)}(\tau_s)\rangle=\mathrm{e}^{\mathrm{i}\phi^{(0)}(\tau_s)}|\Psi^{(0)}(0)\rangle$. The phase $\phi^{(0)}(\tau_s)$ can be written as

$$\phi^{(0)}(\tau_s)=\alpha^{(0)}(\tau_s)+\beta^{(0)}(\tau_s), \tag{93}$$

where $\alpha^{(0)}(\tau_s)$ stands for the dynamical phase and $\beta^{(0)}(\tau_s)$ for the Berry phase [4]:

$$\alpha^{(0)}(\tau_s) \;=\; -\omega_n(s)/v, \tag{94}$$
$$\beta^{(0)}(\tau_s) \;=\; \gamma_n(s). \tag{95}$$

(See Eqs. (5) and (6) for the definition of those quantities.) The Berry phase is a geometrical phase since it only depends on the path described by the varying parameter in the Hamiltonian. More explicitly, if we write $\mathbf{H}(s) = \mathbf{H}(\mathbf{r}(s))$, where $\mathbf{r}(s)$ is the parameter that is changed in the Hamiltonian, then [4] $\gamma_n(\tau_s)$ depends only on the trajectory in parameter space described by $\mathbf{r}(s)$. For a more formal interpretation of the Berry phase in terms of the holonomy of a fiber bundle over the parameter space see Ref. [16].

The concept of a geometric phase is not restricted to systems that start in one of the eigenvectors of $\mathbf{H}(s)$ or to adiabatic evolutions. Indeed, Aharonov and Anandan (AA) [5] generalized the Berry phase to include those two possibilities. As before, we consider a non-degenerate Hamiltonian [17]. The key idea in Ref. [5] was the recognition that by defining the dynamical phase as

$$\alpha(s) = -\frac{\omega(s)}{v} = -\frac{1}{v\hbar}\int_0^s \mathrm{d}s' \langle\Psi(s')|\mathbf{H}(s')|\Psi(s')\rangle, \quad (96)$$

it is possible to show that

$$\beta(\tau_c) = \phi(\tau_c) - \alpha(\tau_c) \quad (97)$$

only depends on the closed path of the curve induced by $|\Psi(s)\rangle$ on its projective Hilbert space [18]. Here $|\Psi(\tau_c)\rangle = \mathrm{e}^{\mathrm{i}\phi(\tau_c)}|\Psi(0)\rangle$. The quantity $\phi(\tau_c)$ is the total phase of the state at $s = \tau_c$ and can be written as

$$\phi(\tau_c) = \mathrm{Im}\ln\langle\Psi(0)|\Psi(\tau_c)\rangle. \quad (98)$$

In the adiabatic regime, the AA phase $\beta(\tau_c)$ reduces to the Berry phase. Note that τ_c is not necessarily the period of the Hamiltonian τ_s.

The AA phase is precisely the concept we need to properly find corrections to the Berry phase in terms of the small parameter v defined in Sec. I and used in Sec. IV to build successive corrections to the adiabatic approximation. However, we need the normalized state that corrects the adiabatic approximation up to order $p = j$,

$$|\Psi(s)\rangle_{N_j} = N_j|\tilde{\Psi}(s)\rangle_j, \quad (99)$$

with

$$|\tilde{\Psi}(s)\rangle_j = \sum_{p=0}^{j} v^p|\Psi^{(p)}(s)\rangle \quad (100)$$

and

$$|N_j|^{-2} = {}_j\langle\tilde{\Psi}(s)|\tilde{\Psi}(s)\rangle_j, \quad (101)$$

where $|\Psi^{(p)}(s)\rangle$ is defined in Eq. (65). Following Ref. [5] and with the aid of Eq. (99) we can define, up to order j, the following geometric phase

$$\beta^{(j)}(\tau_s) = \phi^{(j)}(\tau_s) - \alpha^{(j)}(\tau_s), \quad (102)$$

where now we have

$$\alpha^{(j)}(s) = -\omega^{(j)}(s)/v, \quad (103)$$

$$\phi^{(j)}(s) = \mathrm{Im}\ln\langle\Psi(0)|\Psi(s)\rangle_{N_j}, \quad (104)$$

and

$$\omega^{(j)}(s) = -\frac{1}{\hbar}\int_0^s \mathrm{d}s'\ {}_{N_j}\langle\Psi(s')|\mathbf{H}(s')|\Psi(s')\rangle_{N_j}. \quad (105)$$

In our definition for $\beta^{(j)}$ we have used the period of the Hamiltonian τ_s. This is not mandatory and we could have chosen τ_c as well. But we stick with τ_s since it is closer to what happens in an experimental situation, where the Hamiltonian is slowly changed back and forth from its initial value. Note, however, that if $\tau_c \neq \tau_s$ we lose the meaning of β (Eq. (97)) as given by the closed path of $|\Psi(s)\rangle$ on its projective Hilbert space.

A. Zeroth order correction

Before we show the non-trivial correction to the Berry phase, which is given by the first order term, it is instructive to compute the zeroth order term. This gives us the flavor of what comes next without long calculations and, as a bonus, we are able to check that the zeroth order term is simply the Berry phase. We assume that the system starts at $s = 0$ in the GS of the Hamiltonian,

$$|\Psi(0)\rangle = |0(0)\rangle,$$

although we could as well develop the same analysis for an arbitrary initial condition in a straightforward manner.

The first step is the calculation of $|\Psi(s)\rangle_{N_0}$, as given in Eq. (99) when $j = 0$. Since $|\Psi^{(0)}(s)\rangle$ (Eq. (11)) is normalized it is obvious that $|\Psi(s)\rangle_{N_0} = |\Psi^{(0)}(s)\rangle$. Then, using Eqs. (103) and (105) we get

$$\begin{aligned}\alpha^{(0)}(s) &= -\frac{1}{v\hbar}\int_0^s \mathrm{d}s'\langle 0(s')|\mathbf{H}(s')|0(s')\rangle \\ &= -\frac{1}{v\hbar}\int_0^s \mathrm{d}s' E_0(s') = -\frac{\omega_0(s)}{v}. \quad (106)\end{aligned}$$

On the other hand Eq. (104) gives

$$\phi^{(0)}(s) = -\omega_0(s)/v + \gamma_0(s) + \mathrm{Im}\ln\langle 0(0)|0(s)\rangle. \quad (107)$$

Remembering that for $s = \tau_s$ we have $\mathrm{Im}\ln\langle 0(0)|0(\tau_s)\rangle = 0$ since $|0(\tau_s)\rangle = |0(0)\rangle$, Eq. (102) naturally leads to the Berry phase

$$\beta^{(0)}(\tau_s) = \gamma_0(\tau_s). \quad (108)$$

B. First order correction

We now turn our attention to the first order correction. As before, the first step consists in the computation of the explicit expression for the state $|\Psi(s)\rangle_{N_1}$. Using Eqs. (99) and (100) we have

$$|\Psi(s)\rangle_{N_1} = N_1\left(|\Psi^{(0)}(s)\rangle + v|\Psi^{(1)}(s)\rangle\right), \quad (109)$$

where $|\Psi^{(0)}(s)\rangle$ and $|\Psi^{(1)}(s)\rangle$ are given by Eqs. (11) and (81), respectively. Had we prepared the system in an arbitrary initial state we would need Eqs. (10) and (80) instead.

To calculate the normalization constant we employ Eq. (101)

$$|N_1|^{-2} = 1+2v\mathrm{Re}\langle\Psi^{(0)}(s)|\Psi^{(1)}(s)\rangle+v^2\langle\Psi^{(1)}(s)|\Psi^{(1)}(s)\rangle,$$

where Re means the real part of a complex number. But

$$\langle\Psi^{(0)}(s)|\Psi^{(1)}(s)\rangle = \mathrm{i}\hbar\sum_{n=1} J_{n0}(s)$$

is purely imaginary since $J_{n0}(s)$ is real (Cf. Eq. (52)). Therefore,

$$N_1 = 1/\sqrt{1+v^2\langle\Psi^{(1)}(s)|\Psi^{(1)}(s)\rangle}, \qquad (110)$$

where, without loss of generality, we have set N_1 real. Calculating the scalar product in Eq. (110) with the aid of (81) we get

$$\begin{aligned}\langle\Psi^{(1)}(s)|\Psi^{(1)}(s)\rangle &= \hbar^2\Big(\sum_{n=1} J_{n0}(s)\Big)^2 + \hbar^2\sum_{n=1}\left|\frac{M_{n0}(s)}{\Delta_{n0}(s)}\right. \\ &\quad \left. -\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{n0}(s)}\mathrm{e}^{\mathrm{i}\gamma_{n0}(s)}\frac{M_{n0}(0)}{\Delta_{n0}(0)}\right|^2, \qquad (111)\end{aligned}$$

and assuming that v is small

$$N_1 = 1 - v^2\langle\Psi^{(1)}(s)|\Psi^{(1)}(s)\rangle/2 + \mathcal{O}(v^4), \qquad (112)$$

which leads to

$$N_1 = 1 - \frac{v^2\hbar^2}{2}\left\{\left(\sum_{n=1} J_{n0}(s)\right)^2 + \sum_{n=1}\left|\frac{M_{n0}(s)}{\Delta_{n0}(s)} - \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{n0}(s)}\mathrm{e}^{\mathrm{i}\gamma_{n0}(s)}\frac{M_{n0}(0)}{\Delta_{n0}(0)}\right|^2\right\} + \mathcal{O}(v^4). \qquad (113)$$

Notice that N_1 depends on time although we have not written $N_1(s)$, as we have been doing with all other quantities that depend explicitly on s. Also, we have kept terms up to second order because they give corrections to first order for the dynamical phase. This can be seen looking at Eq. (103), where there exists a factor $1/v$ multiplying $\omega^{(j)}(s)$.

1. *Determination of the total phase*

Inserting Eq. (109) into (104) we get

$$\phi^{(1)}(s) = \mathrm{Im}\ln\left(\langle 0(0)|\Psi^{(0)}(s)\rangle + v\langle 0(0)|\Psi^{(1)}(s)\rangle\right),$$

where we have used $\mathrm{Im}\ln N_1 = 0$ since N_1 is real. When $s=\tau_s$ we know that $\langle 0(0)|n(\tau_s)\rangle = \delta_{n0}$. Thus,

$$\langle 0(0)|\Psi^{(0)}(\tau_s)\rangle = \mathrm{e}^{\mathrm{i}\gamma_0(\tau_s)}\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_0(\tau_s)},$$

$$\langle 0(0)|\Psi^{(1)}(\tau_s)\rangle = \mathrm{i}\hbar\mathrm{e}^{\mathrm{i}\gamma_0(\tau_s)}\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_0(\tau_s)}\sum_{n=1} J_{n0}(\tau_s),$$

and the total phase reads

$$\phi^{(1)}(\tau_s) = -\frac{\omega_0(\tau_s)}{v} + \gamma_0(\tau_s) + \mathrm{Im}\ln\left(1+\mathrm{i}v\hbar\sum_{n=1} J_{n0}(\tau_s)\right). \qquad (114)$$

However, the last term of Eq. (114) can be written as

$$\begin{aligned}\mathrm{Im}\ln\left(1+\mathrm{i}v\hbar\sum_{n=1} J_{n0}(\tau_s)\right) &= \arctan\left(v\hbar\sum_{n=1} J_{n0}(\tau_s)\right) \\ &= v\hbar\sum_{n=1} J_{n0}(\tau_s) + \mathcal{O}(v^3),\end{aligned}$$

which implies that to first order

$$\begin{aligned}\phi^{(1)}(\tau_s) &= -\omega_0(\tau_s)/v + \gamma_0(\tau_s) + v\hbar\sum_{n=1} J_{n0}(\tau_s) \\ &= \phi^{(0)}(\tau_s) + v\hbar\sum_{n=1} J_{n0}(\tau_s). \qquad (115)\end{aligned}$$

If we use Eq. (52) we can rewrite the total phase as

$$\phi^{(1)}(\tau_s) = \phi^{(0)}(\tau_s) + v\hbar\sum_{n=1}\int_0^s \mathrm{d}s'\frac{|M_{n0}(s')|^2}{\Delta_{n0}(s')}. \qquad (116)$$

We should note that the last term above is the first order correction to the Berry phase obtained by Garrison [2] and also in Ref. [3]. However, this conclusion is unsatisfactory for our purposes. Indeed, we are interested in the phase defined by Aharonov and Anandan [5], see Eq. (102), which has a clear geometrical meaning when the state returns to itself (even when the adiabatic approximation fails) and is a natural generalization to the Berry phase [5]. We resolve this state of affairs in the following.

2. Determination of the geometric phase

In order to determine the AA geometric phase we need to calculate, up to first order, the dynamical phase defined in Eq. (103). Then, subtracting it from the total phase computed above, we arrive at the desired AA geometric phase. It is this first order term that we herein call *correction to the Berry phase*.

Looking at Eq. (105) we see that the first quantity we need to obtain is

$$ {}_{N_1}\langle\Psi(s)|\mathbf{H}(s)|\Psi(s)\rangle_{N_1} = N_1^2\left(E_0(s) + v^2\,\langle\Psi^{(1)}(s)|\mathbf{H}(s)|\Psi^{(1)}(s)\rangle\right), \tag{117}$$

where we have used that $\mathrm{Re}\langle\Psi^{(0)}(s)|\Psi^{(1)}(s)\rangle = 0$. The last term of Eq. (117) can be explicitly calculated using Eq. (81),

$$\begin{aligned}\langle\Psi^{(1)}(s)|\mathbf{H}(s)|\Psi^{(1)}(s)\rangle &= \hbar^2 E_0(s)\Big(\sum_{n=1} J_{n0}(s)\Big)^2 + \\ \hbar^2\sum_{n=1} E_n(s)\left|\frac{M_{n0}(s)}{\Delta_{n0}(s)} - \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{n0}(s)}\mathrm{e}^{\mathrm{i}\gamma_{n0}(s)}\frac{M_{n0}(0)}{\Delta_{n0}(0)}\right|^2.\end{aligned} \tag{118}$$

Inserting Eq. (118) into (117), using Eq. (113), and keeping terms up to second order we get

$$\begin{aligned}{}_{N_1}\langle\Psi(s)|\mathbf{H}(s)|\Psi(s)\rangle_{N_1} &= E_0(s) + \\ v^2\hbar^2\sum_{n=1}\Delta_{n0}(s)\left|\frac{M_{n0}(s)}{\Delta_{n0}(s)} - \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{n0}(s)}\mathrm{e}^{\mathrm{i}\gamma_{n0}(s)}\frac{M_{n0}(0)}{\Delta_{n0}(0)}\right|^2,\end{aligned} \tag{119}$$

which, after insertion in (103), leads to

$$\alpha^{(1)}(s) = \alpha^{(0)}(s) - v\hbar\sum_{n=1} J_{n0}(s) - v\hbar^2\sum_{n=1}\frac{|M_{n0}(0)|^2}{\Delta_{n0}^2(0)}\omega_{n0}(s) + 2v\hbar\sum_{n=1}\mathrm{Re}\left(\frac{M_{n0}(0)}{\Delta_{n0}(0)}\int_0^s \mathrm{d}s'\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{n0}(s')}\mathrm{e}^{\mathrm{i}\gamma_{n0}(s')}M_{n0}^*(s')\right), \tag{120}$$

where we have used Eqs. (52) and (106). Notice that the last term has an integral of the form given by Eq. (15)

$$I = \int_0^s \mathrm{d}s' B_{n0}(s')\mathrm{e}^{\frac{1}{v}\int_0^{s'}\mathrm{d}s'' C_{n0}(s'')},$$

with $B_{n0}(s) = \mathrm{e}^{\mathrm{i}\gamma_{n0}(s)}M_{n0}^*(s)$ and $C_{n0}(s) = -\mathrm{i}\Delta_{n0}(s)/\hbar$. But we have shown that this integral is at least order v (see Eq. (18)). Therefore, the overall order of this term is at least v^2. Thus, at $s = \tau_s$, the first order correction to the dynamical phase is

$$\begin{aligned}\alpha^{(1)}(\tau_s) &= \alpha^{(0)}(\tau_s) - v\hbar\sum_{n=1} J_{n0}(\tau_s) \\ &\quad -v\hbar^2\sum_{n=1}\frac{|M_{n0}(0)|^2}{\Delta_{n0}^2(0)}\omega_{n0}(\tau_s).\end{aligned} \tag{121}$$

Finally, the desired geometric phase is obtained by subtracting Eq. (121) from the total phase (115),

$$\begin{aligned}\beta^{(1)}(\tau_s) &= \beta^{(0)}(\tau_s) + 2v\hbar\sum_{n=1} J_{n0}(\tau_s) \\ &\quad +v\hbar^2\sum_{n=1}\frac{|M_{n0}(0)|^2}{\Delta_{n0}^2(0)}\omega_{n0}(\tau_s).\end{aligned} \tag{122}$$

It is worth noting that the zeroth order term above is the Berry phase, i.e., when $v \to 0$ we have $\beta^{(0)}(\tau_s) = \gamma_0(\tau_s)$ as our geometric phase. As mentioned before, this is a property any correction to the Berry phase should satisfy. Remembering that $\omega_{n0}(\tau_s) = \frac{1}{\hbar}\int_0^{\tau_s}\Delta_{n0}(s)\mathrm{d}s$ and using the definition for $J_{n0}(s)$ we can rewrite Eq. (122) as follows

$$\begin{aligned}\beta^{(1)}(\tau_s) &= \gamma_0(\tau_s) + 2v\hbar\sum_{n=1}\int_0^{\tau_s}\frac{|M_{n0}(s)|^2}{\Delta_{n0}(s)}\mathrm{d}s \\ &\quad +v\hbar\sum_{n=1}\frac{|M_{n0}(0)|^2}{\Delta_{n0}^2(0)}\int_0^{\tau_s}\Delta_{n0}(s)\mathrm{d}s.\end{aligned} \tag{123}$$

In Sec. VII we discuss how we can measure this new phase in general and also propose an experiment to probe it for the particular example of that section.

VI. COMPARISON BETWEEN METHODS

In previous sections we have presented four methods that aim to find corrections to the Berry phase and improvements to the adiabatic approximation. The first

one, which we called standard approach, gives different results when compared to the multi-variable expansion method of Garrison [2] and the APT presented in Sec. IV. However, as we have shown, to first order the last two methods agree.

In the next section we show that the standard approach fails to properly correct the adiabatic approximation to first order in the small parameter v. Indeed, we show that the missing term in the standard approach and which is present in the APT is crucial if we want to have the right first order approximation. In other words, the APT developed in Sec. IV gives the following state for the time evolution of a non-degenerate time dependent system that starts at the GS,

$$|\Psi(s)\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_0(s)}\mathrm{e}^{\mathrm{i}\gamma_0(s)}\left\{\left(1+\mathrm{i}v\hbar\sum_{n=1}J_{n0}(s)\right)|0(s)\rangle + \mathrm{i}v\hbar\sum_{n=1}\left(\frac{M_{n0}(s)}{\Delta_{n0}(s)} - \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{n0}(s)}\mathrm{e}^{\mathrm{i}\gamma_{n0}(s)}\frac{M_{n0}(0)}{\Delta_{n0}(0)}\right)|n(s)\rangle\right\} + \mathcal{O}(v^2). \quad (124)$$

This is the state that, to first order in v, properly corrects the adiabatic approximation. Note that it is already normalized to first order since the normalization constant, Eq. (113), is second order in v. Furthermore, as we will show in the following sections, by including the state $|\Psi^{(2)}(s)\rangle$, as derived in Sec. IV, we obtain the right second order correction.

We have also discussed the iterative method of Berry [3], who called it *adiabatic renormalization* [19] because each iteration can be seen as a renormalization map that generates a new Hamiltonian from the previous one. This method, which is also related to other similar approaches [12, 13, 14], cannot be considered a perturbative correction to the adiabatic approximation. This is because at each step of the iteration process v enters to all orders. Of course, if we stop the iteration procedure at a certain point we can use any method at our disposal to solve the transformed problem, including the APT here developed. In other words, we could build a hybrid approach, where we employ both the APT technique and the renormalization method of Berry. This might be an interesting topic to study but its full development is beyond the goal of this paper.

Another method, the usual *time dependent perturbation theory* (TDPT), largely used to solve time dependent problems was not discussed here. The main assumption behind the TDPT is the existence of a time independent Hamiltonian $\mathbf{H}_0$ and a *small* time dependent part $\lambda\mathbf{V}(t)$, where $\lambda \ll 1$. The total Hamiltonian is $\mathcal{H}(t) = \mathbf{H}_0 + \lambda\mathbf{V}(t)$. One then builds a series expansion in λ by using the eigenvectors and eigenvalues of $\mathbf{H}_0$ (not of the snapshot $\mathcal{H}(t)$), with the zeroth order term being the time independent solution to the problem. It is now clear what the main difference between the TDPT and the approaches presented in this paper is: we have never assumed the existence of a *small* time dependent Hamiltonian $\lambda\mathbf{V}(t)$. Actually, the Hamiltonian $\mathcal{H}(t)$ can be seen as a particular choice of $\mathbf{H}(t)$, the general time dependent Hamiltonian used, for instance, in APT.

We want to finish this section explaining why seemingly different approaches such as the multi-variable expansion method and the APT of Sec. IV give the same first order correction to the adiabatic approximation. As we show below there is a discrete linear transformation that connects both approaches. This transformation can be written as follows

$$c_n^{(p)}(\omega, s) = \sum_{m=0}\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}}\mathrm{e}^{\mathrm{i}\gamma_m(s)}b_{nm}^{(p)}(s), \quad (125)$$

where $\gamma_n(s)$ and $\omega_{mn} = \omega_m - \omega_n$ are given by Eqs. (5) and (6), respectively. Note that we will consider in the remaining of this section ω_n as an independent variable ($\omega_n(s) \to \omega_n$) when working with expressions coming from Sec. III A 2. In order to prove that Eq. (125) connects both methods we need to show that we can go from Eq. (27) to (67) and also from Eq. (29) to (72) using Eq. (125).

Let us start with the first part of the proof. Inserting Eq. (125) into (27) we get

$$\begin{aligned}|\Psi(s)\rangle &= \sum_{n=0}\sum_{p=0}^{\infty}v^p\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n} \\ &\quad\times\sum_{m=0}\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}}\mathrm{e}^{\mathrm{i}\gamma_m(s)}b_{nm}^{(p)}(s)|n(s)\rangle \\ &= \sum_{n,m=0}\sum_{p=0}^{\infty}v^p\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m}\mathrm{e}^{\mathrm{i}\gamma_m(s)}b_{nm}^{(p)}(s)|n(s)\rangle,\end{aligned}$$

which is exactly Eq. (67) when ω_m is no longer considered an independent variable.

The second part requires a little more mathematical steps but is nevertheless as straightforward as the previous one. Looking at Eq. (29) we see that it has four terms. We will analyze each one separately. After inserting Eq. (125) into the first term of (29) it results

$$D_\omega c_n^{(p+1)}(\omega, s) = \frac{\mathrm{i}}{\hbar}\sum_{m=0}\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}}\mathrm{e}^{\mathrm{i}\gamma_m(s)}\Delta_{nm}(s)b_{nm}^{(p+1)}(s),$$

where we used $D_\omega(\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}}) = -\mathrm{i}\Delta_{nm}(s)\mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}}/\hbar$ and $\Delta_{mn}(s) = -\Delta_{nm}(s)$. As is easily seen, the fourth term is also given by the previous expression when we set $p = -1$.

The second term gives the following two new terms when we insert Eq. (125) and use that $\mathrm{i}\dot{\gamma}_m(s) = -M_{mm}(s)$,

$$\partial_s c_n^{(p)}(\omega,s) = \sum_{m=0} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} \mathrm{e}^{\mathrm{i}\gamma_m(s)} \Big(\dot{b}_{nm}^{(p)}(s) - M_{mm}(s) b_{nm}^{(p)}(s) \Big).$$

Finally, after employing Eq. (125) the third term can be written as

$$\sum_{m=0} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} M_{nm}(s) c_m^{(p)}(\omega,s) = \\ = \sum_{k,m=0} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}} \mathrm{e}^{\mathrm{i}\gamma_m(s)} M_{nk}(s) b_{km}^{(p)}(s).$$

Putting everything back into Eq. (29), dividing by v, noting that $\omega_{mn} + \omega_n = \omega_m$, and considering again $\omega_n \to \omega_n(s)$, we get exactly Eq. (72). Therefore, Eq. (125) transforms the multi-variable expansion method into the APT of Sec. IV.

Furthermore, we can also go from the APT to the multi-variable expansion method using the transformation

$$b_{nm}^{(p)}(s) = \mathrm{e}^{-\mathrm{i}\gamma_m(s)} \delta_{nm} c_n^{(p)}(\omega,s), \tag{126}$$

where $\delta_{nm} = 1$ if $n = m$ and is zero otherwise. Again the proof is divided into two steps. First we need to show that inserting Eq. (126) into Eq. (67) we get (27),

$$\begin{aligned} |\Psi(s)\rangle &= \sum_{n,m=0} \sum_{p=0}^{\infty} v^p \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_m(s)} \mathrm{e}^{\mathrm{i}\gamma_m(s)} \\ &\quad \times \mathrm{e}^{-\mathrm{i}\gamma_m(s)} \delta_{nm} c_n^{(p)}(\omega,s) |n(s)\rangle \\ &= \sum_{n=0} \sum_{p=0}^{\infty} v^p \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)} c_n^{(p)}(\omega,s) |n(s)\rangle, \end{aligned}$$

which is exactly Eq. (27) when we consider $\omega_n(s)$ as an independent variable. To complete the proof we need to show that Eq. (72), with the aid of (126), leads to (29). As before, we analyze separately each of the five terms in Eq. (72). The first and the last terms are zero after we insert Eq. (126). This is the case since $n = m$ implies $\Delta_{nn} = 0$. The second term should be handled with care since in Eq. (67) the dependence of the variables $\omega_n(s)$ on s must be taken into account. This is important when we take the derivative with respect to s, which, according to the chain rule, is given by

$$\frac{\mathrm{d}}{\mathrm{d}s} = \sum_{n=0} \frac{\mathrm{d}\omega_n}{\mathrm{d}s} \partial_{\omega_n} + \partial_s = \sum_{n=0} \frac{E_n(s)}{\hbar} \partial_{\omega_n} + \partial_s.$$

With this in mind and remembering that $-\mathrm{i}\dot{\gamma}_m(s) = M_{mm}(s)$ we have for the second term

$$\sum_{p=0}^{\infty} v^p \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)} \Big(D_\omega c_n^{(p+1)}(\omega,s) + \partial_s c_n^{(p)}(\omega,s) \\ + M_{nn}(s) c_n^{(p)}(\omega,s) \Big) + v^{-1} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)} D_\omega c_n^{(0)}(\omega,s),$$

where we have used the definition of D_ω given in Sec. III A 2 and written out of the sum the term for $p = 0$. The third and fourth terms can easily be written as

$$-\sum_{p=0}^{\infty} v^p \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)} M_{nn}(s) c_n^{(p)}(\omega,s)$$

and

$$\sum_{p=0}^{\infty} v^p \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_n(s)} \sum_{m=0} \mathrm{e}^{-\frac{\mathrm{i}}{v}\omega_{mn}(s)} M_{nm}(s) c_m^{(p)}(\omega,s)$$

after using Eq. (126). In the last expression, we have also used that $\omega_m(s) = \omega_n(s) + \omega_{mn}(s)$. Finally, adding all the terms above, multiplying the result by v, and considering $\omega_n(s)$ as an independent variable we end up with Eq. (29).

VII. AN ANALYTICALLY SOLVABLE PROBLEM

So far we have presented the general APT formalism. It is time to show some examples that can tell us why the APT of Sec. IV provides the right correction to the adiabatic approximation. For that purpose, it is desirable to start with a non-trivial time dependent problem that is exactly solved in closed form. The exact solution of this problem can then be expanded in terms of the small parameter v and compared with the results given by the APT. As we will see, the missing term in the standard approach of Sec. III A 1, which appears in the APT, also appears in the first order expansion of the exact solution. We also give the second order correction via the APT and show that it is identical to the second order expansion of the exact solution. We end this section comparing the correction to the Berry phase calculated in Sec. V with the first order expansion of the exact geometric phase that can be computed for this problem. As will be shown, both results are identical.

A. Statement of the problem

Let us consider a spin-1/2 (a qubit) with magnetic moment $\mathbf{m}$ subjected to a rotating classical magnetic field $\mathbf{B}$ [20]. The magnitude of the field is fixed and given by $B = |\mathbf{B}|$. Here $\mathbf{m} = eg/(2mc)\,\mathbf{S}$, with e the electric charge of the particle, g its Landé factor, m its mass, c the speed of light in vacuum, and $\mathbf{S}$ its angular momentum operator. Since we have a qubit $\mathbf{S} = (\hbar/2)\boldsymbol{\sigma}$, where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the usual Pauli matrices. The rotating magnetic field can be written as $\mathbf{B}(t) = B\mathbf{r}(t)$, with unit vector written in spherical coordinates $\mathbf{r}(t) = (\sin\theta\cos\varphi(t), \sin\theta\sin\varphi(t), \cos\theta)$, in which $0 \le \theta \le \pi$ and $0 \le \varphi < 2\pi$ are the polar and azimuthal angles, respectively. With this notation the

Hamiltonian describing the system is [20]

$$\mathbf{H}(t) = -\mathbf{m}\cdot\mathbf{B} = b\,\mathbf{r}(t)\cdot\mathbf{S}, \tag{127}$$

where $b = -Bge/(2mc)$ and we set $e > 0$. The snapshot eigenvectors for this problem are

$$|0(t)\rangle = \cos(\theta/2)\,|\uparrow\rangle + \mathrm{e}^{\mathrm{i}\varphi(t)}\sin(\theta/2)\,|\downarrow\rangle, \tag{128}$$
$$|1(t)\rangle = \sin(\theta/2)\,|\uparrow\rangle - \mathrm{e}^{\mathrm{i}\varphi(t)}\cos(\theta/2)\,|\downarrow\rangle, \tag{129}$$

where $\sigma_z|\uparrow\rangle = |\uparrow\rangle$ and $\sigma_z|\downarrow\rangle = -|\downarrow\rangle$. The eigenvalues are respectively

$$E_0 = (\hbar/2)b \;\text{ and }\; E_1 = -(\hbar/2)b. \tag{130}$$

Note that the eigenvalues are time independent and we always have a gap of magnitude $\hbar b$.

B. Exact solution

If $\varphi(t) = w\,t$, where $w > 0$ is the frequency of the rotating magnetic field, the Hamiltonian (127) can be exactly solved [20, 21]. Physically, the component of the field projected onto the xy-plane is rotating counter-clockwise around the z-axes with constant angular frequency w and period $\tau = 2\pi/w$. This suggests that if we rotate clockwise the state $|\Psi(t)\rangle$, which satisfies the SE (1), we could get a new Hamiltonian $\bar{\mathbf{H}}$ that is time independent. Let us define the rotated state as

$$|\bar{\Psi}(t)\rangle = \mathbf{U}^{\dagger}(t)|\Psi(t)\rangle, \tag{131}$$

with

$$\mathbf{U}(t) = \mathrm{e}^{-\frac{\mathrm{i}wt}{\hbar}S_z} = \mathrm{e}^{-\frac{\mathrm{i}wt}{2}\sigma_z}, \tag{132}$$

where $S_z = (\hbar/2)\sigma_z$. Inserting Eq. (131) into the SE (1) we see that $|\bar{\Psi}(t)\rangle$ satisfies a Schödinger-like equation with Hamiltonian

$$\bar{\mathbf{H}} = \mathbf{U}^{\dagger}(t)\mathbf{H}(t)\mathbf{U}(t) - \mathrm{i}\hbar\mathbf{U}^{\dagger}(t)\frac{\mathrm{d}\mathbf{U}(t)}{\mathrm{d}t}. \tag{133}$$

$\bar{\mathbf{H}}$ resembles the transformed Hamiltonians of Berry's iterative approach developed in Sec. III B. Using Eq. (132) and the mathematical identity [20]

$$S_x\cos(wt) + S_y\sin(wt) = \mathrm{e}^{-\mathrm{i}wtS_z/\hbar}S_x\mathrm{e}^{\mathrm{i}wtS_z/\hbar},$$

where $S_{x,y} = (\hbar/2)\sigma_{x,y}$, it is not difficult to show that Eq. (133) can be written as

$$\bar{\mathbf{H}} = \frac{\hbar}{2}(b\cos\theta - w)\sigma_z + \frac{\hbar}{2}(b\sin\theta)\sigma_x = \mathcal{Z}\sigma_z + \mathcal{X}\sigma_x. \tag{134}$$

The important result here is that $\bar{\mathbf{H}}$ is time independent, meaning that the SE for $|\bar{\Psi}(t)\rangle$ can be readily integrated $|\bar{\Psi}(t)\rangle = \mathrm{e}^{-\frac{\mathrm{i}\bar{\mathbf{H}}t}{\hbar}}|\bar{\Psi}(0)\rangle$. Therefore, inverting Eq. (131) and remembering that $|\bar{\Psi}(0)\rangle = |\Psi(0)\rangle$, we have the solution to the original problem

$$|\Psi(t)\rangle = \mathrm{e}^{-\frac{\mathrm{i}wt}{2}\sigma_z}\mathrm{e}^{-\frac{\mathrm{i}\bar{\mathbf{H}}t}{\hbar}}|\Psi(0)\rangle. \tag{135}$$

Although Eq. (135) is the general solution to the problem, we still need to write it in a more practical way. In order to so, we first note that

$$\bar{\mathbf{H}}^{2n} = (\mathcal{X}^2 + \mathcal{Z}^2)^n\sigma_0 \;\text{ and }\; \bar{\mathbf{H}}^{2n+1} = (\mathcal{X}^2 + \mathcal{Z}^2)^n\bar{\mathbf{H}},$$

where σ_0 is the identity matrix and n is a non-negative integer. Also,

$$\mathrm{e}^{-\frac{\mathrm{i}\bar{\mathbf{H}}t}{\hbar}} = 1 - \left(\frac{t}{\hbar}\right)^2\frac{\bar{\mathbf{H}}^2}{2!} + \left(\frac{t}{\hbar}\right)^4\frac{\bar{\mathbf{H}}^4}{4!} - \left(\frac{t}{\hbar}\right)^6\frac{\bar{\mathbf{H}}^6}{6!} + \cdots - \mathrm{i}\left\{\left(\frac{t}{\hbar}\right)\bar{\mathbf{H}} - \left(\frac{t}{\hbar}\right)^3\frac{\bar{\mathbf{H}}^3}{3!} + \left(\frac{t}{\hbar}\right)^5\frac{\bar{\mathbf{H}}^5}{5!} - \cdots\right\}.$$

Combining both results we arrive at

$$\mathrm{e}^{-\frac{\mathrm{i}\bar{\mathbf{H}}t}{\hbar}} = \cos\left(\sqrt{\mathcal{X}^2+\mathcal{Z}^2}\frac{t}{\hbar}\right)\sigma_0 - \frac{\mathrm{i}}{\sqrt{\mathcal{X}^2+\mathcal{Z}^2}}\sin\left(\sqrt{\mathcal{X}^2+\mathcal{Z}^2}\frac{t}{\hbar}\right)\bar{\mathbf{H}}. \tag{136}$$

We now define three vectors that will be used later on to rewrite previous expressions in a more compact way,

$$\mathbf{w} = w\mathbf{z}, \tag{137}$$
$$\mathbf{b} = b\mathbf{r}(t), \tag{138}$$
$$\mathbf{\Omega} = \mathbf{w} - \mathbf{b}, \tag{139}$$

where $\mathbf{z}$ is the unity vector pointing along the z-direction. Since the angle between $\mathbf{w}$ and $\mathbf{b}$ is θ, the magnitude of $\mathbf{\Omega}$ is simply

$$\Omega^2 = w^2 + |b|^2 - 2w|b|\cos\theta. \tag{140}$$

With this new notation Eq. (136) can be recast as

$$\mathrm{e}^{-\frac{\mathrm{i}\bar{\mathbf{H}}t}{\hbar}} = \cos\left(\frac{\Omega t}{2}\right)\sigma_0 - \frac{2\mathrm{i}}{\hbar\Omega}\sin\left(\frac{\Omega t}{2}\right)\bar{\mathbf{H}}. \tag{141}$$

With the aid of Eqs. (134), (135), (141), and remembering that $\sigma_x|\uparrow(\downarrow)\rangle = |\downarrow(\uparrow)\rangle$, we can calculate the evolution of a system that starts either at $|\uparrow\rangle$ or $|\downarrow\rangle$,

$$|\psi^{\uparrow}(t)\rangle = \left[\cos\left(\frac{\Omega t}{2}\right) - \frac{\mathrm{i}}{\Omega}(b\cos\theta - w)\sin\left(\frac{\Omega t}{2}\right)\right]\mathrm{e}^{-\frac{\mathrm{i}wt}{2}}|\uparrow\rangle - \frac{\mathrm{i}b}{\Omega}\sin\theta\sin\left(\frac{\Omega t}{2}\right)\mathrm{e}^{\frac{\mathrm{i}wt}{2}}|\downarrow\rangle, \quad (142)$$

$$|\psi^{\downarrow}(t)\rangle = -\frac{\mathrm{i}b}{\Omega}\sin\theta\sin\left(\frac{\Omega t}{2}\right)\mathrm{e}^{-\frac{\mathrm{i}wt}{2}}|\uparrow\rangle + \left[\cos\left(\frac{\Omega t}{2}\right) + \frac{\mathrm{i}}{\Omega}(b\cos\theta - w)\sin\left(\frac{\Omega t}{2}\right)\right]\mathrm{e}^{\frac{\mathrm{i}wt}{2}}|\downarrow\rangle. \quad (143)$$

The most general initial state is written as $c_\uparrow|\uparrow\rangle + c_\downarrow|\downarrow\rangle$, which implies that its time evolution is simply $c_\uparrow|\psi^{\uparrow}(t)\rangle + c_\downarrow|\psi^{\downarrow}(t)\rangle$. When the system starts at the GS $|0(0)\rangle$ of Eq. (128) the time evolved state is

$$|\Psi(t)\rangle = \cos(\theta/2)\,|\psi^{\uparrow}(t)\rangle + \sin(\theta/2)\,|\psi^{\downarrow}(t)\rangle,$$

or equivalently,

$$|\Psi(t)\rangle = \left[\cos\left(\frac{\Omega t}{2}\right) + \mathrm{i}\frac{w-b}{\Omega}\sin\left(\frac{\Omega t}{2}\right)\right]\cos(\theta/2)\mathrm{e}^{-\frac{\mathrm{i}wt}{2}}|\uparrow\rangle + \left[\cos\left(\frac{\Omega t}{2}\right) - \mathrm{i}\frac{w+b}{\Omega}\sin\left(\frac{\Omega t}{2}\right)\right]\sin(\theta/2)\mathrm{e}^{\frac{\mathrm{i}wt}{2}}|\downarrow\rangle \quad (144)$$

$$= \mathrm{e}^{-\frac{\mathrm{i}wt}{2}}\left\{\left[\cos\left(\frac{\Omega t}{2}\right) + \frac{\mathrm{i}}{\Omega}(w\cos\theta - b)\sin\left(\frac{\Omega t}{2}\right)\right]|0(t)\rangle + \frac{\mathrm{i}w}{\Omega}\sin\theta\sin\left(\frac{\Omega t}{2}\right)|1(t)\rangle\right\}, \quad (145)$$

where, after Eqs. (128) and (129), we have

$$|\uparrow\rangle = \cos(\theta/2)|0(t)\rangle + \sin(\theta/2)|1(t)\rangle, \quad (146)$$

$$|\downarrow\rangle = \sin(\theta/2)\mathrm{e}^{-\mathrm{i}wt}|0(t)\rangle - \cos(\theta/2)\mathrm{e}^{-\mathrm{i}wt}|1(t)\rangle. \quad (147)$$

In order to avoid writing all the time $|b|$ instead of just b, we will consider $b > 0$ in the rest of the paper. The final outcomes for all relevant quantities, nevertheless, are the same had we considered $b < 0$, which is the reason why we will continue calling $|0(s)\rangle$ the GS.

C. Expansion of the exact solution

Since we are looking for corrections to the adiabatic approximation, the frequency $w = v$ of the rotating magnetic field should be small. An important point is the way we need to deal with terms of the form wt and w^2t. If we remember the definition of the rescaled time, $s = vt$, we see that $t \propto 1/v$ in the formalism developed for the APT in Sec. IV. Therefore, the order of magnitude of, for example, w^2t is the same as that of w. In general we have

$$\mathcal{O}(w^{n+1}\,t) = \mathcal{O}(w^n),$$

with n being an integer. This fact should be taken into account when expanding the exact solution.

Let us write Eq. (145) as

$$|\Psi(t)\rangle = \Pi_0|0(t)\rangle + \Pi_1|1(t)\rangle. \quad (148)$$

Using the definition of Ω (Eq. (140)) one can show that

$$\frac{w\cos\theta - b}{\Omega} = -1 + \frac{w^2\sin^2\theta}{2b^2} + \mathcal{O}(w^3),$$

which implies that

$$\Pi_0 = \mathrm{e}^{-\mathrm{i}\frac{(w+\Omega)t}{2}}\left(1 - \frac{w^2\sin^2\theta}{4b^2}(1 - \mathrm{e}^{\mathrm{i}\Omega t})\right) + \mathcal{O}(w^3).$$

In the previous expression, we have to expand the term $\Omega\,t$. But since we now have the time t we need Ω up to third order in w

$$\Omega = b - w\cos\theta + \frac{w^2}{2b}\sin^2\theta + \frac{w^3}{2b^2}\cos\theta\sin^2\theta + \mathcal{O}(w^4).$$

Using the expansion for Ω above and the Taylor expansion for the exponential we get

$$\mathrm{e}^{-\mathrm{i}\frac{(w+\Omega)t}{2}} = \mathrm{e}^{-\mathrm{i}\frac{b\,t}{2}}\mathrm{e}^{-\mathrm{i}wt\sin^2(\theta/2)}\left(1 - \mathrm{i}\frac{w^2t}{4b}\sin^2\theta - \mathrm{i}\frac{w^3t}{4b^2}\cos\theta\sin^2\theta - \frac{w^4t^2}{32b^2}\sin^4\theta\right) + \mathcal{O}(w^3).$$

We also have the term $\mathrm{e}^{\mathrm{i}\Omega t}$ to expand in the expression for Π_0. But since it is multiplied by a second order term, $w^2\sin^2\theta/(4b^2)$, we only need its expansion up to zeroth order

$$\mathrm{e}^{\mathrm{i}\Omega t} = \mathrm{e}^{\mathrm{i}b\,t}\mathrm{e}^{-\mathrm{i}wt\cos\theta} + \mathcal{O}(w).$$

Putting all the pieces together we finally obtain

$$\Pi_0 = \mathrm{e}^{-\mathrm{i}\frac{b\,t}{2}}\mathrm{e}^{-\mathrm{i}wt\sin^2(\theta/2)}\left\{1 - \mathrm{i}\frac{w^2t}{4b}\sin^2\theta - \frac{w^2}{4b^2}\sin^2\theta \times \left(G_-(t) + \frac{w^2\,t^2}{8}\sin^2\theta + \mathrm{i}w\,t\cos\theta\right)\right\} + \mathcal{O}(w^3),$$

where

$$G_{\pm}(t) = 1 \pm \mathrm{e}^{\mathrm{i}bt}\mathrm{e}^{-\mathrm{i}w\,t\cos\theta}. \tag{149}$$

Turning our attention to Π_1, we see that it has an overall w multiplying all its other terms. Therefore, we need to expand $1/\Omega$ up to first order

$$\Omega^{-1} = b^{-1} + \frac{w\cos\theta}{b^2} + \mathcal{O}(w^2),$$

which results in

$$\begin{aligned}\Pi_1 \;=\; & \mathrm{e}^{-\mathrm{i}\frac{(w+\Omega)t}{2}}\left\{-\frac{w}{2b}\sin\theta(1-\mathrm{e}^{\mathrm{i}\Omega\,t})\right.\\ & \left.-\frac{w^2}{4b^2}\sin(2\theta)(1-\mathrm{e}^{\mathrm{i}\Omega\,t})\right\} + \mathcal{O}(w^3).\end{aligned}$$

The second term inside the curly brackets has a w^2 factor, which means that the zeroth order expansion of $\mathrm{e}^{\mathrm{i}\Omega\,t}$ is enough. However, the first term is multiplied by w, implying that we need the first order expansion of $\mathrm{e}^{\mathrm{i}\Omega\,t}$,

$$\mathrm{e}^{\mathrm{i}\Omega t} = \mathrm{e}^{\mathrm{i}b\,t}\mathrm{e}^{-\mathrm{i}wt\cos\theta}\left(1+\mathrm{i}\frac{w^2\,t}{2b}\sin^2\,\theta\right) + \mathcal{O}(w^2).$$

Using the previous expression and the expansion of $\mathrm{e}^{-\mathrm{i}\frac{(w+\Omega)t}{2}}$ up to first order we get after some algebra

$$\begin{aligned}\Pi_1 \;=\; & -\mathrm{e}^{-\mathrm{i}\frac{bt}{2}}\mathrm{e}^{-\mathrm{i}wt\sin^2(\theta/2)}\left\{\frac{w}{2b}G_-(t)\sin\theta + \frac{w^2}{4b^2}\sin(2\theta)\right.\\ & \left.\times\left(G_-(t) - \mathrm{i}\frac{w\,t}{4}G_+(t)\sin\theta\tan\theta\right)\right\} + \mathcal{O}(w^3).\end{aligned}$$

Finally, inserting Π_0 and Π_1 into Eq. (148) and writing it as

$$|\Psi(t)\rangle = |\Psi^{(0)}(t)\rangle + v|\Psi^{(1)}(t)\rangle + v^2|\Psi^{(2)}(t)\rangle + \mathcal{O}(v^3),$$

we obtain

$$|\Psi^{(0)}(t)\rangle \;=\; \mathrm{e}^{-\mathrm{i}\frac{bt}{2}}\mathrm{e}^{-\mathrm{i}wt\sin^2(\theta/2)}|0(t)\rangle, \tag{150}$$

$$\begin{aligned}|\Psi^{(1)}(t)\rangle \;=\; & \mathrm{e}^{-\mathrm{i}\frac{bt}{2}}\mathrm{e}^{-\mathrm{i}wt\sin^2(\theta/2)}\left(-\mathrm{i}\frac{w^2t}{4vb}\sin^2\theta|0(t)\rangle\right.\\ & \left.-\frac{w}{2vb}G_-(t)\sin\theta|1(t)\rangle\right),\end{aligned} \tag{151}$$

and

$$\begin{aligned}|\Psi^{(2)}(t)\rangle \;=\; & \mathrm{e}^{-\mathrm{i}\frac{bt}{2}}\mathrm{e}^{-\mathrm{i}wt\sin^2(\theta/2)}\left\{-\frac{w^2}{4v^2b^2}\sin^2\theta\left(G_-(t)+\frac{w^2\,t^2}{8}\sin^2\theta+\mathrm{i}w\,t\cos\theta\right)|0(t)\rangle\right.\\ & \left.-\frac{w^2}{4v^2b^2}\sin(2\theta)\left(G_-(t)-\mathrm{i}\frac{w\,t}{4}G_+(t)\sin\theta\tan\theta\right)|1(t)\rangle\right\},\end{aligned} \tag{152}$$

with $G_{\pm}(t)$ given by Eq. (149). Equations (150)-(152) represent the expansions up to second order of the exact solution given by Eq. (145).

D. First and second order corrections via the APT

Before determining the first and second order corrections, we want to calculate explicitly the zeroth order term, namely, the adiabatic approximation given by Eq. (11). After Eq. (11) one needs to evaluate two quantities: $\gamma_0(s)$ and $\omega_0(s)$. The last one is easily obtained employing Eqs. (6) and (130)

$$\omega_0(s) = bs/2 = bvt/2.$$

To determine $\gamma_0(s)$ we need $M_{00}(s)$ as given by Eq. (8). Using Eq. (128) for the snapshot eigenvector $|0(s)\rangle$ we get

$$|\dot{0}(s)\rangle = \mathrm{i}\frac{w}{v}\sin(\theta/2)\mathrm{e}^{\mathrm{i}\frac{ws}{v}}|\downarrow\rangle, \tag{153}$$

which implies

$$M_{00}(s) = \mathrm{i}\frac{w}{v}\sin^2(\theta/2). \tag{154}$$

Thus, inserting Eq. (154) into (5) we get

$$\gamma_0(s) = -\frac{w}{v}s\sin^2(\theta/2) = -wt\sin^2(\theta/2), \tag{155}$$

and Eq. (11) reads

$$|\Psi^{(0)}(t)\rangle = \mathrm{e}^{-\mathrm{i}\frac{bt}{2}}\mathrm{e}^{-\mathrm{i}wt\sin^2(\theta/2)}|0(t)\rangle. \tag{156}$$

The first order correction obtained via the APT in Sec. IV is given by Eq. (81). Since we deal with a two-level system, there is no sum and we can set $n = 1$ in all terms of Eq. (81). In addition to $\gamma_0(s)$ and $\omega_0(s)$, we need to compute $\gamma_1(s)$, $\omega_1(s)$, $M_{10}(s)$, $\Delta_{10}(s)$, and $J_{10}(s)$ to determine $|\Psi^{(1)}(s)\rangle$. We start with the gap, which is easily computed using Eq. (130)

$$\Delta_{10}(s) = -\hbar b. \tag{157}$$

Using Eqs. (6) and (130) we immediately get

$$\omega_1(s) = -\omega_0(s) = -bvt/2.$$

The term $\gamma_1(s)$ is obtained after calculating $M_{11}(s)$. Using Eq. (129) we get

$$|\dot{1}(s)\rangle = -\mathrm{i}\frac{w}{v}\cos(\theta/2)\mathrm{e}^{\mathrm{i}\frac{ws}{v}}|\downarrow\rangle. \tag{158}$$

Inserting Eq. (158) into (8) we find that

$$M_{11}(s) = \mathrm{i}\frac{w}{v}\cos^2(\theta/2), \tag{159}$$

which leads to

$$\gamma_1(s) = -wt\cos^2(\theta/2). \tag{160}$$

Using Eqs. (8), (129), and (153) we arrive at

$$M_{10}(s) = -\mathrm{i}\frac{w}{2v}\sin\theta. \tag{161}$$

Finally, with the aid of Eqs. (52), (157), and (161) we obtain

$$J_{10}(s) = -\frac{w^2 t}{4vb\hbar}\sin^2\theta. \tag{162}$$

Therefore, returning to Eq. (81) using that

$$\frac{M_{10}(s)}{\Delta_{10}(s)} = \mathrm{i}\frac{w}{2vb\hbar}\sin\theta, \tag{163}$$

we get

$$\begin{aligned}|\Psi^{(1)}(t)\rangle \;=\; & \mathrm{e}^{-\mathrm{i}\frac{bt}{2}}\mathrm{e}^{-\mathrm{i}wt\sin^2(\theta/2)}\left(-\mathrm{i}\frac{w^2 t}{4vb}\sin^2\theta|0(t)\rangle\right.\\ & \left.-\frac{w}{2vb}G_-(t)\sin\theta|1(t)\rangle\right),\end{aligned} \tag{164}$$

where $G_-(t)$ is given by Eq. (149).

Moving on to the second order term, Eq. (88), whose coefficients are obtained from Eqs. (89) to (92), we see that almost everything we need to explicitly write $|\Psi^{(2)}(t)\rangle$ is already calculated. We are left with only two quantities to compute, which are

$$\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{M_{10}(s)}{\Delta_{10}(s)}\right) = 0,$$

as can be seen from Eq. (163), and

$$W_{10}(s) = \mathrm{i}\frac{w}{v}\cos\theta, \tag{165}$$

where we have employed Eqs. (74), (154), and (159). We are now able to write down explicitly the values of the four coefficients. The first one, Eq. (89), is easily calculated by noting that $M_{01}(s) = M_{01}(0) = -M_{10}^*(0)$. Thus,

$$b_{01}^{(2)}(s) = \frac{w^2}{4v^2b^2}\sin^2\theta. \tag{166}$$

The second one, Eq. (90), is obtained inserting the values of $W_{10}(s)$, $M_{10}(s)$, $\Delta_{10}(s)$, and $J_{10}(s)$,

$$b_{10}^{(2)}(s) = -\frac{w^2\sin(2\theta)}{4v^2b^2}\left(1 - \mathrm{i}\frac{w\,t}{4}\sin\theta\tan\theta\right). \tag{167}$$

The evaluation of the third coefficient, Eq. (91), is just a little more involved. The integrations are easily done since the first integrand is time independent and the second one is a linear polynomial of the rescaled time s. Putting the results of the integration back into Eq. (91) we can rearrange it as follows,

$$b_{00}^{(2)}(s) = -\frac{w^2 sin^2\theta}{4v^2b^2}\left(1 + \frac{w^2t^2\sin^2\theta}{8} + \mathrm{i}w\,t\cos\theta\right). \tag{168}$$

The fourth and last coefficient, Eq. (92), is calculated in the same manner as we did for $b_{10}^{(2)}(s)$. After some algebra we get

$$b_{11}^{(2)}(s) = \frac{w^2\sin(2\theta)}{4v^2b^2}\left(1 + \mathrm{i}\frac{w\,t}{4}\sin\theta\tan\theta\right). \tag{169}$$

Inserting all the coefficients above into Eq. (88) we get after some algebraic manipulations

$$\begin{aligned}|\Psi^{(2)}(t)\rangle \;=\; & \mathrm{e}^{-\mathrm{i}\frac{bt}{2}}\mathrm{e}^{-\mathrm{i}wt\sin^2(\theta/2)}\left\{-\frac{w^2}{4v^2b^2}\sin^2\theta\left(G_-(t) + \frac{w^2\,t^2}{8}\sin^2\theta + \mathrm{i}w\,t\cos\theta\right)|0(t)\rangle\right.\\ & \left.-\frac{w^2}{4v^2b^2}\sin(2\theta)\left(G_-(t) - \mathrm{i}\frac{w\,t}{4}G_+(t)\sin\theta\tan\theta\right)|1(t)\rangle\right\},\end{aligned} \tag{170}$$

with $G_\pm(t)$ given by Eq. (149).

We are now in position to reach interesting and important conclusions. First of all, comparing Eqs. (150)-(152) with Eqs. (156), (164), and (170) we easily realize that they are the same. In other words, the expansion of the exact solution up to second order is identical to the correction to the adiabatic approximation up to second order obtained from the APT of Sec. IV. Second, since Eq. (151) and (164) agree, we can rule out the standard approach of Sec. (III A 1) as the right way of correcting the adiabatic approximation. Indeed, the term proportional to

$$-\mathrm{i}\frac{w^2 t}{4vb}\sin^2\theta|0(t)\rangle$$

is absent in the standard approach first order correction. Although not shown here, we also obtain different second order terms whether we use the standard approach or the

APT. And evidently, the correct term comes from the APT, as Eqs. (152) and (170) demonstrate.

E. The geometric phase

We have demonstrated in the previous paragraphs that the APT gives the right first and second order correction terms to the adiabatic approximation. In this section our goal is to prove that the formalism developed in Sec. V, and which rests on the APT, is also the appropriate one when one is interested in corrections to the Berry phase. We first need to calculate the exact geometric phase for the state given by Eq. (145). We then expand this phase in terms of the small parameter $v = w$, allowing us to compare it with the first order correction obtained via the formalism of Sec. V.

1. The exact geometric phase

We are interested in the geometric phase that the state in Eq. (145) acquires after the Hamiltonian $\mathbf{H}(t)$ returns to itself. Looking at Eq. (127) we see that the period of the Hamiltonian is $\tau = 2\pi/w$, or $\tau_s = 2\pi v/w$ if we work with the rescaled time. The geometric phase we want to calculate is given by Eq. (97). Therefore, we need first the total phase $\phi(\tau)$ and the dynamical phase $\alpha(\tau)$.

The total phase, Eq. (98), is obtained using Eq. (145), which gives the state of the system at $t = \tau$. At $t = 0$, on the other hand, we have $|\Psi(0)\rangle = |0(0)\rangle$. Hence, remembering that $\langle n(0)|m(\tau)\rangle = \delta_{nm}$ we get

$$\begin{aligned}\langle\Psi(0)|\Psi(\tau)\rangle &= \mathrm{e}^{-\mathrm{i}w\tau/2}\left[\cos\left(\frac{\Omega\tau}{2}\right)\right. \\ &\quad \left. +\mathrm{i}\frac{w\cos\theta - b}{\Omega}\sin\left(\frac{\Omega\tau}{2}\right)\right]. \\ &= \mathrm{e}^{-\mathrm{i}w\tau/2}R\,\mathrm{e}^{i\zeta},\end{aligned}$$

with $R = |\langle\Psi(0)|\Psi(\tau)\rangle|$ and $\zeta = \arctan\left(\mathrm{Im}\langle\Psi(0)|\Psi(\tau)\rangle/\mathrm{Re}\langle\Psi(0)|\Psi(\tau)\rangle\right)$. Therefore, using Eq. (98) we get for the total phase $\phi(\tau) = -w\tau/2 + \zeta$, or more explicitly

$$\phi(\tau) = -\frac{w\tau}{2} + \arctan\left[\frac{w\cos\theta - b}{\Omega}\tan\left(\frac{\Omega\tau}{2}\right)\right]. \quad (171)$$

The dynamical phase is given by Eq. (96), which in terms of t is

$$\alpha(\tau) = -\frac{1}{\hbar}\int_0^\tau \mathrm{d}t\langle\Psi(t)|\mathbf{H}(t)|\Psi(t)\rangle.$$

Using the definition of Ω, Eq. (140), we get

$$\langle\Psi(t)|\mathbf{H}(t)|\Psi(t)\rangle = \frac{\hbar b}{2}\left(1 - \frac{2w^2}{\Omega^2}\sin^2\theta\sin^2(\Omega t/2)\right),$$

which results in

$$\alpha(\tau) = -\frac{b\tau}{2} + \frac{w^2 b\tau\sin^2\theta}{2\Omega^2} - \frac{w^2 b\sin(\Omega\tau)\sin^2\theta}{2\Omega^3}. \quad (172)$$

The exact geometric phase, Eq. (97), is calculated subtracting from the total phase the dynamical phase. Thus, using Eqs. (171) and (172) we get

$$\begin{aligned}\beta(\tau) &= -\frac{w\tau}{2} + \arctan\left[\frac{w\cos\theta - b}{\Omega}\tan\left(\frac{\Omega\tau}{2}\right)\right] \\ &+ \frac{b\tau}{2} - \frac{w^2 b\tau\sin^2\theta}{2\Omega^2} + \frac{w^2 b\sin(\Omega\tau)\sin^2\theta}{2\Omega^3}. \quad (173)\end{aligned}$$

2. Expansion of the exact geometric phase

We now proceed with the expansion of the exact results obtained above up to first order in the small parameter $v = w$. Again, we should be careful when doing such an expansion since we are always assuming to be near the adiabatic regime. This implies that the period τ of the Hamiltonian is a large number of order $1/w$. Therefore, terms like $w^2\tau$ are actually $\mathcal{O}(w)$, which means that we need to expand all expressions up to second order in w and then look after terms of this type.

Let us begin with the total phase. Using the definition of Ω and expanding the inverse of the tangent given in Eq. (171) we obtain up to second order in w,

$$\zeta \approx -\frac{b\tau}{2} + \frac{w\tau\cos\theta}{2} - \frac{w^2\tau\sin^2\theta}{4b} + \frac{w^2\sin^2\theta\sin(b\tau)}{4b^2}.$$

The last term is second order in v since $|\sin(b\tau)| \leq 1$, even for large τ. The other term containing w^2 is, nevertheless, $\mathcal{O}(w)$ because it is multiplied by τ. Hence, the total phase expanded up to first order is

$$\phi(\tau) = -\frac{b\tau}{2} - w\tau\sin^2(\theta/2) - \frac{w^2\tau\sin^2\theta}{4b} + \mathcal{O}(w^2). \quad (174)$$

The dynamical phase up to first order is obtained noting that the last term of Eq. (172) is $\mathcal{O}(w^2)$ since

$$\frac{w^2}{\Omega^3}\sin(\Omega\tau) = \frac{w^2}{b^3}\sin(b\tau) + \mathcal{O}(w^3).$$

Then, using that $w^2/\Omega^2 = w^2/b^2 + \mathcal{O}(w^3)$ we get

$$\alpha(\tau) = -\frac{b\tau}{2} + \frac{w^2\tau\sin^2\theta}{2b} + \mathcal{O}(w^2), \quad (175)$$

which leads to the first order expansion of the geometric phase below,

$$\beta(\tau) = -w\tau\sin^2(\theta/2) - \frac{3w^2\tau\sin^2\theta}{4b} + \mathcal{O}(w^2). \quad (176)$$

3. Perturbative correction to the geometric phase

As shown in Sec. V, the zeroth order term of the geometric phase defined in Eq. (102) is simply the Berry

phase. For the particular problem of this section it can be easily calculated using Eqs. (5) and (154),

$$\beta^{(0)}(\tau_s) = -w\tau \sin^2(\theta/2) = -w\tau(1-\cos\theta)/2, \quad (177)$$

where we have used that $\tau_s = v\tau$. Using the value for τ we get $\beta^{(0)}(\tau_s) = -\pi(1-\cos\theta)$. This phase can be interpreted as half of the solid angle subtended by a curve traced on a sphere by the direction of the magnetic field while it goes back and forth to its initial value [4].

The first order correction to the Berry phase is calculated by using directly Eq. (122),

$$\beta^{(1)}(\tau_s) = \beta^{(0)}(\tau_s) + 2v\hbar J_{10}(\tau_s) + v\hbar^2 \frac{|M_{10}(0)|^2}{\Delta_{10}^2(0)}\omega_{10}(\tau_s).$$

Inserting Eqs. (162), (163), and noting that $\omega_{10}(\tau_s) = -b\tau_s = -bv\tau$ we get

$$\beta^{(1)}(\tau_s) = -w\tau \sin^2(\theta/2) - \frac{3w^2\tau\sin^2\theta}{4b}. \quad (178)$$

Comparing Eq. (178) with the expansion of the exact geometric phase given in Eq. (176) we see that they are identical. In other words, the previous result shows that we get the same answer for the correction to the Berry phase either if we expand the exact AA geometric phase or if we calculate the AA geometric phase for the correction to the adiabatic approximation given by the APT. However, and it is here that the usefulness of a perturbative method becomes evident, for the vast majority of problems we do not know their exact geometric phases and we must rely, therefore, on the APT and the methods of Sec. V to go beyond the Berry phase.

4. *Measuring $\beta^{(1)}(\tau_s)$*

The correction to the Berry phase $\beta^{(1)}(\tau_s)$ can be measured as follows. We prepare a beam of particles in the GS $|0(0)\rangle$ of the Hamiltonian $\mathbf{H}(0)$ and split it into two equal parts. Half of it is subjected to the time dependent Hamiltonian $\mathbf{H}(s)$ and the other half to a time independent one, $\tilde{\mathbf{H}}(0)$. In the first beam $\mathbf{H}(s)$ is changed with time in a manner that makes the first order correction to the adiabatic approximation relevant. This is done by adjusting the frequency w of the rotating field. For the other beam, $\tilde{\mathbf{H}}(0)$ is such that it gives the state $|\Phi(\tau_s)\rangle_{N_1} = \mathrm{e}^{\mathrm{i}\alpha(\tau_s)}|\Psi(\tau_s)\rangle_{N_1}$ at $s=\tau_s$, i.e., the state $|\Phi(\tau_s)\rangle_{N_1}$ as given by Eq. (109) with an additional phase equals to the dynamical phase of $|\Psi(\tau_s)\rangle_{N_1}$. This is achieved by $|\Psi(\tau_s)\rangle_{N_1}$ being an eigenvector of $\tilde{\mathbf{H}}(0)$ with an eigenvalue set in a manner that provides the phase $\alpha(\tau_s)$ at τ_s. Then, recombining the two beams we measure its intensity for several orientations of the magnetic field (the angle θ). An interference pattern emerges whose intensity contrast is proportional to $\cos^2(\beta^{(1)}(\theta))$, which can be compared with the contrast predicted by Eq. (178). It is worth noticing that it may not be easy to build experimentally the Hamiltonian $\tilde{\mathbf{H}}(0)$.

We want to end this section analyzing the case where $\tau_s = \tau_c$, i.e., where the periodicity of the Hamiltonian $\tau_s = 2\pi v/w$ equals the time that it takes for the initial state to return to itself up to an overall phase [5]. In Sec. V we emphasized that those two periods are in general different. If one looks at Eq. (145) it is straightforward to see that the exact solution returns to itself (up to an overall phase) after a time $\tau_c = v\tilde{\tau} = 2\pi v/\Omega$. *However, in general we do not know the exact solution and we must rely on the period for the corrected state to return to itself.* To first order the system comes back to the initial state when the term multiplying the state $|1(s)\rangle$ is zero at $s = \tau_s = v\tau$. From Eq. (164) this is the case when $G_-(\tau) = 0$, i.e.,

$$w = \frac{b}{1+\cos\theta} = \frac{-Bge}{2mc(1+\cos\theta)}, \quad (179)$$

after using the values for τ and b. Since $w \ll 1$ this condition can be achieved by choosing a small field. If possible, we can also choose a particle with either a small charge or a big mass, or change the orientation of the field. But assuming this condition is fulfilled the geometric phases defined in Sec. V acquire the geometrical meaning that is inherent to the AA geometric phase [5].

Indeed, using Eq. (179) and $\tau = 2\pi/w$, the first order correction to the Berry phase given by Eq. (178) becomes,

$$\beta^{(1)}(\tau_s) = -2\pi\sin^2(\theta/2) - \frac{3\pi\sin^2\theta}{2(1+\cos\theta)}, \quad (180)$$

which only depends on the angle θ, i.e., the angle of the magnetic field with the z-axis (there is no other dynamical component here such as the small parameter $v = w$). Employing Berry's phase definition we can write Eq. (180) as

$$\beta^{(1)}(\tau_s) = \gamma_0(\tau_s) + \frac{3}{2}\gamma_0(\tau_s) = \frac{5}{2}\gamma_0(\tau_s). \quad (181)$$

This is the geometric phase when the first order correction to the adiabatic approximation is relevant, and it can be probed by using an experimental setup similar to the one developed to test Berry's phase [4] with the following slight modification.

First, a polarized beam of spin-1/2 particles prepared in the GS $|0(0)\rangle$ is split into two beams that are sent to regions with magnetic fields pointing initially in the same direction (see Fig. 2). In one path the direction of the magnetic field is kept constant and its magnitude (B_2) is tuned such that at $s=\tau_s$ the phase of the particles is given by the dynamical phase $\alpha^{(1)}(\tau_s)$ (Eq. (175)) with w satisfying Eq. (179). Note that the GS is independent of the field strength (Eq. (128)). Along the other beam the field (B_1) is slowly rotated with frequency w back and forth around the z-axes. The frequency should be consistent with (179) and chosen in a way that makes the

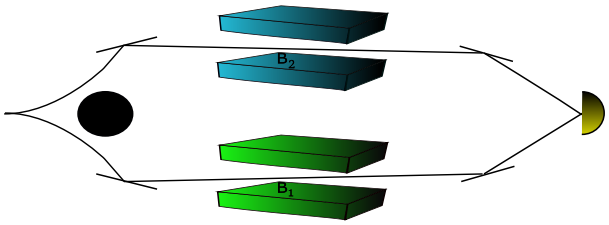

FIG. 2: (Color online) A beam of particles prepared in the GS is split into two equal parts. One (upper beam) goes through a region of constant magnetic field whose strength B_2 is such that at the end it acquires the dynamical phase $\alpha^{(1)}(\tau_s)$ of the lower beam. The latter beam goes through a region where the magnetic field B_1 rotates around the z-axes until it returns to itself. (In the original proposal [4], the field strengths are the same, $B_1 = B_2$.) Finally, the beams are recombined and the intensity measured, allowing us to determine the geometric phase $\beta^{(1)}(\tau_s)$. See text for more details.

first order correction to the adiabatic approximation relevant. Then the beams are recombined and the intensity measured. Repeating this experiment for several values of θ we should see the intensity changing as $\cos^2(\beta^{(1)}(\theta))$, where $\beta^{(1)}(\theta)$ should agree with Eq. (181).

VIII. NUMERICAL EXAMPLES

In this section we want to consider three more examples and compare their exact time evolution with the first and second order corrections to the adiabatic approximation given by the APT. One of the examples can be seen as a particular case of the analytic problem in Sec. VII and another one can also be solved analytically in terms of a special function (See Appendix A). However, here we solve them all numerically.

We again restrict ourselves to a two-level system described by the following Hamiltonian,

$$\mathbf{H}_j(s) = \begin{pmatrix} 0 & E\mathrm{e}^{\mathrm{i}\theta_j(s)} \\ E\mathrm{e}^{-\mathrm{i}\theta_j(s)} & 0 \end{pmatrix}, \tag{182}$$

where $2E$ is the time independent gap of the system and $\theta_j(s)$ is the time dependent part of the Hamiltonian. We choose three polynomials for $\theta_j(s)$, $j = 1, 2, 3$, which define our examples:

$$\theta_j(s) = \theta_j^0 + w_j\, s^j. \tag{183}$$

The parameter θ_j^0 represents the initial condition for $\theta_j(s)$ and $w_j > 0$. For $j = 1$ we recover the example of Sec. VII when the angle of the magnetic field with the z-axes is $\pi/2$. Note that we are already working with the rescaled time [22].

The snapshot eigenvectors and eigenvalues of $\mathbf{H}_j(s)$ are

$$|0(s)\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}\theta_j(s)}|\uparrow\rangle + |\downarrow\rangle\right) \quad \text{with} \quad E_0 = E, \tag{184}$$

$$|1(s)\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}\theta_j(s)}|\uparrow\rangle - |\downarrow\rangle\right) \quad \text{with} \quad E_1 = -E \tag{185}$$

An arbitrary state at s can be represented as

$$|\Psi(s)\rangle = c_\uparrow(s)|\uparrow\rangle + c_\downarrow(s)|\downarrow\rangle. \tag{186}$$

with coefficients satisfying ($\epsilon = E/(v\hbar)$)

$$\dot{c}_\uparrow(s) = -\mathrm{i}\epsilon\mathrm{e}^{\mathrm{i}\theta_j(s)}c_\downarrow(s), \tag{187}$$

$$\dot{c}_\downarrow(s) = -\mathrm{i}\epsilon\mathrm{e}^{-\mathrm{i}\theta_j(s)}c_\uparrow(s). \tag{188}$$

The comparison between the exact time evolution of $|\Psi(s)\rangle$ and the approximate results of the APT simplifies if we rewrite Eq. (186) in terms of the snapshot eigenvectors of $\mathbf{H}(s)$. Using Eqs. (184) and (185)one gets

$$|\uparrow\rangle = \mathrm{e}^{-\mathrm{i}\theta_j(s)}\left(|0(s)\rangle + |1(s)\rangle\right)/\sqrt{2}, \tag{189}$$

$$|\downarrow\rangle = \left(|0(s)\rangle - |1(s)\rangle\right)/\sqrt{2}, \tag{190}$$

so that (186) becomes

$$|\Psi(s)\rangle = c_0(s)|0(s)\rangle + c_1(s)|1(s)\rangle, \tag{191}$$

where

$$c_0(s) = \left(\mathrm{e}^{-\mathrm{i}\theta_j(s)}c_\uparrow(s) + c_\downarrow(s)\right)/\sqrt{2}, \tag{192}$$

$$c_1(s) = \left(\mathrm{e}^{-\mathrm{i}\theta_j(s)}c_\uparrow(s) - c_\downarrow(s)\right)/\sqrt{2}. \tag{193}$$

If the system starts at the eigenvector $|0(0)\rangle$, i.e., $c_0(0) = 1$ and $c_1(0) = 0$, then

$$c_\uparrow(0) = \mathrm{e}^{\mathrm{i}\theta_j^0}/\sqrt{2} \quad \text{and} \quad c_\downarrow(0) = 1/\sqrt{2}. \tag{194}$$

To have a quantitative measure of the closeness of the corrections to the adiabatic approximation to the exact state (191) we compute a quantity called fidelity,

$$F_k(s) = |\langle\Psi(s)|\Psi(s)\rangle_{N_k}|^2, \tag{195}$$

where $|\Psi(s)\rangle_{N_k}$ is the normalized state containing corrections up to order k (Eq. (99)). When the states are the same $F_k = 1$ and $F_k = 0$ when they are orthogonal.

Using the snapshot eigenvectors given by Eqs. (184) and (185), Eqs. (99) and (101), and repeating the same steps of Sec. VII we get

$$|\Psi(s)\rangle_{N_0} = |\Psi^{(0)}(s)\rangle = \mathrm{e}^{-\mathrm{i}\epsilon s}\mathrm{e}^{-\mathrm{i}\Delta\theta_j(s)/2}|0(s)\rangle, \tag{196}$$

with $\Delta\theta_j(s) = \theta_j(s) - \theta_j^0$,

$$|\Psi(s)\rangle_{N_1} = N_1\left(|\Psi^{(0)}(s)\rangle + v|\Psi^{(1)}(s)\rangle\right), \tag{197}$$

where

$$|\Psi^{(1)}(s)\rangle = \mathrm{e}^{-\mathrm{i}\epsilon s}\mathrm{e}^{-\mathrm{i}\Delta\theta_j(s)/2}\left\{-\frac{\mathrm{i}\hbar}{8E}\int_0^s \dot{\theta}_j^2(s')\mathrm{d}s'|0(s)\rangle + \frac{\hbar}{4E}\left(\dot{\theta}_j(s) - \mathrm{e}^{\mathrm{i}2\epsilon s}\dot{\theta}_j(0)\right)|1(s)\rangle\right\}, \tag{198}$$

and

$$|\Psi(s)\rangle_{N_2} = N_2\left(|\Psi^{(0)}(s)\rangle + v|\Psi^{(1)}(s)\rangle + v^2|\Psi^{(2)}(s)\rangle\right), \tag{199}$$

in which $|\Psi^{(2)}(s)\rangle$ is given by Eq. (88). The coefficients of $|\Psi^{(2)}(s)\rangle$, where $\omega_0(s) = -\omega_1(s) = E\,s/\hbar$ and $\gamma_0(s) = \gamma_1(s) = -\Delta\theta_j(s)/2$, are

$$
\begin{aligned}
b_{00}^{(2)}(s) &= \frac{-\hbar^2}{32E^2}\left\{\dot\theta_j^2(0) + \dot\theta_j^2(s) + \frac{1}{4}\left(\int_0^s \dot\theta_j^2(s')\mathrm{d}s'\right)^2\right\},\\
b_{01}^{(2)}(s) &= \frac{\hbar^2}{16E^2}\dot\theta_j(0)\dot\theta_j(s),\\
b_{10}^{(2)}(s) &= \frac{-\mathrm{i}\hbar^2}{8E^2}\left(\ddot\theta_j(s) + \frac{\dot\theta_j(s)}{4}\int_0^s \dot\theta_j^2(s')\mathrm{d}s'\right),\\
b_{11}^{(2)}(s) &= \frac{\mathrm{i}\hbar^2}{8E^2}\left(\ddot\theta_j(0) - \frac{\dot\theta_j(0)}{4}\int_0^s \dot\theta_j^2(s')\mathrm{d}s'\right).
\end{aligned}
$$

By inspection of Eqs. (196), (197), (199), and their coefficients, and using the definition for $\theta_j(s)$, we realize that from one order to the next we have a smaller contribution to the overall state if $\epsilon^{-1} = v\hbar/E < 1$. The previous condition is related to the existence of a gap ($E > 0$) and the near adiabaticity approximation ($v = w_j \ll 1$). When those conditions are satisfied, we should expect the APT to work.

There is one more interesting fact. If we factor out the highly oscillatory dynamical term $\mathrm{e}^{-\mathrm{i}\epsilon s}$, the other oscillatory terms are always multiplied by the first or second order derivatives of θ_j at $s = 0$. This can be seen by looking at Eq. (198), where we have the term $\mathrm{e}^{\mathrm{i}2\epsilon s}\dot\theta_j(0)$. A similar exponential appears in $|\Psi^{(2)}(s)\rangle$, multiplying either $\dot\theta_j(0)$ or $\ddot\theta_j(0)$ (see coefficients $b_{01}^{(2)}(s)$ and $b_{11}^{(2)}(s)$). Therefore, by properly choosing the functional form of θ_j we can eliminate those oscillatory terms. It remains only a global oscillatory phase $\mathrm{e}^{-\mathrm{i}\epsilon s}$ that has no influence on the fidelity or on the probability to find the system out of the GS.

Let us start presenting the results of the numerical calculations. In Fig. 3 we show the value of the infidelity, $|1 - F_k(s)|$, when $\epsilon^{-1} < 1$. For the three cases, as we increase the order of the APT we get closer and closer to the exact solution (small infidelity). In Fig. 4 we show the behavior of the APT as we increase ϵ^{-1}. We computed how much the second order correction differs from the exact solution for all $\theta_j(s)$. It is clear that for $\epsilon^{-1} < 1$ we almost see no difference from the exact solution. For $\epsilon^{-1} > 1$, however, the perturbation theory fails as can be seen from the last panel of Fig. 4.

In all previous calculations it was implicit that $\theta_j(s)$ was a smooth function. It may happen that its first or second (or n-th) order derivative with respect to time becomes discontinuous. This is related to the way we can experimentally control the Hamiltonian [11]. Under those circumstances we can continue using APT to predict the behavior of the exact solution to the SE. The way to circumvent this problem is relatively simple. Let us assume we have the following functional form for $\theta_j(s)$

$$
\theta_j(s) = \begin{cases} \theta_j^0 + w_j s^j & \text{if } \ s \geq 0, \\ \theta_j^0 & \text{if } \ s < 0. \end{cases} \tag{200}
$$

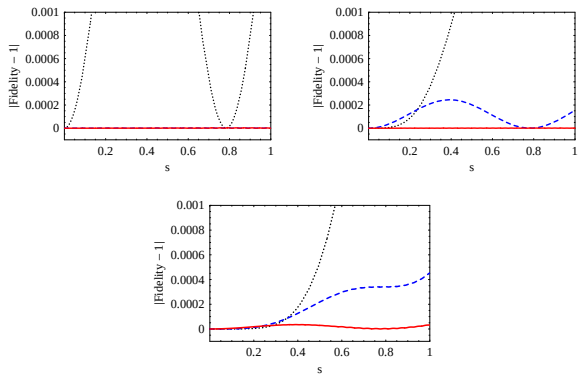

FIG. 3: (Color online) Here $\theta_j^0 = 1$, $E = 2$, and $v = w_j = 0.5$, which gives $\epsilon^{-1} = 0.25$ ($\hbar = 1$). At the top we have $\theta_j(s)$, $j = 1, 2$, and at the bottom $j = 3$. The black/dotted curves represent the infidelity between the zeroth order correction, Eq. (196), and the exact solution, Eq. (191), as a function of the rescaled time s. Both quantities are adimensional. The blue/dashed curves are the infidelity when we go up to first order (Eq. (197)) and the red/solid ones when we include the second order term (Eq. (199)). For $j = 1$, the first and second order curves are indistinguishable and the solid/dotted curves go as high as 0.004.

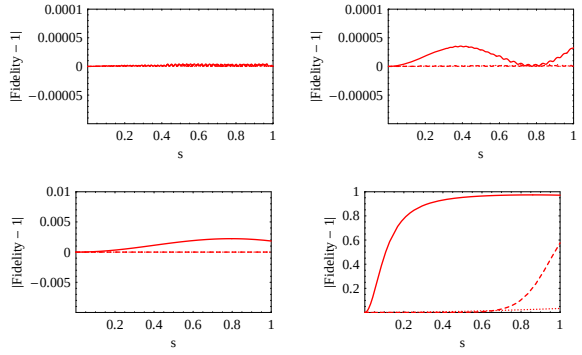

FIG. 4: (Color online) The same parameters of Fig. 3 but with different gaps. Top: $\epsilon^{-1} = 0.125$ and 0.25. Bottom: 0.5 and 5. All curves represent the infidelity between the exact solution and the adiabatic approximation corrected up to second order (Eq. (199)). The solid curve represents $\theta_3(s)$, the dashed $\theta_2(s)$, and the dotted one $\theta_1(s)$. In the first panel all curves coincide while at the next two the dashed and dotted curves are indistinguishable. Note the difference of scale at the bottom panels. For the first three, the APT works beautifully and the results are better the lower ϵ^{-1}. At the last panel we see the three curves and the break down of the APT since $\epsilon^{-1} > 1$.

When $s < 0$, and starting, let us say, at $s = -0.2$, and using the initial condition at that time, we compute the perturbative terms given by the APT using $\theta_j(s) = \theta_j^0$. All terms but the zeroth order vanish since the Hamiltonian is time independent for $s < 0$. Then, at $s = 0$ we start computing the perturbative terms using $\theta_j(s) = \theta_j^0 + w_j s^j$ and as initial state we use the final

state from the previous computation, i.e., we impose the continuity of the wave function at $s = 0$: $\lim_{s\to 0^-} |\Psi(s)\rangle = \lim_{s\to 0^+} |\Psi(s)\rangle$. This procedure allows us to obtain in a perturbative way the right time evolution for the whole range of rescaled time s. We exemplify this approach in Fig. 5. It is clear that this approach (third panel) is the

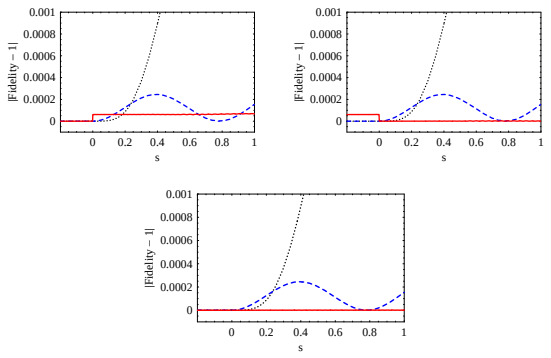

FIG. 5: (Color online) The same parameters and notation of Fig. 3 for the case $\theta_2(s)$. At the top panels we used, for expressions coming from the APT and throughout the whole range of s, $\ddot{\theta}(0) = 0$ for the first panel and $\ddot{\theta}(0) = 2w_2$ for the second one. At the bottom panel we used $\ddot{\theta}(0) = 0$ for $s < 0$ and $\ddot{\theta}(0) = 2w_2$ for $s \geq 0$ plus the continuity of the wave function at $s = 0$.

best option. To second order, we see no appreciable difference between the exact solution and the perturbative solution. In Fig. 5 we worked with $\theta_2(s)$ but the same feature shows up with $\theta_1(s)$, where in this case it is the first order correction that is problematic. The same feature is true if we work with another time dependent Hamiltonian. *In general, a discontinuous derivative of order $k+1$ in the quantity $M_{nm}(s)/\Delta_{mn}(s)$ affects the k-th order in perturbation theory.* The remedy, nevertheless, is the same as before.

IX. DISCUSSIONS AND CONCLUSIONS

In this paper we presented a useful and practical way to find corrections to the adiabatic approximation named, after Garrison [2], adiabatic perturbation theory (APT). Considering the adiabatic approximation as the zeroth order term, we have developed a power series expansion that gives the time evolution of the system. The only assumption made was the existence of a non-degenerate Hamiltonian throughout the time evolution. We have explicitly calculated corrections up to second order in the small parameter v, that is related to the inverse of the relevant time scale of the problem, namely the time required to change the system's Hamiltonian from its initial value to the desired final one.

We have checked the validity of this approach comparing the exact solution of several time dependent problems with the approximate results given by the APT. One of the problems had an exact analytical solution which allowed detailed comparison with the approximate one given by the APT. We got a perfect agreement between both ways of solving the problem. The other time dependent problems were solved numerically. The APT passed all tests for those numerical cases too: the more terms one adds to the approximate solution the closer one gets to the exact solution. We should note, however, that a rigorous general proof of convergence of the APT series expansion was not given, although we believe that it will work in general at least in an asymptotic sense.

In addition, we have compared the APT to other methods that also try to go beyond the adiabatic approximation. The first method we dealt with was what we called the standard approach, since it is based on the straightforward manipulations of the integral equations that one gets when writing formally the exact solution to the time dependent Schrödinger equation (Sec. III A 1). We have shown that the naive expansion of the integral equations in terms of the small parameter v fails to give an accurate correction to the adiabatic approximation. We then studied the iterative rotating-basis method developed in Ref. [3] and which is related to the ones in Refs. [12, 13, 14]. As can be seen in the analysis of Sec. III B, this approach is not a perturbative method in the small parameter v. Rather, it is built on another premise that, loosely speaking, has the goal of finding by an iterative process a new frame of reference where the modified Hamiltonian becomes time independent. We have emphasized that at each iteration step one can in principle use our APT as a way of approximating the solution within that frame.

Most importantly, we have proven that the APT here introduced, and which was inspired by the work of Ponce *et al.* [11], is connected to the multi-variable expansion method developed by Garrison [2]. Indeed, we have shown the formal mathematical equivalence between both methods. Starting with the APT we can obtain the multi-variable expansion method and vice versa. However, the equations obtained from the APT to order p are simple algebraic recursive relations involving the terms of order $p-1$. On the other hand, the multi-variable expansion method requires not only manipulating recursive relations but also solving partial differential equations.

We have also shown how to calculate corrections to the Berry phase [4] to an arbitrary order in the small parameter v. The strategy we adopted had two basic ingredients, one of which was the normalized p-th order correction to the adiabatic approximation. The other one was the Aharonov-Anandan phase, a natural generalization of the Berry phase [5], suited to the calculation of geometric phases away from the adiabatic regime. Moreover, we have explicitly computed the first order correction in a spin-1/2 (qubit) problem, and proposed a specific quantum interference experiment to measure it. We showed that when the first order correction to the adiabatic approximation is relevant, the geometric phase should be two and a half times the Berry phase.

Finally, our results lead naturally to new questions. First, can we build an APT similar in spirit to the one presented here but for open quantum systems where we have non-unitary dynamics [23]? Second, can we employ this open dynamics APT to calculate corrections to all sorts of geometric phases [24]? And third, can we extend our ideas to the case where the Hamiltonian spectrum is degenerate?

Acknowledgments

G. R. thanks the Brazilian agency Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) for funding this research. G. R. and G. O. thank Manny Knill and Armando A. Aligia for several hours of useful discussions at Indiana University and Los Alamos.

APPENDIX A: SOLUTION TO THE $\theta_2(s)$ CASE

For $\theta_2(s) = \theta_2^0 + w_2\, s^2$ Eqs. (187) and (188) are a particular case of the following ones,

$$\begin{aligned} \dot{c}_\uparrow(s) &= V \mathrm{e}^{\mathrm{i}w_2 s^2} c_\downarrow(s), \\ \dot{c}_\downarrow(s) &= -V^* \mathrm{e}^{-\mathrm{i}w_2 s^2} c_\uparrow(s). \end{aligned}$$

Decoupling we get,

$$\ddot{c}_\uparrow(s) - \mathrm{i}2w_2 s \dot{c}_\uparrow(s) - |V|^2 c_\uparrow(s) = 0.$$

Making the change of variable $c_\uparrow(s) = f(s)z(s)$ and imposing that in the new equation the coefficient multiplying $\dot{z}(s)$ be zero we obtain $\ddot{z}(s) + \left(\mathrm{i}w_2 + w_2^2 s^2 + |V|^2\right) z(s) = 0$, with $f(s) = f(0)\mathrm{e}^{\mathrm{i}w_2 s^2/2}$. Making another change of variable, $x = \sqrt{2|w_2|}s$, we get $\mathrm{d}^2 z/\mathrm{d}x^2 + \left(x^2/4 - a\right) z(x) = 0$, where $a = -|V|^2 - \mathrm{i}/2$. The solution to the previous equation are the Weber functions [25],

$$\begin{aligned} z_1(x) &= \sum_{n=0}^{\infty} a_{2n} x^{2n}/(2n)!, \\ z_2(x) &= \sum_{n=0}^{\infty} a_{2n+1} x^{2n+1}/(2n+1)!, \end{aligned}$$

in which $a_0 = a_1 = 1$, $a_2 = a_3 = a$, and $a_{n+2} = a a_n - n(n-1)a_{n-2}/4$. Finally, returning to the original variable we get the solution to the original problem,

$$c_\uparrow(s) = \mathrm{e}^{\mathrm{i}w_2 s^2/2} \left(c_1^0 z_1(2\sqrt{|w_2|}\, s) + c_2^0 z_2(2\sqrt{|w_2|}\, s) \right),$$

with c_1^0 and c_2^0 being fixed by the initial conditions.

[1] A. Messiah, *Quantum Mechanics*, (North-Holland, Amsterdam, 1962), vol. 2.
[2] J. C. Garrison, Preprint UCRL 94267, Lawrence Livermore Laboratory (1986).
[3] M. V. Berry, Proc. R. Soc. Lond. A **414**, 31 (1987).
[4] M. V. Berry, Proc. R. Soc. Lond. A **392**, 45 (1984).
[5] Y. Aharonov and J. Anandan, Phys. Rev. Lett. **58**, 1593 (1987).
[6] K.-P. Marzlin and B. C. Sanders, Phys. Rev. Lett. **93**, 160408 (2004); *ibidem* **97**, 128903 (2006).
[7] D. M. Tong, K. Singh, L. C. Kwek, and C. H. Oh, Phys. Rev. Lett. **95**, 110407 (2005).
[8] S. Jansen, M.-B. Ruskai, and R. Seiler, J. Math. Phys. **48**, 102111 (2007).
[9] R. MacKenzie, A. Morin-Duchesne, H. Paquette, and J. Pinel, Phys. Rev. A **76**, 044102 (2007).
[10] D. M. Tong, K. Singh, L. C. Kwek, and C. H. Oh, Phys. Rev. Lett. **98**, 150402 (2007).
[11] M. V. Ganduglia, E. C. Goldberg, and V. H. Ponce, 70^o Meeting of the Argentine Physics Association (AFA), Rosario; Book of Abstracts and Communications (1985).
[12] L. M. Garrido, J. Mat. Phys. **5**, 335 (1964).
[13] G. Nenciu and G. Rasche, J. Phys. A: Math. Gen. **25**, 5741 (1992).
[14] G. Nenciu, Commun. Math. Phys. **152**, 479 (1993).
[15] It is important to mention again that in Ref. [3] the main author's motivation was to obtain systematic corrections to the Berry phase via the iterative process. What we show in the remaining of Sec. III B, however, is related to corrections to the whole state (not just the phase) via the same iterative process.
[16] B. Simon, Phys. Rev. Lett. **51**, 2167 (1983).
[17] See F. Wilczek and A. Zee, Phys. Rev. Lett **52**, 2111 (1984) for a generalization that includes degenerate subspaces.
[18] Given a Hilbert space $\mathcal{H}$ we can build its associated projective Hilbert space $\mathcal{P}_\mathcal{H}$ as the set of equivalence classes of vectors in $\mathcal{H}$ such that $|\Psi_1\rangle \sim |\Psi_2\rangle$ when $|\Psi_1\rangle = \lambda|\Psi_2\rangle$, with $|\Psi_j\rangle \in \mathcal{H}$, $j = 1, 2$, and $\lambda \neq 0$ complex.
[19] M. V. Berry in *Geometric Phases in Physics*, (World Scientific, 1988), p. 7-28.
[20] A. Bohm, *Quantum Mechanics: Foundations and Applications*, (Springer-Verlag, New York, 1993), p. 587.
[21] I. I. Rabi, N. F. Ramsey, and J. Schwinger, Rev. Mod. Phys. **26**, 167 (1954).
[22] To go from the real time t to the rescaled time s the constants multiplying t, or any function of it, should be properly chosen. For example, had we started with $\tilde{\theta}_3(t) = \tilde{w}_3\, t^3$ and using that $s = v\, t$ we would have $\theta_3(s) = \tilde{w}_3\, s^3/v^3$. Since v is a small number we need to set $\tilde{w}_3$ at least as small as $\tilde{w}_3 = v^3 w_3$ in order to obtain $\theta_3(s)$ as given by Eq. (183).
[23] M. S. Sarandy and D. A. Lidar, Phys. Rev. A **71**, 012331 (2005).
[24] E. I. Duzzioni, R. M. Serra, and M. H. Y. Moussa, Europhys. Lett. **82**, 20007 (2008).
[25] M. Abramowitz and I. A. Stegun (Eds.), *Handbook of Mathematical Functions*, (New York, Dover, 1965), p. 692.