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Assessing Errors in the Adiabatic Approximation via Bures Angle

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Resumo

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Resumo da Dissertação de Mestrado apresentada ao Programa de Pós-Graduação em Física do Instituto de Física da Universidade Federal do Rio de Janeiro - UFRJ, como parte dos requisitos necessários à obtenção do título de Mestre em Ciências (Física).

A aproximação quântica adiabática desempenha um papel importante em mecânica quântica. Essa aproximação afirma que, para um sistema inicialmente preparado num auto-estado de um Hamiltoniano que varia no tempo, a evolução governada pela equação de Schrödinger manterá o estado do sistema no correspondente auto-estado do Hamiltoniano no limite de uma variação infinitamente lenta. Entretanto, para aplicações práticas, como a computação quântica adiabática (CQA), é crucial determinar, para processos em tempo finito, o erro, ou distância, entre o estado real do sistema e o estado-alvo, a saber, o auto-estado instantâneo do Hamiltoniano. Em especial, é importante determinar quão longo deve ser o tempo total T da evolução para que o erro final não seja maior que um certo valor pequeno fixo. Inicialmente, a maioria dos estudos em CQA se apoiou na versão tradicional da aproximação quântica adiabática, o que é insuficiente para tal estimativa. Mesmo as estimativas recentes, que levam em conta correções à aproximação quântica adiabática, ainda deixam espaço para aperfeiçoamento. Neste trabalho apresentamos estimativas para este erro, quantificando-o pelo ângulo de Bures entre o estado real

do sistema e o estado-alvo. Mais precisamente, apresentamos limites superior e inferior a esta distância que se mostram altamente precisos. Nossa abordagem é baseada numa teoria de perturbação adiabática que expande e fornece correções à aproximação quântica adiabática tradicional. Além disso, apresentamos um teorema que prescreve o comportamento do ângulo de Bures quando um número de derivadas do Hamiltoniano vai a zero nos instantes inicial e final. Obtém-se que o erro diminui quando mais derivadas são tomadas como nulas. Este efeito é desejável e pode ser aplicado à CQA, pois os Hamiltonianos envolvidos são supostos controláveis.

Palavras-chave: 1. Computação Quântica Adiabática, 2. Teoria de Perturbação Adiabática, 3. Ângulo de Bures.

Abstract

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Abstract of the Master Dissertation presented to the Graduate Program in Physics of the Institute of Physics of the Federal University of Rio de Janeiro - UFRJ, as part of the requirements to the obtention of the title of Master in Sciences (Physics).

The quantum adiabatic approximation plays an important role in quantum mechanics. This approximations states that, if a system is initially prepared in an eigenstate of a time-dependent Hamiltonian, the time evolution governed by the Schrödinger equation will keep the state of the system in a corresponding eigenstate of the Hamiltonian in the limit of a infinitely slow change. However, for practical reasons, like those encountered in Adiabatic Quantum Computation (AQC), it is crucial to determine the error, or the distance between the actual state of the system and the target state, namely, the instantaneous eigenstate of the Hamiltonian for finite-time processes. In particular it is important to determine how long the process must last in order to obtain a final error which is not greater than a small fixed value. Most AQC studies have relied on the traditional quantum adiabatic approximation, which is unsatisfactory for such estimates. Even recent estimates, which take into account corrections to the quantum adiabatic approximation, leave room for improving. In this work we present estimates of this error through the Bures angle between

the actual state of the system and the target state. More precisely we present upper and lower bounds on this distance which turn out to be very accurate. Our approach is based on an adiabatic perturbation theory which expands and provides corrections to traditional quantum adiabatic approximation. Furthermore we present a theorem which prescribes the behaviour of the Bures distance when a number of derivatives of the Hamiltonian vanishes at initial and final times of the physical process, namely, the error decreases. This effect is desirable and it can be applied to AQC, since the Hamiltonians involved are assumed to be controllable.

Keywords: 1. Adiabatic Quantum Computation, 2. Adiabatic Perturbation Theory, 3. Bures Angle.

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Chapter 1

Introduction

The adiabatic approximation of quantum mechanics states that if we prepare a system in an eigenstate of a Hamiltonian which varies slowly enough, the time evolution of the system, which is governed by the Schrödinger equation, will approximately keep the actual state of the system in a corresponding eigenstate of the Hamiltonian [1]. This approximation plays a fundamental role in applications, for instance, in Adiabatic Quantum Computation (AQC) [13] which offers a paradigm for exploiting quantum mechanics in order to obtain a speedup for classically difficult computational problems. The idea is to solve a problem by adiabatically modifying a Hamiltonian whose initial ground state $|\phi(0)\rangle$ encodes the input and the whose final ground state encodes the output $|\phi(\mathrm{T})\rangle$. The time taken to reach the final ground state is the running time of the quantum adiabatic algorithm. In this scenario we would like to minimize the error, or distance, between the actual final state of the system $|\psi(\mathrm{T})\rangle$ and the desired final ground state while at the same time minimizing the running time. Nevertheless the adiabatic approximation of the quantum mechanics is not sufficient in applications and we would like to quantify this error in a more precise way, which constitutes the aim of this work. Some references to this subject are the works [4], [10], [9] and [11]. As a introduction to this subject we present the results of [4], which is our main reference.

The notion of error in [4] is quantified by the distance

$$\delta = || \ |\psi(\mathrm{T})\rangle \text{ - } e^{\mathrm{i}\chi}|\phi(\mathrm{T})\rangle \ ||, \tag{1.1}$$

between the actual state of the system $|\psi\rangle$ and the ground state of the Hamiltonian $|\phi\rangle$, the target state. This distance is considered at the final time of the physical process $t = T$, as denoted in (1.1). Here χ represents a dynamical phase, which will become clear in the following discussion. Now we introduce a theorem, which is the central result of that work, then we discuss the hypothesis about this result and its proof.

Theorem If the first N ≥ 1 derivatives of the Hamiltonian vanish at $\tau = 0$ and $\tau = 1$ (the initial and final times of the evolution of the system), a final time which scales with

$$\mathrm{T} = \frac{q}{\gamma}\mathrm{N}\ \frac{\xi^2}{d^3}, \tag{1.2}$$

where the *time dilation* q is a free parameter, yields an adiabatic approximation error which satisfies

$$\delta \leq (\mathrm{N}+1)^{\gamma+1} q^{-N}. \tag{1.3}$$

They [4] express the dimensionless Hamiltonian of the system as H = h / J, where J is an arbitrary energy unit and the Hamiltonian of the system h obeys the Schrödinger equation

$$i\frac{\partial}{\partial t}|\psi(\mathrm{t})\rangle = \mathrm{h(t)}|\psi(\mathrm{t})\rangle \ , \tag{1.4}$$

because they work in units of $\hbar$=1. They define the dimensionless parameter τ= t/T = ϵJt , where $\epsilon = 1/(\mathrm{JT})$. Thus for a given T it always possible to choose J so that ϵ is a small number, which is needed for the asymptotic expansion below. The Schrödinger equation in dimensionless units reads

$$\mathrm{i}\epsilon\frac{\partial}{\partial \tau}|\psi(\tau)\rangle = \mathrm{H}(\tau)|\psi(\tau)\rangle \ . \tag{1.5}$$

They are concerned with analytic continuations of the Hamiltonian, so that γ is the distance to the pole or branch point of H(τ) that is nearest to the real τ-axis, that is, they suppose H(τ) admits an analytic continuation to an open set which contains the real τ-axis. They additionally suppose that it is possible to set any given number of the derivatives of the Hamiltonian to zero at the initial and final times. Furthermore they consider that the target state $|\phi(\tau)\rangle$, with the corresponding eigenvalue E(τ), is a non-degenerate and isolated eigenstate of H(τ). Other quantities which need to be defined are the norm of an operator A, which is the largest of the eigenvalues of $\sqrt{A^\dagger A}$ and denoted by $||A||$, and the minimum dimensionless gap during the whole evolution Δ. They express

$$\mathrm{d} = \mathrm{J}\Delta \tag{1.6}$$

and

$$\xi = \max_{\tau} || \frac{\mathrm{dh}}{\mathrm{d}\tau} ||. \tag{1.7}$$

The quantity they want to bound is (1.1), where χ =- $\int_0^1 \mathrm{E}(\tau)\mathrm{d}\tau/\epsilon$, so that their strategy will be consider the following two distances separately, that is,

$$\delta_1 = || \ |\psi(1)\rangle \text{ - } |\Psi_N(1,\epsilon)\rangle \ || \tag{1.8}$$

and

$$\delta_2 = || \ e^{i\int_0^1 E(\tau)\mathrm{d}\tau/\epsilon}|\Psi_N(1,\epsilon)\rangle \text{ - } |\phi(1)\rangle||. \tag{1.9}$$

In the equations (1.8) and (1.9) the final time of the physical process $t = T$ is denoted by $\tau = 1$, because they have made the substitution τ = t/T. Furthermore they are considering a perturbative approximation whose zeroth order term is the target state, namely,

$$\big|\Psi_N(\tau,\epsilon)\rangle = |\phi(\tau)\rangle+\epsilon|\psi_1(\tau)\rangle+\epsilon^2\big|\,\psi_2(\tau)\rangle+...+\epsilon^N|\psi_N(\tau)\rangle+\epsilon^{N+1}|\psi^{\perp}_{N+1}(\tau)\rangle, \tag{1.10}$$

where

$$\big|\psi_j(\tau)\rangle = f_j(\tau)|\phi(\tau)\rangle+|\psi^{\perp}_j(\tau)\rangle \ , \tag{1.11}$$

for 1≤ j ≤ N. The vector $\left|\psi_j^{\perp}(\tau)\right\rangle$ can be obtained from

$$\left|\psi_j^{\perp}(\tau)\right\rangle = G_r(\tau)(f_j(\tau)|\dot{\phi}(\tau)\rangle + P_{\perp}(\tau)|\dot{\psi}_{j-1}(\tau)\rangle) \,, \tag{1.12}$$

and $\left|\psi_0^{\perp}(\tau)\right\rangle = 0$. The functions $f_j(\tau)$ are determined from

$$\dot{f}_j(\tau) = \text{-} \, \langle\phi(\tau)|\dot{\psi}_j^{\perp}(\tau)\rangle \tag{1.13}$$

and from the conditions $f_0(\tau) \equiv 1$ and $f_j(1) = 0$, $1 \leq \text{j} \leq \text{N}$. The operator $P_{\perp}(\tau)$ is a projector onto the orthogonal complement of the target subspace, therefore $P_{\perp}(\tau)$ = 1 - $|\phi(\tau)\rangle\langle\phi(\tau)|$. The operator G_r is a map from the full Hilbert space to the orthogonal complement of the target subspace, it is a reduced resolvent of the Hamiltonian given by

$$G_r(\tau)=\frac{i}{H(\tau) - E(\tau)}. \tag{1.14}$$

The triangle inequality results in

$$\delta \leq \delta_1 + \delta_2, \tag{1.15}$$

therefore their strategy is to bound (1.8) and (1.9) separately in order to obtain a bound on (1.1).

The distance (1.9) vanishes by imposing that the first $(N + 1)$ derivatives of the Hamiltonian vanish at the initial and final times of the physical process [4]. The error in (1.8) was estimated in [11] as

$$|| \, |\phi(1)\rangle \text{ - } |\Psi_N(1,\epsilon)\rangle \, || \leq \text{A}(1)\epsilon^{N+1}, \tag{1.16}$$

where

$$A_N(\tau) = \int_0^{\tau} \| \frac{\text{d}\psi_N^{\perp}}{\text{d}\zeta} || \text{d}\zeta. \tag{1.17}$$

The derivative of the vector $\left|\psi_N^{\perp}\right\rangle$ can be evaluated by making use of the Cauchy integral formula, because this vector is an analytic function within the domain of analyticity of the Hamiltonian [4]. In fact they prove by induction that

$$|| \, \psi_N^{\perp}|| \leq \text{C(N)g(N)}A^{3N-1}\beta^{2N-1}, \tag{1.18}$$

where

$$\mathrm{g(N)} = (\frac{N-1}{\gamma})^{N-1}, \tag{1.19}$$

$$\mathrm{C(N)} = \prod_{j=1}^{N-1}(1+ \gamma \ \frac{(j-1)^{j-1}}{j^j} \ ), \tag{1.20}$$

$$A = 1/\Delta \tag{1.21}$$

and

$$\beta = \xi/\mathrm{J}. \tag{1.22}$$

The Cauchy integral formula is then used to obtain an upper bound on $\left\| \frac{\mathrm{d}\psi_N^{\perp}}{\mathrm{d}\tau} \right\|$, namely,

$$|| \ \dot{\psi}_N^{\perp}|| \leq \mathrm{C(N)g(N+1)}A^{3N}\beta^{2N}. \tag{1.23}$$

This last result provides

$$A_N(1) \leq \mathrm{(N+2)}^{\gamma+1}(\ \frac{(N+1)A^3\beta^2}{\gamma})^{N+1}. \tag{1.24}$$

Therefore they obtain an upper bound on the error (1.16) as

$$\delta_1 \leq \mathrm{(N+2)}^{\gamma+1}(\ \frac{(N+1)\xi^2}{\gamma \mathrm{Td}^3})^{N+1}, \tag{1.25}$$

where they have reinserted dimensional units. Thus they pick T as

$$\mathrm{T} = \frac{q}{\gamma}\mathrm{(N+1)}\frac{\xi^2}{d^3}, \tag{1.26}$$

where q is a free parameter whose value can be chosen arbitrarily. This choice furnishes

$$\delta_1 \leq \mathrm{(N+2)}^{\gamma+1}q^{-(N+1)}. \tag{1.27}$$

The substitution N $\rightarrow$ (N - 1) together with the assumption about the derivatives of the Hamiltonian then reproduce (1.2) and (1.3), so that the theorem is proved. These results constitute the main motivation to the results derived below.

The next chapter introduces some ideas which constitute the backbone of our results, which are presented in the third chapter. An adiabatic perturbation theory is introduced together with a notion of distance between two quantum states which is different from (1.1). In the third chapter we present bounds on the distance between two quantum states and make a estimate about the running time.

Chapter 2

An Adiabatic Perturbation Theory

In this chapter we present the adiabatic approximation in a more formal way than that of the previous chapter, then we develop an adiabatic perturbation theory (APT), which furnishes corrections to this approximation. Finally we introduce some concepts related to the notion of distance between two pure quantum states.

2.1 Adiabatic approximation

In this section we follow [1]. We consider a physical process which lasts a time interval T, so that we define $s = vt$ ($v = 1/T$) as a dimensionless parameter. Let P_0, P_1,...,P_i,... be a complete set of orthonormal projectors which satisfy

$$\mathrm{H(s)}P_i\mathrm{(s)}{=}E_i\mathrm{(s)}P_i\mathrm{(s)}, \tag{2.1}$$

where $H(s)$ is the time-dependent Hamiltonian of the system, which varies continuously during the process from an initial value $H(0)$ to a final value $H(1)$. Additionally we suppose: (i) the derivatives of first and second order of the projectors above are piecewise continuous during the process and (ii) the energy eigenvalues remain distinct throughout the transition of the Hamiltonian, that is, $E_i\mathrm{(s)}{\neq}E_k\mathrm{(s)}$. Thus under these assumptions we want to prove that the time evolution operator of the system exhibits the following asymptotic behaviour

$$\lim_{T\to\infty} U_T\mathrm{(s)}P_j(0){=}P_j\mathrm{(s)}\lim_{T\to\infty} U_T\mathrm{(s)}, \tag{2.2}$$

since (2.2) is completely equivalent to the adiabatic approximation. Before proving (2.2) we need to introduce an additional apparatus.

2.1.1 Rotating axis representation

We introduce a unitary operator $A(s)$ having the property

$$P_j(\mathrm{s}) = \mathrm{A(s)}P_j(0)A^{\dagger}(\mathrm{s}), \tag{2.3}$$

which takes any set of eigenvectors of $H(0)$ over into a set of eigenvectors of $H(s)$. It is unambiguously defined by the initial condition

$$\mathrm{A}(0) = 1 \tag{2.4}$$

and the differential equation

$$\mathrm{i}\hbar\frac{\mathrm{dA}(s)}{\mathrm{ds}} = \mathrm{K(s)A(s)}, \tag{2.5}$$

where $K(s)$ may be chosen as the hermitian operator

$$\mathrm{K(s)} = \mathrm{i}\hbar \sum_j \frac{dP_j(s)}{ds}P_j(\mathrm{s}) \ . \tag{2.6}$$

For (2.3) to be satisfied it is necessary and sufficient that $K(s)$ obey the commutation relations

$$[\mathrm{K(s)},P_j(\mathrm{s})] = \mathrm{i}\hbar\frac{dP_j(s)}{ds}. \tag{2.7}$$

The unitary transformation $A(s)$ carries the vectors and operators of the Schrödinger representation over into the vectors and operators of a new representation, the *rotating axis representation*. The Hamiltonian transforms into

$$H^{(A)}(\mathrm{s}) = A^{\dagger}(\mathrm{s})\mathrm{H(s)A(s)}, \tag{2.8}$$

similarly $K(s)$ becomes

$$K^{(A)}(\mathrm{s}) = A^{\dagger}(\mathrm{s})\mathrm{K(s)A(s)}. \tag{2.9}$$

The time evolution operator in this new representation is

$$U^{(A)}(\mathrm{s}) = A^{\dagger}(\mathrm{s})U_T(\mathrm{s}), \tag{2.10}$$

then it satisfies

$$U^{(A)}(0) = 1, \tag{2.11}$$

furthermore

$$\frac{\mathrm{dU}^{(A)}(s)}{\mathrm{ds}} = \frac{\mathrm{dA}^{\dagger}(s)}{\mathrm{ds}}U_T(\mathrm{s}) + A^{\dagger}(\mathrm{s})\,\frac{dU_T(s)}{\mathrm{ds}}, \tag{2.12}$$

but $U_T(\mathrm{s})$ obeys the Schrödinger equation, namely,

$$\mathrm{i}\hbar\,\frac{dU_T(s)}{\mathrm{ds}} = \mathrm{TH(s)}U_T(\mathrm{s}), \tag{2.13}$$

so that it provides

$$\mathrm{i}\hbar\,\frac{\mathrm{dU}^{(A)}(s)}{\mathrm{ds}} = \text{-}A^{\dagger}(\mathrm{s})\mathrm{K(s)A(s)}A^{\dagger}(\mathrm{s})U_T(\mathrm{s}) + A^{\dagger}(\mathrm{s})\mathrm{TH(s)A(s)}A^{\dagger}(\mathrm{s})U_T(\mathrm{s}), \tag{2.14}$$

which also follows from (2.5) and from the unitarity of $A(s)$. Now (2.8), (2.9) and (2.10) allow us to write

$$\mathrm{i}\hbar\,\frac{\mathrm{dU}^{(A)}(s)}{\mathrm{ds}} = [\mathrm{TH}^{(A)}(\mathrm{s}) \text{ - } K^{(A)}(\mathrm{s})]U^{(A)}(\mathrm{s}), \tag{2.15}$$

which is the Schrödinger equation in this new representation.

2.1.2 A proof of the adiabatic approximation

In order to prove (2.2) we start introducing the operator

$$\mathrm{W} = \Phi_T^{\dagger}U^{(A)}, \tag{2.16}$$

where Φ_T is completely defined by

$$\mathrm{i}\hbar\frac{\mathrm{d}\Phi_T(s)}{\mathrm{ds}} = \mathrm{TH}^{(A)}(\mathrm{s})\Phi_T(\mathrm{s}) \tag{2.17}$$

and

$$\Phi_T(0) = 1, \tag{2.18}$$

namely

$$\Phi_T(\mathrm{s}) = \sum_j e^{-\mathrm{iT}\phi_j(s)/\hbar} P_j(0), \tag{2.19}$$

where $\phi_j(\mathrm{s}) = \int_0^s E_j(\mathrm{q})\mathrm{dq}$. In fact the Hamiltonian $H^{(A)}$ can be written as

$$H^{(A)}(\mathrm{s}) = \sum_j E_j(\mathrm{s}) P_j(0), \tag{2.20}$$

because of (2.3) and (2.8), then (2.17) can be readily integrated. Now (2.15) and (2.17) provide

$$\mathrm{i}\hbar \frac{\mathrm{dW}(s)}{\mathrm{ds}} = \bar{K}(\mathrm{s})\mathrm{W}(\mathrm{s}), \tag{2.21}$$

where

$$\bar{K}(\mathrm{s}) = \Phi_T^{\dagger}(\mathrm{s}) K^{(A)}(\mathrm{s}) \Phi_T(\mathrm{s}). \tag{2.22}$$

Therefore (2.21) can be written as a Volterra equation in the following form

$$\mathrm{W(s)} = 1 + \frac{i}{\hbar} \int_0^s \bar{K}(\mathrm{q})\mathrm{W(q)dq}, \tag{2.23}$$

so that we need to show the integral above possesses the following property

$$\int_0^s \bar{K}(\mathrm{q})\mathrm{W(q)dq} = \mathrm{O}(\ \frac{1}{T}\ ), \tag{2.24}$$

because then $U^{(A)}(\mathrm{s}) = \Phi_T(\mathrm{s})(\ 1 + \mathrm{O}(\ \frac{1}{T}\ )\ )$ and (2.2) follows from this last result. Thus we should notice that (2.24) can be written, after integration by parts,

$$\mathrm{F(s)W(s)} - \int_0^s \mathrm{F(q)} \frac{\mathrm{dW}(q)}{\mathrm{dq}} \mathrm{dq}, \tag{2.25}$$

or

$$\mathrm{F(s)W(s)} + \frac{i}{\hbar} \int_0^s \mathrm{F(q)} \bar{K}(\mathrm{q})\mathrm{W(q)dq}, \tag{2.26}$$

because of (2.21). Here

$$\mathrm{F(s)} = \int_0^s \bar{K}(\mathrm{q})\mathrm{dq}, \tag{2.27}$$

which in fact possesses the property F(s) = O($\frac{1}{T}$), so in order to check this affirmative we are going to obtain the matrix elements of $F(s)$. We can decompose any operator Q as

$$\mathrm{Q} = \sum_i \sum_j P_i(0)\mathrm{Q}P_j(0) \tag{2.28}$$

thus henceforth we will employ the notation

$$Q_{\mathrm{jk}} = P_j(0)\mathrm{Q}P_k(0). \tag{2.29}$$

Now from (2.3), (2.17) and (2.19) we obtain

$$\bar{K}_{\mathrm{jk}} = e^{\mathrm{iT}(\phi_j - \phi_k)} K^{(A)}_{\mathrm{jk}}, \tag{2.30}$$

where

$$K^{(A)}_{\mathrm{jk}}(\mathrm{s}) = A^{\dagger}(\mathrm{s})P_j(\mathrm{s})\mathrm{K}(\mathrm{s})P_k(\mathrm{s})\mathrm{A}(\mathrm{s}). \tag{2.31}$$

On the other hand, the choice (2.9) results in

$$\bar{K}_{\mathrm{jj}} = 0, \tag{2.32}$$

thus the diagonal terms of K are identically zero. Therefore we can write the matrix elements of $F(s)$ as

$$F_{\mathrm{jk}}(\mathrm{s}) = \int_0^s e^{\mathrm{iT}(\phi_j - \phi_k)} K^{(A)}_{\mathrm{jk}} \mathrm{dq}, \tag{2.33}$$

and $F_{\mathrm{jj}}(\mathrm{s}) \equiv 0$. But such an integral is known to go to zero when $\mathrm{T} \to \infty$, indeed, integrating by parts, it becomes

$$F_{\mathrm{jk}}(\mathrm{s}) = \frac{\hbar}{\mathrm{iT}}\Big[\, e^{\mathrm{iT}(\phi_j - \phi_k)} \frac{K^{(A)}_{\mathrm{jk}}}{E_j - E_k}\Big|_0^s - \int_0^s e^{\mathrm{iT}(\phi_j - \phi_k)} \frac{d}{\mathrm{dq}}\Big(\frac{K^{(A)}_{\mathrm{jk}}}{E_j - E_k} \Big)\, \mathrm{dq}\Big], \tag{2.34}$$

therefore $|F_{\mathrm{jk}}(\mathrm{s})| \longrightarrow 0$, if $\mathrm{T} \longrightarrow \infty$ and the property F(s) = O($\frac{1}{T}$) follows. Thus we conclude that

$$\mathrm{W}(\mathrm{s}) = 1 + \mathrm{O}\Big(\frac{1}{T} \Big), \tag{2.35}$$

from which we obtain

$$U_T(\mathrm{s}) = \mathrm{A}(\mathrm{s})\Phi_T(\mathrm{s})\Big(1 + \mathrm{O}\Big(\frac{1}{T} \Big) \Big), \tag{2.36}$$

according to (2.10) and (2.16). Now since $\Phi_T(\mathrm{s})$ commutes with the projectors $P_j(0)$ and since the operator $A(s)$ has the property (2.3), the asymptotic property (2.2) follows.

2.2 An adiabatic perturbation theory (APT)

An approach to the problem of improving the adiabatic approximation of quantum mechanics which we present here can be found in [7]. We write the solutions of the Schrödinger's Equation,

$$\mathrm{i}\hbar\mathrm{v}\frac{d|\psi(s)\rangle}{ds}=\mathrm{H(s)}|\psi(\mathrm{s})\rangle, \tag{2.37}$$

as

$$|\psi(\mathrm{s})\rangle=\sum_{n=0} e^{\mathrm{i}\gamma_n(s)}e^{-\frac{i}{v}\omega_n(s)}b_n(\mathrm{s})|\mathrm{n(s)}\rangle, \tag{2.38}$$

where the sum is over eigenstates of the Hamiltonian of the system, which satisfy the eigenvalue expression

$$H(\mathrm{s})|\mathrm{n(s)}\rangle=E_n(\mathrm{s})|\mathrm{n(s)}\rangle. \tag{2.39}$$

We are supposing the spectrum of the Hamiltonian $H(s)$ is completely non-degenerate, though this last assumption can be restricted to the ground state only. Moreover we observe that the equation (2.38) displays dynamical and geometric phases explicitly, where these quantities are defined as

$$\omega_n(\mathrm{s})=\frac{1}{\hbar}\int_0^s E_n(\mathrm{q})\mathrm{dq} \tag{2.40}$$

and

$$\gamma_n(\mathrm{s})=\mathrm{i}\int_0^s \langle\mathrm{n(q)}|\frac{d}{dq}\mathrm{n(q)}\rangle\mathrm{dq}, \tag{2.41}$$

respectively. So in order to develop a perturbative theory we decompose the coefficients in (2.38) in the following form

$$b_n(\mathrm{s})=\sum_{p=0}^{\infty} v^p b_n^{(p)}(\mathrm{s}), \tag{2.42}$$

where we can distinguish several orders of perturbation whose individual contributions are written as

$$b_n^{(p)}(\mathrm{s}) = \sum_{m=0} e^{\frac{i}{v}\omega_{\mathrm{nm}}(s)} e^{-\mathrm{i}\gamma_{\mathrm{nm}}(s)} b_{\mathrm{nm}}^{(p)}(\mathrm{s}), \tag{2.43}$$

where $\omega_{\mathrm{nm}} = \omega_n - \omega_m$, $\gamma_{\mathrm{nm}} = \gamma_n - \gamma_m$. Now we can combine equations (2.38), (2.42) and (2.43) to obtain

$$|\psi(\mathrm{s})\rangle = \sum_{n,m=0} \sum_{p=0} v^p e^{-\frac{i}{v}\omega_m(s)} e^{\mathrm{i}\gamma_m(s)} b_{\mathrm{nm}}^{(p)}(\mathrm{s}) |\mathrm{n(s)}\rangle. \tag{2.44}$$

At this point we impose that all contributions of the adiabatic perturbation theory must be zero at the initial instant except the zeroth order contribution, namely,

$$b_n^{(0)}(0) = b_n(0), \tag{2.45}$$

where

$$|\psi(0)\rangle = \sum_{n=0} b_n(0) |\mathrm{n}(0)\rangle, \tag{2.46}$$

but

$$b_n^{(p)}(0) = \sum_{m=0} b_{\mathrm{nm}}^{(p)}(0) = 0, \ (\mathrm{p} \geq 1). \tag{2.47}$$

Our basic idea is to replace (2.44) into (2.37) to obtain a recursive relation, then the adiabatic approximation is used to calculate the first order correction, which can be used to generate the second order correction and so on. Therefore the adiabatic approximation plays the role of zeroth order correction and we have to impose this condition explicitly, thus

$$b_{\mathrm{nm}}^{(0)}(\mathrm{s}) = b_{\mathrm{nm}}^{(0)}(0) = b_n(0)\delta_{\mathrm{nm}}. \tag{2.48}$$

In other words we mean that up to zeroth order contribution this condition assures that if the state of the system is initially prepared as an eigenstate of the Hamiltonian, it remains as an eigenstate during the time evolution of the system, so this condition constitutes the adiabatic approximation itself. Now replacing (2.44) into (2.37) and left multiplying by

$\langle \mathrm{k(s)}|$ we get

$$\sum_{m,p} v^p e^{-\frac{i}{v}\omega_m(s)} e^{\mathrm{i}\gamma_m(s)} \left(\frac{i}{\mathrm{v}\hbar}\Delta_{\mathrm{km}}(\mathrm{s}) b^{(p)}_{\mathrm{km}}(\mathrm{s}) + \frac{db^{(p)}_{\mathrm{km}}(s)}{\mathrm{ds}} + \mathrm{i}\frac{\mathrm{d}\gamma_m(s)}{\mathrm{ds}} b^{(p)}_{\mathrm{km}}(\mathrm{s}) + \sum_n M_{\mathrm{kn}}(\mathrm{s}) b^{(p)}_{\mathrm{nm}}(\mathrm{s})\right) = 0, \tag{2.49}$$

where $M_{\mathrm{nm}}(\mathrm{s})=\langle \mathrm{n(s)}|\frac{d}{ds}\mathrm{m(s)}\rangle$ and $\Delta_{\mathrm{nm}}(\mathrm{s})= E_n(\mathrm{s})\text{-}E_m(\mathrm{s})$. Then after some simple manipulations we are led to a sufficient condition to satisfy the preceding equation, that is,

$$\frac{i}{\hbar}\Delta_{\mathrm{nm}}(\mathrm{s}) b^{(p+1)}_{\mathrm{nm}}(\mathrm{s}) + \frac{db^{(p)}_{\mathrm{nm}}(s)}{ds} + W_{\mathrm{nm}}(\mathrm{s}) b^{(p)}_{\mathrm{nm}}(\mathrm{s}) + \sum_{k\neq n} M_{\mathrm{nk}}(\mathrm{s}) b^{(p)}_{\mathrm{km}}(\mathrm{s}) = 0, \tag{2.50}$$

which is a *recursive relation* to be used to generate perturbative corrections, where $W_{\mathrm{nm}}(\mathrm{s})=M_{\mathrm{nn}}(\mathrm{s})\text{-}M_{\mathrm{mm}}(\mathrm{s})$. When $n \neq m$ this last equation can be cast in the form

$$b^{(p+1)}_{\mathrm{nm}}(\mathrm{s}) = \frac{\mathrm{i}\hbar}{\Delta_{\mathrm{nm}}(s)} \left(\frac{db^{(p)}_{\mathrm{nm}}(s)}{ds} + W_{\mathrm{nm}}(\mathrm{s}) b^{(p)}_{\mathrm{nm}}(\mathrm{s}) + \sum_{k\neq n} M_{\mathrm{nk}}(\mathrm{s}) b^{(p)}_{\mathrm{km}}(\mathrm{s})\right), \tag{2.51}$$

whereas for $n = m$ this equation becomes

$$\frac{db^{(p+1)}_{\mathrm{nn}}(s)}{ds} + \sum_{k\neq n} M_{\mathrm{nk}}(\mathrm{s}) b^{(p+1)}_{\mathrm{kn}}(\mathrm{s}) = 0. \tag{2.52}$$

The general procedure to calculate the $(p+1)th$ order of correction is to obtain non-diagonal terms from (2.51) to use them to obtain diagonal terms from the differential equation (2.52). As an illustration of this procedure we are going to obtain the first contribution of this theory to the general correction (2.42). The system starts at the ground state, so

$$b_n(0) = \delta_{\mathrm{n0}}. \tag{2.53}$$

Equations (2.48), (2.51) and (2.53) then provide

$$b^{(1)}_{\mathrm{nm}}(\mathrm{s}) = (\mathrm{i}\hbar)\frac{M_{\mathrm{n0}}(s)}{\Delta_{\mathrm{n0}}(s)}\delta_{\mathrm{n0}},\ (\mathrm{n}\neq\mathrm{m}). \tag{2.54}$$

The next step is to solve (2.52), therefore we get

$$b^{(1)}_{\mathrm{nn}}(\mathrm{s}) = (\mathrm{i}\hbar)\sum_{m\neq n}\left(J_{\mathrm{m0}}(\mathrm{s})\delta_{\mathrm{n0}} - \frac{M_{\mathrm{n0}}(0)}{\Delta_{\mathrm{n0}}(0)}\delta_{\mathrm{m0}}\right), \tag{2.55}$$

where $J_{\mathrm{m0}}(\mathrm{s})=\int_0^s \frac{|M_{\mathrm{m0}}(q)|^2}{\Delta_{\mathrm{m0}}(q)}\mathrm{dq}$. To obtain this solution we replace (2.54) into (2.52), then we integrate the resulting equation. As a final step the initial condition $b_{\mathrm{nn}}^{(1)}(0)$, which is a constant of integration, can be obtained with help of (2.47). The second order correction can be calculated in a similar manner from the coefficients of the first order correction.

2.3 Some geometric notions about distances between two pure quantum states

How close are two quantum states? A good idea to answer this question is to define the *fidelity* between them,

$$\mathrm{F}(|\psi\rangle,|\phi\rangle)=|\langle\psi|\phi\rangle|^2, \tag{2.56}$$

which satisfies[1] $0 \leqslant \mathrm{F}(|\psi\rangle,|\phi\rangle) \leqslant 1$, because this quantity measures how much these states are overlapping. As an illustrative example we consider the quantum harmonic oscillator, whose Hamiltonian is $\mathrm{H}=\hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$. From quantum mechanics we know there are *quasi classical states* of this system, which are eigenstates of the annihilation operator

$$a|\alpha\rangle=\alpha|\alpha\rangle. \tag{2.57}$$

It is straightforward to show that

$$|\alpha\rangle= \exp\left(-\frac{1}{2}|\alpha|^2 \right)\sum_{n=0}^{\infty}\frac{\alpha^n}{n!}|\mathrm{n}\rangle \tag{2.58}$$

where $|\mathrm{n}\rangle$ is an eigenvector of the Hamiltonian, which follows from (2.57). Now in the Heisenberg picture

$$(\mathrm{i}\hbar)\frac{da}{dt}= [a,\mathrm{H}] \ , \tag{2.59}$$

which provides[2] $a(\mathrm{t})=a(0)e^{-\mathrm{i}\omega\mathrm{t}}$, so that (2.57) furnishes

$$\alpha(\mathrm{t})=\alpha(0)e^{-\mathrm{i}\omega\mathrm{t}}. \tag{2.60}$$

[1] From Cauchy-Schwarz inequality $|\langle\psi|\phi\rangle|^2 \leqslant \langle\psi|\psi\rangle\langle\phi|\phi\rangle = 1$.

[2] An initial phase was chosen to be zero.

Then we calculate the *fidelity* between both the initial coherent state and the coherent state at some time t from (2.56), (2.58) and (2.60), namely,

$$\mathrm{F}(|\alpha(\mathrm{t})\rangle,|\alpha(0)\rangle)=e^{-4(|\alpha(0)|)^2\sin^2\left(\frac{\omega \mathrm{t}}{2}\right)}, \tag{2.61}$$

whose graph is depicted below. We can observe that this graph represents a periodic func-

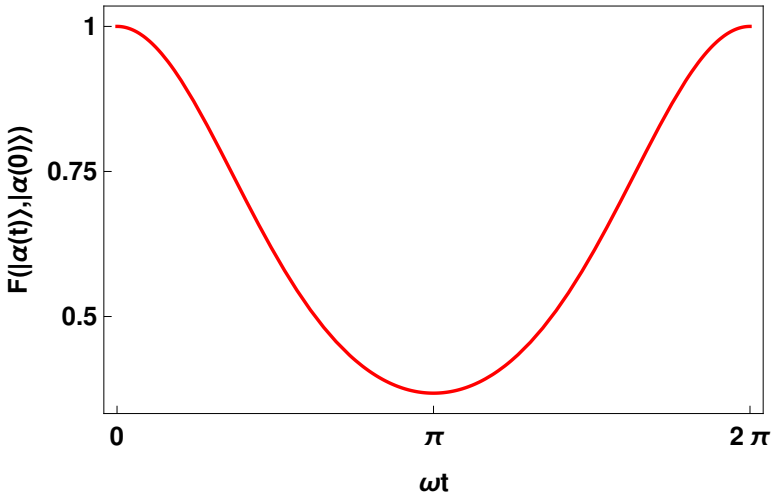

Figure 2.1: Fidelity between coherent states of a quantum mechanical oscillator.

tion whose initial value is one, because the wavepacket $\psi(\mathrm{q})=\langle \mathrm{q}|\alpha(\mathrm{t})\rangle$ oscillates back and forth, like a classical oscillator, so that at $\mathrm{t}=\pi/\omega$ the *fidelity* reaches its minimum value, because the overlap is then minimum and the classical oscillator reaches its maximum distance from the initial position, and then its value returns to one at $\mathrm{t}=2\pi/\omega$, when the overlap is maximum again and the classical oscillator comes back to its initial position.

Despite its physical significance (2.56) does not define a metric on physical states. In fact a distance is a function of two elements of a set of objects $X, Y, Z, ...$ which possesses some properties, namely, (i)$\mathrm{D(X,Y)} \geq 0$ and $\mathrm{D(X,Y)} = 0 \Leftrightarrow \mathrm{X} = \mathrm{Y}$,(ii) $D(X, Y) = D(Y, X)$ and (iii) $\mathrm{D(X,Z)} + \mathrm{D(Z,Y)} \geq \mathrm{D(X,Y)}$, so that (2.56) cannot satisfy all of these properties. On the other hand, a distance between two quantum states can be defined as

$$\mathrm{D}(|\psi\rangle,|\phi\rangle) = \sqrt{F(|\psi\rangle, |\phi\rangle)}, \tag{2.62}$$

known as *Bures angle*, because it possesses all the preceding properties and, in fact, it will be used throughout this work to quantify our notion about distance between two physical

states. In order to verify the preceding properties we start observing that we restrict ourselves to the principal branch of cosine inverse function, that is, $0 \leq \arccos z \leq \pi$, so $0 \leqslant D(|\psi\rangle,|\phi\rangle) \leqslant \pi/2$, because $0 \leqslant F(|\psi\rangle,|\phi\rangle) \leqslant 1$. If $D(|\psi\rangle,|\phi\rangle)=0$, then $|\langle\psi|\phi\rangle|= 1$, but these states are both normalized, therefore $|\phi\rangle=e^{i\delta}|\psi\rangle$, which represents the same physical state, whereas the reciprocal property is obvious. The second property above is trivial, because the *fidelity* is symmetric in its inputs. For the third property above we invoke the image of a sphere of unit radius such that each point on this sphere represents a physical state. Let $|\phi\rangle$,$|\psi\rangle$ and $|\eta\rangle$ be three points on this sphere, so three angles, whose measurements are $D(|\phi\rangle,|\psi\rangle)$, $D(|\psi\rangle,|\eta\rangle)$ and $D(|\eta\rangle,|\phi\rangle)$, are drawn on this surface. Now from this picture follows that [3, p. 413] $D(|\phi\rangle,|\psi\rangle)+ D(|\psi\rangle,|\eta\rangle) \geqslant D(|\phi\rangle,|\eta\rangle)$. Actually for pure states the proof of these properties is very simple, but in the general case involving mixed states we need the concept of purification and an additional result known as Uhlmann's theorem, moreover the description of physical states involves density operators [3]. As an illustration we plot the graph of the Bures angle between coherent states described above, but now we observe the Bures angle reaches its maximum value when the classical oscillator reaches its maximum distance from the initial position, whereas this distance is zero when the classical oscillator is at extremal points of its trajectory, since then the overlap of both the initial state and the final state is maximum.

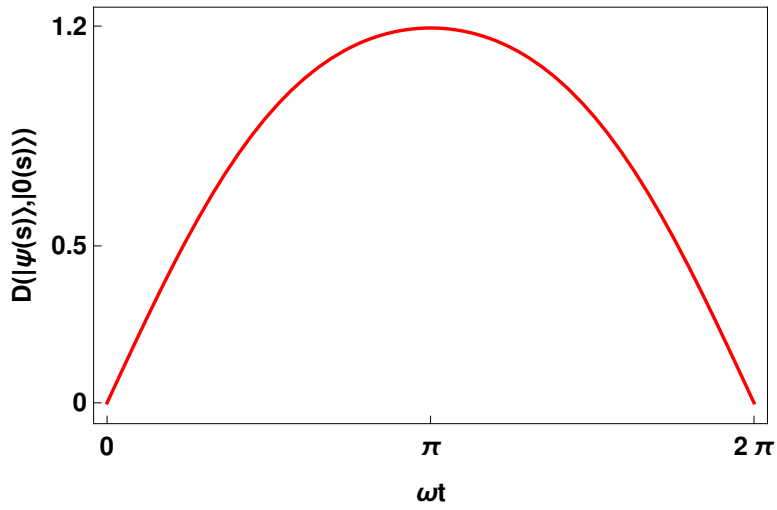

Figure 2.2: Bures angle between coherent states of a quantum mechanical oscillator.

Some observations

1) A particular problem treated here is to obtain bounds on the Bures angle between the ideal state, the eigenstate of the Hamiltonian, and the actual state of the system at some instant of its evolution[3]

$$|\psi(\mathrm{s})\rangle = \sum_{n=0} b_n(\mathrm{s})|\mathrm{n(s)}\rangle. \tag{2.63}$$

Equation (2.62) then provides

$$\mathrm{D}(|\psi(\mathrm{s})\rangle,|0(\mathrm{s})\rangle) = \arccos|b_0(\mathrm{s})|, \tag{2.64}$$

so that an adiabatic perturbation theory allow us to expand this distance in terms of the parameter v

$$\mathrm{D}(|\psi(\mathrm{s})\rangle,|0(\mathrm{s})\rangle) = f_1(\mathrm{s})\ v + f_2(\mathrm{s})\ v^2 + f_3(\mathrm{s})\ v^3 + ..., \tag{2.65}$$

where f_1(s), f_2(s), f_3(s), ... are bounded and continuous functions of the parameter s. Actually these functions still depend on v, but that parameter is always part of an argument of a complex exponential function, thus the modulus of these functions does not depend on the parameter v.

2) We take the derivative of both sides of (2.39), then we left multiply by $\langle$m(s)|, thus we obtaining

$$M_{\mathrm{nm}}(\mathrm{s}) = \frac{\left\langle n(s) \left| \frac{\mathrm{dH}(s)}{\mathrm{ds}} \right| m(s) \right\rangle}{\Delta_{\mathrm{mn}}(s)}. \tag{2.66}$$

3) As a final remark we notice that in the next chapter we will make the following approximation

$$\cos^2\left[\mathrm{D}(|\psi(\mathrm{s})\rangle,|0(\mathrm{s})\rangle)\right] \simeq 1 - D^2(|\psi(\mathrm{s})\rangle,|0(\mathrm{s})\rangle), \tag{2.67}$$

which constitutes an acceptable approximation for our purposes, since we are interested in distances which are typically much smaller than the maximum distance between two quantum states ($\pi/2$).

[3]The set $|\mathrm{n(s)}\rangle$ constitutes the energy representation.

4) The Bures angle also defines a Riemannian distance between two quantum states.

Chapter 3

Some Results

In the first section of this chapter we present two theorems of paramount importance to prove the results of the second section, which constitute the main subject of this work, namely, bounds on the Bures angle between the actual state of the system and the eigenstate of the Hamiltonian and a theorem about the behaviour of this distance under certain conditions.

3.1 Two theorems about coefficients of the perturbative series

We are supposing that the system starts at the ground state (2.53). The results would also hold if the initial state were a different eigenstate of the Hamiltonian.

Theorem 1: If n≠m, then the general form of the coefficients $b^{(p)}_{\mathrm{nm}}(\mathrm{s})$ in (2.43) is

$$b^{(p)}_{\mathrm{nm}}(\mathrm{s})=(\mathrm{i}\hbar)^p \sum_{q=0}^{p-1} \sum_{k\neq m} \chi^{pq}_{\mathrm{nmk}}(\mathrm{s}) \frac{d^q \lambda_{\mathrm{km}}(s)}{ds^q} \tag{3.1}$$

where $\lambda_{\mathrm{nm}}(\mathrm{s})=\frac{M_{\mathrm{nm}}(s)}{\Delta_{\mathrm{nm}}(s)}$ and $\chi^{pq}_{\mathrm{nmk}}(\mathrm{s})$ are functions of the parameter s.

Proof (by induction): We replace (3.1) into (2.51), then we set

$$\chi_{\rm nmk}^{p+1,q} = \frac{1}{\Delta_{\rm nm}} \, (\frac{{\rm d}\chi_{\rm nmk}^{\rm pq}}{\rm ds} + \, (1 \, - \, \delta_{\rm q0} \,)\chi_{\rm nmk}^{p,q-1} + W_{\rm nm}\chi_{\rm nmk}^{\rm pq} + \sum_{l\neq n,m} M_{\rm nl}\chi_{\rm lmk}^{\rm pq} + \delta_{\rm q0}\delta_{\rm nk}c_{\rm mm}^{(p)}\Delta_{\rm nm} \,), \tag{3.2}$$

where $c_{\rm mm}^{(p)}({\rm s}) = b_{\rm mm}^{(p)}({\rm s})/({\rm i}\hbar)$ and $q = 0, 1, 2, ..., p-1$, whereas for $q = p$

$$\chi_{\rm nmk}^{p+1,p} = \frac{\chi_{\rm nmk}^{p,p-1}}{\Delta_{\rm nm}}. \tag{3.3}$$

Thus we obtain

$$b_{\rm nm}^{(p+1)}({\rm s}) = ({\rm i}\hbar)^{p+1} \sum_{q=0}^{p} \sum_{k\neq m} \chi_{\rm nmk}^{p+1,q}({\rm s}) \frac{d^q \lambda_{\rm km}(s)}{ds^q}. \tag{3.4}$$

Notice that can rewrite (2.54) as

$$b_{\rm nm}^{(1)}({\rm s}) = ({\rm i}\hbar)^{1} \sum_{q=0}^{0} \sum_{k\neq m} \chi_{\rm nmk}^{1q}({\rm s}) \frac{d^q \lambda_{\rm km}(s)}{ds^q}, \tag{3.5}$$

where

$$\chi_{\rm nmk}^{10}({\rm s}) = \delta_{\rm kn}\delta_{\rm m0}, \tag{3.6}$$

so that the affirmative is valid for $p = 1$, then it must be valid for $p = 2$ and so on.

Corollary 1: If $\frac{{\rm dH(1)}}{\rm ds} = \frac{d^2H(1)}{{\rm ds}^2} = ... = \frac{d^pH(1)}{{\rm ds}^p} = 0$, the derivatives of the Hamiltonian at the final time of the physical process, then $b_{\rm nm}^{(1)}(1) = b_{\rm nm}^{(2)}(1) = ... = b_{\rm nm}^{(p)}(1) = 0$, n≠m.

We notice that Leibniz rule for derivatives yields

$$\frac{d^k \lambda_{\rm nm}(s)}{{\rm ds}^k} = \sum_{j=0}^{k} \frac{k!}{j!(k-j)!} \frac{d^{k-j} M_{\rm nm}(s)}{{\rm ds}^{k-j}} \frac{d^j}{{\rm ds}^j} \left(\frac{1}{\Delta_{\rm nm}(s)} \right), \tag{3.7}$$

so that if we take $\frac{{\rm dH(1)}}{\rm ds} = \frac{d^2H(1)}{{\rm ds}^2} = ... = \frac{d^pH(1)}{{\rm ds}^p} = 0$, then $\frac{d\lambda_{\rm nm}(1)}{\rm ds} = \frac{d^2\lambda_{\rm nm}(1)}{{\rm ds}^2} = ... = \frac{d^{p-1}\lambda_{\rm nm}(1)}{{\rm ds}^{p-1}} = 0$ and the theorem 1 implies $b_{\rm nm}^{(1)}(1) = b_{\rm nm}^{(2)}(1) = ... = b_{\rm nm}^{(p)}(1) = 0$, because

$$\lambda_{\rm nm}({\rm s}) = \frac{M_{\rm nm}(s)}{\Delta_{\rm nm}(s)} = \frac{\left\langle n(s) \left| \frac{{\rm dH}(s)}{\rm ds} \right| m(s) \right\rangle}{\Delta_{\rm nm}(s)\Delta_{\rm mn}(s)}. \tag{3.8}$$

Theorem 2: If m $\neq 0$ and $\frac{\mathrm{dH(0)}}{\mathrm{ds}} = \frac{d^2H(0)}{\mathrm{ds}^2}$=...=$\frac{d^pH(0)}{\mathrm{ds}^p}$= 0, the derivatives of the Hamiltonian at the initial time of the physical process, then $\chi^{\mathrm{p+1,q}}_{\mathrm{nmk}}$ is identically zero.

Proof (by induction): Let us initially suppose that $\chi^{\mathrm{pq}}_{\mathrm{nmk}} \sim \delta_{\mathrm{m0}}$. This implies from (3.2) and (3.3), which express $\chi^{p+1,q}_{\mathrm{nmk}}$ in terms of χ^{pq}_{nmk}, that the only term which is not zero is that proportional to $c^{(p)}_{\mathrm{mm}}$(s)= $b^{(p)}_{\mathrm{mm}}$(s)/(i$\hbar$). This term can be obtained from (2.52), namely,

$$\frac{db^{(p)}_{\mathrm{mm}}(s)}{ds} + \sum_{n\neq m} M_{\mathrm{mn}}(\mathrm{s}) b^{(p)}_{\mathrm{nm}}(\mathrm{s})=0, \tag{3.9}$$

where $b^{(p)}_{\mathrm{nm}}$(s) are obtained from (3.1), therefore are identically zero according to our assumptions. This implies

$$b^{(p)}_{\mathrm{mm}}(\mathrm{s}) = -\sum_{n\neq m} b^{(p)}_{\mathrm{mn}}(0), \tag{3.10}$$

from (2.47), or

$$b^{(p)}_{\mathrm{mm}}(\mathrm{s}) \equiv 0 \ , \tag{3.11}$$

according to (3.1). Thus we conclude that

$$\chi^{p+1,q}_{\mathrm{nmk}} \sim \delta_{\mathrm{m0}}. \tag{3.12}$$

Since, from (3.6), $\chi^{1q}_{\mathrm{nmk}} \sim \delta_{\mathrm{m0}}$, taking $\frac{\mathrm{dH(0)}}{\mathrm{ds}} = 0$ results in $\chi^{2q}_{\mathrm{nmk}} \sim \delta_{\mathrm{m0}}$. In the same way, taking $\frac{\mathrm{dH(0)}}{\mathrm{ds}} = \frac{d^2H(0)}{\mathrm{ds}^2} = 0$ implies $\chi^{3q}_{\mathrm{nmk}} \sim \delta_{\mathrm{m0}}$ and so on, so that the theorem is proved.

Corollary 2: If $\frac{\mathrm{dH(0)}}{\mathrm{ds}} = \frac{d^2H(0)}{\mathrm{ds}^2}$=...=$\frac{d^pH(0)}{\mathrm{ds}^p}$= 0, then $b^{(1)}_{\mathrm{nn}}$(s)= $b^{(2)}_{\mathrm{nn}}$(s)= ...= $b^{(p)}_{\mathrm{nn}}$(s)$\equiv$ 0, for n$\neq$ 0.

The $b^{(p)}_{\mathrm{nn}}$(s) must be a constant of motion according to (3.9), because $b^{(p)}_{\mathrm{nm}}$(s) $\sim \delta_{\mathrm{m0}}$, but this constant must depend on the derivatives of the Hamiltonian at the initial instant according to (3.10), (3.1) and (3.7), which are equal to zero, so that it follows trivially.

3.2 Bures angle and APT

In the following discussion we derive an expansion for the Bures angle in terms of the adiabatic perturbation theory (APT) developed in the preceding chapter, then we present the main results of this work, which are bounds on the Bures angle between the actual state of the system and the eigenstate of the Hamiltonian and a theorem which prescribes the behaviour of this distance when a number of derivatives of the Hamiltonian of the system vanishes.

3.2.1 A perturbative expansion

The distance of our interest is (2.64), which we can rewrite as

$$\cos \mathrm{D} = \mid b_0(\mathrm{s})|, \tag{3.13}$$

but $|\psi(\mathrm{s})\rangle$ is normalized, which implies, given (2.63),

$$\mid b_0(\mathrm{s})|^2 = 1 - \sum_{n=1} \mid b_n(\mathrm{s})|^2. \tag{3.14}$$

Now we expand the coefficients on the right according to (2.42), which yields

$$\sum_{n=1} \mid b_n(\mathrm{s})|^2 = v^2 \sum_{\mu=1}^{\infty} \xi_\mu v^{\mu-1}, \tag{3.15}$$

where

$$\xi_\mu(\mathrm{s}) = \sum_{n=1} \sum_{q=1}^{\mu} \overline{b_n^{(q)}(s)} b_n^{(\mu-q+1)}(\mathrm{s}). \tag{3.16}$$

So we can rewrite (3.13) as

$$\cos^2 \mathrm{D} = 1 - v^2 \sum_{\mu=1}^{\infty} \xi_\mu v^{\mu-1}. \tag{3.17}$$

Using the approximation (2.67), we obtain

$$D^2(|\psi(\mathrm{s})\rangle, |0(\mathrm{s})\rangle) = v^2 \sum_{\mu=1} \xi_\mu v^{\mu-1}, \tag{3.18}$$

or

$$D(|\psi(s)\rangle, |0(s)\rangle) = v\ \xi_1^{1/2}(1+z), \tag{3.19}$$

where

$$z = \sum_{\mu=2} \frac{\xi_\mu}{\xi_1} v^{\mu-1} \tag{3.20}$$

and we are supposing $\xi_1 \neq 0$. We would like to expand (3.19) in a power series of the parameter v, or equivalently in a power series in z, but the function f(z) = $(1+z)^{1/2}$ possesses a branch point at $z = -1$, so the only expansion about the origin (a Taylor series) converges if |z| < 1. Thus under this assumption we expand this distance as

$$D(|\psi(s)\rangle, |0(s)\rangle) = v\xi_1^{1/2}(s)(1 + \frac{1}{2}\frac{\xi_2(s)}{\xi_1(s)}v + (\frac{1}{2}\frac{\xi_3(s)}{\xi_1(s)} - \frac{1}{8}\frac{\xi_2^2(s)}{\xi_1^2(s)})v^2 + ...). \tag{3.21}$$

Actually (3.21) is not a genuine power series in v, because its coefficients still depend on v, but this parameter is always part of an argument of a complex exponential function, that is, the coefficients are continuous and bounded functions of the parameter s with modulus independent of the small parater. The only exception would be when $\xi_1 = 0$, but in this case the expansion (3.21) is no longer valid, as will be discussed soon. Now we consider the running time T large enough so that the only appreciable term in the preceding series is that of lowest power in v. Therefore we write

$$\mathrm{D}(|\psi(\mathrm{s})\rangle, |0(\mathrm{s})\rangle) = v\xi_1^{1/2}(\mathrm{s}), \tag{3.22}$$

where, from (3.16), we have

$$\xi_1 = \sum_{n=1} \overline{b_n^{(1)}(s)} b_n^{(1)}(\mathrm{s}). \tag{3.23}$$

An expression for $b_n^{(1)}(\mathrm{s})$ is obtained from (2.43), (2.54) and (2.55), which yields

$$b_n^{(1)}(\mathrm{s}) = (\mathrm{i}\hbar)\ (\ e^{\frac{i}{v}\omega_{\mathrm{n0}}(s)} e^{-\mathrm{i}\gamma_{\mathrm{n0}}(s)} \frac{M_{\mathrm{n0}}(s)}{\Delta_{\mathrm{n0}}(s)} - \frac{M_{\mathrm{n0}}(0)}{\Delta_{\mathrm{n0}}(0)}\ ), \tag{3.24}$$

where we are supposing $\mathrm{n} \neq 0$. Thus the triangle inequality $|z_1 + z_2| \leq |z_1| + |z_2|$ implies

$$|\ b_n^{(1)}(\mathrm{s})| \leq \hbar(\ \frac{|M_{\mathrm{n0}}(s)|}{\Delta_{\mathrm{n0}}(s)} + \frac{|M_{\mathrm{n0}}(0)|}{\Delta_{\mathrm{n0}}(0)}\ ), \tag{3.25}$$

whereas $|z_1 - z_2| \geq ||z_1|$ - $|z_2||$ yields

$$| \, b_n^{(1)}(\mathrm{s})| \geq \hbar \, |\frac{|M_{\mathrm{n0}}(s)|}{\Delta_{\mathrm{n0}}(s)} - \frac{|M_{\mathrm{n0}}(0)|}{\Delta_{\mathrm{n0}}(0)} \, |. \tag{3.26}$$

These two last expressions together with (3.22) and (3.23) furnish an upper bound and a lower bound on the Bures angle respectively, which are

$$\mathrm{D}(|\psi(\mathrm{s})\rangle,|0(\mathrm{s})\rangle) \leq \frac{\hbar}{T}(\sum_{n=1} (\frac{|M_{\mathrm{n0}}(s)|}{\Delta_{\mathrm{n0}}(s)} + \frac{|M_{\mathrm{n0}}(0)|}{\Delta_{\mathrm{n0}}(0)})^2)^{1/2} \tag{3.27}$$

and

$$\mathrm{D}(|\psi(\mathrm{s})\rangle,|0(\mathrm{s})\rangle) \geq \frac{\hbar}{T}(\sum_{n=1} | \, \frac{|M_{\mathrm{n0}}(s)|}{\Delta_{\mathrm{n0}}(s)} - \frac{|M_{\mathrm{n0}}(0)|}{\Delta_{\mathrm{n0}}(0)}|^2)^{1/2}. \tag{3.28}$$

Some comments

1) We consider as an example the Hamiltonian $\mathrm{H(t)} = \hbar\omega \, [(1 - \frac{t}{T})\mathrm{X} + \frac{t}{T}\mathrm{Z}]$, where X and Z denote Pauli spin matrices. This Hamiltonian connects X at $t = 0$ to Z at $\mathrm{t = T}$. A graph of the Bures angle, which was obtained numerically, is depicted below. The broken lines represent the bounds obtained above. In the numerical simulations $\mathrm{v} = 0.002 \, \omega$ and $\hbar = 1$.

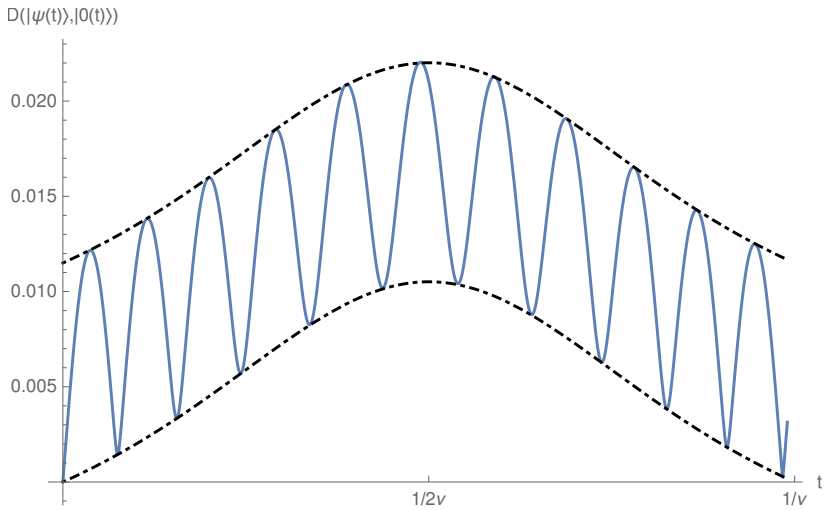

Figure 3.1: Bounds on the Bures angle for a linear Hamiltonian.

2) If $\frac{\mathrm{dH(0)}}{\mathrm{ds}} = 0$, then (3.27) and (3.28) become identical and constitute an expression for the Bures angle itself, namely,

$$\mathrm{D}(|\psi(\mathrm{s})\rangle,|0(\mathrm{s})\rangle) = \frac{\hbar}{T}\Big(\sum_{n=1}\Big(\frac{|M_{\mathrm{n0}}(s)|}{\Delta_{\mathrm{n0}}(s)}\Big)^2\Big)^{1/2}. \tag{3.29}$$

As an example we consider a modified version of the preceding Hamiltonian, namely, $\mathrm{H(t)} = \hbar\omega\ [\ (1 - 3\ (\frac{t}{T})^2 + 2\ (\frac{t}{T})^3)\mathrm{X} + (\ 3\ (\frac{t}{T})^2 + 2\ (\frac{t}{T})^3)\ \mathrm{Z}]$. A graph of the Bures angle is depicted in the figure 3.2. The small paramater $\mathrm{v} = 0.002\ \omega$ and $\hbar = 1$. We notice that we cannot visually distinguish bounds (broken line) from the distance (continuous line).

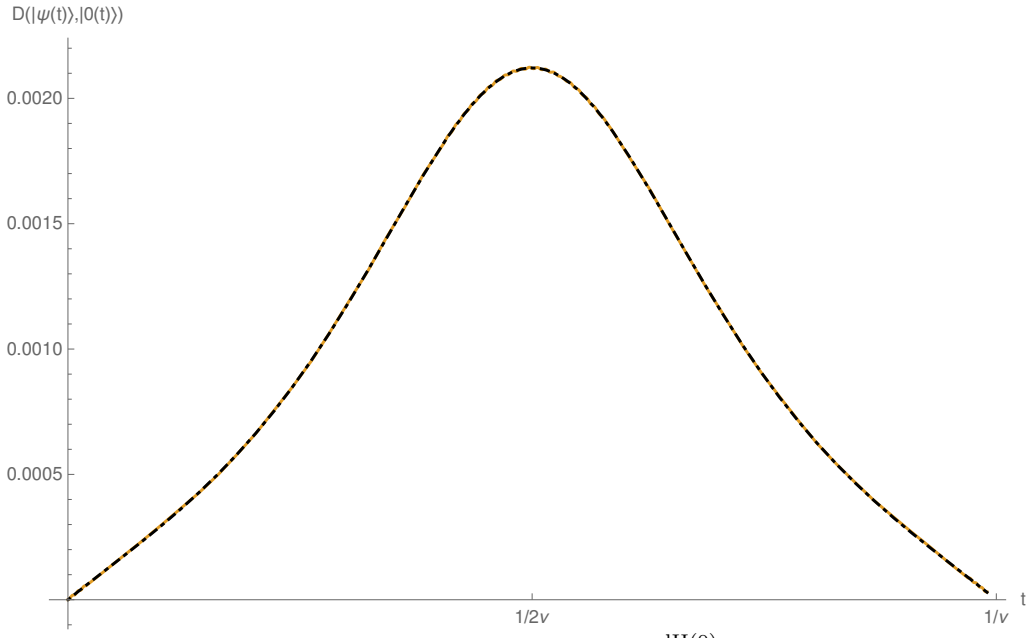

Figure 3.2: Bures angle when $\frac{\mathrm{dH(0)}}{\mathrm{ds}} = 0$.

3) When the derivatives of the Hamiltonian are different from zero at the initial instant and equal to zero at the final instant, the bounds above converge to a unique bound at the final instant as exhibited in the figure 3.3.

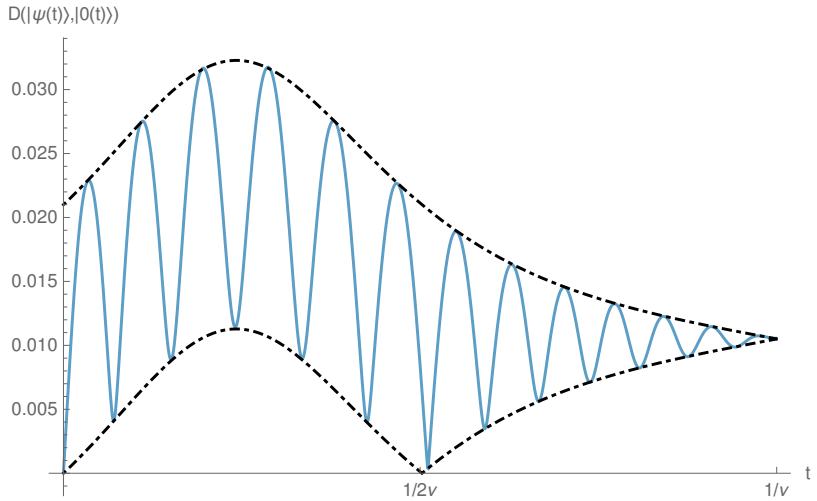

Figure 3.3: Bures angle when $\frac{\mathrm{dH(1)}}{\mathrm{ds}} = 0$.

4) We can think about (3.22) as a first perturbative contribution to the distance. Obviously if this contribution is zero for some value of the parameter s, then we have to consider the next non-vanishing contribution as dominant. Thus we obtain bounds on this distance in a similar manner of that above. In a sense the next theorem prescribes the behaviour of the Bures angle when a number of perturbative contributions vanishes.

3.2.2 Fundamental Theorem

Theorem 3: If $\frac{\mathrm{dH(0)}}{\mathrm{ds}} = \frac{d^2H(0)}{\mathrm{ds}^2}$=...=$\frac{d^pH(0)}{\mathrm{ds}^p}$= 0 and $\frac{\mathrm{dH(1)}}{\mathrm{ds}} = \frac{d^2H(1)}{\mathrm{ds}^2}$=...=$\frac{d^pH(1)}{\mathrm{ds}^p}$= 0, then the distance (2.64) is bounded in the following way

$$\mathrm{D}(|\psi(\mathrm{s})\rangle,|0(\mathrm{s})\rangle) \leq \frac{\hbar^{p+1}}{T^{p+1}}\Big(\sum_{n=1}\Big(\frac{\left|\lambda^{(p)}_{\mathrm{n0}}(s)\right|}{\Delta^p_{\mathrm{n0}}(s)} + \frac{\left|\lambda^{(p)}_{\mathrm{n0}}(0)\right|}{\Delta^p_{\mathrm{n0}}(0)}\Big)^2\Big)^{1/2} \tag{3.30}$$

and

$$\mathrm{D}(|\psi(\mathrm{s})\rangle,|0(\mathrm{s})\rangle) \geq \frac{\hbar^{p+1}}{T^{p+1}}\Big(\sum_{n=1}\Big|\frac{\left|\lambda^{(p)}_{\mathrm{n0}}(s)\right|}{\Delta^p_{\mathrm{n0}}(s)} - \frac{\left|\lambda^{(p)}_{\mathrm{n0}}(0)\right|}{\Delta^p_{\mathrm{n0}}(0)}\Big|^2\Big)^{1/2}, \tag{3.31}$$

where $\lambda^{(p)}_{\mathrm{n0}}(\mathrm{s}) \equiv \frac{d^p\lambda_{\mathrm{n0}}(s)}{\mathrm{ds}^p}$.

Proof: We observe that $\xi_1(1) = \xi_2(1) = ... = \xi_{2p-1}(1) = \xi_{2p}(1) = 0$ as a consequence

of the corollaries of the preceding section, therefore (3.18) yields

$$\mathrm{D}(|\psi(1)\rangle,|0(1)\rangle) = v^{p+1}\xi_{2p+1}^{1/2}(1)(\ 1 + \frac{1}{2}\frac{\xi_{2p+2}(1)}{\xi_{2p+1}(1)}v + ...), \tag{3.32}$$

thus we consider again the lowest power of v as the only appreciable term in (3.32), namely,

$$\mathrm{D}(|\psi(1)\rangle,|0(1)\rangle) = v^{p+1}\xi_{2p+1}^{1/2}(1)\ , \tag{3.33}$$

where $\xi_{2p+1}(1) \neq 0$, given by

$$\xi_{2p+1}(1) = \sum_{n=1} \overline{b_n^{(p+1)}(1)} b_n^{(p+1)}(1), \tag{3.34}$$

is assumed to be different from zero. In order to calculate $b_n^{(p+1)}(1)$ we obtain $b_{\mathrm{nm}}^{(p+1)}(1)$ from (3.4)

$$b_{\mathrm{nm}}^{(p+1)}(1) = (\mathrm{i}\hbar)^{p+1} \sum_{k\neq m} \chi_{\mathrm{nmk}}^{p+1,p}(1) \frac{d^p \lambda_{\mathrm{km}}(1)}{\mathrm{ds}^p}, \tag{3.35}$$

where, by iterating (3.3), we have

$$\chi_{\mathrm{nmk}}^{p+1,p}(1) = \frac{\delta_{\mathrm{kn}}\delta_{\mathrm{m0}}}{\Delta_{\mathrm{nm}}^p(1)}. \tag{3.36}$$

We are led then to

$$b_{\mathrm{nm}}^{(p+1)}(1) = (\mathrm{i}\hbar)^{p+1} \frac{\lambda_{\mathrm{nm}}^{(p)}(1)}{\Delta_{\mathrm{nm}}^p(1)} \delta_{\mathrm{m0}},\ (\mathrm{n} \neq \mathrm{m}). \tag{3.37}$$

In order to obtain $b_{\mathrm{nn}}^{(p+1)}(\mathrm{s})$, $\mathrm{n} \neq 0$, we need to solve (2.52), which results in

$$b_{\mathrm{nn}}^{(p+1)}(\mathrm{s}) = \text{-}(\mathrm{i}\hbar)^{p+1} \frac{\lambda_{\mathrm{n0}}^{(p)}(0)}{\Delta_{\mathrm{nm}}^{(p)}(0)},\ (\mathrm{n} \neq 0). \tag{3.38}$$

Now we replace (3.37) and (3.38) into (2.43), so that we obtain

$$b_n^{(p+1)}(1) = (\mathrm{i}\hbar)^{p+1}(\ e^{\frac{i}{v}\omega_{\mathrm{n0}}(1)} e^{-\mathrm{i}\gamma_{\mathrm{n0}}(1)} \frac{\lambda_{\mathrm{n0}}^{(p)}(1)}{\Delta_{\mathrm{nm}}^p(1)} \text{ - } \frac{\lambda_{\mathrm{n0}}^{(p)}(0)}{\Delta_{\mathrm{nm}}^p(0)}),\ (\mathrm{n} \neq 0), \tag{3.39}$$

then the triangle inequalities furnish

$$|\ b_n^{(p+1)}(1)|^2 \leq \hbar^{2p+2}\ (\ \frac{\left|\lambda_{\mathrm{n0}}^{(p)}(1)\right|}{\Delta_{\mathrm{nm}}^p(1)} + \frac{\left|\lambda_{\mathrm{n0}}^{(p)}(0)\right|}{\Delta_{\mathrm{nm}}^p(0)})^2 \tag{3.40}$$

and

$$\mid b_n^{(p+1)}(1)|^2 \geq \hbar^{2p+2} \; (\; \frac{\left|\lambda_{\rm n0}^{(p)}(1)\right|}{\Delta_{\rm nm}^p(1)} \; - \; \frac{\left|\lambda_{\rm n0}^{(p)}(0)\right|}{\Delta_{\rm nm}^p(0)})^2, \tag{3.41}$$

which concludes the proof.

Comments

1) When $p = 0$ the formulas (3.30) and (3.31) recover (3.27) and (3.28), because then none of the derivatives of the Hamiltonian are assumed to be zero.

2) If $\frac{\rm dH(0)}{\rm ds} = \frac{d^2H(0)}{\rm ds^2} = ... = \frac{d^pH(0)}{\rm ds^p} = 0$ and $\frac{\rm dH(s^*)}{\rm ds} = \frac{d^2H(s^*)}{\rm ds^2} = ... = \frac{d^pH(s^*)}{\rm ds^p} = 0$, for some s^*, where $0 < s^* \leqslant 1$, then we can write

$$\rm D(|\psi(s^*)\rangle,|0(s^*)\rangle) \leq \frac{\hbar^{p+1}}{T^{p+1}}(\sum_{n=1} (\frac{\left|\lambda_{\rm n0}^{(p)}(s^*)\right|}{\Delta_{\rm n0}^p(s^*)} + \frac{\left|\lambda_{\rm n0}^{(p)}(0)\right|}{\Delta_{\rm n0}^p(0)})^2)^{1/2} \tag{3.42}$$

and

$$\rm D(|\psi(s^*)\rangle,|0(s^*)\rangle) \geq \frac{\hbar^{p+1}}{T^{p+1}}(\sum_{n=1} (\mid \frac{|\lambda_{\rm n0}(s^*)|}{\Delta_{\rm n0}(s^*)} - \frac{|\lambda_{\rm n0}(0)|}{\Delta_{\rm n0}(0)} \mid)^2))^{1/2}, \tag{3.43}$$

which follows from the preceding proof.

3) As an illustration we consider some Hamiltonians H_p(t) = (1-f_p(t/T))X + f_p(t/T)Z, where the functions f_p(x) possess the following properties: (i) $f_p(0) = 0$ and $f_p(1) = 1$ and (ii) $\frac{\rm df_p(0)}{\rm dx} = \frac{d^2f_p(0)}{\rm dx^2} = ... = \frac{d^pf_p(0)}{\rm dx^p} = \frac{\rm df_p(1)}{\rm dx} = \frac{d^2f_p(1)}{\rm dx^2} = ... = \frac{d^pf_p(1)}{\rm dx^p} = 0$. Two graphs are depicted in the figures 3.4 and 3.5. The parameter v is smaller than v = 0.002 ω. The first graph shows the first-order contribution of the adiabatic perturbation theory to the Bures angle ((3.27) or (3.28)) (broken line), which furnishes the distance during the evolution of the system except at $s = 1, (t = 1/v)$, because then this contribution vanishes. The second graph shows the upper bound (3.30) (broken line) and the distance

around $s = 1$. The lower bounds (3.31) are zero. We notice the distance satisfies the bounds obtained from higher-order contributions of the APT.

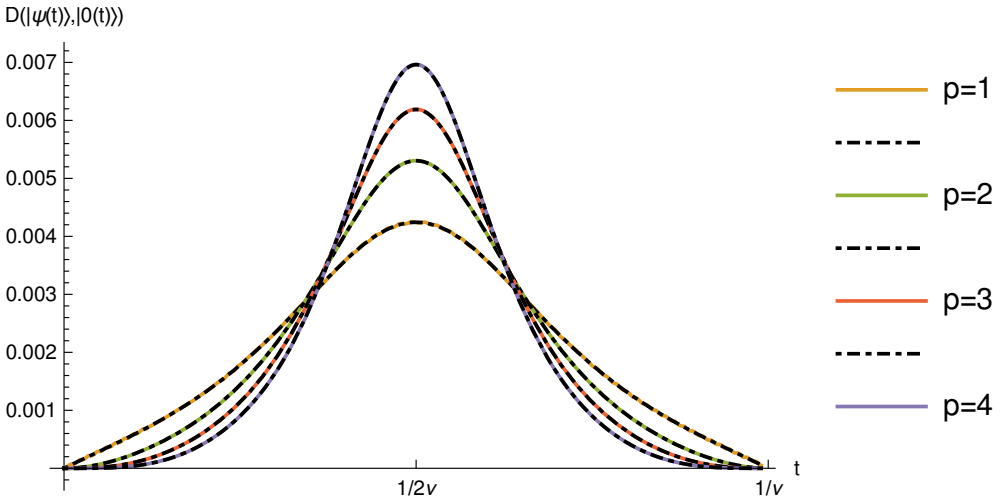

Figure 3.4: Bures angle when $\frac{\mathrm{dH}_p}{\mathrm{ds}}|_{s=0,1} = \frac{d^2 H_p}{\mathrm{ds}^2}|_{s=0,1} = ... = \frac{d^p H_p}{\mathrm{ds}^p}|_{s=0,1} = 0$.

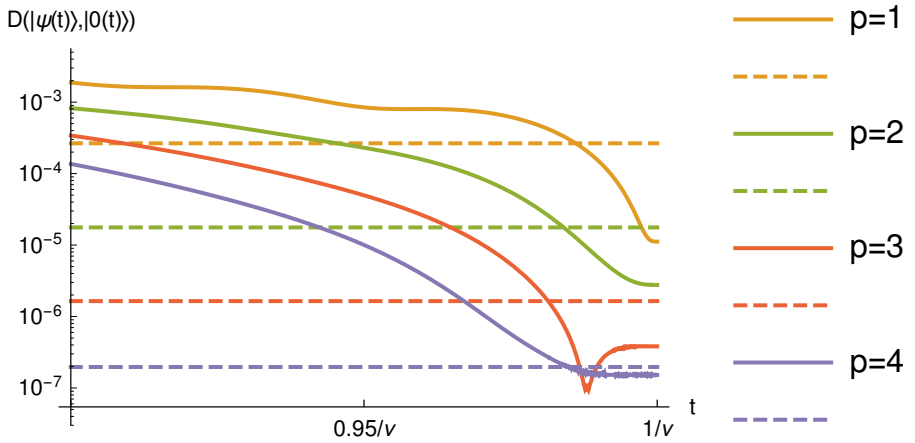

Figure 3.5: Bures angle: contributions of higher-orders of perturbation.

3.2.3 A Calculation of the Running Time T

We want to obtain expressions for the duration of the physical process T which make the preceding expressions for the distance work. We consider (3.21). The first term in this expansion becomes the main contribution when all other contributions are much smaller than it, in particular the second term must satisfy

$$\frac{1}{2}\frac{\xi_2(s)}{\xi_1(s)}v \ll 1, \tag{3.44}$$

or

$$T \gg \frac{1}{2}\frac{\xi_2(s)}{\xi_1(s)}, \tag{3.45}$$

where ξ_1 and ξ_2 are obtained from (3.16). Now we define the vectors

$$b^{(1)} = (b_1^{(1)}, b_2^{(1)},...,b_{N-1}^{(1)}\ ) \tag{3.46}$$

and

$$b^{(2)} = (b_1^{(2)}, b_2^{(2)},...,b_{N-1}^{(2)}\ ). \tag{3.47}$$

The inner product

$$\langle\ b^{(1)}, b^{(2)}\ \rangle = \sum_{n=1}^{N-1} \overline{b_n^{(1)}} b_n^{(2)} \tag{3.48}$$

allow us to rewrite (3.45) as

$$\mathrm{T} \gg \frac{\left\langle b^{(1)}, b^{(2)}\right\rangle + \left\langle b^{(2)}, b^{(1)}\right\rangle}{2\left\langle b^{(1)}, b^{(1)}\right\rangle}. \tag{3.49}$$

We notice that

$$\left\langle b^{(1)}, b^{(2)}\right\rangle + \left\langle b^{(2)}, b^{(1)}\right\rangle = 2\ \mathrm{Re}(\left\langle b^{(1)}, b^{(2)}\right\rangle) \leq 2 \mid \left\langle b^{(1)}, b^{(2)}\right\rangle \mid . \tag{3.50}$$

Furthermore the Cauchy-Schwarz inequality provides

$$\mid \left\langle b^{(1)}, b^{(2)}\right\rangle \mid \leq \sqrt{\left\langle b^{(1)}, b^{(1)}\right\rangle}\sqrt{\left\langle b^{(2)}, b^{(2)}\right\rangle}. \tag{3.51}$$

Therefore from (3.50), (3.51) and (3.49) we obtain

$$\mathrm{T} \gg \sqrt{\frac{\left\langle b^{(2)}, b^{(2)}\right\rangle}{\left\langle b^{(1)}, b^{(1)}\right\rangle}}. \tag{3.52}$$

In a similar manner when p pairs of derivatives of the Hamiltonian vanish at $s = 0$ and $s = 1$, an analogous reasoning involving (3.32) lead us to

$$\mathrm{T} \gg \sqrt{\frac{\langle b^{(p+2)}, b^{(p+2)} \rangle}{\langle b^{(p+1)}, b^{(p+1)} \rangle}}, \tag{3.53}$$

this last expression evaluated at $s = 1$. Now in order to obtain an upper bound on the quantities (3.52) and (3.53) we obtain upper bounds on the numerators of these expressions and lower bounds on their denominators, then we combine them to obtain an upper bound on these expressions.

Expression (3.52)

In order to reduce the number of oscillatory terms of the perturbative coefficients we assume that $\dot{H}(0) = \ddot{H}(0) = 0$. The APT developed in the preceding chapter then provides

$$b_n^{(1)}(\mathrm{s}) = (\mathrm{i}\hbar)\, e^{\frac{i}{v}\omega_{\mathrm{n0}}(s)} e^{-\mathrm{i}\gamma_{\mathrm{n0}}(s)} \frac{M_{\mathrm{n0}}(s)}{\Delta_{\mathrm{n0}}(s)} \tag{3.54}$$

and

$$b_n^{(2)}(\mathrm{s}) = (\mathrm{i}\hbar)^2 e^{\frac{i}{v}\omega_{\mathrm{n0}}(s)} e^{-\mathrm{i}\gamma_{\mathrm{n0}}(s)} \frac{1}{\Delta_{\mathrm{n0}}(s)} \Big(\frac{d}{\mathrm{ds}} \Big(\frac{M_{\mathrm{n0}}(s)}{\Delta_{\mathrm{n0}}(s)} \Big) + W_{\mathrm{n0}}(\mathrm{s}) \frac{M_{\mathrm{n0}}(s)}{\Delta_{\mathrm{n0}}(s)} + \sum_{k \neq n} \frac{M_{\mathrm{nk}}(s) M_{\mathrm{k0}}(s)}{\Delta_{\mathrm{k0}}(s)} \Big). \tag{3.55}$$

We write the inner product in the denominator of (3.45) as

$$\langle\, b^{(1)}, b^{(1)} \rangle = \hbar^2 \sum_{n=1}^{N-1} \frac{\Big| \Big\langle n(s) \Big| \dot{H}(s) \Big| 0(s) \Big\rangle \Big|^2}{\Delta_{\mathrm{n0}}^2(s)}. \tag{3.56}$$

Let $\bar{\Delta}$ denote the maximum gap during the whole evolution of the system. In terms of this quantity we can derive from the preceding equation the inequality

$$\langle\, b^{(1)}, b^{(1)} \rangle \geq \frac{\hbar^2}{\bar{\Delta}^2} \sum_{n=1}^{N-1} |\langle \mathrm{n(s)} | \dot{H}(\mathrm{s}) | 0(\mathrm{s}) \rangle\, |^2. \tag{3.57}$$

Now the closure relation,

$$\sum_{n=1}^{N-1} |\mathrm{n(s)}\rangle\langle \mathrm{n(s)}| = 1 \text{ - } |0(\mathrm{s})\rangle\langle 0(\mathrm{s})|, \tag{3.58}$$

when inserted in (3.57) furnishes

$$\langle\ b^{(1)}, b^{(1)}\rangle \geq \frac{\hbar^2}{\bar{\Delta}^2}(\delta\dot{H})_0^2, \tag{3.59}$$

where

$$(\delta\dot{H})_0^2 = \langle 0(\mathrm{s})|\dot{H}^2(\mathrm{s})|0(\mathrm{s})\rangle \text{ - } |\langle 0(\mathrm{s})|\dot{H}(\mathrm{s})|0(\mathrm{s})\rangle\ |^2. \tag{3.60}$$

Our next task is to determine an upper bound on the numerator of (3.45), then for this purpose we obtain upper bounds on each term of (3.55). The term

$$\sum_{k\neq n} \frac{M_{\mathrm{nk}}(s)M_{\mathrm{k0}}(s)}{\Delta_{\mathrm{k0}}(s)} \tag{3.61}$$

can be rewritten as

$$\langle \mathrm{n}|\dot{H}\sum_{k\neq n} \frac{|k\rangle\langle k|}{\Delta_{\mathrm{k0}}\Delta_{\mathrm{kn}}\Delta_{0n}}\dot{H}|0\rangle, \tag{3.62}$$

or

$$\langle \mathrm{n}|\dot{H}A_n\dot{H}|0\rangle, \tag{3.63}$$

where

$$A_n = \sum_{k\neq n} \frac{|k\rangle\langle k|}{\Delta_{\mathrm{k0}}\Delta_{\mathrm{kn}}\Delta_{0n}}. \tag{3.64}$$

The expression (A.1) and the theorem in the appendix A result in

$$|\langle \mathrm{n}|\dot{H}A_n\dot{H}|0\rangle| \leq ||\ \dot{H}A_n\dot{H}\ || \leq ||\ \dot{H}\ ||\ ||\ A_n\ ||\ ||\ \dot{H}\ ||, \tag{3.65}$$

but (3.64) provides

$$||\ A_n\ || \leq \frac{1}{\Delta^3}, \tag{3.66}$$

where Δ denotes the minimum gap during the whole evolution of the system. Therefore

$$|\ \sum_{k\neq n} \frac{M_{\mathrm{nk}}(s)M_{\mathrm{k0}}(s)}{\Delta_{\mathrm{k0}}(s)}\ | \leq \frac{\|\dot{H}\|^2}{\Delta^3}. \tag{3.67}$$

The term involving W_{n0} can be rewritten as

$$W_{\mathrm{n0}}\frac{M_{\mathrm{n0}}}{\Delta_{\mathrm{n0}}} = (\ \langle n|\dot{n}\rangle - \langle 0|\dot{0}\rangle)\frac{\left\langle n\left|\dot{H}\right|0\right\rangle}{\Delta_{\mathrm{n0}}\Delta_{0n}}. \tag{3.68}$$

At this point we define

$$q_1 = \max_{\{s,n\}} | \langle n|\dot{n}\rangle |, \tag{3.69}$$

so that

$$| \langle n|\dot{n}\rangle - \langle 0|\dot{0}\rangle | \leq | \langle n|\dot{n}\rangle | + | \langle 0|\dot{0}\rangle | \leq 2q_1. \tag{3.70}$$

On the other hand,

$$| \frac{\left\langle n \left| \dot{H} \right| 0 \right\rangle}{\Delta_{\mathrm{n}0}\Delta_{0n}} | \leq \frac{\|\dot{H}\|}{\Delta^2}. \tag{3.71}$$

Therefore we consider an upper bound on the modulus of (3.68) as

$$| W_{\mathrm{n}0}\frac{M_{\mathrm{n}0}}{\Delta_{\mathrm{n}0}} | \leq 2q_1\frac{\|\dot{H}\|}{\Delta^2}. \tag{3.72}$$

The term

$$\frac{d}{\mathrm{d}s}\left(\frac{M_{\mathrm{n}0}(s)}{\Delta_{\mathrm{n}0}(s)}\right) \tag{3.73}$$

can be rewritten as

$$\frac{\dot{M}_{\mathrm{n}0}(s)}{\Delta_{\mathrm{n}0}(s)} - \frac{M_{\mathrm{n}0}(s)}{\Delta_{\mathrm{n}0}(s)}\frac{\dot{\Delta}_{\mathrm{n}0}(s)}{\Delta_{\mathrm{n}0}(s)}. \tag{3.74}$$

If we define

$$q_2 = \max_{\{n,s\}} | \frac{\dot{\Delta}_{\mathrm{n}0}(s)}{\Delta_{\mathrm{n}0}(s)} |, \tag{3.75}$$

then

$$| \frac{M_{\mathrm{n}0}(s)}{\Delta_{\mathrm{n}0}(s)}\frac{\dot{\Delta}_{\mathrm{n}0}(s)}{\Delta_{\mathrm{n}0}(s)} | \leq q_2\frac{\|\dot{H}\|}{\Delta^2}. \tag{3.76}$$

Finally the term

$$\frac{\dot{M}_{\mathrm{n}0}}{\Delta_{\mathrm{n}0}}, \tag{3.77}$$

which appear in (3.74), can be cast in the form

$$\frac{\left\langle \dot{n} \left| \dot{H} \right| 0 \right\rangle}{\Delta_{\mathrm{n}0}\Delta_{0n}} + \frac{\left\langle n \left| \ddot{H} \right| 0 \right\rangle}{\Delta_{\mathrm{n}0}\Delta_{0n}} + \frac{\left\langle n \left| \dot{H} \right| \dot{0} \right\rangle}{\Delta_{\mathrm{n}0}\Delta_{0n}} + \frac{\left\langle n \left| \dot{H} \right| 0 \right\rangle}{\Delta_{0n}^2}\frac{\dot{\Delta}_{0n}}{\Delta_{0n}}. \tag{3.78}$$

We write immediately

$$| \frac{\left\langle n \left| \dot{H} \right| 0 \right\rangle}{\Delta_{0n}^2}\frac{\dot{\Delta}_{0n}}{\Delta_{0n}} | \leq q_2\frac{\|\dot{H}\|}{\Delta^2} \tag{3.79}$$

and

$$| \frac{\left\langle n \left| \ddot{H} \right| 0 \right\rangle}{\Delta_{\mathrm{n}0}\Delta_{0n}} | \leq \frac{\|\ddot{H}\|}{\Delta^2}. \tag{3.80}$$

In order to derive an upper bound on the modulus of

$$\frac{\left\langle \dot{n} \left| \dot{H} \right| 0 \right\rangle}{\Delta_{\mathrm{n}0}\Delta_{0n}} \tag{3.81}$$

we consider an upper bound on the expression

$$|\langle \dot{n}|\dot{H}|0\rangle|. \tag{3.82}$$

From the property (A.2) presented in the appendix A we deduce that

$$|| \ (|\dot{n}\rangle\langle\dot{n}|)\dot{H}(|0\rangle\langle 0|) \ || = |\langle\dot{n}|\dot{H}|0\rangle| \ || \ |\dot{n}\rangle\langle 0| \ || = \sqrt{\langle\dot{n}|\dot{n}\rangle} \ |\langle\dot{n}|\dot{H}|0\rangle|, \tag{3.83}$$

whereas the property (A.1) provides

$$|| \ (|\dot{n}\rangle\langle\dot{n}|)\dot{H}(|0\rangle\langle 0|) \ || \leq || \ |\dot{n}\rangle\langle\dot{n}| \ || \ || \ \dot{H} \ || \ || \ |0\rangle\langle 0| \ || = \langle\dot{n}| \, \dot{n}\rangle \ || \ \dot{H} \ ||. \tag{3.84}$$

We define

$$q_3 = \max_{\{s,n\}} \sqrt{\langle\dot{n}|\dot{n}\rangle}, \tag{3.85}$$

so that (3.83) and (3.84) furnish

$$|\langle\dot{n}|\dot{H}|0\rangle| \leq q_3 \ || \ \dot{H} \ ||. \tag{3.86}$$

Therefore we obtain

$$| \ \frac{\left\langle \dot{n} \left| \dot{H} \right| 0 \right\rangle}{\Delta_{\mathrm{n}0}\Delta_{0n}} \ | \leq q_3 \frac{\|\dot{H}\|}{\Delta^2}. \tag{3.87}$$

In a similar way we derive

$$| \ \frac{\left\langle n \left| \dot{H} \right| \dot{0} \right\rangle}{\Delta_{\mathrm{n}0}\Delta_{0n}} \ | \leq q_3 \frac{\|\dot{H}\|}{\Delta^2}. \tag{3.88}$$

The equations (3.79), (3.80), (3.87), (3.88) and the triangle inequality imply

$$| \ \frac{\dot{M}_{\mathrm{n}0}(s)}{\Delta_{\mathrm{n}0}(s)} \ | \leq (q_2 + 2q_3) \ \frac{\|\dot{H}\|}{\Delta^2} + \frac{\|\ddot{H}\|}{\Delta^2}. \tag{3.89}$$

An upper bound on the modulus of (3.74) can be written as

$$| \frac{d}{\mathrm{ds}}(\frac{M_{\mathrm{n0}}(s)}{\Delta_{\mathrm{n0}}(s)})| \leq 2(q_2+q_3) \frac{\|\dot{H}\|}{\Delta^2} + \frac{\|\ddot{H}\|}{\Delta^2}. \tag{3.90}$$

The results (3.67), (3.72), (3.90) and the triangle inequality provide

$$| b_n^{(2)}(\mathrm{s}) | \leq \frac{\hbar^2}{\Delta^2}(2 \ (\ q_1 + q_2 + q_3\ ) \frac{\|\dot{H}\|}{\Delta} + \frac{\|\ddot{H}\|}{\Delta} + \frac{\|\dot{H}\|^2}{\Delta^2}\ ). \tag{3.91}$$

The norm of $b^{(2)}$ possesses the following upper bound

$$\sqrt{\langle b^{(2)}, b^{(2)}\rangle} \leq \frac{\hbar^2}{\Delta^2}\sqrt{N-1}\ (2 \ (\ q_1 + q_2 + q_3\ ) \frac{\|\dot{H}\|}{\Delta} + \frac{\|\ddot{H}\|}{\Delta} + \frac{\|\dot{H}\|^2}{\Delta^2}\ ). \tag{3.92}$$

Therefore an expression for the running time (3.52) is

$$\mathrm{T} \gg \hbar \ \frac{\sqrt{N-1}}{\sqrt{\left(\delta\dot{H}\right)_0^2}}\ (\frac{\bar{\Delta}}{\Delta})^2(2 \ (\ q_1 + q_2 + q_3\ ) \frac{\|\dot{H}\|}{\Delta} + \frac{\|\ddot{H}\|}{\Delta} + \frac{\|\dot{H}\|^2}{\Delta^2}\ ), \tag{3.93}$$

derived from (3.59) and (3.92), where N denotes the dimension of the vector space. We take

$$\bar{q} = \max\{2 \ (\ q_1 + q_2 + q_3\ ),1\}, \tag{3.94}$$

then (3.93) is rewritten as

$$\mathrm{T} \gg \hbar \ \frac{\sqrt{N-1}}{\sqrt{\left(\delta\dot{H}\right)_0^2}}\ (\frac{\bar{\Delta}}{\Delta})^2\bar{q}(\ \frac{\|\dot{H}\|}{\Delta} + \frac{\|\ddot{H}\|}{\Delta} + \frac{\|\dot{H}\|^2}{\Delta^2}\ ). \tag{3.95}$$

Expression (3.53)

Analogously to the preceding case we assume that $H^{(p+1)}(0) = H^{(p+2)}(0) = 0$, which reduces the number of oscillatory terms in the expressions for the perturbative coefficients. We also assume that $\mathrm{p} \geq 1$. The APT and the tools developed in the first section of this chapter furnish

$$b_n^{(p+1)}(1) = (\mathrm{i}\hbar)^{p+1} e^{\frac{i}{v}\omega_{\mathrm{n0}}(1)} e^{-\mathrm{i}\gamma_{\mathrm{n0}}(1)} \frac{\lambda_{\mathrm{n0}}^{(p)}(1)}{\Delta_{\mathrm{n0}}^p(1)} \tag{3.96}$$

and

$$b_n^{(p+2)}(1) = (\mathrm{i}\hbar)^{p+2} e^{\frac{i}{v}\omega_{\mathrm{n0}}(1)} e^{-\mathrm{i}\gamma_{\mathrm{n0}}(1)} \frac{1}{\Delta_{\mathrm{n0}}(1)} \Big(\frac{d}{\mathrm{ds}} \Big(\frac{\lambda_{\mathrm{n0}}^{(p)}(s)}{\Delta_{\mathrm{n0}}^{p}(s)} \Big)\Big|_{s=1}$$
$$+ \big((\mathrm{p+1}) W_{\mathrm{n0}}(1) - \frac{p(p-1)}{2} \frac{\dot{\Delta}_{\mathrm{n0}}(1)}{\Delta_{\mathrm{n0}}(1)} \big) \frac{\lambda_{\mathrm{n0}}^{(p)}(1)}{\Delta_{\mathrm{n0}}^{p}(1)} \Big), \tag{3.97}$$

where $\dot{\Delta}_{\mathrm{n0}}(\mathrm{s}) = \frac{\mathrm{d}\Delta_{\mathrm{n0}}(s)}{\mathrm{ds}}$. This last expression can be obtained from (2.43). The diagonal terms are identically zero as a consequence of the corollary 2 of the first section of this chapter. The non-diagonal terms can be obtained from the recursive relation (2.51). The derivative $\dot{b}_n^{(p+1)}(1)$ can be evaluated from the equations (3.1) and (3.2). The inner product $\left\langle b^{(p+1)}, b^{(p+1)} \right\rangle$ is then given by

$$\left\langle\, b^{(p+1)}, b^{(p+1)} \right\rangle = \hbar^{2p+2} \sum_{n=1}^{N-1} \frac{\left| \left\langle n(1) \left| H^{(p+1)}(1) \right| 0(1) \right\rangle \right|^2}{\Delta_{\mathrm{n0}}^{2p+2}(1)}, \tag{3.98}$$

so that we are led to

$$\left\langle\, b^{(p+1)}, b^{(p+1)} \right\rangle \geq \frac{\hbar^{2p+2}}{\bar{\Delta}^{2p+2}} (\, \delta \mathrm{H}^{(p+1)})_0^2, \tag{3.99}$$

where

$$(\, \delta \mathrm{H}^{(p+1)})_0^2 = \langle 0(1)|(H^{(p+1)}(1))^2|0(1)\rangle - |\langle 0(1)|H^{(p+1)}(1)|0(1)\rangle\,|^2. \tag{3.100}$$

We can derive an upper bound on (3.97) by making use of the same techniques already presented, namely,

$$|\, b_n^{(p+2)}(1)| \leq \hbar^{p+2} \Big(\big(2(\mathrm{p+1}) q_1 + (\frac{p^2}{2} + \frac{3p}{2} + 2) q_2 + 2q_3 \big) \frac{\left\| H^{(p+1)}(1) \right\|}{\Delta^{p+3}} + \frac{\left\| H^{(p+2)}(1) \right\|}{\Delta^{p+3}} \Big). \tag{3.101}$$

From the equations (3.59) and (3.101) we write the following expression for the running time

$$\mathrm{T} \gg \hbar \, \frac{\sqrt{N-1}}{\sqrt{\Big(\delta \mathrm{H}^{(p+1)} \Big)_0^2}} \Big(\frac{\bar{\Delta}}{\Delta} \Big)^{p+2} \bar{r} \, \Big(\frac{\left\| H^{(p+1)}(1) \right\|}{\Delta} + \frac{\left\| H^{(p+2)}(1) \right\|}{\Delta} \Big), \tag{3.102}$$

where

$$\bar{r} = \max\{ (\, 2(\mathrm{p+1}) q_1 + (\frac{p^2}{2} + \frac{3p}{2} + 2) q_2 + 2q_3 \,), 1\}. \tag{3.103}$$

Chapter 4

Final Comments

The distance

$$\delta = || \, |\psi(\mathrm{T})\rangle - e^{\mathrm{i}\chi} |\phi(\mathrm{T})\rangle \, ||, \tag{4.1}$$

presented in [4], is not a distance in the Hilbert projective space, therefore it is not an appropriate definition of distance between two quantum states. In fact if the relative phase between the vectors $|\psi\rangle$ and $|\phi\rangle$ changes, the distance (4.1) is altered, but both the vectors still represent the same physical state.

Some works suggest the result presented in the theorem 3 of the preceding chapter, for instance, [4] states that the error decreases exponentially when a number of derivatives of the Hamiltonian vanishes at the initial and final times of the physical process. The work [9] provides evidence of this same behaviour, but the notion of distance, or error, is different from [4].

We have obtained lower and upper bounds on the distance between the actual state of the system and the target state which are extremely accurate, furthermore under certain conditions our bounds become an estimate for the distance itself. This accuracy is not reached neither in the results presented in [4] nor in the works cited in the introduction, which deal with exponential estimates.

We still hope to obtain better estimates for the running time than those presented in the equations (3.95) and (3.102), which overestimate this quantity.

Appendix A

Some Properties of the Norm of an Operator

The norm of an operator A was defined in the introduction as the largest of the eigenvalues of the operator $\sqrt{A^\dagger A}$. It possesses some useful properties [12] like

$$||\mathrm{AB}|| \leq ||\mathrm{A}||\ ||\mathrm{B}|| \tag{A.1}$$

and

$$||\mathrm{cA}|| \leq |\mathrm{c}|\ ||\mathrm{A}||, \tag{A.2}$$

where A and B are operators and c is a complex number. An additional result is stated in the following theorem.

Theorem: Let $|\Psi_1\rangle$ and $|\Psi_2\rangle$ be both normalized vectors, then

$$|\langle\Psi_1|\mathrm{A}|\Psi_2\rangle| \leq ||\mathrm{A}||. \tag{A.3}$$

Proof: Let us consider the following projectors,

$$P_1 = |\Psi_1\rangle\langle\Psi_1| \tag{A.4}$$

and

$$P_2 = |\Psi_2\rangle\langle\Psi_2|\,. \tag{A.5}$$

From (A.2) we can write

$$\|P_1 \mathrm{A} P_2\| = |\langle \Psi_1 | \mathrm{A} | \Psi_2 \rangle| \; || \; |\Psi_1\rangle\langle\Psi_2| \; || \; , \tag{A.6}$$

therefore

$$\|P_1 \mathrm{A} P_2\| = |\langle \Psi_1 | \mathrm{A} | \Psi_2 \rangle| \quad . \tag{A.7}$$

On the other hand, from (A.1) we obtain

$$|| \; P_1 \mathrm{A} P_2 \; || \leq || \; P_1 \; || \; || \; \mathrm{A} \; || \; || \; P_2 \; || = || \; \mathrm{A} \; ||. \tag{A.8}$$

We conclude that the statement holds by comparing (A.7) and (A.8).

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