Classical manipulation of a quantum system
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The post-adiabatic corrections to the adiabatic wave function of a fast quantum system coupled to a slow classical system was calculated in the previous chapter. In this chapter some dynamical properties of a slow classical system coupled to a fast quantum system is considered. In particular, the result of the previous chapter is employed in order to calculate the postadiabatic forces exerted by the quantum system on the classical one. Up to higher orders in the small parameter \( \epsilon \), which represents the ratio of the time-scales of the two systems, the exerted force can be derived from a Lagrangian. However, at orders higher than two the Lagrangian is not just a functional of the coordinate and velocity of the classical system but it also depends on the acceleration and higher time-derivatives of the slowly varying coordinates. This brings new physical concepts such as spin and zitterbewegung effect in the purely classical regime.

5.1 Introduction

In this chapter we employ the results of the previous chapter and study the dynamics of the classical slow part of the quantum-classical (also called
mean-field or hybrid) dynamics, which describes coupled quantum and classical systems in the adiabatic regime where the characteristic time scale of the system of interest is much slower than that of its fast counterpart. [2,3]. We focus on the slow classical system adiabatically exclude the quantum system and construct an autonomous dynamics for the classical particle in successive orders of the small ratio $\epsilon$ of the characteristic times.

One of the well-established results in this direction known from 1922 is the Darwin Lagrangian [85,99] for a system of slowly moving charges. We know that in electrodynamics the propagation velocity is finite and the fields must be considered as independent systems with their own degrees of freedom. As a result, if we want to build up a Lagrangian for a system of interacting charges in a rigorous way, we have to encounter the quantities related to the internal degrees of freedom of the fields as well as the velocity and the coordinates of the particles in the Lagrangian. However, if the velocities of all the particles in the system are small compared to the velocity of light, the system can be described by a certain approximate Lagrangian called Darwin Lagrangian, named after Charles Galton Darwin a grandson of the great naturalist and has important applications in plasma physics and astrophysics [85]. It turns out to be possible to derive the equation of motion for the particles through a Lagrangian up to $(v/c)^2$ order. This can be done since the radiation of electromagnetic waves by moving charges occurs only in third order of $(v/c)$.

Here, we assume the classical system is slow — a condition that is normally fulfilled in practice. We introduce a small parameter $\epsilon$ defined as the ratio of the characteristic times for the quantum over the classical system, respectively. Then we exclude the fast quantum system and study to which extent the ensuing dynamics of the slow classical system can be described by an autonomous Lagrangian-generated equations for the classical coordinates. In the leading order and order of $\epsilon^1$ this includes respectively the Born-Oppenheimer potential and an effective magnetic field related to the Berry phase. Within the order $\epsilon^2$ the motion of the classical particle is described by a Lagrangian that depends on its coordinate and momenta. We show that in the order $\epsilon^3$ the motion of the classical particle is still described by a Lagrangian, but the latter linearly depends on the particle’s acceleration [98]. This implies the existence of a spin tensor [non-orbital angular momentum] for the particle. This spin tensor is related to the momentum via an analogue of the zitterbewegung effect. The Hamiltonian structure of the classical system is non-trivial and is defined via non-linear Poisson brackets.
The linear dependence of the effective classical Lagrangian on higher-order derivatives is seen as well in the higher orders $\epsilon^n$ [98].

This chapter is organized as the following. In section 5.2 we introduce the quantum-classical dynamics. Section 5.3 is devoted to derivation of the higher order corrections to the post-adiabatic force. In section 5.4 we review the derivation of the classical Lagrangian in the orders $\epsilon$. In particular, we reproduce in a systematic way the results obtained by Berry and Robbins [2]. It is well known that at the zero order of $\epsilon$ the influence of the quantum system on the classical one can be described by the Born-Oppenheimer potential energy term [2, 3, 94, 95, 100, 101].

It was shown by Berry and Robbins that in the first order of $\epsilon$ one gets an effective magnetic field, which manifests itself as the velocity-dependent term in the classical Lagrangian [2].

Section 5.5 describes the second-order post-adiabatic force using the adiabatic perturbation theory outlined in the previous chapter. In this chapter we reproduce the results recently shown by Goldhaber [3]. Namely, in the second order $\epsilon^2$ one gets in the Lagrangian of the classical system an additional kinetic energy term, i.e., a quadratic form in slow velocities [3]. A very similar result on the order $\epsilon^2$ was obtained earlier by Weigert and Littlejohn for two coupled (fast and slow) quantum systems [100]. Moreover, we show that at the order $\epsilon^2$ the classical Lagrangian corresponds to a classical particle moving along the geodesics of a curved manifold. We calculate the curvature for the simplest non-trivial case and work out its implications for the stability of the effective classical motion at the order $\epsilon^2$. Here we also point out at an unusual scenario related to the metric of the manifold changing its signature [i.e., changing from a Riemannian to a pseudo-Riemannian manifold]. It appears that the slow classical motion within this order can be reduced to a free motion (“geodesic motion”) on a Riemannian space with a signature-indefinite metric tensor. This offers the possibility of interchanging time-like and space-like coordinates. Recall in this context that within non-relativistic classical mechanics the geodesic motion on a curved surface proceeds according to a positively-defined metric tensor, while the geodesic motion in the general theory of relativity has a metric tensor with signature $(1, -1, -1, -1)$ [99]. In both cases the signature is fixed.

We are also interested in knowing what happens in the next orders. In particular, we want to understand how far we can continue the expansion over $\epsilon$, still keeping the classical system Lagrangian. Most importantly, we are interested to know whether there are new physical effects essentially related
to post-adiabatic corrections. These questions are answered in sections 5.6 and 5.7. It appears that at every order over \( \epsilon \) one can derive Lagrange equations for the dynamics of the classical system. However, there is an important difference between the orders \( \epsilon \) and \( \epsilon^2 \) and all successive orders. At the order \( \epsilon^3 \) the classical dynamics is Lagrangian, but the Lagrangian starts to depend on the higher-order time-derivatives of the classical coordinates. It is important to note that the classical Lagrangians normally depend on the coordinates and their first-order time-derivatives (velocities). In section 5.6 we show that at the order \( \epsilon^3 \) we get a Lagrangian that is linear over the second order time-derivatives, i.e., classical accelerations. This fact is of conceptual relevance. The classical physics is essentially based on the Newton’s second law that equates acceleration to the force, which depends only on coordinates and velocities. As a consequence, the trajectory of the classical motion is fixed via initial coordinates and initial velocities. In its turn, the Newton’s second law is generated by a Lagrangian, which depends on coordinates and velocities. A Lagrangian depending on higher-order derivatives enlarges the amount of the initial data needed to fix the classical trajectory and produces equations of motion that go beyond the Newton’s law. Our result seems to be the first example where a higher-derivative Lagrangian emerges for an open classical system due to time-scale separation. Dependence on higher-order derivatives in the Lagrangian implies a number of essential changes in the kinematics of the classical system: the momentum of the classical system depends on the acceleration, while the full angular momentum tensor is a sum of the usual orbital part and a term that can be interpreted as the spin of the classical system. In the simplest non-trivial case this spin is proportional to the velocity square of the classical particle. We show that this implies the existence of the zitterbewegung effect, where the momentum of the classical particle (system) is governed by the projected time-derivative of the spin. So far the zitterbewegung effect was known only in the physics of relativistic Dirac electron, while we show the same effect appears in a purely non-relativistic slowly evolved classical system due to its coupling to a fast quantum system. It appears now that this effect is a part of the physics generated by higher-order post-adiabatic corrections. We conjecture that similar dependence on higher-order derivatives is expected at higher orders \( \epsilon^n \) with \( n \geq 4 \), though we restrict ourselves with deriving the effective classical Lagrangian up to the order \( \epsilon^4 \). In section 5.7 we deduce the classical Lagrangian at the order \( \epsilon^4 \) and show that it also depends linearly on higher-order derivatives of the classical coordinates.
5.2 Quantum-classical dynamics

In this section we derive the equation of motion for a classical system coupled to a quantum system. In doing so, we consider the mean-field classical dynamics. In this approach the classical variables are treated as parameters in the Hamiltonian of the quantum system. The dynamics of the quantum system, is described by the Schrödinger equation while the dynamics of the classical system is given by the Newton equation of motion supplemented by the average force acting from the quantum part. As a result, the classical particle experiences an averaged force exerted by the quantum system.

It is important to note that in general this force is not generated by an averaged potential. This would only be the case in the adiabatic regime and the first order adiabatic perturbation theory.

As a model we consider a $K$-degree of freedom classical system with coordinates $q = (q_1, \ldots, q_K)$ and with Lagrangian

$$\mathcal{L}_0 = \frac{M}{2} \sum_{\alpha=1}^K \left( \frac{dq_\alpha}{dt} \right)^2 - V(q),$$

(5.1)

where $M$ is the mass, and $V(q) = V(q_1, \ldots, q_K)$ is the potential energy of the classical system.

Now this classical system (or particle) couples to a quantum system with Hamiltonian operator $\hat{H}(q(t))$, which parametrically depends on the classical coordinates. The quantum system evolves in time according to the Schrödinger equation (for simplicity we put $\hbar = 1$)

$$i \frac{\partial}{\partial t} |\Psi\rangle = \hat{H}(q(t)) |\Psi\rangle,$$

(5.2)

where $|\Psi\rangle$ is the wave-function, and where $\partial_t = \frac{\partial}{\partial t}$.

We can calculate the force exerted by the quantum system on the classical one as

$$F_\mu = \langle \Psi | \partial_\mu \hat{H}(q(t)) |\Psi\rangle,$$

(5.3)

where we defined $^1$:

$$\partial_\mu = \frac{\partial}{\partial q_\mu(t)}.$$

(5.4)

For the simplicity of notation we absorb the minus sign in the force.

$^1$ Note that $\partial_\mu = \partial_{q_\mu(t)}$ acts only on the coordinates, but not on the velocities, e.g., $\partial_\mu \dot{q}_\alpha = 0$. In particular, $\partial_\mu$ commutes with the total time-derivative $\frac{d}{dt}$.  

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The classical part of the dynamics is written as [94,95,101]

\[ M \frac{d^2 q_\mu}{dt^2} + \partial_\mu V + \langle \Psi | \partial_\mu \hat{H} (q(t)) | \Psi \rangle = 0, \quad \mu = 1, \ldots, K. \tag{5.5} \]

Eq. (5.5) is the Newton equation of motion, where besides the classical force \( -\partial_\mu V \), the classical particle experiences an average force \( -\langle \Psi(t) | \partial_\mu H (q(t)) | \Psi(t) \rangle \) exerted by the quantum systems. In this sense the classical coordinates play a role of a mean-field [101]. The main purpose of the present chapter is to understand to which extent this force can be generated by a Lagrangian which depends on the classical coordinates \( q_\alpha(t) \) and their time-derivatives.

It should be clear from (5.2) and (5.5) that the total average energy is conserved in time:

\[ \frac{d}{dt} \left( \frac{M}{2} \sum_{\alpha=1}^{K} \left( \frac{dq_\alpha}{dt} \right)^2 + V(q) + \langle \Psi | \hat{H} (q(t)) | \Psi \rangle \right) = 0. \tag{5.6} \]

We note that the quantum-classical equations of motion (5.2, 5.5) can be derived from a Lagrangian

\[ \tilde{\mathcal{L}} = \frac{1}{2i} \langle \partial_t | \Psi \rangle - \frac{1}{2i} \langle \Psi | \partial_t \Psi \rangle - \langle \Psi | \hat{H} (q(t)) | \Psi(t) \rangle \]

\[ + \frac{M}{2} \sum_{\alpha=1}^{K} \left( \frac{dq_\alpha}{dt} \right)^2 - V(q), \]

where as a set of independently varying parameters one should take \( | \Psi \rangle \) and \( q(t) \) (or alternatively \( \langle \Psi | \) and \( q(t) \))^2. It is seen that \( \tilde{\mathcal{L}} \) is simply a sum of the corresponding quantum and classical Lagrangians, which points out that combination of classical and quantum degrees of freedom does not violate the Lagrangian formalism. However, In section 5.2.1 we briefly discuss the possibility of derivation of the quantum-classical dynamics from a full quantum-quantum dynamics.

### 5.2.1 Derivation

The quantum-classical dynamics can be derived from a full quantum-quantum dynamics in the following fashion [94,101–105].

\[ \frac{d}{dt} \langle \delta \Psi | \Psi \rangle. \]

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\(^2\) As usual, when varying (5.7) we put aside the total time-derivatives, e.g., \( \frac{d}{dt} \langle \delta \Psi | \Psi \rangle \).
We first consider both coupled systems are on equal footing. Therefore, we assume we are given a two-degree of freedom quantum system with the following Hamiltonian

\[ \hat{H}_{\text{tot}} = \frac{\hat{p}^2}{2M} + \hat{V}(q) + \hat{H}(q, x) + \frac{\hat{\pi}^2}{2M}, \]

where \((q, p)\) and \((x, \pi)\) are two degrees of freedom.

For simplicity we shall assume that the initial state is factorized for these two degrees of freedom.

The Heisenberg equation generated by this Hamiltonian reads:

\[ \frac{d\hat{q}}{dt} = \frac{\hat{p}}{M}, \quad \frac{d\hat{p}}{dt} = -\partial_q \hat{V}(q) - \partial_q \hat{H}(q, x), \]

\[ \frac{d\hat{x}}{dt} = \frac{\hat{\pi}}{M}, \quad \frac{d\hat{\pi}}{dt} = -\partial_x \hat{H}(q, x). \]

We separate the motion of \((\hat{q}, \hat{p})\) degrees of freedom into two parts:

\[ \hat{p}(t) = \bar{p}(t) + \hat{p}_f, \quad \hat{q}(t) = \bar{q}(t) + \hat{q}_f, \]

where \(\bar{p}(t)\) and \(\bar{q}(t)\) are the averages over the initial state, and where \(\hat{p}_f\) and \(\hat{q}_f\) are the fluctuations. Then we make two assumptions:

- The \((\hat{q}, \hat{p})\) degrees of freedom are Gaussian which means they satisfy

\[ \bar{p}_f = \bar{q}_f = 0. \]

- The fluctuations of \((\hat{q}, \hat{p})\) degrees of freedom are small.

Keeping these assumptions in mind, we substitute (5.12) into (5.8, 5.9, 5.11) and expand (5.8) and (5.11) over small \(\hat{q}_f\):

\[ \frac{d\bar{q}}{dt} + \frac{d\hat{q}_f}{dt} = \frac{\bar{p}}{M} + \frac{\hat{p}_f}{M}, \]

\[ \frac{d\bar{p}}{dt} + \frac{d\hat{p}_f}{dt} = -\partial_q \hat{V}(\bar{q}) - \partial_q \hat{H}(\bar{q}, x) \]

\[- \partial^2_q \hat{V}(\bar{q}) q_f - \partial^2_q \hat{H}_{qq}(\bar{q}, x) q_f + O(\hat{q}^2_f), \]

\[ \frac{d\bar{x}}{dt} = -\partial_x \hat{H}(\bar{q}, x) - \partial^2_{xq} \hat{H}(\bar{q}, x) q_f + O(\hat{q}^2_f). \]
Averaging (5.14)-(5.16) over the initial states we obtain

$$\frac{dq}{dt} = \frac{\overline{p}}{M},$$  \hspace{1cm} (5.17)
$$\frac{dp}{dt} = -\partial_q V(\overline{q}) - \partial_q \overline{H}(\overline{q}, x) - \partial^2_q \overline{H}(\overline{q}, x) q_f + \mathcal{O}(\overline{q}_f^2),$$ \hspace{1cm} (5.18)
$$\frac{d\pi}{dt} = -\partial_x \overline{H}(\overline{q}, x) - \partial^2_{xq} \overline{H}(\overline{q}, x) q_f + \mathcal{O}(\overline{q}_f^2).$$ \hspace{1cm} (5.19)

Based on our second assumption, if in (5.18, 5.19) the terms proportional to $\mathcal{O}(q_f)$ are neglected we get into a quantum-classical equations, where $(\overline{p}, \overline{q})$ is considered as the classical degree of freedom. Thus, from (5.18) we arrive at the Newton equation of motion for the classical part of the system:

$$M \frac{d^2 q}{dt^2} + \partial_q V + \langle \Psi | \partial_q \overline{H} (q(t)) | \Psi \rangle = 0.$$  

We conclude this section by emphasizing that the main assumption involved in the quantum-classical dynamics derivation is that the quantum fluctuation of the classical coordinate(s) are small. The validity of the (mean-field) quantum-classical dynamics is not related to the classical sub-system being slow. The derivations of the quantum-classical dynamics need not neglect fluctuations of all pertinent variables, i.e., it need not impose the full quantum trajectories. It will be sufficient that the to-be classical sector of the dynamics is approximated via suitable Gaussian density matrices [106]. Then, the parameters of this matrices satisfy the equations of motion for some effective classical systems [106].

### 5.3 Post-adiabatic force

In this section we concentrate on the adiabatic limit of the quantum-classical system, where the classical system is slow and the quantum system is fast, and derive an autonomous equations of motion for the classical part. To this end, we shall solve the time-dependent Schrödinger equation for the fast quantum system under the adiabatic assumption and determine via its solution, the structure of the averaged force.

We employ the adiabatic perturbation theory described in the previous chapter. For the sake of brevity, instead of $|n; q(s)\rangle$ we simply write $|n\rangle$ but
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we keep in mind that $|n\rangle$ parametrically depends on the slow time $s$ through the classical parameters $q(s)$. This notation holds for higher order corrections as well. We will also write $\hat{H}(s)$, and $E_n(s)$ instead of $\hat{H}(q(s))$ and $E_n(q(s))$.

Assuming the quantum system initially starts its evolution from an eigenstate of the Hamiltonian $\hat{H}(s)$, the slow component of the wave-function can be expanded over the small dimensionless parameter $\epsilon$. Let us recall

$$|\psi_n\rangle = e^{\int_0^s du \langle \hat{n}|n\rangle} |\phi_n\rangle,$$

$$|\phi_n\rangle = |n\rangle + \epsilon |n_1\rangle + \epsilon^2 |n_2\rangle + \epsilon^3 |n_3\rangle + \ldots.$$  (5.20)

The zero order term $|\phi_n\rangle = |n\rangle$ in the expansion (5.21) is the statement of the adiabatic theorem. In (5.20), $e^{\int_0^s du \langle \hat{n}|n\rangle}$ is the Berry phase factor; it was separated out for ensuring the proper gauge-covariance [96]; see also below. Note that $\langle \hat{n}|n\rangle$ is purely imaginary (due to $\langle n|n\rangle = 1$). An alternative representation of $|\phi_n\rangle$ is

$$|\phi_n\rangle = \sum_{k=1}^d c_{kn} |k\rangle,$$

$$c_{kn} = \delta_{kn} + \epsilon c_{kn}^{[1]} + \epsilon^2 c_{kn}^{[2]} + \epsilon^3 c_{kn}^{[3]} + \ldots.$$  (5.22)

$c_{kn}^{[m]}$ and $c_{nn}^{[m]}$ are given by

$$c_{kn}^{[m]} = \frac{i\langle n|\hat{n}\rangle}{\Delta_{nk}} c_{k\neq n}^{[m-1]} - i\langle k|\hat{n}_{m-1}\rangle,$$  (5.24)

$$c_{nn}^{[m]} = -\sum_{k}^{'} \int_0^s du c_{kn}^{[m]} \langle n|\hat{k}\rangle,$$  (5.25)

where

$$\Delta_{kn}(s) = E_k(s) - E_n(s).$$

The expression for the exerted force from the fast quantum system to the slow classical system reads

$$F_\mu = \langle \psi_n | \partial_\mu \hat{H}(s) | \psi_n \rangle, \quad \mu = 1, \ldots, K,$$  (5.26)

where $K$ is the number of degrees of freedom of the classical system. Inserting the expression for $|\psi_n\rangle$ from (5.20) into (5.26) we get

$$F_\mu = \partial_\mu \langle \phi_n | \hat{H}(s) | \phi_n \rangle - 2 \Re \langle \partial_\mu \phi_n | \hat{H}(s) | \phi_n \rangle.$$  (5.27)
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We add and subtract $\partial_\mu E_n(s)$ from (5.27). Employing the time-dependent Schrödinger equation for $\hat{H}(s)|\phi_n\rangle$ we get

$$\hat{H}(s)|\phi_n\rangle = i\epsilon \langle \hat{n}|\phi_n\rangle + i\epsilon |\dot{\phi}_n\rangle + E_n(s)|\phi_n\rangle. \tag{5.28}$$

Multiplying both sides of (5.28) from left by $\langle \partial_\mu \phi_n |$, and taking into account that $\langle \phi_n | \partial_\mu \phi_n \rangle$ is purely imaginary since $\langle \phi_n | \phi_n \rangle = 1$, the general expression for the force $F_\mu$ acting on the classical system reads

$$F_\mu(s) = \partial_\mu E_n(s) + 2\epsilon \Im \langle \partial_\mu \phi_n | \dot{\phi}_n \rangle + \partial_\mu \langle \phi_n | \hat{H}(s)|\phi_n\rangle - E_n(s). \tag{5.29}$$

We note from (5.22) and (5.23) that the last term of (5.29) is of second order in $\epsilon$ and higher:

$$\langle \phi_n | \hat{H}(s)|\phi_n\rangle - E_n(s) = \sum_k' \Delta_{kn}|c_{kn}|^2 = O(\epsilon^2). \tag{5.30}$$

The factor $\partial_\mu E_n$ is the force generated by the adiabatic (Born-Oppenheimer) potential $E_n(s)$. Thus the last two terms in (5.29) represent the non-adiabatic force. We denote

$$F_\mu = F_\mu^{[0]} + \epsilon F_\mu^{[1]} + \epsilon^2 F_\mu^{[2]} + \epsilon^3 F_\mu^{[3]} + \ldots, \tag{5.31}$$

where $F_\mu^{[0]}(s) = \partial_\mu E_n(s)$.

In the following sections we derive expressions for higher-order post-adiabatic forces and show that they can be generated by a Lagrangian.

### 5.4 First order post-adiabatic force

The first order post-adiabatic force can be calculated through the only first order term in the general expression for the force, (5.29), given by

$$2\epsilon \Im \langle \partial_\mu \phi_n | \dot{\phi}_n \rangle,$$

where according to (5.21)

$$|\phi_n\rangle = |n\rangle + O(\epsilon). \tag{5.32}$$

Therefore the first order post-adiabatic force reads

$$F_\mu^{[1]} = 2\epsilon \Im \langle \partial_\mu n | \dot{n} \rangle. \tag{5.33}$$
5.4. First order post-adiabatic force

From now on, for the sake of simplicity, we drop the argument $s$.

The expression for the first order post-adiabatic force given by (5.33) can be simplified more. Taking into account that $|\dot{n}\rangle = \dot{q}_\alpha |\partial_\alpha n\rangle$, and assuming implicit summation from 1 to $K$ over the repeated Greek indices, the first order post-adiabatic force, $F^{[1]}_\mu$, reads

$$F^{[1]}_\mu = 2\dot{q}_\alpha \Im \langle \partial_\mu n | \partial_\alpha n \rangle.$$ (5.34)

We notice $\Im \langle \partial_\mu n | \partial_\alpha n \rangle = -\Im \langle \partial_\alpha n | \partial_\mu n \rangle$, therefore the first order force is antisymmetric. Moreover, the presence of $\dot{q}_\alpha$, which represents the slow velocity of the classical system, suggests that $F^{[1]}$ is effective Lorentz [or gyroscopic] type force [2]. This force emerges from a vector potential whose elements are

$$A_\alpha = \Im \langle \partial_\alpha n | n \rangle.$$ (5.35)

Therefore, we see that the first order averaged force can be generated by the following Lagrangian

$$\mathcal{L}^{[1]}(\dot{q}, q) = \epsilon A_\alpha(q) \dot{q}_\alpha.$$ (5.36)

Now the complete classical Lagrangian to the first order represented by $L_1$ is obtained by adding $\mathcal{L}^{[1]}(\dot{q}, q)$ and the Born-Oppenheimer potential $E_n(q)$ to the initial (bare) classical Lagrangian $L_0$, given by (5.1):

$$L_1 = \frac{M}{2} \sum_{\alpha=1}^{K} \left( \frac{dq_\alpha}{dt} \right)^2 - V(q) - E_n(q) + \epsilon A_\alpha(q) \dot{q}_\alpha.$$ (5.37)

If we rescale the kinetic energy to the slow time, we will get

$$L_1 = \epsilon^2 \frac{M}{2} \sum_{\alpha=1}^{K} (\dot{q}_\alpha)^2 + \epsilon A_\alpha(q) \dot{q}_\alpha - V(q) - E_n(q).$$ (5.38)

The generalized momenta then reads

$$p_\alpha = \frac{\partial L_1}{\partial \dot{q}_\alpha} = \epsilon^2 M \dot{q}_\alpha + \epsilon A_\alpha(q).$$ (5.39)
The effective Hamiltonian governing the slow classical system up to the first order, denoted by $H_1$, can be calculated using the Legendre transformation of the Lagrangian (5.39):

$$H_1 = \frac{1}{2M\epsilon^2} \sum_{\alpha=1}^{K} [p_{\alpha} - \epsilon A_{\alpha}(q)]^2 + E_n(q) + V(q),$$  \hspace{1cm} (5.41)

which has the similar structure of the Hamiltonian of a moving electric charge in an electromagnetic field.

### 5.5 Second order post-adiabatic force

In this section we calculate the second-order post-adiabatic force and prove that this force can be produced by a kinetic term in the second-order post-adiabatic Lagrangian —and not a potential term— which has a coordinate-dependent mass tensor.

Inserting (5.22) in the third term in the general expression of post-adiabatic force given by (5.29) and considering the second order terms we obtain:

$$\epsilon \mathfrak{H} \langle \partial_{\mu} \phi_n | \hat{H}(s) | \phi_n \rangle = \epsilon^2 \frac{d}{ds} \mathfrak{H} \langle \partial_{\mu} n | n_1 \rangle + \epsilon^2 \partial_{\mu} \mathfrak{H} \langle n_1 | \dot{n} \rangle + O(\epsilon^3).$$  \hspace{1cm} (5.42)

The second term in (5.29) leads to

$$\partial_{\mu} \left[ \langle \phi_n | \hat{H}(s) | \phi_n \rangle - E_n \right] = \epsilon^2 \sum_k' \Delta_{kn} | c_{kn}^{[1]} |^2 + O(\epsilon^3).$$  \hspace{1cm} (5.43)

Therefore, the second order post-adiabatic force can be written as

$$F_\mu^{[2]} = \partial_{\mu} \sum_k' \Delta_{kn} | c_{kn}^{[1]} |^2 + 2\mathfrak{H} \{ \langle \partial_{\mu} n_1 | \dot{n} \rangle + \langle \partial_{\mu} n | \dot{n}_1 \rangle \}$$
$$= \partial_{\mu} \sum_k' \langle k | \dot{n} \rangle \langle \dot{n} | k \rangle \Delta_{kn} + 2\mathfrak{H} \left\{ \frac{d}{ds} \langle \partial_{\mu} n_1 | n_1 \rangle + \partial_{\mu} \langle n_1 | \dot{n} \rangle \right\}. \hspace{1cm} (5.44)$$

Let us recall the expression for $|n_1\rangle$ from the previous chapter:

$$|n_1\rangle = c_{n_1 n}^{[1]} |n\rangle + |n_1^\perp\rangle,$$  \hspace{1cm} (5.46)

$$|n_1^\perp\rangle = \sum_{k \neq n} c_{kn}^{[1]} |k\rangle,$$  \hspace{1cm} (5.47)

where

$$c_{k \neq n}^{[1]} = \frac{\langle k | \dot{n} \rangle}{i\Delta_{nk}}.$$  \hspace{1cm} (5.48)
5.5. Second order post-adiabatic force

Inserting (5.46) into the second expression of (5.45) yields

\[
\frac{d}{ds} \langle \partial_\mu n | n_1 \rangle = \frac{d}{ds} \Im \langle \partial_\mu n | n_1^- \rangle = \frac{d}{ds} \sum' k \Im \left\{ c_{kn}^{[1]} \langle \partial_\mu n | k \rangle \right\}, \tag{5.49}
\]

\[
\partial_\mu \langle n_1 | \dot{n} \rangle = \partial_\mu \langle n_1^- | \dot{n} \rangle = \partial_\mu \sum' k \Im \left\{ c_{kn}^{[1]*} \langle k | \dot{n} \rangle \right\}, \tag{5.50}
\]

where we have inserted the expression (5.47) for \( | n_1^- \rangle \).

We notice that the non-local (time-integral) contribution \( c_{kn}^{[1]} \) drops out from (5.49), and (5.50) since \( c_{kn}^{[1]} \) and \( \langle n | \partial_\mu n \rangle \) are both purely imaginary. This means that the second order post-adiabatic mean-field force can be interpreted as a local force acting on the classical (slow) system.

Given the expression for \( c_{kn}^{[1]} \) by (5.48) and employing the fact that \( | \dot{k} \rangle = \dot{q}_\alpha | \partial_\alpha k \rangle \), (5.52) the second order post-adiabatic force can be written as

\[
F_{[2]}^\mu = -2\dot{q}_\alpha \Re \left\{ \sum' k \frac{\langle n | \partial_\mu k \rangle \langle \partial_\alpha k | n \rangle}{\Delta_{nk}} \right\} + \dot{q}_\alpha \dot{q}_\beta \partial_\mu \Re \left\{ \sum' k \frac{\langle n | \partial_\alpha k \rangle \langle \partial_\beta k | n \rangle}{\Delta_{nk}} \right\}, \tag{5.52}
\]

We recognize in (5.52) the acceleration contribution. Defining

\[
G_{\mu\alpha}(q) \overset{\text{def}}{=} -2\sum' k \frac{1}{\Delta_{nk}(q)} \Re \left\{ \langle n(q) | \partial_\mu k(q) \rangle \langle \partial_\alpha k(q) | n(q) \rangle \right\}, \tag{5.53}
\]

where \( G_{\mu\alpha}(q) \) plays the role of a coordinate dependent mass tensor, the second order force reads

\[
F_{[2]}^\mu = G_{\mu\alpha} \dot{q}_\alpha + \dot{q}_\alpha \dot{q}_\beta \left( \frac{1}{2} \partial_\beta G_{\alpha\mu} + \frac{1}{2} \partial_\alpha G_{\beta\mu} - \frac{1}{2} \partial_\mu G_{\alpha\beta} \right). \tag{5.54}
\]

We notice from (5.53) that \( G_{\alpha\beta} \) is a symmetric matrix: \( G_{\alpha\beta} = G_{\beta\alpha} \). It is also a positive matrix, i.e., \( G_{\alpha\beta} \phi_\alpha \phi_\beta \geq 0 \), for any vector \( \phi_\alpha \), provided that the quantum system starts its evolution from the ground state: \( \Delta_{kn} \geq 0 \). But \( G_{\alpha\beta} \) cannot be a positive matrix for all initial states of the quantum system, since, e.g., when the quantum system is a two-level system with \( d = 2 \), one has \( G_{\alpha\beta}[\text{excited state}] = -G_{\alpha\beta}[\text{ground state}] \). This case will be explicitly studied in the next section.
It is clear that the force given by (5.54) is generated by the following Lagrangian

\[ L^{[2]}(\dot{q}, q) = \frac{1}{2} G_{\alpha\beta}(q) \dot{q}_\alpha \dot{q}_\beta. \]  

Therefore, the dynamics of the slowly evolving classical system under the influence of a fast quantum system up to the second order is described by

\[ L_2 = \frac{M}{2} \sum_{\alpha=1}^{K} \left( \frac{dq_\alpha}{dt} \right)^2 - V(q) - E_n(q) + \epsilon L^{[1]}(\dot{q}, q) + \epsilon^2 L^{[2]}(\dot{q}, q), \]

where \( L^{[1]}(\dot{q}, q) \) is given by (5.37).

Note that when the time-scale separation is enforced by a large [bare] mass \( M \) of the classical particle, the post-adiabatic Lagrangian \( L^{[1]}(\dot{q}, q) \), and \( L^{[2]}(\dot{q}, q) \) are small as compared to the large kinetic energy \( M \sum_{\alpha=1}^{K} \left( \frac{dq_\alpha}{dt} \right)^2 \); to make this fact explicit, we rescale this kinetic energy to the slow time via \( \epsilon \sim 1/\sqrt{M} \):

\[ L_2 = \frac{\epsilon^2}{2} \left[ M\delta_{\alpha\beta} + G_{\alpha\beta}(q) \right] \dot{q}_\alpha \dot{q}_\beta + \epsilon A_\alpha(q) \dot{q}_\alpha - V(q) - E_n(q). \]  

### 5.5.1 Metric tensor and curvature

The kinetic part \( \frac{\epsilon^2}{2} \left[ M\delta_{\alpha\beta} + G_{\alpha\beta}(q) \right] \dot{q}_\alpha \dot{q}_\beta \) of the second-order Lagrangian (5.57) corresponds to a free particle moving on a Riemannian manifold with metric tensor [99]:

\[ g_{\alpha\beta}(q) \equiv \epsilon^2 \left[ M\delta_{\alpha\beta} + G_{\alpha\beta}(q) \right]. \]

There is an important particular case, where the complete Lagrangian (5.57) just reduces to this kinetic energy. This happens when

- the eigenvectors \( |n\rangle \) can be chosen real, which then nullify the vector potential \( A_\alpha(q) \),

- the bare potential \( V(q) \) and the Born-Oppenheimer potential \( E_n(q) \) compensate each other, \( V(q) + E_n(q) = 0 \), or \( V(q) \) is zero from the outset, while \( E_n(q) \) turns to zero, since the eigenvalues of the quantum Hamiltonian \( \hat{H}[q] \) do not depend on the coordinates \( q \) (though the eigen-vectors do).
Thus we focus on the purely kinetic Lagrangian

\[ \frac{1}{2} g_{\alpha \beta}(q) \dot{q}^\alpha \dot{q}^\beta. \] (5.59)

Once we are going to exercise on the Riemannian geometry, we recover for the velocities the explicitly contravariant notations \([99]\) \(dq^\alpha\). The metric tensor \(g_{\alpha \beta}\) is then naturally covariant. The Lagrangian (5.57) yields the following equations of motion

\[ \ddot{q}^\alpha + \Gamma^\alpha_{\mu \nu} \dot{q}^\mu \dot{q}^\nu = 0. \] (5.60)

This is the geodesic equation \(\frac{d\bar{q}^\alpha}{d\sigma} = 0\), where the covariant differential of any vector \(C^\alpha\) is defined as

\[ DC^\alpha = dC^\alpha + \Gamma^\alpha_{\nu \mu} C^\nu dq^\mu, \] (5.61)

and where the connections \(\Gamma^\alpha_{\mu \nu}\) are related to the metric tensor via \([99]\):

\[ \Gamma^\alpha_{\mu \nu} = \frac{1}{2} g^{\alpha \sigma} \left( \partial_\mu g_{\sigma \nu} + \partial_\nu g_{\sigma \mu} - \partial_\sigma g_{\mu \nu} \right). \] (5.62)

Here \(g^{\alpha \sigma}\) is the inverse of the metric tensor: \(g^{\alpha \sigma} g_{\sigma \beta} = \delta^\alpha_\beta\), and where \(\delta^\alpha_\beta\) is the Kronecker delta-symbol.

The first important question is whether the resulting Riemannian manifold is curved or not. In the case of a flat manifold it is possible to bring \(g_{\alpha \beta}\) to a diagonal and coordinate independent form by going to some new coordinates \(q'\). The criterion of this is the Riemannian curvature tensor \(R^\mu_{\nu \alpha \beta}\) \([99]\). The explicit formula for the covariant curvature tensor is \([99]\)

\[ R^\alpha_{\beta \gamma \delta} = \frac{1}{2} \left[ \partial^2_{\beta \gamma} g_{\alpha \delta} + \partial^2_{\alpha \delta} g_{\beta \gamma} - \partial^2_{\beta \delta} g_{\alpha \gamma} - \partial^2_{\alpha \gamma} g_{\beta \delta} \right] + g^{\mu \nu} \left[ \Gamma^\nu_{\beta \gamma} \Gamma^\mu_{\alpha \delta} - \Gamma^\nu_{\beta \delta} \Gamma^\mu_{\alpha \gamma} \right], \] (5.63)

where \(\Gamma^\mu_{\nu \beta \gamma} = g_{\mu \alpha} \Gamma^\alpha_{\beta \gamma}\). Eq. (5.63) implies the following symmetry relations:

\[ R^\alpha_{\beta \gamma \delta} = -R^\beta_{\alpha \gamma \delta} = -R^\gamma_{\alpha \beta \delta} = R^\gamma_{\beta \alpha \delta} = R^\delta_{\alpha \beta \gamma}. \] (5.64)

The manifold is not curved, if and only if

\[ R^\mu_{\nu \alpha \beta} = 0. \] (5.65)
For any vector $C^\alpha$, the curvature tensor determines the non-commutativity degree of the covariant derivatives [99]:

$$C^\alpha_{;\beta;\gamma} - C^\alpha_{;\gamma;\beta} = -C^\sigma R^\alpha_{\sigma\beta\gamma}, \quad C^\alpha_{;\beta} \equiv \frac{DC^\alpha}{\partial q^\beta}. \quad (5.66)$$

It is known that the curvature tensor determines the local behavior of geodesics with respect to perturbing their initial conditions [99]. Let $x^\alpha(s, \phi)$ be a family of geodesics, where $s$ is the time, and $\phi$ is a scalar continuous parameter which distinguishes the members of the family. Thus by the definition of the geodesic:

$$\frac{Du^\alpha}{ds} = 0, \quad u^\alpha \equiv \frac{\partial x^\alpha}{\partial s}. \quad (5.67)$$

Let us introduce a vector $v^\alpha \equiv \frac{\partial x^\alpha}{\partial \phi}$, which determines the deviation of two geodesics with slightly perturbed initial conditions. This vector satisfies the following Jacobi-Levi-Civita equation [99]:

$$D_2^2 v^\alpha ds^2 = R^\alpha_{\beta\gamma\delta} u^\beta u^\gamma v^\delta. \quad (5.68)$$

The vector $v^\alpha$ can be separated into two components $v^\alpha = v^\alpha_{[1]} + v^\alpha_{[2]}$: one orthogonal to $u^\alpha (u^\alpha v^\alpha_{[1]} = 0)$ and another one parallel to $u^\alpha$. One can check with help of (5.64, 5.67) that the orthogonal component $v^\alpha_{[1]}$ satisfies the same equation (5.68), while the parallel component $v^\alpha_{[2]}$ satisfies the geodesic equation (5.67).

Below we calculate the curvature for the simplest example of two classical coordinates $q^1$ and $q^2$. The fact of having only two coordinates simplifies the formulas for the curvature. Eqs. (5.64) imply that there is only one independent component of the [covariant] curvature tensor, which can be chosen to be $R_{1212}$. All other components are either zero or equal to $\pm R_{1212}$. Now $R_{\alpha\beta\gamma\delta}$ is expressed as

$$R_{\alpha\beta\gamma\delta} = \frac{R}{2} [g_{\alpha\gamma} g_{\beta\delta} - g_{\alpha\delta} g_{\beta\gamma}], \quad (5.69)$$

$$R = g^{\alpha\gamma} g^{\beta\delta} R_{\alpha\beta\gamma\delta} = \frac{2R_{1212}}{g_{11} g_{22} - g_{12}^2}, \quad (5.70)$$

\[3\]To derive Eq. (5.68) note that the very definitions of $u^\alpha$ and $v^\alpha$ imply $v^\beta \partial_\beta u^\alpha = w^\beta \partial_\beta v^\alpha$, which amounts to $u^\alpha_{;\beta} v^\beta = v^\alpha_{;\beta} u^\beta$. Now calculate directly $\frac{D^2 v^\alpha}{ds^2}$ recalling (5.66) and noting that $u^\alpha_{;\beta} u^\beta = 0$ due to (5.67).
5.5. Second order post-adiabatic force

where \( R \) is the scalar curvature.
The latter thus determines the whole curvature tensor for the present two-dimensional situation. Substituting (5.69) into (5.68) and recalling that one can take \( u_\alpha v^\alpha = 0 \) in this equation, we get

\[
\frac{D^2 v^\alpha}{ds^2} = -\frac{R}{2} v^\alpha (u_\beta u^\beta). \tag{5.71}
\]

Note that \( u_\beta u^\beta \) does not depend on \( s \); see (5.67).

We now set to calculate the curvature tensor \( R^\mu_{\nu\alpha\beta} \) for the simplest possible example, where there are only two classical coordinates \( q^1, q^2 \) and the quantum system is a two-level system. For further simplicity we assume that the quantum Hamiltonian is real. This means that the Hamiltonian is a linear combination of the first and third Pauli matrices:

\[
\hat{H}[q] = \begin{pmatrix} q^2 & q^1 \\ q^1 & -q^2 \end{pmatrix}. \tag{5.72}
\]

The eigenvalues and eigenvectors of \( \hat{H} \) read respectively

\[
E_+ = \sqrt{(q^1)^2 + (q^2)^2} \equiv \rho, \quad (\rho > 0) \tag{5.73}
\]
\[
E_- = -\sqrt{(q^1)^2 + (q^2)^2} \equiv -\rho, \tag{5.74}
\]
\[
|+\rangle = \frac{1}{\sqrt{2\rho}} \begin{pmatrix} q^1 \\ \sqrt{\rho - q^2} \end{pmatrix}, \tag{5.75}
\]
\[
|\rangle = \frac{1}{\sqrt{2\rho}} \begin{pmatrix} q^1 \\ -\sqrt{\rho + q^2} \end{pmatrix}. \tag{5.76}
\]

It is seen that the adiabatic energies \( E_+ \) and \( E_- \) cross at \( \rho = 0 \).

We shall study in separate the case when the quantum system starts at \( t = 0 \) from its ground state \( |\rangle \), and from the excited state \( +\rangle \).

**Ground state**

The metric reads form (5.58) and (5.73–5.76):

\[
g_{11} = \epsilon^2 \left[ M + \frac{(q^2)^2}{4\rho^5} \right], \quad g_{22} = \epsilon^2 \left[ M + \frac{(q^1)^2}{4\rho^5} \right], \tag{5.77}
\]
\[
g_{12} = g_{21} = -\epsilon^2 \left( \frac{q^1 q^2}{4\rho^5} \right).
\]
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The determinant and trace of the metric read

\[ \text{det}[g] = \epsilon^4 M \left( M + \frac{1}{4\rho^3} \right), \quad \text{tr}[g] = \epsilon^2 \left( M + \frac{1}{4\rho^3} \right). \]  

(5.78)

It is seen from (5.77–5.78) that both the determinant and the trace of \( g_{\alpha\beta} \) are positive; thus the eigenvalues are positive as well. This situation refers to a usual classical mechanical particle, which is enforced to move on a two-dimensional surface. For the scalar curvature we get from (5.62, 5.63, 5.70) and (5.77–5.78)

\[ R = -\frac{3(1 + 16M\rho^3)}{2\epsilon^2 M\rho^2 (1 + 4M\rho^3)^2}. \]  

(5.79)

Thus \( R \) is strictly negative. Returning to (5.71) we see that since the metric is positively defined [see (5.77–5.78)] \( u^\alpha u_\alpha \) is always non-negative. Then the negativity of \( R \) in (5.79) implies that the geodesics are unstable with respect to small perturbation of initial conditions, because (5.71) corresponds to a harmonic oscillator with an inverted (though space-dependent) frequency\(^4\). We see that \( R \) is singular at \( \rho = 0 \), where the adiabatic energy levels cross.

**Excited state**

Now we assume that the two-level quantum system starts its evolution from the excited state \( |+\rangle \). This case leads to more interesting possibilities, since now the metric reads:

\[ g_{11} = \epsilon^2 \left[ M - (\frac{q_2^2}{4\rho^5}) \right], \quad g_{22} = \epsilon^2 \left[ M - (\frac{q_1^2}{4\rho^5}) \right], \]

\[ g_{12} = g_{21} = \epsilon^2 (q_1 q_2)^2 / 4\rho^5. \]  

(5.80)

Hence the determine and trace of \( g \) read, respectively,

\[ \text{det}[g] = \epsilon^4 M \left[ M - \frac{1}{4\rho^3} \right], \quad \text{tr}[g] = \epsilon^2 \left[ M - \frac{1}{4\rho^3} \right]. \]  

(5.81)

\(^4\)Such a local instability leads to chaos, if the \((q_1, q_2)\)-manifold is compact. This is not the case for the considered situation, though it is presumably not very difficult to compactify the manifold, keeping the conclusion on the local instability of geodesics.
Since the metric (5.80) relates to (5.77) with transformation $M \rightarrow -M$ and $\epsilon \rightarrow i\epsilon$ ($i^2 = -1$), we get for the scalar curvature directly from (5.79)

$$R = \frac{3(16M\rho^3 - 1)}{2\epsilon^2 M\rho^2 (1 - 4M\rho^3)^2}. \quad (5.82)$$

When the particle moves sufficiently far from the origin $q^1 = q^2 = 0$ (i.e., when $4M\rho^3 > 1$), the metric is positively defined and the curvature is positive. According to (5.71) this means that the geodesics are not sensitive to perturbations in initial conditions. At $4M\rho^3 = 1$ the metric tensor changes its signature, so that for $4M\rho^3 < 1$ it has one positive and one negative eigenvalue. At $4M\rho^3 = 1$ the scalar curvature is singular. We expect that the adiabatic assumption will become problematic in the vicinity of the singularity, but it seems that it is possible for the particle to “tunnel” between subspaces of different signature.

Since the metric tensor is not positively defined for $4M\rho^3 < 1$, (5.71, 5.82) show that for $\frac{1}{4} < 4M\rho^3 < 1$ the geodesics with initial condition $u_\alpha u^\alpha < 0$ can become unstable.

For even smaller values of $\rho$ with $16M\rho^3 < 1$ the curvature becomes negative. Now the unstable geodesics have $u_\alpha u^\alpha > 0$, while those with $u_\alpha u^\alpha < 0$ are (at least locally) stable.

It is thus seen that the initial ground versus the excited state of the quantum system produces rather different dynamic behavior for the classical system.

### 5.6 Third order post-adiabatic force

We now turn to study the post-adiabatic force at the order $\epsilon^3$. The calculations here are more involved, though their general pattern—employing the adiabatic perturbation theory and then reconstructing the effective Lagrangian—remains the same.

In order to calculate the third-order post-adiabatic force given by (5.29), we have to calculate two terms of (5.29) namely, $\langle \phi_n | H | \phi_n \rangle - E_n = \sum_k \Delta_k \epsilon |c_k|^2$ and $\epsilon^3 \langle \partial_\mu \phi_n | \phi_n \rangle$ up to the third order in $\epsilon$.

---

5In the General Theory of Relativity $u_\alpha u^\alpha < 0$ is prohibited by causality; for massive particles $u_\alpha u^\alpha > 0$ and can be normalized to $u_\alpha u^\alpha = 1$, while for photons $u_\alpha u^\alpha = 0$ [99]. However, for the present classical theory with a well-defined global time $s$ nothing prohibits us to consider the class of geodesics with $u_\alpha u^\alpha < 0$. 

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Employing \((5.23)\) we see that \(|c_{kn}|^2\) in the third order of \(\epsilon\) reads

\[
|c_{kn}|^2 = 2\epsilon^3 \Re\{c_{kn}^{[2]} c_{kn}^{[1]*}\}. \tag{5.83}
\]

Inserting (5.83) into the last expression of the post-adiabatic force (5.29) for the third-order correction we get

\[
\partial_\mu[(\phi_\mu|\hat{H}(s)|\phi_\mu) - E_\mu] = \partial_\mu \sum_k' \Delta_{kn}|c_{kn}|^2 = 2\epsilon^3 \partial_\mu \sum_k' \Delta_{kn} \Re\{c_{kn}^{[2]} c_{kn}^{[1]*}\}. \tag{5.84}
\]

Now let us calculate the other part of the general expression of the third-order post-adiabatic force given by \(\epsilon \Im\langle \partial_\mu \phi_\mu | \dot{\phi}_\mu \rangle\) for the third-order correction:

\[
2\epsilon \Im\langle \partial_\mu \phi_\mu | \dot{\phi}_\mu \rangle = 2 \frac{d}{ds} \Im \{\langle \partial_\mu n | n_2 \rangle \} + 2 \partial_\mu \Im \{\langle n_2 | \dot{n} \rangle \} + 2 \Im \{\langle \partial_\mu n_1 | \dot{n}_1 \rangle \}. \tag{5.85}
\]

Then the expression for the third-order force reads

\[
\frac{F_{\mu}^{[3]}}{2} = \partial_\mu \sum_k' \Delta_{kn} \Re\{c_{kn}^{[2]} c_{kn}^{[1]*}\} + \frac{d}{ds} \Im \{\langle \partial_\mu n | n_2 \rangle \} + \partial_\mu \Im \langle n_2 | \dot{n} \rangle + \Im \langle \partial_\mu n_1 | \dot{n}_1 \rangle. \tag{5.86}
\]

Inserting

\[
|n_2\rangle = c_{mn}^{[2]} |n\rangle + \sum_k' c_{kn}^{[2]} |k\rangle, \tag{5.87}
\]

For the expression \(\Im \langle n_2 | \dot{n} \rangle\) we get

\[
\Im \langle n_2 | \dot{n} \rangle = \Im \{c_{mn}^{[2]*} \langle n | \dot{n} \rangle \} + \sum_k' \Delta_{nk} \Re\{c_{kn}^{[2]} c_{kn}^{[1]*}\}, \tag{5.88}
\]

where we used

\[
c_{k\neq n}^{[1]*} = i \frac{\langle \dot{n} | k \rangle}{\Delta_{nk}} \tag{5.89}
\]

in obtaining (5.88).

Therefore the third term of (5.86) reads

\[
\partial_\mu \Im \langle n_2 | \dot{n} \rangle = \partial_\mu \Im \{c_{mn}^{[2]*} \langle n | \dot{n} \rangle \} - \partial_\mu \sum_k' \Delta_{kn} \Re\{c_{kn}^{[2]} c_{kn}^{[1]*}\}, \tag{5.90}
\]

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where we used $\Delta_{nk} = -\Delta_{kn}$.

Then the third order post-adiabatic force reads

$$
\frac{F^{[3]}_{\mu}}{2} = \frac{d}{ds} \Im \langle \partial_\mu n | n_2 \rangle + \partial_\mu \Im \langle \{ c_{mn}^{[2]} \} | n \dot{n} \rangle + \Im \langle \partial_\mu n_1 | \dot{n}_1 \rangle. \quad (5.91)
$$

Now we work out $\Im \langle \partial_\mu n | n_2 \rangle$. This can be done by inserting the expression for $|n_2\rangle$, given by (5.87), in the first term of the above expression for the third-order force. Having (5.87) in mind the first term of (5.91) can be written as

$$
\frac{d}{ds} \Im \langle \partial_\mu n | n_2 \rangle = \Im \left\{ c_{mn}^{[2]} \langle \partial_\mu \dot{n} | n \rangle \right\} + \Im \left\{ c_{mn}^{[2]} \langle \partial_\mu n | \dot{n} \rangle \right\} + \Im \left\{ \left( \frac{d}{ds} c_{mn}^{[2]} \right) \langle \partial_\mu n | n \rangle \right\} + \frac{d}{ds} \Im \left\{ \sum_k c_{kn}^{[2]} \langle \partial_\mu n | k \rangle \right\}. \quad (5.92)
$$

Since $\langle \partial_\mu n | n \rangle$ is purely imaginary, we get

$$
\frac{d}{ds} \Im \langle \partial_\mu n | n_2 \rangle = \Im \left\{ c_{mn}^{[2]} \langle \partial_\mu \dot{n} | n \rangle \right\} + \Im \left\{ c_{mn}^{[2]} \langle \partial_\mu n | \dot{n} \rangle \right\} + \Im \left\{ \left( \frac{d}{ds} c_{mn}^{[2]} \right) \langle \partial_\mu n | n \rangle \right\} + \frac{d}{ds} \Im \left\{ \sum_k c_{kn}^{[2]} \langle \partial_\mu n | k \rangle \right\} \cdot \quad (5.93)
$$

The second term of (5.87) reads

$$
\partial_\mu \Im \left\{ c_{mn}^{[2]} \langle \dot{n} | n \rangle \right\} = -\partial_\mu \Im \left\{ c_{mn}^{[2]} \langle \dot{n} | n \rangle \right\} = -\Im \left\{ \langle \partial_\mu c_{mn}^{[2]} \rangle \langle \dot{n} | n \rangle \right\} - \Im \left\{ c_{mn}^{[2]} \langle \partial_\mu \dot{n} | n \rangle \right\} - \Im \left\{ c_{mn}^{[2]} \langle \dot{n} | \partial_\mu n \rangle \right\}. \quad (5.94)
$$

Adding (5.92) and (5.94) together yields

$$
\frac{d}{ds} \Im \langle \partial_\mu n | n_2 \rangle + \partial_\mu \Im \left\{ c_{mn}^{[2]} \langle \dot{n} | n \rangle \right\} = 2 \Im \langle \partial_\mu n | \dot{n} \rangle \Re \left\{ c_{mn}^{[2]} \right\} + \Im \langle \partial_\mu n | n \rangle \frac{d}{ds} \Re \left\{ c_{mn}^{[2]} \right\} - \Im \langle \dot{n} | n \rangle \partial_\mu \Re \left\{ c_{mn}^{[2]} \right\} + \frac{d}{ds} \Im \left\{ \sum_k c_{kn}^{[2]} \langle \partial_\mu n | k \rangle \right\} \cdot \quad (5.95)
$$

where we noticed $\langle \dot{n} | n \rangle$ is purely imaginary. Thus

$$
\Im \left\{ \langle \partial_\mu c_{mn}^{[2]} \rangle \langle \dot{n} | n \rangle \right\} = \Im \langle \dot{n} | n \rangle \partial_\mu \Re \left\{ c_{mn}^{[2]} \right\}. \quad (5.96)
$$
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We also used the fact that
\[
\Im \left\{ c_{nn}^{[2]} \langle \partial_\mu n | \dot{n} \rangle \right\} - \Im \left\{ c_{nn}^{[2]} \langle \dot{n} | \partial_\mu n \rangle \right\} = 2 \Im \langle \partial_\mu n | \dot{n} \rangle \Re \left\{ c_{nn}^{[2]} \right\}.
\] (5.97)

Let us recall the normalization condition in the second order of \( \epsilon \):
\[
\Re \left\{ c_{nn}^{[2]} \right\} = -\frac{1}{2} \langle n_1 | n_1 \rangle.
\] (5.98)

Thus, the third-order post-adiabatic force reads
\[
\frac{F^{[3]}}{2} = -\Im \left\{ \langle \partial_\mu n | \dot{n} \rangle \right\} \langle n_1 | n_1 \rangle - \frac{1}{2} \Im \left[ \langle \partial_\mu n | n \rangle \right] \frac{d}{ds} \langle n_1 | n_1 \rangle
\] (5.99)
\[
- \frac{1}{2} \Re \left[ \langle n | \dot{n} \rangle \right] \partial_\mu \langle n_1 | n_1 \rangle + \Re \langle \partial_\mu n_1 | \dot{n}_1 \rangle
\] + \frac{d}{ds} \Im \left\{ \sum_k c_{kn}^{[2]} \langle \partial_\mu n | k \rangle \right\}.
\]

In order to simplify (5.99) we first work out the terms containing \( |n_1\rangle \). Let us recall the expression for \( |n_1\rangle \) and \( c_{k\neq n}^{[2]} \) from the previous chapter:
\[
|n_1\rangle = c_{nn}^{[1]} |n\rangle + |n_1^\perp\rangle,
\] (5.100)
\[
c_{k\neq n}^{[2]} = c_{nn}^{[1]} c_{k\neq n}^{[1]} + c_{k\neq n}^{[2]},
\] (5.101)
where \( |n_1^\perp\rangle \) and \( c_{k\neq n}^{[2]} \) are given by
\[
|n_1^\perp\rangle = \sum_k c_{kn}^{[1]} |k\rangle, \quad c_{kn}^{[1]} = -i \frac{\langle k | \dot{n} \rangle}{\Delta_{nk}},
\] (5.102)
and
\[
c_{k\neq n}^{[2]} = \frac{i}{\Delta_{nk}} \left[ c_{kn}^{[1]} \left( \langle n | \dot{n} \rangle - \langle k | \dot{k} \rangle \right) - \frac{d}{ds} \left( c_{kn}^{[1]} \right) + \sum_{l(\neq k)}' c_{ln}^{[1]} \langle k | l \rangle \right].
\] (5.103)

We also notice that
\[
\langle n_1 | n_1 \rangle = |c_{nn}^{[1]}|^2 + |n_1^\perp | n_1^\perp \rangle,
\] (5.104)
\[
|\dot{n}_1 \rangle = \left( \frac{d}{ds} c_{nn}^{[1]} \right) |n\rangle + c_{nn}^{[1]} |\dot{n}\rangle + \frac{d}{ds} |n_1^\perp \rangle,
\] (5.105)
\[
\langle \partial_\mu n_1 \rangle = \langle \partial_\mu c_{nn}^{[1]} \rangle |n\rangle + c_{nn}^{[1]} \langle \partial_\mu n \rangle + \langle \partial_\mu n_1^\perp \rangle.
\] (5.106)
5.6. Third order post-adiabatic force

Inserting (5.101), and (5.104)-(5.106) into (5.99) we notice that all the non-local terms consisting $c_{[1]n}$ are canceled out and we are left with

$$F_\mu^{[3]} = -\langle n_1^+|n_1^+\rangle \Im \langle \partial_\mu n|\hat{n}\rangle - \frac{1}{2} \frac{d}{ds} \left( \langle n_1^+|n_1^+\rangle \right) \Im \langle \partial_\mu n|n\rangle - \frac{1}{2} \partial_\mu \left( \langle n_1^+|n_1^+\rangle \right) \Im \langle n|\hat{n}\rangle + \Im \langle \partial_\mu n_1^+|\hat{n}_1^+\rangle + \frac{d}{ds} \left( \Im \left[ \sum_k' \tilde{c}_kn \langle \partial_\mu n|k\rangle \right] \right),$$

where $\tilde{c}_kn$ is given by (5.104).

The first three terms of (5.107) can be written in terms of the derivatives of each of the expressions. Therefore the third-order post-adiabatic force reads:

$$\frac{F_\mu^{[3]}}{2} = -\frac{1}{2} \frac{d}{ds} \left[ \langle n_1^+|n_1^+\rangle \Im \langle \partial_\mu n|n\rangle \right] - \frac{1}{2} \frac{d}{ds} \left( \langle n_1^+|n_1^+\rangle \right) \Im \langle \partial_\mu n|\hat{n}\rangle + \Im \langle \partial_\mu n_1^+|\hat{n}_1^+\rangle + \frac{d}{ds} \left\{ \sum_k' \left( \frac{-i}{\Delta_{nk}} \frac{d}{ds} \left[ \tilde{c}_kn \langle \partial_\mu n|k\rangle \right] + \frac{i}{\Delta_{nk}} \sum_l \langle \tilde{c}_ln |l\rangle \langle \partial_\mu n|k\rangle \right) \right\},$$

where we have used $\frac{i}{\Delta_{nk}} \tilde{c}_kn$ in simplifying the last term of (5.107) such that the term $-\langle k|\hat{n}\rangle \tilde{c}_kn$ in the expression (5.104) is absorbed in the summation over the index $l$ and the condition $l \neq k$ is removed.

Defining

$$|n_1^\perp\rangle = -i\hat{q}_\alpha |N_\alpha\rangle \quad |N_\alpha\rangle \overset{def}{=} \sum_k \langle \tilde{c}_kn |k\rangle,$$

and inserting this expression for $|n_1\rangle$ into the first three terms of the expression (5.108), after some algebra it is straightforward to see that those terms
Post Adiabatic Forces

can be generated by a Lagrangian

\[ -\frac{1}{2} \frac{d}{ds} \left[ \langle n^+_1|n^+_1 \rangle \Im \langle \partial_\mu n|n \rangle \right] - \frac{1}{2} \partial_\mu \left[ \langle n^+_1|n^+_1 \rangle \Im \langle n|\dot{n} \rangle \right] \\
+ \frac{d}{ds} \left[ \Re \left( \sum_k' \langle \partial_\mu n|k \rangle \langle k|\dot{n} \rangle / \Delta_{nk}^2 \right) \Im \langle n|\dot{n} \rangle \right] = \\
\left( \frac{d}{ds} \frac{\partial}{\partial \dot{q}_\mu} - \frac{\partial}{\partial q_\mu} \right) \frac{1}{3} h_{\alpha\beta\gamma} \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma, \tag{5.110} \]

where

\[ h_{\alpha\beta\gamma} = \frac{1}{2} \Im \langle n|\partial_\gamma n \rangle \Re \langle N_\alpha|N_\beta \rangle \tag{5.111} \]

\[ + \frac{1}{2} \Im \langle n|\partial_\alpha n \rangle \Re \langle N_\gamma|N_\beta \rangle + \frac{1}{2} \Im \langle n|\partial_\beta n \rangle \langle N_\alpha|N_\gamma \rangle. \]

\( h_{\alpha\beta\gamma} \) is symmetric with respect to any permutation of indices \( \alpha, \beta \) and \( \gamma \), so that

\[ \frac{1}{3} h_{\alpha\beta\gamma} \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma = \frac{1}{2} \Im \langle n|\partial_\gamma n \rangle \Re \langle N_\alpha|N_\beta \rangle \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma. \tag{5.112} \]

Working out the term \( \Im \langle \partial_\mu n^+_1|\dot{n}^+_1 \rangle \) in the expression (5.108) for the third order post-adiabatic force yields

\[ \Im \langle \partial_\mu n^+_1|\dot{n}^+_1 \rangle = \Im \langle \partial_\mu N_\beta|N_\alpha \rangle \dot{q}_\alpha \dot{q}_\beta + \Im \langle \partial_\mu N_\beta|\partial_\beta N_\alpha \rangle \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma. \tag{5.113} \]

It is straightforward to show that the last term of (5.108) can be written as

\[ \frac{d}{ds} \Im \left\{ \sum_k' \left( -i \frac{d}{\Delta_{nk} d} \frac{c_{[k]}^{[n]}}{c_{[k]}^{[n]}} + i \frac{d}{\Delta_{nk} d} \sum_l' c_{[k]}^{[n]} \langle k|l \rangle \right) \langle \partial_\mu n|k \rangle \right\} = \frac{d}{ds} \Im \{ -i \langle N_\mu|\dot{n}^+_1 \rangle \} = -\frac{d}{ds} \left[ \Im \langle N_\mu|N_\alpha \rangle \dot{q}_\alpha + \Im \langle N_\mu|\partial_\beta N_\alpha \rangle \dot{q}_\alpha \dot{q}_\beta \right] \\
= \frac{d^2 q_\alpha}{ds^2} \Im \langle N_\alpha|N_\mu \rangle + \dot{q}_\alpha \dot{q}_\beta \Im \{ \partial_\beta \langle N_\alpha|N_\mu \rangle + \langle \partial_\beta N_\alpha|N_\mu \rangle + \langle \partial_\beta N_\alpha|N_\mu \rangle \} \\
+ \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma \Im \{ \partial_\gamma \langle \partial_\beta N_\alpha|N_\mu \rangle \}. \tag{5.114} \]
5.6. Third order post-adiabatic force

combining \((5.113)\) and \((5.114)\) together we get
\[
\frac{d}{ds} \Im \left\{ \sum_{k} \left( -\frac{i}{\Delta n_{k}} \frac{d}{ds} [c_{kn}^{[1]}] + \frac{i}{\Delta n_{k}} \sum_{l} c_{ln}^{[1]} \langle k|l \rangle \right) \langle \partial_{\mu} n|k \rangle \right\}
+ \Im \langle \partial_{\mu} n_{1}^{+}|n_{1}^{+} \rangle = \frac{d^{3}q_{\alpha}}{ds^{3}} \Im \langle N_{\alpha}|N_{\mu} \rangle
+ \dot{q}_{\alpha} \dot{q}_{\beta} \Im \left\{ \langle \partial_{\beta} N_{\alpha}|N_{\mu} \rangle + \langle \partial_{\beta} N_{\alpha}|N_{\mu} \rangle + \langle \partial_{\mu} N_{\beta}|N_{\alpha} \rangle \right\}
+ \dot{q}_{\alpha} \dot{q}_{\beta} \dot{q}_{\gamma} \Im \left\{ \langle \partial_{\gamma} \partial_{\beta} N_{\alpha}|N_{\mu} \rangle + \langle \partial_{\gamma} \partial_{\beta} N_{\alpha}|N_{\mu} \rangle \right\}.
\tag{5.115}
\]
working out these two terms of the third-order post-adiabatic force, after some algebra, we see that it can be produced by the following Lagrangian
\[
\frac{d}{ds} \Im \left\{ \sum_{k} \left( -\frac{i}{\Delta n_{k}} \frac{d}{ds} [c_{kn}^{[1]}] + \frac{i}{\Delta n_{k}} \sum_{l} c_{ln}^{[1]} \langle k|l \rangle \right) \langle \partial_{\mu} n|k \rangle \right\}
+ \Im \langle \partial_{\mu} n_{1}^{+}|n_{1}^{+} \rangle = \left[ -\frac{d^{2}}{ds^{2}} \frac{\partial}{\partial \dot{q}_{\mu}} + \frac{d}{ds} \frac{\partial}{\partial \dot{q}_{\mu}} - \frac{\partial}{\partial \dot{q}_{\mu}} \right] \left( -z_{\alpha\beta} \dot{q}_{\alpha} \dot{q}_{\beta} + \frac{1}{3} \lambda_{\alpha\beta\gamma} \dot{q}_{\alpha} \dot{q}_{\beta} \dot{q}_{\gamma} \right),
\tag{5.116}
\]
where we define the antisymmetric tensor \(z_{\alpha\beta}\) as
\[
z_{\alpha\beta} \overset{\text{def}}{=} \frac{1}{2} \Im \langle N_{\beta}|N_{\alpha} \rangle,
\tag{5.117}
\]
and the symmetric tensor \(\lambda_{\alpha\beta\gamma}\) as
\[
\lambda_{\alpha\beta\gamma} \overset{\text{def}}{=} \frac{1}{4} \Im \left\{ \langle \partial_{\beta} N_{\gamma}|N_{\alpha} \rangle + \langle \partial_{\beta} N_{\gamma}|N_{\alpha} \rangle + \langle \partial_{\alpha} N_{\gamma}|N_{\beta} \rangle \right. \\
+ \left. \langle \partial_{\gamma} N_{\alpha}|N_{\beta} \rangle + \langle \partial_{\gamma} N_{\alpha}|N_{\beta} \rangle + \langle \partial_{\gamma} N_{\alpha}|N_{\beta} \rangle \right\}
= \frac{6}{4} \Im \langle \partial_{\alpha} N_{\beta}|N_{\gamma} \rangle.
\tag{5.118}
\]
In obtaining the above result we employed:
\[
\Im \langle \partial_{\beta} N_{\mu}|N_{\alpha} \rangle = \frac{1}{2} \Im \langle \partial_{\beta} N_{\mu}|N_{\alpha} \rangle + \frac{1}{2} \Im \langle \partial_{\beta} N_{\mu}|N_{\alpha} \rangle
= \frac{1}{2} \Im \langle \partial_{\beta} N_{\mu}|N_{\alpha} \rangle - \frac{1}{2} \Im \langle N_{\alpha}|\partial_{\beta} N_{\mu} \rangle
= \frac{1}{2} \Im \langle \partial_{\beta} N_{\mu}|N_{\alpha} \rangle + \frac{1}{2} \Im \langle \partial_{\beta} N_{\alpha}|N_{\mu} \rangle + \frac{1}{2} \partial_{\beta} \Im \langle N_{\mu}|N_{\alpha} \rangle.
\tag{5.119}
\]
Combining the above results for the last two terms of the third-order post-adiabatic force (5.116) with those we got for the first three terms given by (5.110) yields

\[
\frac{F^{[3]}_{\mu}}{2} = \left[ -\frac{d^2}{ds^2} \frac{\partial}{\partial \dot{q}_\mu} + \frac{d}{ds} \frac{\partial}{\partial q_\mu} - \frac{\partial}{\partial q_\mu} \right] \left( -z_{\alpha\beta\gamma} \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma + \frac{1}{3} [h_{\alpha\beta\gamma} + \lambda_{\alpha\beta\gamma}] \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma \right).
\] (5.120)

Thus the third-order post-adiabatic force is purely Lagrangian though containing higher-order derivatives.\(^6\) We can write the third order Lagrangian as

\[
L^{[3]}[q, \dot{q}, \ddot{q}] = \epsilon^3 \left[ f_{\alpha\beta\gamma}(q) \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma - z_{\alpha\beta}(q) \dot{q}_\alpha \dot{q}_\beta \right],
\] (5.121)

where \(f_{\alpha\beta\gamma}(q)\) is defined as

\[
f_{\alpha\beta\gamma}(q) = \frac{1}{2} \Im \left\{ \langle n | \partial_\gamma n \rangle \langle N_\beta | N_\alpha \rangle + \langle \partial_\gamma N_\beta | N_\alpha \rangle \right\}.
\] (5.122)

It is seen that besides the expected third-order polynomial in the velocities \(f_{\alpha\beta\gamma} \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma\), the third-order Lagrangian \(L^{[3]}\) contains a linear dependence on the accelerations \(\dot{q}_\alpha\). The corresponding coupling matrix \(z_{\alpha\beta}(q)\) is antisymmetric \(z_{\alpha\beta}(q) = -z_{\beta\alpha}(q)\) as it should be, since any term \(\phi_{\alpha\beta}(q) \dot{q}_\alpha \dot{q}_\beta\) with a symmetric \(\phi_{\alpha\beta} = \phi_{\beta\alpha}\), can be reduced (up to a total differential in time) to a third-order polynomial in the velocities.

The total Lagrangian describing the classical system including the higher-order terms up to \(\epsilon^3\), \(L_3[q, \dot{q}, \ddot{q}]\), will include the previous order post-adiabatic Lagrangians and the bare classical Lagrangian,

\[
L_3[q, \dot{q}, \ddot{q}] = -V(q) - E_n(q) + \epsilon A_\alpha(q) \dot{q}_\alpha + \frac{\epsilon^2}{2} [M \delta_{\alpha\beta} + G_{\alpha\beta}(q)] \dot{q}_\alpha \dot{q}_\beta
\]

\[+ \epsilon^3 \left[ f_{\alpha\beta\gamma}(q) \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma - z_{\alpha\beta}(q) \dot{q}_\alpha \dot{q}_\beta \right],
\] (5.123)

\(^6\)Let we are given a classical system with action \(L = L[q, \dot{q}, \ddot{q}, s]\), where \(L\) is the Lagrangian, \(q\) is the vector of (generalized) coordinates, and \(\dot{q} = \frac{dq}{ds}\). The Euler-Lagrange variational equations of motion \(\frac{d}{ds} \frac{\partial L}{\partial \dot{q}_\mu} - \frac{\partial L}{\partial q_\mu} = 0\), are obtained when varying the action over the coordinate-path \(q(s)\) assuming that the end-points are fixed: \(\delta q(0) = \delta q(S) = 0\). This well-known set-up has a straightforward generalization for a Lagrangian \(L_3[q, \dot{q}, \ddot{q}, s]\) that depend on the acceleration [or more generally on higher-order derivatives of coordinates]. The corresponding Euler-Lagrange equations of motion read: \(\frac{d}{ds} \frac{\partial L}{\partial \dot{q}_\mu} - \frac{\partial L}{\partial q_\mu} - \frac{d^2}{ds^2} \frac{\partial L}{\partial \dot{q}_\mu} = 0\), where now we assume that \(\delta q(0) = \delta q(S) = \delta \dot{q}(0) = \delta \ddot{q}(S) = 0\).
while the equations of motion it generates is [see Footnote 6]
\[
\left[ \frac{d}{ds} \frac{\partial}{\partial \dot{q}_\mu} - \frac{d^2}{ds^2} \frac{\partial}{\partial \ddot{q}_\mu} - \frac{\partial}{\partial q_\mu} \right] \mathcal{L}_3[q, \dot{q}, \ddot{q}] = 0. \tag{5.124}
\]

These equations of motion contain third-order time-derivatives \(q^{(3)}_\alpha\) of coordinates, i.e., they can be written as
\[
2\epsilon^3 z_{\alpha\beta} q^{(3)}_\beta = \varphi_\alpha(q, \dot{q}, \ddot{q}). \tag{5.125}
\]

Thus when the determinant of the matrix \(z_{\alpha\beta}(q)\) is non-zero—and this is generically the case for even number of classical coordinates—the third-derivatives can be expressed through \((q, \dot{q}, \ddot{q})\). This means that the dynamics described by (5.124) needs three independent sets of initial conditions at the initial (slow) time \(s_i = \epsilon t_i\):
\[
(q(s_i), \dot{q}(s_i), \ddot{q}(s_i)). \tag{5.126}
\]

For an odd number \(K\) of classical coordinates, the determinant of \(z_{\alpha\beta}(q)\) vanishes, since \(z_{\alpha\beta}\) is anti-symmetric. Generically, the matrix \(z_{\alpha\beta}(q)\) will only have one eigenvalue equal to zero. Let us denote the related eigenvector by \(y_{(0)}^\alpha\), where
\[
y_{(0)}^\alpha z_{\alpha\beta} = 0, \tag{5.127}
\]
and let \(y_{(\gamma)}^\alpha\) with \(\gamma = 1, \ldots, K - 1\) be the eigenvector of \(z_{\alpha\beta}\) with non-zero eigenvalues \(\lambda^{(\gamma)}\). Eq. (5.125) produces
\[
2\epsilon^3 \lambda^{(\gamma)} y_{(\gamma)}^\alpha q^{(3)}_\beta = y_{(\gamma)}^\alpha \varphi_\alpha(q, \dot{q}, \ddot{q}), \quad \text{for} \quad \gamma = 1, \ldots, K - 1, \tag{5.128}
\]
\[
0 = y_{(0)}^\alpha \varphi_\alpha(q, \dot{q}, \ddot{q}). \tag{5.129}
\]

Now the initial conditions \((q(s_i), \dot{q}(s_i), \ddot{q}(s_i))\) at the initial time \(s_i\) cannot be anymore taken independently from each other, because (5.129) imposes a constraint on them. Provided that \((q(s_i), \dot{q}(s_i), \ddot{q}(s_i))\) satisfy this constraint, (5.128) gives \(K - 1\) equations for components of \(q^{(3)}_\alpha\). Another equation for components of \(q^{(3)}_\alpha\) can be obtained by differentiating (5.129) over time \(t\) and taking \(t \to t_i\).

The construction described by (5.128), and (5.129) is conceptually not very different from its simplest analog: Consider two classical degrees of
freedom with coordinates $x$ and $q$. Let the corresponding Lagrangian be $\frac{\dot{q}^2}{2} - V(q, x)$. Note that this Lagrangian does not contain the kinetic energy for the $x$-particle, i.e., the kinetic energy matrix is degenerate. The Lagrange equations of motion read: $\ddot{q} = -V'_q(q, x)$ and $V'_x(q, x) = 0$. The second equation is a constraint on admissible values of $q$ and $x$ at any time. In particular, it confines their initial values. Now the initial conditions amount to $q(s_i)$, $\dot{q}(s_i)$ and $x(s_i)$ provided that the constraint is satisfied. One is not free in choosing the initial velocity $\dot{x}(s_i)$. The latter is determined from differentiating the constraint over time $s$ and taking $s \to s_i$.

Before closing this discussion on the initial conditions let us note the following aspect. The quantum-classical equations (5.2, 5.5) have the following well-defined initial conditions at the initial moment $t = 0$ of the fast time $t$: $|\Psi(0)\rangle$, $q(0)$ and $\dot{q}(0)$. On the other hand, as we saw above, the autonomous classical dynamics starts to depend on higher-derivatives of the coordinate(s). The reason of this difference is that the initial conditions of the autonomous classical dynamics are to be imposed at an initial value $s_i = \epsilon t_i$ of the slow time, where $t_i$ should be still sizable larger than $t = 0$. The difference between the original initial conditions of the slow variables and their effective initial conditions after eliminating the fast variables is known as the initial slip problem. It is well recognized in theories dealing with elimination of fast variables [107–109]. There also exist more or less regular procedures of relating the original initial conditions to effective ones [107–109]. In this work, we are interested in autonomous classical dynamics for sufficiently large (fast) times, where the precise relation with the original initial conditions is not directly relevant.

### 5.6.1 Kinematics

The dependence of $L_3[q, \dot{q}, \ddot{q}]$ on accelerations implies conceptual changes in the kinematics of the classical system, as we now proceed to show.

First we note that the momentum of the classical system is defined via the response of $L_3$ to an infinitesimal coordinate shift $q_\mu \to q_\mu + \delta q_\mu$, where $\delta q_\mu$ does not depend on time [99]:

$$
\delta L_3 = \frac{\partial L_3}{\partial q_\mu} \delta q_\mu = \delta q_\mu \frac{d}{ds} \left[ \frac{\partial L_3}{\partial \dot{q}_\mu} - \frac{d}{ds} \frac{\partial L_3}{\partial \ddot{q}_\mu} \right],
$$

(5.130)
where we used (5.124). Thus the momentum is defined as

\[ p_\mu = \frac{\partial L_3}{\partial \dot{q}_\mu} - \frac{d}{ds} \frac{\partial L_3}{\partial \ddot{q}_\mu}, \]  

(5.131)

implying that the equations of motion can be written as \( \dot{p}_\mu = \frac{\partial L_3}{\partial q_\mu} \).

If \( L_3 \) would not depend on \( q_\mu \) (which is generically not the case), the corresponding momentum \( p_\mu \) would be conserved in time. We note that \( p_\mu \) consists of the usual part \( \frac{\partial L_3}{\partial \dot{q}_\mu} \) and the anomalous part \( -\frac{d}{ds} \frac{\partial L_3}{\partial \ddot{q}_\mu} \) that comes solely from the dependence of the Lagrangian on the acceleration. Using (5.123) we get for the momentum

\[ p_\mu = \epsilon A_\mu + \epsilon^2 [M \dot{q}_\mu + G_{\mu\alpha} \dot{q}_\alpha] + 3\epsilon^3 f_{\mu\alpha\beta}^{(\text{sym})} \dot{q}_\alpha \dot{q}_\beta + 2\epsilon^3 z_{\mu\alpha} \ddot{q}_\alpha + \epsilon^3 \{\partial_\gamma z_{\mu\beta}\} \dot{q}_\gamma \dot{q}_\beta, \]  

(5.132)

where \( f_{\alpha\beta\gamma}^{(\text{sym})} \), defined as

\[ f_{\alpha\beta\gamma}^{(\text{sym})} \overset{\text{def}}{=} \frac{1}{6} \sum_{\Pi} f_{\Pi[\alpha\beta\gamma]}, \]  

(5.133)

is the completely symmetrized expression (5.122); the sum is taken over all six permutations \( \Pi \) of three elements. It is seen that the expression for the momentum does depend linearly on the acceleration. One half of the acceleration-dependence comes from usual part \( \frac{\partial L_3}{\partial \dot{q}_\mu} \), while another half comes through the anomalous part \( -\frac{d}{ds} \frac{\partial L_3}{\partial \ddot{q}_\mu} \), resulting altogether in \( 2\epsilon^3 z_{\mu\alpha} \ddot{q}_\alpha \) in (5.132).

The energy corresponding to the Lagrangian \( L_3[q, \dot{q}, \ddot{q}] \) is obtained via looking at the total time-derivative of \( L_3[q, \dot{q}, \ddot{q}] \):

\[ \frac{d}{ds} L_3[q, \dot{q}, \ddot{q}] = \frac{\partial L_3}{\partial \dot{q}_\mu} \ddot{q}_\mu + \frac{\partial L_3}{\partial \dot{q}_\mu} \dot{q}_\mu + \frac{\partial L_3}{\partial \ddot{q}_\mu} \ddot{q}_\mu, \]  

(5.134)

where we noted that \( L_3[q, \dot{q}, \ddot{q}] \) does not have any explicit time-dependence. Employing equations of motion \( \dot{p}_\mu = \frac{\partial L_3}{\partial q_\mu} \), (5.134) results into energy conservation:

\[ \frac{dE}{ds} = 0, \quad E \equiv p_\mu \dot{q}_\mu + \frac{\partial L_3}{\partial \dot{q}_\mu} \ddot{q}_\mu - L_3. \]  

(5.135)
Thus the energy of the classical particle reads:

\[
E = \frac{\epsilon^2}{2} [M\delta_{\alpha\beta} + G_{\alpha\beta}] \dot{q}_\alpha \dot{q}_\beta + 2\epsilon^3 f_{\alpha\beta\gamma} \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma + 2\epsilon^3 z_{\mu\alpha} \dot{q}_\alpha \dot{q}_\mu + V(q) + E_n(q). \tag{5.136}
\]

Note that the vector-potential \( A_\alpha(q) \) expectedly drops out from the expression of energy [99]. However, the acceleration-dependent part of the Lagrangian does contribute directly into the energy. In fact, the whole third-order Lagrangian (5.121) is multiplied by a factor 2 and enters into the energy expression.

Let us now turn to the generalized angular momentum tensor, which is defined via the response of \( L_3 \) to an infinitesimal rotation (i.e., a distance conserving linear transformation) [99]:

\[
q_\mu \rightarrow q_\mu + \omega_{\mu\sigma} \delta q_\sigma, \quad \text{where} \quad \omega_{\mu\sigma} = -\omega_{\sigma\mu}:
\]

\[
\delta L_3 = \omega_{\alpha\beta} \left[ \frac{\partial L_3}{\partial q_\alpha} q_\beta + \frac{\partial L_3}{\partial \dot{q}_\alpha} \dot{q}_\beta + \frac{\partial L_3}{\partial \ddot{q}_\alpha} \ddot{q}_\beta \right] = \omega_{\alpha\beta} \frac{d}{ds} \left[ p_\alpha q_\beta + \frac{\partial L_3}{\partial \dot{q}_\alpha} \dot{q}_\beta \right],
\]

\[
\tag{5.137}
\]

where we again used (5.124). The full angular momentum tensor is now defined as [recalling \( \omega_{\mu\sigma} = -\omega_{\sigma\mu} \) :]

\[
M_{\alpha\beta} = p_\alpha q_\beta - p_\beta q_\alpha + \frac{\partial L_3}{\partial \dot{q}_\alpha} \dot{q}_\beta - \frac{\partial L_3}{\partial \dot{q}_\beta} \dot{q}_\alpha = L_{\alpha\beta} + S_{\alpha\beta},
\]

\[
\tag{5.138}
\]

\[
\tag{5.139}
\]

so that when \( L_3 \) is rotationally invariant, \( M_{\alpha\beta} \) is conserved in time. One part of this tensor is the usual orbital momentum \( L_{\alpha\beta} = p_\alpha q_\beta - p_\beta q_\alpha \). The remainder—non-orbital momentum, or spin—arises due to the dependence of the Lagrangian on the accelerations, and it is a second-order polynomial over the velocities:

\[
S_{\alpha\beta} = \frac{\partial L_3}{\partial \ddot{q}_\alpha} \ddot{q}_\beta - \frac{\partial L_3}{\partial \dot{q}_\beta} \dot{q}_\alpha = \epsilon^3 [z_{\beta\gamma} \dot{q}_\gamma q_\alpha - z_{\alpha\gamma} \dot{q}_\gamma \dot{q}_\beta].
\]

\[
\tag{5.140}
\]

\[
\tag{5.141}
\]

In the simplest two-coordinate situation \( S_{12} = -S_{21} = \epsilon^3 z_{21}(\dot{q}_1^2 + \dot{q}_2^2) \), which means that the spin tensor is proportional to the velocity square.
5.6. Third order post-adiabatic force

Zitterbewegung effect

From the expression of the momentum given by (5.132) and the expression for the spin given by (5.140,5.141) and using the fact that \( z_{\alpha\beta} \) is antisymmetric, we can write

\[
p_{\mu} = \frac{\partial L_3}{\partial \dot{q}_\mu} + \frac{d}{ds} \left[ \frac{S_{\alpha\mu} \dot{q}_\alpha}{\dot{q}^2} \right], \quad \dot{q}^2 \equiv \dot{q}_\alpha \dot{q}_\alpha,
\]

which means that the anomalous part \( p_{\mu} - \frac{\partial L_3}{\partial \dot{q}_\mu} \) of the momentum is driven by the time-derivative of the velocity-projected spin-tensor.

An expression similar to (5.142)—relating the momentum to the projected time-derivative of the spin—appears in the (relativistic) Dirac electron theory [110]. There the fact that the total angular momentum is a sum of the orbital part and the spin part, as well as the fact that the velocity and the momentum are different objects and are not simply proportional to each other via the mass, are the consequence of the relativistic invariance for the electron. The very effect of the spin time-derivative contributing into the momentum was named *zitterbewegung*, since for the free Dirac electron this contribution brings in an additional oscillatory motion [110]. In a more recent literature, the zitterbewegung effect is also derived via Lagrangians containing the higher-order derivatives of coordinates [111,112].

There are, however, several aspects that distinguish (5.142) from the zitterbewegung effects already known in literature.

- First, we do not have a relativistic invariant theory; for us relation (5.142) emerges due to the fact that the classical system is open.

- Second, we do not have to have the conservation of momentum and of angular momentum for deriving (5.142). Both these quantities are generically non-conserved in our situation (ultimately since the system is open), but relation (5.142) still holds generally due to the specific, anti-symmetric form (5.121) of the acceleration-dependent part of the Lagrangian.

We close this part by emphasizing its main findings: due to interaction with the fast quantum system the classical system gets a spin [non-orbital angular momentum], which is related to its momentum via zitterbewegung effect.
5.6.2 Hamiltonian description

In this section we study the Hamiltonian description. Within the order $\epsilon^2$ the Hamiltonian description is straightforward. However, the third-order dynamics has a non-trivial Hamiltonian structure, as seen below.

Let us first explicitly separate out the higher-derivative term of the Lagrangian given by (5.123). Thus we have

$$L_3[q, \dot{q}, \ddot{q}] = L_3[q, \dot{q}] - \epsilon^3 z_{\alpha\beta} \ddot{q}_\alpha \dot{q}_\beta.$$  \hspace{1cm} (5.143)

In general, we can introduce three sets of variables

$$q = (q_1, \ldots, q_K), \quad v = (v_1, \ldots, v_K), \quad \pi = (\pi_1, \ldots, \pi_K),$$  \hspace{1cm} (5.144)

and instead of (5.143) introduce the following extended Lagrangian:

$$L[q, v, \pi] = L_3(q, v) - \epsilon^3 z_{\alpha\beta} \dot{v}_\alpha v_\beta + \pi_\alpha (\dot{q}_\alpha - v_\alpha).$$  \hspace{1cm} (5.145)

It should be clear that if we treat $q$, $v$ and $\pi$ as coordinates, then the Lagrange equations generated by $L[q, v, \pi]$ are equivalent to those generated by $L_3[q, \dot{q}, \ddot{q}]$. At this point $\pi$ is considered as a part of the overall set of coordinates. It may be equivalently viewed as Lagrange multipliers. If $L[q, v, \pi]$ were not dependent on $\dot{v}$—that is, $L_3[q, \dot{q}, \ddot{q}]$ would not depend on $\ddot{q}$—we would write the velocities $v = v(q, \pi)$ as functions of the coordinates and momenta, and end up with the usual Hamiltonian description with $q$ and $\pi$ being the canonical coordinates and momenta, respectively. Though $L[q, v, \pi]$ does depend on $\dot{v}$, it can be still related to a Hamiltonian in the following way [113].

Once the triplet $q, v, \pi$ is considered as coordinates, we introduce a separate notation for it

$$Q = (Q_1, \ldots, Q_{3K}) = (q_\alpha, v_\alpha, \pi_\alpha).$$  \hspace{1cm} (5.146)

Now the Lagrangian (5.145) reads

$$L[Q] = L_3[Q] + A_a[Q] \dot{Q}_a, \quad a = 1, \ldots, 3K,$$  \hspace{1cm} (5.147)

where

$$A[Q] = (\pi_\alpha, \epsilon^3 z_{\beta\alpha}, 0).$$  \hspace{1cm} (5.148)

Below we shall show that the expression $L_3[Q]$ plays the role of the Hamiltonian.
Eq. (5.147) generates the following Lagrange equations of motion:

\[
\Omega_{ab}(Q) \dot{Q}_b = \frac{\partial L_3}{\partial Q_a}, \quad (5.149)
\]

where

\[
\Omega_{ab}(Q) \overset{\text{def}}{=} \frac{\partial A_a}{\partial Q_b} - \frac{\partial A_b}{\partial Q_a}. \quad (5.150)
\]

In block-matrix notations \( \Omega \) reads

\[
\Omega = \begin{pmatrix}
0 & Y & I \\
-Y^T & Z & 0 \\
-I & 0 & 0
\end{pmatrix}, \quad (5.151)
\]

where each element in the above matrix is a \( K \times K \) matrix, with \( K \) being the number of classical degrees of freedom:

\[
Y_{\alpha\beta} = \epsilon^3 v_\gamma \partial_\alpha z_{\gamma\beta}, \quad Z_{\alpha\beta} = -2\epsilon^3 z_{\alpha\beta}, \quad I_{\alpha\beta} = \delta_{\alpha\beta}, \quad (5.152)
\]

and where \( I \) is the \( K \times K \) unit matrix. Provided \( Z \) is invertible, the inverse of \( \Omega \) reads [block-matrix notations]

\[
\Omega^{-1} = \begin{pmatrix}
0 & 0 & -I \\
0 & Z^{-1} & -Z^{-1}Y^T \\
I & -YZ^{-1} & YZ^{-1}Y^T
\end{pmatrix}. \quad (5.153)
\]

For an even \( K \) the matrix \( Z \) is generically invertible; as we discussed before. In this case \( \Omega_{ab} \) is invertible and antisymmetric. Moreover, from its definition given by (5.150) we see that

\[
\frac{\partial}{\partial Q_c} \Omega_{ab} + \frac{\partial}{\partial Q_b} \Omega_{ca} + \frac{\partial}{\partial Q_a} \Omega_{bc} = 0. \quad (5.154)
\]

Therefore it ensures that the Poisson brackets defined via \( \Omega_{ab} \) does not change in time [114]. In fact, \( \Omega_{ab} \) defines a symplectic structure [114].

Then \( L_3[Q] \) plays the role of the Hamiltonian.

Now for any two functions \( C(Q) \) and \( D(Q) \) the Poisson bracket is defined as

\[
\{C(Q), D(Q)\}_{PB} = \Omega^{-1}_{ab} \frac{\partial C}{\partial Q_a} \frac{\partial D}{\partial Q_b}. \quad (5.155)
\]

The equations of motion (5.149) can now be written as

\[
\dot{Q}_a = \{ Q_a, L_3[Q] \}_{PB}. \quad (5.156)
\]
Post Adiabatic Forces

In this case the Poisson brackets are non-linear. It is seen from (5.151, 5.155) that $z_{\alpha\beta}$ and its derivatives define a non-trivial symplectic structure for the system.

The matrix $Z$ is not invertible for an odd $K$. The Hamiltonian description in this case is still possible, but it requires more care in explicitly accounting for constraints.

5.7 The Fourth order Lagrangian

In this section we discuss a specific example on the fourth-order Lagrangian. Since the calculations now become very complicated, we shall restrict ourselves to the situation where the classical system has just one single coordinate $q$. For further simplicity we assume the quantum system has real adiabatic eigenstates. In fact, the main purpose of this section is to illustrate that the fourth-order Lagrangian again depends linearly on the highest-order time-derivatives of the classical coordinate.

Following the same lines of calculation for the third order non-adiabatic force presented in section 5.6, and assuming a single coordinate classical system and real eigenstates for the quantum system, the non-adiabatic force acting on the classical system in the fourth order is described by the following Lagrangian

$$
\epsilon^4 F^{[4]} = \left( \frac{d^3}{ds^3} \frac{\partial}{\partial q(3)} - \frac{d^2}{ds^2} \frac{\partial}{\partial \dot{q}} + \frac{d}{ds} \frac{\partial}{\partial \ddot{q}} - \frac{\partial}{\partial q} \right) L^{[4]}[q, \dot{q}, \ddot{q}, q^{(3)}],
$$

where

$$
L^{[4]}[q, \dot{q}, \ddot{q}, q^{(3)}] = \epsilon^4 \left[ a\dot{q}^4 + b\ddot{q}^2 + wq^{(3)} \right],
$$

where $q^{(3)}$ stands for the third order time derivative of $q$, and where $L^{[4]}$ represents the fourth-order Lagrangian. We notice the same pattern in the higher-order Lagrangian, i.e., that the dependence on the higher-order time
5.8. Summary

We have studied the post-adiabatic equations of motion for a slow classical system which is coupled to a fast quantum system. The slow versus fast motion is controlled by a small ratio $\epsilon$ of the characteristic times. The general problem we addressed is to find an effective Lagrangian that describes the dynamics of the classical system. The post-adiabatic reaction force is proved to be Lagrangian up to the fifth order of $\epsilon$. We conjecture that at every order of $\epsilon$ the effective dynamics of the classical system can be derived from a Lagrangian.

In the order $\epsilon^0$ the effective Lagrangian differs from the bare one by the Born-Oppenheimer potential energy. In the first order correction the effective...
Lagrangian corresponds to a magnetic field, which is related to the geometric phase [2].

In the order $\epsilon^2$ the effective Lagrangian gets an additional kinetic energy term, which is a second-order polynomial over the classical velocities [3,100]. We showed that in the second order of $\epsilon$, the motion generated by the effective classical Lagrangian can be mapped on to geodesic curves on a suitable Riemannian manifold. Operating with the simplest possible example—two classical coordinates interacting with a two-level quantum system—we show that the Riemannian manifold is essentially curved solely due to the kinetic energy generated by the fast quantum system. The scalar curvature is frequently negative indicating that the classical trajectories [geodesic curves] are unstable with respect to small variations of the initial conditions. The metric tensor generated by the fast quantum system can change its signature as a function of the two coordinates. Physically this means a transition from an Euclidean to pseudo-Euclidean manifold, emergence of a time-like coordinate.

Within the order $\epsilon^3$ the effective Lagrangian linearly depends on the accelerations of the classical system.

We argued that this result is important, because it provides a physically well-motivated scenario for the emergence of higher-derivative Lagrangians for open classical systems. This result should be contrasted to the usual open-system approaches, which can also produce forces depending on higher-order derivatives (e.g., the Abraham-Lorentz force in electrodynamics), but those forces are dissipative (non-Lagrangian).

The presence of higher-derivative terms can be tested by essential influences they bring on the kinematics of the system. First, they modify initial conditions; in our case this means that the trajectory of the classical system on the slow (coarse-grained) time starts to depend on acceleration. Second, the conserved energy of the slow classical motion does depend on the acceleration. And third, the presence of higher-derivative terms naturally separates the total angular momentum into the sum of orbital momentum and spin. We show that this spin satisfies an exact analogue of the zitterbewegung relation.