A.E. Allahverdyan$^1$ and B. Mehmaui$^2$

$^1$ Yerevan Physics Institute, Alikhanian Brothers St. 2, Yerevan 375036, Armenia and

$^2$ Institute for Theoretical Physics, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands

We study a slow classical system [particle] coupled to a fast quantum system with discrete energy spectrum. We 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 in order to uncover new physical phenomena. It is known that in the order $\epsilon^0$ the particle gets an additional [Born-Oppenheimer] potential, while in the order $\epsilon^1$ it feels an effective magnetic field related to the Berry phase. In the order $\epsilon^2$ the motion of the classical particle can be reduced to a free [geodesic] motion on a curved Riemannian manifold, with the metric generated by the excluded quantum system. This motion has a number of unusual features, e.g., it combines subspaces of different (Riemannian and pseudo-Riemannian) signature for the metric tensor. 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. 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 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 $\epsilon^n$.

PACS numbers:

I. INTRODUCTION

A recurrent theme in modern physics is to derive autonomous equations of motion for an open system, i.e., a system that interacts with its environment [1–3]. Depending on the type of environment, there are different conditions under which this procedure is possible. A group of methods, which goes under the name of system-bath interaction, amounts to isolating a relatively small system in contact to an equilibrium environment (thermal bath) [1, 2]. The prerequisite of applying the model reduction in this case is that the reaction of the system on its environment is in a sense weak [1, 2]. One of the main consequences of this approach is the Langevin equation, which supplements the Newton equation of motion for the small system by a (random) conservative and non-conservative (i.e., non-Lagrangian), velocity-dependent friction force [1, 2].

There is another set-up that allows deriving autonomous equations for an open system. Here the essential condition is that the target system is much slower than its environment [3–9]. One of the oldest results in this direction is the Darwin Lagrangian [3, 4]: when the characteristic speed $v$ of charges is slow as compared to the speed $c$ of the electromagnetic field, the latter can be adiabatically excluded, producing at the order $(v/c)^2$ the Darwin Lagrangian for the charges, which has important applications in plasma physics and astrophysics; see [4] for a recent review.

In this paper we shall study the quantum-classical (also called mean-field or hybrid) dynamics, which describes coupled quantum and classical systems [5, 6]. This is the most used set-up for coupling quantum and classical variables [10], and has numerous applications, e.g., in chemical physics [11] and in (semi)quantum gravity [12]. Assuming that the classical system is slow—a condition that is normally met in practice—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. For example, in the above Darwin problem, the autonomous dynamics exists up to higher orders in $(v/c)$, but already at the order $(v/c)^3$ the dynamics of the charges is not Lagrangian due to the friction (Abraham-Lorentz) force related to radiation damping, i.e., to emission of electromagnetic field by the charges [3]. (In some special cases this friction force is suppressed and the Darwin Lagrangian can be written including the order $(v/c)^4$ [3]).

For the quantum-classical dynamics it is well known that at the zero order of $\epsilon$—where $\epsilon$ is the small ratio of the characteristic times for the quantum over the classical system, respectively—the influence of the quantum system on the classical one can be described by the Born-Oppenheimer potential energy term [5–7, 10–12]. 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 [5]. Goldhaber has recently shown that in the second order $\epsilon^2$ one gets in the Lagrangian an additional kinetic energy term, i.e., a quadratic form in slow velocities [6]. A very similar result on the order $\epsilon^2$ was obtained earlier by Weigert and Littlejohn for two coupled (fast and slow) quantum systems [7].

What happens in the next orders? In particular, how far we can continue the expansion over $\epsilon$, still keeping the classical system Lagrangian? Most importantly, are there new physical effects essentially related to post-adiabatic
corrections?

Here we answer these questions. 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: While the classical Lagrangians normally depend on the coordinates and their first-order time-derivatives (velocities), at the order $\epsilon^3$ we get a Lagrangian that is linear over the 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. Such Lagrangians were phenomenologically introduced at various places and for various purposes (see, e.g., Ref. [6] for a sample of references), but our result seems to be the first example where a higher-derivative Lagrangian emerges for an open classical system due to time-scale separation. We should like to stress that the fast system being quantum is not important for obtaining the above result. What is important is that the fast system is integrable, i.e., it admits a full and globally well-defined set of action-angle variables.

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; see [14] for a review, while we show the same effect appears in a purely non-relativistc 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. Similar dependence on higher-order derivatives is expected at higher orders $\epsilon^n$ with $n \geq 4$, though in the present paper we restrict ourselves with deriving the effective classical Lagrangian up to the order $\epsilon^3$.

While these results concern higher-order (three and more) post-adiabatic corrections, we found an interesting effect already in the second-order post-adiabatic correction, which was formally known since Ref. [6, 7]. It appears that the slow classical motion within this order can be reduced to a free motion on a Riemannian space with a signature-indefinite metric tensor. This implies a possibility of interchanging between 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 $(1, -1, -1, -1)$ [3]. In both cases the signature is fixed.

This paper is organized as follows. In section II we introduce the quantum-classical dynamics. The next section, section III outlines the adiabatic perturbation theory, which differs from the standard text-book presentations by a careful accounting of the higher-order terms. In section IV we review the derivation of the classical Lagrangian in the orders $\epsilon$ and $\epsilon^2$. In particular, we reproduce in a systematic way the results obtained by Berry and Robbins [5] and Goldhaber [6]. At the order $\epsilon^2$ this 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]. Section V derives the classical Lagrangian at the order $\epsilon^3$, and shows that the classical Lagrangian in this case depends linearly on the third-derivative of the classical coordinates. In this section we explore kinematical consequences of this result and explore its Hamiltonian description. In section VI 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. The last section presents our conclusions and summarizes the present work. Several technical question are discussed in appendices.

II. QUANTUM-CLASSICAL DYNAMICS

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

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

where $M$ is the mass, and $V(q) = V(q_1, \ldots, q_K)$ is the potential energy.
Now this classical system (or particle) couples to a quantum system with Hamiltonian operator $H[q(t)]$, which parametrically depends on the classical coordinates. The quantum system evolves in time according to the Schrödinger equation (for simplicity we put $\hbar = 1$)

$$i\partial_t |\Psi\rangle = H[q(t)]|\Psi(t)\rangle,$$

where $|\Psi\rangle$ is the wave-function, and where $\partial_t = \frac{\partial}{\partial t}$. The classical part of the dynamics is written as [10–12] (see [10] for a derivation)

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

where we defined $^1$

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

Eq. (3) 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 [10]. The main purpose of the present paper is to understand to which extent this force can be generated by a Lagrangian which depends on the classical coordinates $q_\alpha$ and their time-derivatives.

It should be clear from (2, 3) that the total average energy is conserved in time:

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

We note that the quantum-classical equations of motion (2, 3) can be derived from a Lagrangian

$$\tilde{\mathcal{L}} = \frac{1}{2t} \langle \partial_t |\Psi\rangle - \frac{1}{2t} \langle |\partial_t \Psi\rangle - \langle |H|\Psi\rangle + \frac{M}{2} \sum_{\alpha=1}^{K} \left( \frac{dq_\alpha}{dt} \right)^2 - V(q),$$

where as a set of independently varying parameters one should take $|\Psi\rangle$ and $q$ (or alternatively $\langle \Psi|q\rangle$) $^2$. It is seen that $\tilde{\mathcal{L}}$ is simply a sum of the corresponding quantum and classical Lagrangians, which points out at the naturalness of quantum-classical equations of motion (2, 3).

Let us briefly comment on derivations of the quantum-classical dynamics from a full quantum-quantum dynamics. Such a derivation was carried out in literature several times; see, e.g., [10, 15–17]. Moreover, many derivations of the (semi)classical mechanics from the quantum mechanics can be adopted for deriving quantum-classical dynamics; see in this context [18, 19] in addition to the above references. The main assumption involved in all these derivations is that fluctuations of classical coordinate(s) are small [10, 15–19]. For deriving the quantum-classical dynamics it is not necessary that the classical motion as such is slow $^3$. Note that 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 suffice that the to-be classical sector of the dynamics is approximated via suitable Gaussian density matrices [18]. Then, the parameters of this matrices satisfy the equations of motion for some effective classical systems [18] $^4$. In Appendix A we briefly remind the main argument involved in the derivation of quantum-classical dynamics.

$^1$ 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 $\frac{\partial}{\partial t}$.

$^2$ As usual, when varying (6) we put aside the total time-derivatives, e.g., $\frac{\partial}{\partial t} (\delta |\Psi\rangle \rangle$.

$^3$ It is not excluded that there are situations, where both the classical limit and adiabatic limit—where the classical motion is slow—are taken simultaneously. Our consideration does not apply to such situations, because when looking for post-adiabatic corrections one should simultaneously account for post-classical corrections, which is something we do not do.

$^4$ A general remarks is in order here. The quantum-classical dynamics is just an approximation which holds under suitable conditions. There are, however, controversial aspects related to this dynamics, which emerged when people wanted to get a non-perturbative generalization of the mean-field quantum-classical dynamics; see, e.g., [20] for examples. These generalizations are supposed to be closed and self-consistent theories, where one part of variables is quantum and another is classical. Such theories (if they exist) would somehow get the same fundamental status as their limiting cases, i.e., as quantum and classical mechanics. Numerous attempts to formulate such fundamental quantum-classical theories met with severe difficulties [20]. Those difficulties do not seem to be insurmountable, as witnessed by a recent proposal by Hall and Regginato [21].
A. Classical representation for the quantum system

Below we are going to 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. A natural question is that why specifically we need the fast system to be quantum, and would it be possible to obtain the same result assuming that also the fast system is classical. (Then we would not need additional conditions for the applicability of the quantum-classical dynamics, and we could start from the outset with an overally classical dynamics).

The answer to this question is that in principle only one feature of the fast quantum dynamics is needed, that is its integrability [in the sense of [22]]. To support this answer we may note that all the results of the quantum Hamiltonian dynamics [30]. The Schrödinger equation (2) can be mapped to a classical dynamics if one introduces a classical variable. This is a classical integrable dynamics, because it has globally well-defined action-angle variables with trivial Poisson brackets [22]. Eq. (9) makes clear that the adiabatic theory for the quantum Schrödinger equation can be alternatively developed from the viewpoint of classical integrable systems [30].

For definiteness, in the present paper we shall confine ourselves with the quantum fast system.

III. TIME-SCALE SEPARATION AND ADIABATIC PERTURBATION THEORY

We shall now assume that there is a time-scale separation: the quantum system evolves much faster than the classical particle. To make this assumption more precise and to investigate its consequences, let us recall that the adiabatic energy levels \( \{ E_k(q) \} \) and the corresponding eigen-vectors \( \{ |k(q)\rangle \} \) are defined via the eigen-resolution of the Hamiltonian \( H[q] \) at fixed values of \( q = (q_1, \ldots, q_K) \):

\[
H[q]|k(q)\rangle = E_k(q)|k(q)\rangle, \quad \langle k(q)|l(q)\rangle = \delta_{kl}, \quad k = 1, \ldots, d,
\]

where \( d \) is the total number of energy levels. We shall assume that the adiabatic energy levels are not degenerate. Then qualitative sufficient condition for the time-scale separation is that the characteristic time of the classical motion is much larger than \( \frac{\Delta}{\Delta} \), where \( \Delta \) is the minimal adiabatic energy gap: \( \Delta \equiv \min_{k \neq l} \{ |E_k - E_l| \} \).

Note that the adiabatic representation (10) has a gauge freedom:

\[
|k(q)\rangle \rightarrow e^{i\alpha_k(q)}|k(q)\rangle,
\]

where \( \alpha_k(q) \) is an arbitrary single-values function of \( q = (q_1, \ldots, q_N) \). Hence all physical observables have to be gauge-invariant.

To reflect mathematically the fact of time-scale separation we shall write the dependence of the quantum Hamiltonian on the classical coordinates as

\[
H[q_1(\ell t), q_2(\ell t), \ldots],
\]

This condition is sufficient, but not necessary for the validity of the time-scale separation and the consequent adiabatic approach, e.g., the latter can still hold if certain level-crossings are allowed. We shall not consider this more general situation in the present paper.
where $\epsilon$ is a small dimensionless parameter

$$\epsilon \ll 1. \quad (13)$$

The time-scale separation, i.e., condition (13), can be generated, e.g., by a large mass $M$ of the classical particle. Then the classical particle moves slowly—provided that its initial velocity is small—and $\epsilon \sim 1/\sqrt{M}$. This scenario of time-scale separation is normally met in chemical physics (heavy classical nuclei versus light quantum electrons) [11] and semi-quantum gravity [12].

In the Schrödinger equation (2) we shall assume that the initial state $|\Psi(0)\rangle$ is equal to an eigenstate:

$$|\Psi(0)\rangle = |n(0)\rangle. \quad (14)$$

Within the adiabatic approach the choice (14) does not imply any serious loss of generality; see Footnote 6.

Our program is now to solve the Schrödinger equation (2) under the adiabatic assumption (12, 13), and determine, via this solution, the structure of the averaged force in (3). To this end, we shall need the adiabatic perturbation theory, which was developed in [23, 24], and which is explained in detail in Appendix B. Now we shall recall some basic facts from this theory. As in any theory that is based on time-scale separation, we should start with dividing the sought solution into fast and slow components:

$$|\Psi(t)\rangle = e^{-i\int_0^t da E_n(u(t))} |\psi_n(\epsilon t)\rangle$$

$$= e^{-iA} \int_0^t da E_n(u) |\psi_n(s)\rangle, \quad (15)$$

where in (16) we introduced the slow time $s = \epsilon t$, and where $|\psi_n\rangle$ satisfies [see (2)]

$$i\epsilon \langle \dot{\psi}_n(s) \rangle = [H(s) - E_n(s)] \langle \psi_n(s) \rangle. \quad (17)$$

Here dots denote differentiation over the slow time

$$s = \epsilon t, \quad \dot{A} \equiv \frac{dA}{ds}, \quad (18)$$

and the lower index $n$ in (15, 16, 17) refers to the initial state (14). Depending on the context we shall write $H[q(s)]$ as $H(s)$, etc.

Eqs. (15, 16) extend to the adiabatic situation the usual formula for a stationary state of a time-independent quantum Hamiltonian. This analogy also explains why $|\psi_n\rangle$ in (15, 16) depends only on the slow coordinate. We see that the dynamical phase $e^{-i\epsilon \int_0^t da E_n(u)}$ is the fast component of the wave-vector, since due to $\epsilon \ll 1$ it strongly oscillates at slow times $^6$.

Within the adiabatic perturbation theory, the solution of (17) can be sought for via expanding over $\epsilon$ (see [23, 24] and Appendix B)

$$|\psi_n(s)\rangle = e^{\int_0^s du \langle \dot{n}(u)|n(u)\rangle} |\phi_n(s)\rangle,$$

$$|\phi_n\rangle = |n(s)\rangle + \epsilon |n_1(s)\rangle + \epsilon^2 |n_2(s)\rangle + \epsilon^3 |n_3(s)\rangle + \ldots \quad (19)$$

The zero order term $|\phi_n\rangle = |n(s)\rangle$ in this expansion is the statement of the adiabatic theorem. In (19), $e^{\int_0^s du \langle \dot{n}(u)|n(u)\rangle}$ is the Berry phase factor; it was separated out for ensuring the proper gauge-covariance [24]; see also below. Note that $\langle \dot{n}(u)|n(u)\rangle$ is purely imaginary (due to $\langle n(u)|n(u)\rangle = 1$), so that this phase factor nullifies, if $|n(u)\rangle$ can be chosen to be real. An alternative representation of $|\phi_n(s)\rangle$ is

$$|\phi_n(s)\rangle = \sum_{k=1}^d c_{kn}(s)|k(s)\rangle, \quad c_{kn}(0) = \delta_{kn}, \quad (21)$$

$$c_{kn}(s) = \delta_{kn} + \epsilon c_{kn}^1(s) + \epsilon^2 c_{kn}^2(s) + \epsilon^3 c_{kn}^3(s) + \ldots \quad (22)$$

---

$^6$ This fact also explains why in (14) it suffices to take a single initial wave-vector and not a superposition of them. Any superposition will bring in the adiabatic limit strong oscillations for non-diagonal elements of the resulting density matrix. This will reduce the superposition to the mixture of adiabatic eigen-vectors, which amounts to studying the consequences of (14), and then taking the average over the index $n$ with certain time-independent weights.
Let us quote from Appendix B several basic formulas of the adiabatic perturbation theory:

\[ c_{k\neq n}^{[1]}(s) = \frac{\langle k(s)|\dot{n}(s)\rangle}{i\Delta_{nk}(s)}, \quad \Delta_{kl}(s) \equiv E_k(s) - E_l(s), \]  
\[ c_{nn}^{[1]}(s) = -\frac{1}{2} \sum_k \epsilon \int_0^s \frac{|\langle k(u)|\dot{n}(u)\rangle|^2}{\Delta_{nk}(u)}, \]  
\[ c_{k\neq n}^{[2]}(s) = \frac{i}{\Delta_{nk}} \left[ c_{k\neq n}^{[1]} \langle n|\dot{n}\rangle - \langle k|\dot{n}\rangle \right] \]  

where \( \sum' \) means that \( k = n \) is excluded from the summation \( \sum_{k=1}^d \).

Eq. (23) for the first-order adiabatic correction is especially well-known [5, 6]. It is certainly less well-known that the consistent adiabatic perturbation theory generates another \( O(\epsilon) \) term, i.e., \( c_{nn}^{[1]} \); see however [24]. This term is purely imaginary and it drops out from the lowest-order post-adiabatic corrections to the averaged force in (3).

The representation (21) is gauge-covariant \( \langle \phi_n(s)|e^{i\alpha_n(s)}|\phi_n(s)\rangle \) due to (23–25). Eq. (19) is also gauge-covariant \( |\psi_n(s)\rangle \rightarrow e^{i\alpha_n(0)}|\psi_n(s)\rangle \), and shows that the relative phase \( \arg(|\langle n|\phi_n(s)\rangle|) \) is gauge-invariant. Hence it can be observed [25, 26]. Note that Berry phase factor in (19) is not gauge-invariant as such, apart of a certain specific case [25–27].

A. Compact expression for the non-adiabatic force

Employing (17, 19) we now calculate:

\[ F_\mu \equiv \langle \psi_n|\partial_\mu H|\psi_n\rangle = \langle \phi_n|\partial_\mu H|\phi_n\rangle \]  
\[ = \partial_\mu \langle \phi_n|H|\phi_n\rangle - 2\Re\langle \partial_\mu \phi_n|H|\phi_n\rangle - E_n + 2\epsilon \Im \langle \partial_\mu \phi_n|\phi_n\rangle, \]  

where \( \Re \) and \( \Im \) mean, respectively, the real and imaginary parts. The factor \( \partial_\mu E_n \) is the force generated by the adiabatic (Born-Oppenheimer) potential \( E_n = E_n(q) \). Thus the last two expressions in (28) represent the non-adiabatic force. We denote

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

where \( F_\mu^{[0]} = \partial_\mu E_n \). In this context note from (21) that

\[ \langle \phi_n|H|\phi_n\rangle - E_n = \sum' \Delta_{kn} |c_{kn}|^2 = O(\epsilon^2). \]  

IV. FIRST- AND SECOND-ORDER POST-ADIABATIC FORCE.

Using (22) and (28) we get for the first-order post-adiabatic force:

\[ F_\mu^{[1]} = 2\Im\langle \partial_\mu n|\dot{n}\rangle = 2\partial_\alpha \Im\langle \partial_\alpha n|\partial_\alpha n\rangle, \]  

where we always assume implicit summation from 1 to \( K \) over the repeated Greek (not Latin!) indices:

\[ A_\alpha B_\alpha \equiv \sum_{\alpha=1}^K A_\alpha B_\alpha. \]  

Since \( \Im\langle \partial_\mu n|\partial_\alpha n\rangle = -\Im\langle \partial_\alpha n|\partial_\mu n\rangle \), Eq. (31) leads to an effective Lorentz [or gyroscopic] force [5].

Employing (21, 23) we obtain at the second order:

\[ F_\mu^{[2]} = \partial_\mu \sum' \Delta_{kn} |c_{kn}^{[1]}|^2 + 2\Im \left( \langle \partial_\mu n|\dot{n}\rangle + \langle \partial_\mu n|\dot{n}\rangle \right) \]  
\[ = \partial_\mu \sum' \frac{|\langle k|\dot{n}\rangle|\langle \dot{n}|k\rangle|}{\Delta_{kn}} + 2\Im \left( \frac{d}{ds} \langle \partial_\mu n|n_1\rangle + \partial_\mu \langle n_1|n\rangle \right). \]  

Note that the non-local contribution \( c_{nn}^{[1]} \) drops out from (34), since both \( c_{nn}^{[1]} \) and \( \langle n|\partial_\mu n\rangle \) are purely imaginary.
Working out \((33, 34)\) and taking the result together with \((31)\), we obtain that in the first and second orders the averaged force can be generated by the following Lagrangian \(^7\)

\[
\epsilon F^{[1]}_{\mu} + \epsilon^2 F^{[2]}_{\mu} = \frac{d}{ds} \frac{\partial L^{[12]}_{\mu}}{\partial \dot{q}_{\mu}} - \frac{\partial L^{[12]}_{\mu}}{\partial q_{\mu}},
\]

\[
L^{[12]}(\dot{q}, q) = \frac{\epsilon^2}{2} G_{\alpha\beta}(q) \dot{q}_{\alpha} \dot{q}_{\beta} + \epsilon A_{\alpha}(q) \dot{q}_{\alpha},
\]

\[
A_{\alpha} = \Im \{\langle n| \partial_{\beta} n| k \rangle \langle \partial_{\alpha} k| n \rangle \}.
\]

Here \(A_{\alpha}\) is the vector potential that corresponds to the effective magnetic field \((31)\) \([5]\), and \(G_{\alpha\beta}\) plays the role of a coordinate-dependent mass tensor, which is generated from \((34)\) \([6]\). Note that \(G_{\alpha\beta}\) is 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: \(\Delta_{kn} \geq 0\). Now \(G_{\alpha\beta}\) cannot be a positive matrix for all initial states of the quantum system, since, e.g., when \(d = 2\) (two level situation), one has \(G_{\alpha\beta}[\text{excited state}] = -G_{\alpha\beta}[\text{ground state}]\).

The complete classical Lagrangian to the second order is obtained by adding \(L^{[12]}(\dot{q}, q)\) and the Born-Oppenheimer potential \(E_n(q)\) to the initial (bare) classical Lagrangian \(L_0\), given by \((1)\):

\[
L_2 = \frac{M}{2} \sum_{\alpha=1}^{K} \left( \frac{dq_{\alpha}}{dt} \right)^2 - V(q) - E_n(q) + L^{[12]}(\dot{q}, q).
\]

Note that when the time-scale separation is enforced by a large [bare] mass \(M\) of the classical particle, the post-adiabatic Lagrangian \(L^{[12]}(\dot{q}, q)\) is 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 \(\epsilon \sim 1/\sqrt{M}\).

### A. Second-order post-adiabatic force, metric tensor and curvature.

The kinetic part \(\sum_{i=1}^{K} [M \delta_{\alpha\beta} + G_{\alpha\beta}(q)] \dot{q}_{\alpha} \dot{q}_{\beta}\) of the second-order Lagrangian \((39)\) corresponds to a free particle moving on a Riemannian manifold with metric tensor \([3]\):

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

There is an important particular case, where the complete Lagrangian \((39)\) just reduces to this kinetic energy. This happens when \(ij\) the eigenvectors \([n]\) can be chosen real, which then nullifies the vector potential \(A_{\alpha}\), \(ii)\) the bare potential \(V(q)\) and the Born-Oppenheimer potential \(E_n(q)\) compensate each other, \(V(q) + E_n(q) = 0\), e.g., \(V(q)\) is zero from the outset, while \(E_n(q)\) turns to zero, since the eigenvalues of the quantum Hamiltonian \(H[q]\) do not depend on the coordinates \(q\) (though the eigen-vectors do).

Thus we focus on the purely kinetic Lagrangian

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

Once we are going to excersise on the Riemannian geometry, we recover for the velocities the explicitly contravariant notations \([3]\) \(q^\alpha\). The metric tensor \(g_{\alpha\beta}\) is then naturally covariant. The Lagrangian \((41)\) yields the following equations of motion

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

\(^7\) Let us be given a classical system with action \(\int_{\alpha}^{\beta} ds L[\dot{q}(s), q(s)]\), where \(L\) is the Lagrangian, \(q\) is the vector of (generalized) coordinates, and \(\dot{q} = \frac{dq}{dt}\). The Euler-Lagrange variational equations of motion \(\frac{d}{ds} \frac{\partial L_{\mu}}{\partial \dot{q}_{\mu}} - \frac{\partial L_{\mu}}{\partial q_{\mu}} = 0\), are obtained when varying the action over the coordinate-path \(q(s)\) assuming that the end-points are fixed: \(\delta q(0) = \delta q(\beta) = 0\). This well-known set-up has a straightforward generalization for a Lagrangian \(L[\dot{q}(s), q(s), q(s)]\) that depend on the acceleration or more generally on higher-order derivatives of coordinates. The corresponding Euler-Lagrange equations of motion read \(\frac{d}{ds} \frac{\partial L}{\partial \dot{q}_{\mu}} - \frac{\partial L}{\partial q_{\mu}} - \frac{d^2}{ds^2} \left[ \frac{\partial L}{\partial q_{\mu}} \right] = 0\), where now we assume that \(\delta q(0) = \delta q(\beta) = \delta \ddot{q}(0) = \delta \ddot{q}(\beta) = 0\).
This is the geodesic equation $\frac{Du^\alpha}{ds} = 0$, where the covariant differential of any vector $C^\alpha$ is defined as

$$DC^\alpha = dC^\alpha + \Gamma^\alpha_{\mu\nu} C^\nu dq^\mu,$$

and where the connections $\Gamma^\alpha_{\mu\nu}$ relate to the metric tensor as [3]:

$$\Gamma^\alpha_{\mu\nu} = \frac{1}{2} g^{\alpha\sigma} (\partial_\mu g_{\sigma\nu} + \partial_\nu g_{\sigma\mu} - \partial_\sigma g_{\mu\nu}).$$

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

The first important question is whether the Riemannian manifold is curved or not. In the latter case 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 $R^\mu_{\nu\alpha\beta}$ [3]. It will be more convenient to present the explicit formula for the covariant curvature tensor [3]

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

where $\Gamma^\mu_{\nu\alpha} = g_{\mu\sigma} \Gamma^\alpha_{\nu\sigma}$. Eq. (45) implies the following symmetry relations:

$$R^\alpha_{\beta\gamma\delta} = -R^\alpha_{\gamma\beta\delta} = -R^\alpha_{\delta\beta\gamma} = R^\alpha_{\gamma\delta\beta}.$$

If the curvature tensor is non zero the manifold is curved. The manifold is not curved, if and only if $R^\mu_{\nu\alpha\beta} = 0$. Recall that for any vector $C^\alpha$, the curvature tensor determines the non-commutativity degree of the covariant derivatives [3]:

$$C^\alpha_{\beta;\gamma} - C^\alpha_{\gamma;\beta} = -C^\alpha R^\alpha_{\nu\beta\gamma}, \quad C^\alpha_{\beta;\gamma} = \frac{DC^\alpha}{\partial q^\nu}.$$

It is known that the curvature tensor determines the local behaviour of geodesics with respect to perturbing their initial conditions [3]. 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:

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

Introduce a vector $v^\alpha = \frac{\partial x^\alpha}{\partial \phi}$, which determines the deviation of two geodesics with slightly perturbed initial conditions. This vector satisfies the following Jacobi-Levi-Civita equation [3]:

$$\frac{D^2 v^\alpha}{ds^2} = R^\alpha_{\beta\gamma\delta} u^\beta u^\gamma v^\delta.$$

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 (46, 48) that the orthogonal component $v^\alpha_{[1]}$ satisfies the same equation (49), while the parallel component $v^\alpha_{[2]}$ satisfies the geodesic equation (48).

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. (46) 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 ±$R_{1212}$. One can check that now $R^\alpha_{\beta\gamma\delta}$ is expressed as

$$R^\alpha_{\beta\gamma\delta} = \frac{1}{2} \left[ g^\alpha_{\beta\gamma} g^\delta_{\delta\gamma} - g^\alpha_{\beta\delta} g^\delta_{\gamma\gamma} \right],$$

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

To derive Eq. (49) note that the very definitions of $u^\alpha$ and $v^\alpha$ imply $v^\beta \partial_\beta u^\alpha = u^\beta \partial_\beta v^\alpha$, which amounts to $u^\alpha_{\beta} v^\beta = v^\alpha_{\beta} u^\beta$. Now calculate directly $\frac{\partial^2 v^\alpha}{\partial s^2}$ recalling (47) and noting that $u^\alpha_{\beta} v^\beta = 0$ due to (48).
where $R$ is the scalar curvature. The latter thus determines the whole curvature tensor for the present two-dimensional situation. Substituting (50) into (49) and recalling that one can take $u_\alpha v^\alpha = 0$ in this equation, we get

$$\frac{D^2 v^\alpha}{ds^2} = -\frac{R}{2} v^\alpha (u_\beta u^\beta).$$

(52)

Note that $u_\beta u^\beta$ does not depend on $s$; see (48).

We now set to calculate the curvature tensor $R_{\alpha\nu\beta}^\mu$ for the simplest possible example, where there are only two classical coordinates $q^1, q^2$ and the quantum system has only two energy levels. 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:

$$\hat{H} = \left( q^2 q^1 - q^2 q^1 \right).$$

(53)

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

$$E_+ = \sqrt{(q^1)^2 + (q^2)^2} \equiv \rho, \quad (\rho > 0)$$

$$E_- = -\sqrt{(q^1)^2 + (q^2)^2} \equiv -\rho,$$

$$|+\rangle = \frac{1}{\sqrt{2\rho}} \left[ q^1 \sqrt{\rho-q^2} \right],$$

$$|\rangle = \frac{1}{\sqrt{2\rho}} \left[ q^1 \sqrt{\rho+q^2} - q^2 \right].$$

(54–57)

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 $|+\rangle$.

1. The ground state.

The metric reads form (40) and (54–57):

$$g_{11} = \epsilon^2 \left[ M + \frac{(q^2)^2}{4\rho^3} \right], \quad g_{22} = \epsilon^2 \left[ M + \frac{(q^1)^2}{4\rho^3} \right],$$

$$g_{12} = g_{21} = -\epsilon^2 \left( \frac{q^1 q^2}{4\rho^3} \right).$$

(58–59)

The determinant and trace of the metric read

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

(60–61)

It is seen from (58–61) 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 (44, 45, 51) and (58–61)

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

(62)

$R$ is strictly negative. Returning to (52) we see that since the metric is positively defined [see (58–61)] $u^\alpha u_\alpha$ is always non-negative. Then the negativity of $R$ in (62) implies that the geodesics are unstable with respect to small
perturbation of initial conditions, because (52) corresponds to a harmonic oscillator with an inverted (though space-dependent) frequency. This instability might have implications for the validity of the adopted adiabatic assumption, a question which we plan to study elsewhere. Note as well that $R$ is singular at $\rho = 0$, where the adiabatic energy levels cross.

2. The excited initial 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:

$$
g_{11} = \epsilon^2 \left[ M - \frac{(q^1)^2}{4\rho^3} \right], \quad g_{22} = \epsilon^2 \left[ M - \frac{(q^2)^2}{4\rho^3} \right],
$$

$$
g_{12} = g_{21} = \epsilon^2 \frac{q^1 q^2}{4\rho^3}.
$$

Hence the determinant and trace of $g$ read, respectively,

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

Since the metric (63, 65) relates to (58, 60) with transformation $M \rightarrow -M$ and $\epsilon \rightarrow i\epsilon$ ($i^2 = -1$), we get for the scalar curvature directly from (62)

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

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 (52) 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 the possibility for the particle to “tunnel” between subspaces of different signature is striking and deserves a more detailed investigation.

Since the metric tensor is not positively defined for $4M\rho^3 < 1$, (52, 67) 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 $16M\rho^3 < 1$ of $\rho$ 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 produce rather different dynamic behaviour for the classical system.

V. THIRD-ORDER POST-ADIABATIC FORCE.

We now turn to studying 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. The calculation details being presented in Appendix C, we shall quote the main result: At the order $\epsilon^3$ the non-adiabatic force acting on the classical system is still Lagrangian [see Footnote 7]:

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

$$
\mathcal{L}^{[3]}[q, \dot{q}, \ddot{q}] = \epsilon^3 \left[ f_{\alpha\beta\gamma} \dot{q}^\alpha \ddot{q}^\beta \dot{q}^\gamma - z_{\alpha\beta\gamma} \dddot{q}^\alpha \dot{q}^\beta \dot{q}^\gamma \right],
$$

---

9 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.

10 In 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 $u_\alpha u^\alpha = 0$ [3]. However, for the present classical theory with a well-defined global time $s$ nothing prohibits us to consider the class of geodesics with $u_\alpha u^\alpha < 0$. 
where $L^{[3]}$ stands for the third-order Lagrangian, and where we defined

$$f_{\alpha\beta\gamma} = 3 \left\langle n | \partial_{\alpha} n \rangle \langle N_{\beta} | N_{\alpha} \rangle + \langle \partial_{\gamma} N_{\beta} | N_{\alpha} \rangle \right\rangle,$$

$$z_{\alpha\beta} = 3 \left\langle N_{\beta} | N_{\alpha} \rangle \right\rangle,$$

$$|N_{\mu}\rangle = \sum_{k} \left( \frac{\langle k | \partial_{\mu} n \rangle}{\Delta_{nk}} \right) |k\rangle.$$

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

The total Lagrangian describing the classical system including the three-times terms will include the previous order non-adiabatic forces and the bare classical Lagrangian, $L_3[q, \dot{q}, \ddot{q}] = (39) + L^{[3]}[q, \dot{q}, \ddot{q}]$, or

$$L_3[q, \dot{q}, \ddot{q}] = -V(q) - E_{\alpha}(q) + eA_{\alpha}(q)\dot{q}_{\alpha} + \frac{e^2}{2} \left[ M\delta_{\alpha\beta} + G_{\alpha\beta}(q) \right] \dot{q}_{\alpha} \dot{q}_{\beta} + e^3 \left[ f_{\alpha\beta\gamma} q_{\alpha} q_{\beta} q_{\gamma} - z_{\alpha\beta}\dot{q}_{\alpha} \dot{q}_{\beta} \right],$$

while the equations of motion it generates is [see Footnote 7]

$$\left( \frac{d}{ds} \frac{\partial}{\partial \dot{q}_{\mu}} - \frac{d^2}{ds^2} \frac{\partial}{\partial \dot{q}_{\mu}} \right) L_3[q, \dot{q}, \ddot{q}] = 0.$$

These equations of motion contain third-order time-derivatives $q_{(3)}^{(3)}$ of coordinates, i.e., they can be written as

$$2e^3 z_{\alpha\beta}\dot{q}_{(3)}^{(3)} = \varphi_{\alpha}(q, \dot{q}, \ddot{q}).$$

Thus when $\text{det}[z_{\alpha\beta}] \neq 0$—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 (74) needs three independent (sets of) initial conditions at the initial (slow) time $s_i$: 

$$(q(s_i), \dot{q}(s_i), \ddot{q}(s_i)).$$

For an odd number $K$ of classical coordinates, one has $\text{det}[z_{\alpha\beta}] = 0$, since $z_{\alpha\beta}$ is anti-symmetric. Generically, the matrix $z_{\alpha\beta}$ will have only one eigenvalue equal to zero. Let us denote this eigenvector by $y_{\alpha}^{[0]}, y_{\alpha}^{[6]} = 0$, and let $y_{\alpha}^{[\gamma]}$ with $\gamma = 1, \ldots, K - 1$ be the eigenvector of $z_{\alpha\beta}$ with non-zero eigenvalues $\lambda^{[\gamma]}$. 11 Eq. (75) produces

$$2e^3 \lambda^{[\gamma]} y_{\alpha}^{[\gamma]} \dot{q}_{(3)}^{(3)} = y_{\alpha}^{[\gamma]} \varphi_{\alpha}(q, \dot{q}, \ddot{q}), \quad \text{for} \quad \gamma = 1, \ldots, K - 1,$$

$$0 = y_{\alpha}^{[6]} \varphi_{\alpha}(q, \dot{q}, \ddot{q}).$$

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 (78) imposes a constraint on them. Provided that $(q(s_i), \dot{q}(s_i), \ddot{q}(s_i))$ satisfy this constraint, (77) gives $K - 1$ equations for components of $q_{(3)}^{(3)}$. Another equation for components of $q_{(3)}^{(3)}$ can be obtained by differentiating (78) over time $t$ and taking $t \to t_i$.

Before closing this discussion on the initial conditions let us note the following aspect. The quantum-classical equations (2, 3) have the following well-defined initial conditions at the initial moment $t = 0$ of the fast time $t$: $(\Psi(0)), q(0)$ 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 $s_i = ct_i$ of the slow time, where $t_i$ should be still sizable larger than $t = 0$. The difference between the 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 [35]. There also exist more or less regular procedures of relating the original initial conditions to effective ones [35]. We shall not dwell into this issue anymore, because in the present paper we are interested by autonomous classical dynamics for sufficiently large (fast) times, where the precise relation with the original initial conditions is not directly relevant.

---

11 The construction described around (77, 78) 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 $\frac{1}{2} (\frac{d^2}{dt^2} - V(q, x))$. 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: $\ddot{q} = -V_{x}^{\prime}(q, x)$ and $V_{x}^{\prime}(q, x) = 0$. 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 $s \to s_i$. 
A. Kinematics.

The dependence of \( \mathcal{L}_3[q, \dot{q}, \ddot{q}] \) 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 \( \mathcal{L}_3 \) to an infinitesimal coordinate shift \( q_\mu \to q_\mu + \delta q_\mu \), where \( \delta q_\mu \) does not depend on time \([3]\):

\[
\delta \mathcal{L}_3 = \frac{\partial \mathcal{L}_3}{\partial q_\mu} \delta q_\mu = \frac{d}{ds} \left[ \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu} - \frac{d}{ds} \frac{\partial \mathcal{L}_3}{\partial \ddot{q}_\mu} \right] \tag{79}
\]

where we used (74). Thus the momentum is defined as

\[
p_\mu = \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu} - \frac{d}{ds} \frac{\partial \mathcal{L}_3}{\partial \ddot{q}_\mu}, \tag{80}
\]

implying that the equations of motion can be written as \( \dot{p}_\mu = \frac{\partial \mathcal{L}_3}{\partial q_\mu} \).

If \( \mathcal{L}_3 \) would not depend on \( q_\mu \) (which is generically not the case), the corresponding momentum \( p_\mu \) will be conserved in time. Note that \( p_\mu \) consists of the usual part \( \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu} \) and the anomalous part \(- \frac{d}{ds} \frac{\partial \mathcal{L}_3}{\partial \ddot{q}_\mu} \) that comes solely from the dependence of the Lagrangian on the acceleration. Using (73) we get for the momentum

\[
p_\mu = \epsilon A_\mu + \epsilon^2 \left[ M \dot{q}_\mu + G_{\mu\alpha\beta} \dot{q}_\alpha \dot{q}_\beta \right] + 3 \epsilon^3 f^{(sym)}_{\mu\alpha\beta} \dot{q}_\alpha \dot{q}_\beta + 2 \epsilon^3 z_{\mu\alpha} \dot{q}_\alpha \dot{q}_\mu + \epsilon^3 \left[ \partial_\gamma z_{\mu\beta} \right] \dot{q}_\gamma \dot{q}_\beta. \tag{81}
\]

where \( f^{(sym)}_{\alpha\beta\gamma} \equiv \frac{1}{6} \sum_\Pi f_{\Pi[\alpha\beta\gamma]} \) is the completely symmetrized expression (70); 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 \( \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu} \), while another half comes through the anomalous part \(- \frac{d}{ds} \frac{\partial \mathcal{L}_3}{\partial \ddot{q}_\mu} \), resulting altogether in \( 2 \epsilon^3 z_{\mu\alpha} \dot{q}_\alpha \) in (81).

The energy corresponding to the Lagrangian \( \mathcal{L}_3[q, \dot{q}, \ddot{q}] \) is obtained via looking at the total time-derivative of \( \mathcal{L}_3[q, \dot{q}, \ddot{q}] \):

\[
\frac{d}{dt} \mathcal{L}_3[q, \dot{q}, \ddot{q}] = \frac{\partial \mathcal{L}_3}{\partial q_\mu} \dot{q}_\mu + \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu} \ddot{q}_\mu + \frac{\partial \mathcal{L}_3}{\partial \ddot{q}_\mu} \dddot{q}_\mu, \tag{82}
\]

where we noted that \( \mathcal{L}_3[q, \dot{q}, \ddot{q}] \) does not have any explicit time-dependence. Employing equations of motion \( \dot{p}_\mu = \frac{\partial \mathcal{L}_3}{\partial q_\mu} \), (82) results into energy conservation:

\[
\frac{dE}{dt} = 0, \quad E \equiv p_\mu \dot{q}_\mu + \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu} \ddot{q}_\mu - \mathcal{L}_3. \tag{83}
\]

For our case the energy \( E \) reads

\[
E = \frac{\epsilon^2}{2} \left[ M \delta_{\alpha\beta} + G_{\alpha\beta} \dot{q}_\alpha \dot{q}_\beta + 2 \epsilon^3 f_{\alpha\beta\gamma} \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma + 2 \epsilon^3 z_{\mu\alpha} \dot{q}_\alpha \dot{q}_\mu + V(q) + E_n(q) \right]. \tag{84}
\]

Note that the vector-potential \( A_\alpha(q) \) expectedly drops out from the expression of energy [3]. However, the acceleration-dependent part of the Lagrangian does contribute directly into the energy. In fact, the whole third-order Lagrangian (69) is multiplied by 2 and enters into the energy.

Let us now turn to the angular momentum tensor, which is defined via the response of \( \mathcal{L}_3 \) to an infinitesimal rotation (i.e., a distance conserving linear transformation) [3]: \( q_\mu \to q_\mu + \omega_{\mu\sigma} \delta q_\sigma \), where \( \omega_{\mu\sigma} = -\omega_{\sigma\mu} \):

\[
\delta \mathcal{L}_3 = \omega_{\alpha\beta} \left[ \frac{\partial \mathcal{L}_3}{\partial q_\alpha} \ddot{q}_\beta + \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\alpha} \dddot{q}_\beta + \frac{\partial \mathcal{L}_3}{\partial \ddot{q}_\alpha} \dot{q}_\beta \right] = \omega_{\alpha\beta} \frac{d}{dt} \left[ p_\alpha \dot{q}_\beta + \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\alpha} \ddot{q}_\beta \right], \tag{85}
\]

where we again used (74). The full momentum tensor is now defined as [recalling \( \omega_{\mu\sigma} = -\omega_{\sigma\mu} \)]:

\[
M_{\alpha\beta} = p_\alpha \dot{q}_\beta - p_\beta \dot{q}_\alpha + \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\alpha} \ddot{q}_\beta - \frac{\partial \mathcal{L}_3}{\partial \ddot{q}_\alpha} \dot{q}_\beta = L_{\alpha\beta} + S_{\alpha\beta}, \tag{86}
\]
so that when $\mathcal{L}_3$ 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:

$$S_{\alpha \beta} = \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\beta} q_\alpha - \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\alpha} q_\beta = \epsilon^{\alpha \beta \gamma} \dot{q}_\gamma q_\alpha - z_{\alpha \gamma} \dot{q}_\alpha q_\beta. \quad (88)$$

In the simplest two-coordinate situation $S_{12} = -S_{21} = \epsilon^2 z_{21} (q_1^2 + q_2^2)$, which means that the spin tensor is proportional to the velocity square.

1. Zitterbewegung effect.

Now note from (80, 88, 89) and from $z_{\beta \alpha} = -z_{\alpha \beta}$ that the momentum can be written as

$$p_\mu = \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu} + \frac{d}{dt} \left[ \frac{S_{\alpha \mu} q_\alpha}{q^2} \right], \quad \dot{q}^2 \equiv \dot{q}_\beta \dot{q}_\beta, \quad (90)$$

which means that the anomalous part $p_\mu - \frac{\partial \mathcal{L}_3}{\partial \dot{q}_\mu}$ of the momentum is driven by the time-derivative of the velocity-projected spin-tensor.

An expression similar to (90)—relating the momentum to the projected time-derivative of the spin—appears in the (relativistic) Dirac electron theory; see [14] for a review. 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 [14]. In a more recent literature, the zitterbewegung effect is also derived via Lagrangians containing the higher-order derivatives of coordinates [28, 29].

There are, however, several aspects that distinguish (90) from the zitterbewegung effects already known in literature. First, we do not have a relativistic invariant theory; for us relation (90) 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 (90). Both these quantities are generically non-conserved in our situation (ultimately since the system is open), but relation (90) still holds generally due to the specific, anti-symmetric form (69) of the acceleration-dependent part of the Lagrangian.

We close this part by re-iterating 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.

B. Hamiltonian description.

Further insight into the structure of the effective classical dynamics is gained by studying its 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. Rewrite (73) as

$$\mathcal{L}_3(q, \dot{q}, \dot{\bar{q}}) = \mathcal{L}_3(q, \dot{q}) - \epsilon^3 z_{\alpha \beta} \dot{q}_\alpha \dot{q}_\beta, \quad (91)$$

where the higher-derivative term is explicitly separated out. Instead of (91) we now introduce the following extended Lagrangian:

$$\mathcal{L}(q, v, \pi) = \pi_\alpha (\dot{q}_\alpha - v_\alpha) - \epsilon^3 z_{\alpha \beta} \dot{v}_\alpha v_\beta + \mathcal{L}_3(q, v), \quad (92)$$

which is a function of three set of variables: $q = (q_1, \ldots, q_K)$, $v = (v_1, \ldots, v_K)$ and $\pi = (\pi_1, \ldots, \pi_K)$. It should be clear that if we treat $q$, $v$ and $\pi$ as coordinates, then the Lagrange equations generated by $\mathcal{L}[q, v, \pi]$ are equivalent to those generated by $\mathcal{L}_3(q, \dot{q}, \dot{\bar{q}})$. At this point $\pi$ is considered as a part of the overall set of coordinates. It may be equivalently viewed as Lagrange multipliers. If $\mathcal{L}[q, v, \pi]$ were not depend on $\dot{v}$—that is $\mathcal{L}_3(q, \dot{q}, \dot{\bar{q}})$ were not depend on $\dot{q}$—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 $\mathcal{L}[q, v, \pi]$ does depend on $\dot{v}$, it can be still Hamiltonized following to the method advocated in [31].
Once the triple $q, v, \pi$ is considered as coordinates, we introduce a separate notation for it

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

Now the Lagrangian (92) reads

$$L[Q] = A_a[Q]Q_a + H[Q], \quad H \equiv L_3[Q],$$

where the index $a$ runs from 1 to $3K$, and where $A_a = (\pi_\alpha, e^3 z_\alpha v_\beta, 0)$ is deduced from (92). As we show below, $H[Q]$ will play the role of Hamiltonian. Eq. (94) generates the following Lagrange equations of motion:

$$\Omega_{ab}(Q) \dot{Q}_b = \frac{\partial H}{\partial Q_a},$$

$$\Omega_{ab}(Q) = \frac{\partial A_a}{\partial Q_b} - \frac{\partial A_b}{\partial Q_a}.$$ 

In block-matrix notations $\Omega$ reads

$$\Omega = \begin{pmatrix} 0 & Y & I \\ -Y^T & Z & 0 \\ -I & 0 & 0 \end{pmatrix},$$

where each element in the above matrix is $K \times K$ matrix:

$$Y_{\alpha\beta} = e^3 v_\gamma \partial_\alpha z_\gamma \beta, \quad Z_{\alpha\beta} = -2e^3 z_\alpha \beta, \quad I_{\alpha\beta} = \delta_{\alpha\beta},$$

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

$$\Omega^{-1} = \begin{pmatrix} 0 & 0 & -I \\ 0 & Z^{-1} & -Z^{-1}Y^T \\ -I & Z^{-1}Y^T & Y Z^{-1}Y^T \end{pmatrix}.$$ 

For an even $K$ the matrix $Z$ is generically invertible; compare with our discussion after (74). Since $\Omega_{ab}$ is invertible, antisymmetric, closed \(^{12}\) and it satisfies (95), $\Omega_{ab}$ defines a symplectic structure [22]. Then $H[Q]$ plays the role of Hamiltonian. These two ingredients are necessary and sufficient for the Hamiltonian description [22]. In particular, for any two functions $C(Q)$ and $D(Q)$ the Poisson bracket is defined as

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

The equations of motion (95) are now written as

$$\dot{Q}_a = \{ Q_a, H[Q] \}_{PB}.$$ 

The matrix $Z$ is not invertible for an odd $K$. The Hamiltonian description in this case is still possible, but requires more care in explicitly accounting for constraints; compare with our discussion after (74).

**VI. THE FOURTH ORDER LAGRANGIAN.**

Here we briefly report 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.

\(^{12}\) Closed means that $\frac{\partial}{\partial Q_a} \Omega_{ab} + \frac{\partial}{\partial Q_b} \Omega_{ca} + \frac{\partial}{\partial Q_c} \Omega_{bc} = 0$. This feature is automatic from the definition (96), and it ensures that the Poisson brackets defined via $\Omega_{ab}$ does not change in time [22].
Following the same lines of calculation for the third order non-adiabatic force presented in Appendix C, 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

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

(102)

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

(103)

where \( q^{(3)} \) stands for the third order time derivative of \( q \), and where \( L^{[4]} \) represents the fourth-order Lagrangian. Note that the dependence on the higher-order time derivatives \( q \) and \( q^{(3)} \) is linear. The coefficients \( a, b, \) and \( d \) are given as

\[ a(q) = \sum_k \frac{\langle k \mid \partial_N \mid k \rangle^2}{\Delta_{nk}}, \]  

(104)

\[ b(q) = -\sum_k \frac{\langle k \mid \partial_q \mid n \rangle^2}{\Delta_{nk}^{-1}}, \]  

(105)

\[ w(q) = -\sum_k \frac{\langle k \mid \partial_q \mid n \rangle^2}{\Delta_{nk}^3}, \]  

(106)

where \( |N \rangle \) is given by (72): \( |N \rangle = \sum_k \frac{\langle k \mid \partial_N \mid k \rangle}{\Delta_{nk}} |k \rangle \).

Then the total Lagrangian describing the one dimensional classical system reads

\[ L_4[q, \dot{q}, \ddot{q}, q^{(3)}] = -V(q) - E_n(q) + \frac{\epsilon^2}{2} (M + G) q^2 + \epsilon^4 \left( a\dot{q}^4 + b\ddot{q}^2 + wq q^{(3)} \right), \]  

(107)

where the first and the third order terms vanish due to the assumption of real eigenstates of the quantum system, and where \( a, b, \) and \( w \) are given by (104)-(106) and \( G \) is defined as

\[ G = -2\sum_k \frac{\langle n \mid \partial_q \mid k \rangle^2}{\Delta_{nk}}. \]  

(108)

The kinematics of this Lagrangian can be developed along the same lines as in the previous section.

**VII. 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 following facts were known for this problem: (1.) In the order \( \epsilon^0 \) the effective Lagrangian differs from the bare one by the Born-Oppenheimer potential energy. (2.) Berry and Robbins have shown that the \( \epsilon \)-force term in the effective Lagrangian corresponds to a magnetic field, which is related to the geometric phase [5]. (3.) Weigert and Littlejohn and Goldhaber have recently shown that in the order \( \epsilon^3 \) the effective Lagrangian gets an additional kinetic energy term, which is a second-order polynomial over the classical velocities [6, 7].

In this work we obtain the following new results.

**i)** The post-adiabatic reaction force is proved to be Lagrangian up to the fifth order in \( \epsilon \). We conjecture that at every order of \( \epsilon \) the effective dynamics of the classical system can be derived form a Lagrangian.

**ii)** 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). We also explained that this result does not depend on the quantum character of the fast system, and will be present as well if the fast system is classical and integrable [in the sense of [22]].

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; see our discussion around (75–78). 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.

iii) We also found interesting results for the classical autonomous dynamics within the order $\epsilon^2$, where the motion generated by the effective classical Lagrangian can be mapped 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 and etc. This result deserves a careful elaboration.

Acknowledgments

We are grateful to Armen Nersissian for several discussions and for explaining us the Hamiltonization procedure given in section V B. Ruben Manvelian is acknowledged for making several critical remarks. Last but not least, we thank Theo Nieuwenhuizen for his kind support.

[1] Yu. L. Klimontovich, Statistical Theory of Open Systems (Kluwer, Dordrecht 1997).
[2] U. Weiss, Quantum Dissipative Systems (World Scientific, 1993).
[3] L. D. Landau and E.M. Lifshitz, The Classical Theory of Fields (Elsevier Science, 1980).
[4] H. Essen, Eur. J. Phys. 30, 515 (2009).
[5] M. V. Berry and J. M. Robbins, Proc. R. Soc. Lond. A, 442, 659 (1993).
[6] A. S. Goldhaber, Phys. Rev. A, 71, 062102 (2005).
[7] S. Weigert and R. G. Littlejohn, Phys. Rev. A, 47, 3506 (1993).
[8] C. Jarzynski, Phys. Rev. Lett. 74, 2937 (1995).
[9] A. Krakovsky and J. L. Birman, Phys. Rev. A, 51, 50 (1995).
[10] A.O. Barut and A. J. Bracken, Phys. Rev. D, 23, 2454 (1981).
[11] B. Sundaram and P. W. Milonni, Phys. Rev. E, 51, 1971 (1995).
[12] L. Diosi et al., Phys. Rev. A 61, 022108 (2000).
[13] M. Plyushchay, Phys. Lett. B 243, 383 (1990).

References
APPENDIX A: ON THE DERIVATION OF THE QUANTUM-CLASSICAL DYNAMICS

The argument follows basically to [19, 32]. Let we are given a two-degrees-of-freedom quantum system with Hamiltonian 
\[ \frac{p^2}{2M} + V(q) + H(q, x) + \frac{\pi^2}{2M}, \]
where \( q \) and \( x \) are operator coordinates, and where \( p \) and \( \pi \) are operator momenta. For simplicity we shall assume that the initial state is factorized over these two degrees of freedom.

The Heisenberg equation generated by this Hamiltonian read:
\[ \frac{dq}{dt} = \frac{p}{M}, \]
\[ \frac{dp}{dt} = -V'(q) - H'_q(q, x), \]
\[ \frac{dx}{dt} = \frac{\pi}{m}, \]
\[ \frac{d\pi}{dt} = -H'_x(q, x). \]

Now the motion of the \( (p, q) \) degree of freedom is separated into two part:
\[ p(t) = \overline{p}(t) + p_f, \quad q(t) = \overline{q}(t) + q_f, \]
where \( \overline{p}(t) \) and \( \overline{q}(t) \) are the averages over the initial state, and where \( p_f \) and \( x_f \) are the fluctuations. By definition these operators satisfy
\[ p_f = q_f = 0. \]

We now substitute (A5) into (A1, A2, A4) and expand (A2, A4) over the small \( q_f \):
\[ \frac{d\overline{q}}{dt} + \frac{dq_f}{dt} = \frac{\overline{p}}{M} + \frac{p_f}{M}, \]
\[ \frac{d\overline{q}}{dt} + \frac{dp_f}{dt} = -V'(\overline{q}) - H'_q(\overline{q}, x) - V''(\overline{q})q_f - H''_{qq}(\overline{q}, x)q_f + O(q_f^2), \]
\[ \frac{d\pi}{dt} = -H'_x(\overline{q}, x) - H''_{qx}(\overline{q}, x)q_f + O(q_f^2). \]

Averaging these equations over the initial state we obtain
\[ \frac{d\overline{q}}{dt} = \frac{\overline{p}}{M}, \]
\[ \frac{d\overline{q}}{dt} = -V'(\overline{q}) - H'_q(\overline{q}, x) - H''_{qq}(\overline{q}, x)q_f + O(q_f^2), \]
\[ \frac{d\pi}{dt} = -H'_x(\overline{q}, x) - H''_{qx}(\overline{q}, x)q_f + O(q_f^2). \]
If in (A11, A12) the terms proportional to $O(q_f)$ are neglected we get into a quantum-classical equations, where (7,7) is the classical degree of freedom. If, however, there are physical reasons to expect that the initial state will remain factorized over the considered range of times [see 10 for a detailed discussion of such situations], then we have to neglect only terms $O(q^2_f)$, because the terms $O(q_f)$ drop out due to (A6).

APPENDIX B: ADIABATIC PERTURBATION THEORY.

Here we outline the adiabatic perturbation theory as developed in [23, 24]. This appendix is completely self-contained and can be read independently from the main text.

Consider the non-stationary Schrödinger equation

$$i\hbar \partial_t |\Psi(t)\rangle = H(\epsilon t)|\Psi(t)\rangle,$$  \hspace{1cm} (B1)

where $\hbar = 1$, $\epsilon \ll 1$ is a small parameter, and where $H(\epsilon t)$ is the slowly changing Hamiltonian. Let us define

$$s = \epsilon t,$$  \hspace{1cm} (B2)

for the slow time. Let $E_n(s)$ and $|n(s)\rangle$ be the adiabatic eigen-energies and eigenvectors, respectively:

$$H(s)|n(s)\rangle = E_n(s)|n(s)\rangle,$$  \hspace{1cm} (B3)

We assume that the adiabatic energy spectrum is non-degenerate for all $s$. Let us also assume for simplicity that the system starts from the initial state equal to one of the adiabatic eigen-states:

$$|\Psi(0)\rangle = |n(0)\rangle.$$  \hspace{1cm} (B4)

The first step in any adiabatic approach is to separate the slowly changing quantities from the fast ones. To this end we look for the solution of (B1) as

$$|\Psi(\epsilon, t)\rangle = |\psi_n(\epsilon, s)\rangle e^{i\alpha_n(t)}, \hspace{1cm} \alpha_n(t) \equiv -\int_0^t \mathrm{d}\tilde{t} E_1(\epsilon \tilde{t}),$$  \hspace{1cm} (B5)

where $\alpha_n(t)$ is the dynamical phase. It is clear that $e^{i\alpha_n(t)}$ changes fast, i.e., as $\sim e^{i/\epsilon}$, for slow times $s$. Putting (B5) into (B1) we get

$$i\epsilon \dot{|\psi_n(\epsilon, s)\rangle} = [H(s) - E_n(s)]|\psi_n(\epsilon, s)\rangle,$$  \hspace{1cm} (B6)

where dot means differentiation over $s$. Now we expand the slow wave-function, $\psi_n(\epsilon, s)$, over $\epsilon$

$$|\psi_n(\epsilon, s)\rangle = e^{i\gamma_n(s)} \left[ |n(s)\rangle + \epsilon |n_1(s)\rangle + \epsilon^2 |n_2(s)\rangle + \ldots \right],$$  \hspace{1cm} (B7)

where

$$\gamma_n(s) = i \int_0^s \mathrm{d}u \langle n(s)|\dot{n}(u)\rangle,$$  \hspace{1cm} (B8)

is the Berry phase factor. We separated it out to facilitate further calculations.

Substituting power series expansion (B7) into (B6) and comparing terms of equal order of $\epsilon$, we get

$$0 = (H - E_n) |n\rangle,$$  \hspace{1cm} (B9)

$$i|\dot{n}\rangle - i\langle n|\dot{n}\rangle |n\rangle = (H - E_n) |n_1\rangle,$$  \hspace{1cm} (B10)

$$i|\dot{n}_1\rangle - i\langle n_1|\dot{n}\rangle |n_1\rangle = (H - E_n) |n_2\rangle,$$  \hspace{1cm} (B11)

$$\vdots$$

Eq. (B9) holds automatically. To solve the higher order equations we introduce the projection operators $P$ and $Q$:

$$P = |n\rangle\langle n|, \hspace{1cm} Q = \sum_k |k\rangle\langle k|,$$  \hspace{1cm} (B12)

$$P + Q = 1, \hspace{1cm} PQ = QP = 0.$$  \hspace{1cm} (B13)
where \( \sum_k \) means the term \( k = n \) is excluded from the summation \( \sum_{k=1}^{d} \).

Operating \( Q \) from left to the both sides of (B10), we get

\[
i \sum_k' |k\rangle \langle k| = \sum_k' \Delta_{kn} |k\rangle \langle k|, \quad \Delta_{kn} \equiv E_k - E_n. \tag{B14}
\]

Since \( \Delta_{k \neq n} \) is non-zero [energy levels are not degenerate], we get

\[
\langle k|n_1 \rangle \equiv c_{kn}^{[1]} = -i \langle k|\dot{n} \rangle \Delta_{nk}. \tag{B15}
\]

This determines \( Q|n_1 \rangle \), but we still have to find \( P|n_1 \rangle \). Let us define

\[
|n_1 \rangle = c_{nn}^{[1]} |n \rangle + |n_1^+ \rangle, \tag{B16}
\]

\[
|n_1^+ \rangle \equiv \sum_k' c_{kn}^{[1]} |k\rangle, \tag{B17}
\]

\[
c_{nn}^{[1]} \equiv \langle n|n_1 \rangle, \tag{B18}
\]

where \( c_{nn}^{[1]} \) has to be found. To this end we multiply both sides of (B11) from left by \( P \) [recall that (B11) is obtained from \( \epsilon^2 \) term in expansion (B7)]

\[
\langle n|\dot{n}_1 \rangle = \langle n|n_1 \rangle \langle n|\dot{n} \rangle, \tag{B19}
\]

where \( \dot{n}_1 \) is found from (B16):

\[
\dot{n}_1 = c_{nn}^{[1]} |n \rangle + c_{nn}^{[1]} |\dot{n} \rangle + |n_1^+ \rangle. \tag{B20}
\]

Using (B19) we get

\[
c_{nn}^{[1]}(s) = -\langle n(s)|\dot{n}_1^+(s) \rangle, \tag{B21}
\]

which together with (B4) solves as

\[
c_{nn}^{[1]}(s) = -\int_0^s du \langle n(u)|\dot{n}_1^+(u) \rangle = -i \sum_k' \int_0^s du \frac{|\langle k(u)|\dot{n}(u) \rangle|^2}{\Delta_{nk}(u)}. \tag{B22}
\]

It is seen that \( c_{nn}^{[1]}(s) \) is purely imaginary.

Analogous argument gives the higher order non-adiabatic corrections \( |n_m(s) \rangle, (m > 1) \) in (B7)

\[
|n_m \rangle = \sum_k' c_{km}^{[m]}|k \rangle + c_{nn}^{[m]} |n \rangle, \tag{B23}
\]

\[
c_{kn}^{[m]} = \frac{i \langle n|\dot{n} \rangle c_{k\neq n}^{[m-1]} - i \langle k|\dot{n}_{m-1} \rangle}{\Delta_{nk}}, \tag{B24}
\]

\[
c_{nn}^{[m]} = -\sum_k' \int_0^s du c_{kn}^{[m]}(u) \langle n(u)|\dot{k}(u) \rangle. \tag{B25}
\]

Altogether \( |\psi_n(\epsilon, s) \rangle \) in (B7) can be written as

\[
|\psi_n(\epsilon, s) \rangle = e^{i\gamma_n(s)} \sum_k c_{kn}|k \rangle, \tag{B26}
\]

\[
c_{kn} = \delta_{kn} + c_{kn}^{[1]} + \epsilon^2 c_{kn}^{[2]} + \cdots. \tag{B27}
\]

Some relations between coefficients \( c_{kn} \) can be uncovered without knowing their explicit form, but rather looking at the normalization condition:

\[
\sum_k |c_{nk}|^2 = 1, \tag{B28}
\]

which should be satisfied at each order of \( \epsilon \). For the first two orders

\[
|c_{nn}|^2 = 1 + 2\epsilon \Re\{c_{nn}^{[1]} \} + 2\epsilon^2 \Re\{c_{nn}^{[2]} \} + \epsilon^2 |c_{nn}^{[1]}|^2 + \mathcal{O}(\epsilon^3), \tag{B29}
\]

\[
|c_{nn}|^2 + |c_{nn}^{[1]}|^2 |c_{nn}^{[2]}|^2 + \cdots + \mathcal{O}(\epsilon^3).
\]
which brings in the following two relations in the orders $\epsilon$ and $\epsilon^2$, respectively,

$$\Re\{c_{nn}^{[1]}\} = 0,$$
$$2\Re\{c_{nn}^{[2]}\} + |c_{nn}^{[1]}|^2 + \sum_k |c_{kn}^{[1]}|^2 = 2\Re\{c_{nn}^{[2]}\} + \langle n_1|n_1 \rangle = 0.$$

(B30)\hspace{1cm} (B31)

Let us work out explicitly the second-order coefficient $c_{k\neq n}^{[2]}(s)$. Using in (B27), $\langle k|\hat{n}_1 \rangle = \frac{d}{ds}\langle k|n_1 \rangle - \langle k|n_1 \rangle$ we get

$$c_{k\neq n}^{[2]}(s) = c_{k\neq n}^{[1]}(s)c_{nn}^{[1]}(s) + \frac{i}{\Delta n_k(s)} c_{k\neq n}^{[1]} \left( \langle n|\hat{n}_1 \rangle - \langle k|\hat{k} \rangle \right) - \frac{d}{ds} \left[ c_{k\neq n}^{[1]} \right] + \sum_l (l\neq k) c_{l\neq n}^{[1]} \langle k|l \rangle .$$

(B32)

1. Precision of the adiabatic approximation

An important problem of precision of the adiabatic approximation was studied in [23, 33, 34]. Simplifying previous results on this problem, Hagedorn and Joye have proven the following result [23]. Following to (B7) let us define

$$|\psi^N(\epsilon, s)\rangle = e^{i\gamma_n(s)} \sum_{k=0}^N c_k|n_k(s)\rangle.$$

(B33)

Let $\{a\}$ define the integer part of a real number $a$, and let we are given a positive number $g$. Then it is shown that [23]:

$$\left| |\psi^{\lfloor g/\epsilon \rfloor}(\epsilon, s)\rangle - |\psi_{\text{exact}}(\epsilon, s)\rangle \right| \leq C(g)e^{-\Gamma(g)/\epsilon},$$

(B34)

where $|\psi_{\text{exact}}(\epsilon, s)\rangle$ is the exact solution of the original equation (B6) $|\psi^{\lfloor g/\epsilon \rfloor}(\epsilon, 0)\rangle = |\psi_{\text{exact}}(\epsilon, 0)\rangle$ at the initial time, and where $C(g)$ and $\Gamma(g)$ are bounded positive functions of $g$. This results implies that the precision of the adiabatic approximation is exponential over $\epsilon$.

APPENDIX C: CALCULATION OF THE THIRD-ORDER POST-ADIABATIC FORCE.

Within the present Appendix $\sum'_k$ means $\sum_{k=1, k\neq n}^d$, and $\dot{A} = A' = \frac{4\Delta}{ds}$, where $s$ is the slow time.

The third-order post-adiabatic force is given by (28), where for $\langle \phi_n|H|\phi_n \rangle - E_n$ we should employ (30) and then (22), while for $\Im\partial_{\mu} \phi_n \phi_n^*$ we directly use (20). Having done these, we select terms $\propto \epsilon^3$ and end up with

$$\frac{F^{[3]}}{2} = \partial_\mu \sum_k \Delta kn \Re\{c_{kn}^{[2]}c_{kn}^{[1]^*}\} + \frac{d}{ds} \Im\partial_{\mu} n_1 n_2 + \partial_{\mu} \Im\langle n_2|n' \rangle + \Im\partial_{\mu} \langle n_1|n' \rangle$$

$$= \frac{d}{ds} \Im\langle n_2|n_1 \rangle + \partial_{\mu} \Im\langle c_{kn}^{[2]}c_{kn}^{[1]^*} \langle n|n' \rangle \rangle + \Im\partial_{\mu} \langle n_1|n' \rangle ,$$

(C1)\hspace{1cm} (C2)

where we additionally employed (B15) and $|n_2| = c_{nn}^{[2]}|n| + \sum_k c_{kn}^{[2]}|k|$ when going from (C1) to (C2).

Looking at (B32) we introduce the following notation

$$c_{k\neq n}^{[2]} = c_{kn}^{[1]}c_{nn}^{[1]} + c_{k\neq n}^{[2]}.$$ \hspace{1cm} (C3)

Using (B31) we exclude $\Re c_{nn}^{[2]}$ and get

$$\frac{F^{[3]}}{2} = -\Im\langle [\partial_{\mu} n|n' \rangle \langle n_1|n_1 \rangle - \frac{1}{2} \Im\langle [\partial_{\mu} n|n \rangle \frac{d}{ds} \langle n_1|n_1 \rangle - \frac{1}{2} \Im\langle [n|n' \rangle \partial_{\mu} \langle n_1|n_1 \rangle$$

$$+ \Im\partial_{\mu} \langle n_1|n_1 \rangle + \frac{d}{ds} \Im\sum_k [\partial_{\mu} n|k \rangle \langle n_1|n_1 \rangle \rangle .$$

(C4)\hspace{1cm} (C5)

Let us denote:

$$|n_1\rangle = c_{nn}^{[1]}|n| + |n_1^+\rangle.$$ \hspace{1cm} (C6)
Using this notation and expanding $\Im(\partial_{n_1} n_1')$ we get after some algebraic steps that all non-local terms in (C4, C5) are cancelled out. This means that (C4, C5) are written as

$$\frac{F^{[3]}}{2} = -\Im [(\partial_{n_1} n_1') \langle n_1^+ | n_1^+ \rangle - \frac{1}{2} \Im [(\partial_{n_1} n_1) \frac{d}{ds} n_1^+ | n_1^+ \rangle] - \frac{1}{2} \Im [(n | n') \partial_{n_1} n_1^+ | n_1^+]$$

$$+ \Im (\partial_{n_1} n_1^+ | n_1^+ \rangle + \frac{d}{ds} \Im \sum_k \langle k | n \rangle (\partial_{n_1} n_1 | k \rangle).$$

(C7)

Using (B32) (C7, C8) can be represented as

$$\frac{F^{[3]}}{2} = -\frac{1}{2} \frac{d}{ds} \Im (\langle n | \partial_{n_1} n \rangle \langle n_1^+ | n_1^+ \rangle) - \frac{1}{2} \partial_{n_1} \Im (\langle n | n' \rangle \langle n_1^+ | n_1^+ \rangle) + \frac{d}{ds} \Im \sum_k \langle k | n \rangle (\partial_{n_1} n_1 | k \rangle)$$

$$+ \Im (\partial_{n_1} n_1^+ | n_1^+ \rangle + \frac{d}{ds} \Im \sum_k \langle k | n \rangle (\partial_{n_1} n_1 | k \rangle).$$

(C9)

After some algebra one can show that (C9) can be generated by a Lagrangian

$$(C9) = \left( \frac{d}{ds} \partial_{\tilde{q}_1} - \frac{\partial}{\partial \tilde{q}_1} \right) \frac{1}{3} h_{\alpha \beta \gamma} \tilde{q}_\alpha \tilde{q}_\beta \tilde{q}_\gamma,$$

(C11)

where

$$h_{\alpha \beta \gamma} = \frac{1}{2} \Im (\langle n | \partial_{n_1} n \rangle) \Re (\langle N_\alpha | N_\beta \rangle) + \frac{1}{2} \Im (\langle n | \partial_{n_1} n \rangle) \Re (\langle N_\alpha | N_\beta \rangle) + \frac{1}{2} \Im (\langle n | \partial_\beta n \rangle) \Re (\langle N_\alpha | N_\beta \rangle).$$

(C12)

Here we defined

$$| n_1^+ \rangle = -i \tilde{q}_\alpha | N_\alpha \rangle, \quad | N_\mu \rangle = \sum_k \frac{\langle k | n \rangle}{\Delta_{nk}} | k \rangle,$$

(C13)

Recall that an implicit summation is carried over indices $\alpha, \beta$ and $\gamma$. Note that $h_{\alpha \beta \gamma}$ is symmetric with respect to any permutation of indices $\alpha, \beta$ and $\gamma$, so that

$$\frac{1}{3} h_{\alpha \beta \gamma} \tilde{q}_\alpha \tilde{q}_\beta \tilde{q}_\gamma = \frac{1}{2} \Im (\langle n | \partial_{n_1} n \rangle) \Re (\langle N_\alpha | N_\beta \rangle) \tilde{q}_\alpha \tilde{q}_\beta \tilde{q}_\gamma.$$

(C14)

We now work out (C10): Then

$$\Im \left[ \sum_k \langle k | n \rangle (\partial_{n_1} n_1 | k \rangle) \right] = \Im \left[ \Im \sum_k \langle k | n \rangle (\partial_{n_1} n_1 | k \rangle) \right] = -\Im \left[ \langle N_\mu | N_\alpha \rangle \tilde{q}_\alpha + \tilde{q}_\alpha \tilde{q}_\beta \langle N_\mu | \partial_{\beta} N_\alpha \rangle \right],$$

(C15)

$$\Im (\partial_{n_1} n_1^+ | n_1^+ \rangle + \frac{d}{ds} \Im \sum_k \langle k | n \rangle (\partial_{n_1} n_1 | k \rangle).$$

(C16)

Combining together (C17, C18) we get

$$\frac{d}{ds} \Im [\langle N_\beta | N_\alpha \rangle \tilde{q}_\alpha \tilde{q}_\beta + \langle \partial_{\beta} N_\alpha | \partial_{\alpha} N_\beta \rangle]$$

(C19)

We define

$$z_{\alpha \beta} \equiv \frac{1}{2} \Im \langle N_\beta | N_\alpha \rangle$$

(C22)
and write

\[
(C20) + (C21) = \left[ \frac{d^2}{ds^2} \frac{\partial}{\partial \dot{q}_\mu} - \frac{d}{ds} \frac{\partial}{\partial q_\mu} + \frac{\partial}{\partial q_\mu} \right] z_{\alpha\beta} \dot{q}_\alpha \dot{q}_\beta
\]  
(C23)

\[+ \dot{q}_\alpha \dot{q}_\beta \frac{1}{2} \Im \left\{ \langle \partial_\beta N_\mu | N_\alpha \rangle + \langle \partial_\beta N_\alpha | N_\mu \rangle + \langle \partial_\alpha N_\beta | N_\mu \rangle + \langle \partial_\alpha N_\mu | N_\beta \rangle + \langle \partial_\mu N_\alpha | N_\beta \rangle + \langle \partial_\mu N_\beta | N_\alpha \rangle \right\} \]  
(C24)

\[+ \dot{q}_\alpha \dot{q}_\beta \Im \left[ \partial_\gamma (\partial_\beta N_\alpha | N_\mu \rangle + \langle \partial_\mu N_\beta | \partial_\gamma N_\alpha \rangle - \frac{1}{2} \partial_\gamma^2 \langle N_\beta | N_\mu \rangle \right], \]  
(C25)

where in obtaining (C24) we employed:

\[
\Im \langle \partial_\beta N_\mu | N_\alpha \rangle = \frac{1}{2} \Im \langle \partial_\beta N_\mu | N_\alpha \rangle + \frac{1}{2} \Im \langle \partial_\beta N_\mu | N_\alpha \rangle
\]  
(C26)

\[
= \frac{1}{2} \Im \langle \partial_\beta N_\mu | N_\alpha \rangle - \frac{1}{2} \Im \langle N_\alpha | \partial_\beta N_\mu \rangle
\]  
(C27)

\[
= \frac{1}{2} \Im \langle \partial_\beta N_\mu | N_\alpha \rangle + \frac{1}{2} \Im \langle \partial_\beta N_\alpha | N_\mu \rangle + \frac{1}{2} \Im \langle \partial_\beta N_\mu | N_\alpha \rangle.
\]  
(C28)

The quantity inside of the square brackets in (C24) is symmetric with respect to permutation of indices \(\mu, \alpha\) and \(\beta\). We now define

\[
\lambda_{\alpha\beta\gamma} = \frac{1}{4} \Im \left\{ \langle \partial_\beta N_\gamma | N_\alpha \rangle + \langle \partial_\beta N_\alpha | N_\gamma \rangle + \langle \partial_\alpha N_\gamma | N_\beta \rangle + \langle \partial_\alpha N_\beta | N_\gamma \rangle + \langle \partial_\gamma N_\alpha | N_\beta \rangle + \langle \partial_\gamma N_\beta | N_\alpha \rangle \right\}
\]  
(C29)

\[
\lambda_{\alpha\beta\gamma} \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma = \frac{6}{4} \Im \left\{ \langle \partial_\alpha N_\beta | N_\gamma \rangle \right\}
\]  
(C30)

and obtain

\[
(C24) + (C25) = \left[ \frac{d}{ds} \frac{\partial}{\partial \dot{q}_\mu} - \frac{\partial}{\partial \dot{q}_\mu} \right] \frac{1}{3} \lambda_{\alpha\beta\gamma}
\]  
(C31)

\[+ \dot{q}_\alpha \dot{q}_\beta \Im \left[ \partial_\gamma (\partial_\beta N_\alpha | N_\mu \rangle + \langle \partial_\mu N_\beta | \partial_\gamma N_\alpha \rangle - \frac{1}{2} \partial_\gamma^2 \langle N_\beta | N_\mu \rangle \right] \]  
(C32)

\[+ \frac{1}{2} \partial_\beta \langle \partial_\alpha N_\beta | N_\gamma \rangle - \frac{1}{2} \partial_\gamma \langle \partial_\alpha N_\beta | N_\mu \rangle - \frac{1}{2} \partial_\gamma \langle \partial_\beta N_\alpha | N_\mu \rangle - \frac{1}{2} \partial_\gamma \langle \partial_\mu N_\alpha | N_\beta \rangle \]  
(C33)

Working out (C32, C33) we finally obtain:

\[(C32) + (C33) = 0. \]  
(C34)

Thus the third-order post-adiabatic force is purely Lagrangian (though containing higher-order derivatives):

\[
\frac{F^{[3]}}{2} = \left( \frac{d}{ds} \frac{\partial}{\partial \dot{q}_\mu} - \frac{d^2}{ds^2} \frac{\partial}{\partial q_\mu} - \frac{\partial}{\partial q_\mu} \right) \left[ \frac{1}{3} (\delta_{\alpha\beta\gamma} + \lambda_{\alpha\beta\gamma}) \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma - \frac{1}{2} \partial_{\alpha\beta\gamma} \dot{q}_\alpha \dot{q}_\beta \dot{q}_\gamma \right]. \]  
(C35)