Induced geometry in quantum-classical systems from adiabatic perturbation theory

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Geometry in effective dynamics

Slow dynamics from fast–slow systems

Two vastly different time scales, weakly coupled — but weak couplings accumulate over time.

- Huygens' clocks synchronise.
- The swing plane of Foucault's pendulum slowly rotates.

Integrating Newton's law directly is possible but

- computationally costly.
- unilluminating: it does not explain why the slow motion looks the way it does.

Goal

Eliminate fast variables & obtain a closed set of effective equations of motion for slow ones.

Reduced descriptions repeatedly turn out to be geometric:

- Foucault's swing plane $\leftrightarrow$ parallel transport on a sphere.
- Molecular nuclei feel the Berry–Mead–Truhlar gauge potential / induced Riemannian metric.
- Slowly driven (adiabatic) quantum states acquire the Berry phase.

Observation

Geometry from low-order adiabatic approximations is well understood.
The geometry of higher-order approximations is almost completely unexplored.

This talk: push the expansion to third order — meet a new geometry, beyond Riemann.
Potential future application: efficient calculation of response properties in materials.

Quick summary of results

Mixed quantum–classical system (e.g. electrons and nuclei)
$\longrightarrow$ adiabatically eliminate the quantum part, order by order in a parameter ϵ.

order	effective force	induced geometry
ϵ^0	Born–Oppenheimer $-\partial_\mu \mathrm{E_n}$	potential on $\mathcal{M}$
ϵ^1	Berry–Lorentz force	gauge field A_μ
ϵ^2	mass renormalisation	Riemannian $(\mathrm{M}^\star_{\mu\nu})$
ϵ^3	jerk: depends on $\dddot{\mathrm{x}}$	Kawaguchi (KL^2)

The third order results in an equation of motion which is third order in time.
It induces Kawaguchi geometry — arc length depending on acceleration, not just velocity.

Quantum–classical dynamics

Classical (nuclear) coordinates $\mathrm{x}^\mu(\mathrm{t})$, $\mu = 1, \dots, \mathrm{N}$ — on a (parameter) manifold $\mathcal{M}$.
Quantum (electronic) state $|\psi(\mathrm{t})\rangle$ with Hamiltonian $\mathrm{H}(\mathrm{x})$ depending parametrically on x.

Action

$$\mathrm{S}[\mathrm{x}, |\psi\rangle] = \int \mathrm{d}\mathrm{t} \left[\tfrac{1}{2} \mathrm{M}_{\mu\nu}(\mathrm{x})\, \dot{\mathrm{x}}^\mu \dot{\mathrm{x}}^\nu + \langle\psi| \Big(\mathrm{i} \tfrac{\mathrm{d}}{\mathrm{d}\mathrm{t}} - \mathrm{H}(\mathrm{x}) \Big) |\psi\rangle \right]$$

$\mathrm{M}_{\mu\nu}(\mathrm{x})$: the bare mass tensor = a Riemannian metric on $\mathcal{M}$.

Euler–Lagrange equations ⇒ Ehrenfest molecular dynamics equations:

$$\mathrm{M}_{\mu\nu}\, \mathrm{a}^\nu = -\langle\psi|\partial_\mu \mathrm{H}|\psi\rangle, \qquad \mathrm{i} \tfrac{\mathrm{d}}{\mathrm{d}\mathrm{t}} |\psi\rangle = \mathrm{H}(\mathrm{x})|\psi\rangle.$$

RHS: the force. LHS: the acceleration vector, built with the Levi-Civita connection for M,

$$\mathrm{a}^\mu = \ddot{\mathrm{x}}^\mu + \mathring{\Gamma}^\mu_{\nu\rho}[\mathrm{M}]\, \dot{\mathrm{x}}^\nu \dot{\mathrm{x}}^\rho, \qquad \mathring{\Gamma}^\mu_{\nu\rho}[\mathrm{M}] = \tfrac{1}{2} \mathrm{M}^{\mu\sigma} \big(\partial_\nu \mathrm{M}_{\sigma\rho} + \partial_\rho \mathrm{M}_{\sigma\nu} - \partial_\sigma \mathrm{M}_{\nu\rho} \big).$$

Task: reduce these two coupled equations to a single effective equation for x^μ.

Adiabatic perturbation theory & quantum geometry

APT: method to approximate quantum systems with slowly-varying t-dependent Hamiltonians. Nuclei are slow because they are heavy.

Introduce a (dimensionless) adiabatic parameter ϵ, controlling the accuracy of approximations. An approximate solution $|\psi^{\mathrm{approx,p}}\rangle$ is a pth-order adiabatic approximation to the actual $|\psi\rangle$ if

$$\lim_{\epsilon\to 0} \frac{1}{\epsilon^{\mathrm{p}}} \, |||\psi^{\mathrm{approx,p}}\rangle - |\psi\rangle|| = 0\,.$$

Scale the mass tensor $\mathrm{M}_{\mu\nu} \to \epsilon^{-2}\mathrm{M}_{\mu\nu}$ and pass to "slow time" $\mathrm{t}' = \epsilon\mathrm{t}$.
The Schrödinger equation becomes singularly perturbed, (Newton's law stays the same,)

$$\mathrm{i}\,\epsilon\,\tfrac{\mathrm{d}}{\mathrm{dt}'}|\psi\rangle = \mathrm{H}(\mathrm{x})|\psi\rangle.$$

Different in scope from ordinary perturbation theory (weakness vs. slowness.)

The zeroth order adiabatic approximation to the Schrödinger equation, $|\psi^{\mathrm{approx},0}\rangle$:

Berry's zeroth-order solution

$$|\psi^{\mathrm{approx},0}\rangle = \mathrm{e}^{\,\mathrm{i}\epsilon^{-1}\phi(\mathrm{t})}\,\mathrm{e}^{\,\mathrm{i}\gamma(\mathrm{t})}\,|\mathrm{n}\rangle, \qquad \mathrm{H}(\mathrm{x})|\mathrm{n}\rangle = \mathrm{E}_\mathrm{n}(\mathrm{x})|\mathrm{n}\rangle.$$

$|\mathrm{n}\rangle = |\mathrm{n}(\mathrm{x})\rangle$ is the normalized nth eigenstate of $\mathrm{H} = \mathrm{H}(\mathrm{x})$, $\langle \mathrm{n}|\mathrm{n}\rangle = 1$ (adiabatic eigenstates.)
The solution contains the dynamical and geometric phases:

$$\phi(\mathrm{t}) = -\int_{\mathrm{t}_0}^{\mathrm{t}} \mathrm{ds}\,\mathrm{E}_\mathrm{n}(\mathrm{x}(\mathrm{s})), \qquad \gamma(\mathrm{t}) = \int_{\mathrm{t}_0}^{\mathrm{t}} \mathrm{ds}\,\mathrm{A}_\mu \frac{\mathrm{dx}^\mu}{\mathrm{ds}}, \qquad \boxed{\mathrm{A}_\mu = \mathrm{i}\langle \mathrm{n}|\partial_\mu \mathrm{n}\rangle}$$

A_μ: Berry–Mead–Truhlar connection on a principal circle bundle over $\mathcal{M}$. Berry curvature:

$$\mathrm{B}_{\mu\nu} = \partial_\mu \mathrm{A}_\nu - \partial_\nu \mathrm{A}_\mu.$$

Splitting $\partial_\mu|\mathrm{n}\rangle$ into horizontal + vertical parts gives the gauge-covariant derivative (hor)

$$\mathrm{D}_\mu = \partial_\mu + \mathrm{i}\mathrm{A}_\mu\,, \qquad \langle \mathrm{n}|\mathrm{D}_\mu \mathrm{n}\rangle = 0\,.$$

Physical states live in the ray space; a (Hermitian) metric measuring the distance between them.

Definition

$$\mathrm{h}_{\mu\nu} = \langle \mathrm{D}_\mu \mathrm{n} | \mathrm{D}_\nu \mathrm{n} \rangle = \mathrm{g}_{\mu\nu} - \tfrac{\mathrm{i}}{2} \mathrm{B}_{\mu\nu}.$$

Real part $\mathrm{g}_{\mu\nu}$:
a Riemannian metric.

Imaginary part $\mathrm{B}_{\mu\nu}$:
the Berry curvature.

It is the pullback of the Fubini–Study metric of $\mathbb{P}\mathcal{H}$ under $\psi : \mathcal{M} \to \mathbb{P}\mathcal{H}$,

$$\mathrm{ds}^2_{\mathrm{FS}} = \langle \mathrm{d}\psi | \mathrm{d}\psi \rangle - |\langle \psi | \mathrm{d}\psi \rangle|^2, \qquad \mathrm{h}_{\mu\nu} = \psi^* (\mathrm{h}^{\mathrm{FS}})_{\mu\nu}.$$

NB: higher orders produce higher analogues, built from powers of the resolvent $(\mathrm{E_n} - \mathrm{H})^{-1}$.
QGT need not be Kähler. The dimension of $\mathcal{M}$ is not necessarily = to that of the ray space.

Find a hierarchy of effective electronic Hamiltonians ⇒ increasingly accurate effective actions.
Diagonalise H with a unitary tranformation U_0, then apply a sequence of near-identity unitaries

$$U_0^\dagger H U_0 = E = \mathrm{diag}(E_1, E_2, \dots), \qquad U_k = e^{i\epsilon^k G_k}, \qquad k = 1, 2, \dots$$

chosen so the off-diagonal (nonadiabatic) couplings are pushed to ever higher order in ϵ.

- The diagonal part defines the effective Hamiltonian at each order.
- Generators G_k are fixed by the Baker–Campbell–Hausdorff formula.

- $H^{(0)} = E - i\epsilon U_0^\dagger \dot{U}_0 \quad \Rightarrow \quad H^{\mathrm{eff}(0)} = E - \epsilon \sum_n A_{\mu,nn}\dot{x}^\mu |n\rangle\langle n| \,.$
- $H^{(1)} = U_1^\dagger E U_1 - i\epsilon U_1^\dagger U_0^\dagger \dot{U}_0 U_1 - i\epsilon U_1^\dagger \dot{U}_1 \quad \Rightarrow \quad H_{nn}^{\mathrm{eff}(1)} = E_n - \epsilon A_{\mu,nn}\dot{x}^\mu - \frac{\epsilon^2}{2} M_{2\mu\nu}\dot{x}^\mu \dot{x}^\nu \,.$
- $H^{(2)} = U_2^\dagger H^{(1)} U_2 - i\epsilon U_2^\dagger \dot{U}_2 \quad \Rightarrow \quad H_{nn}^{\mathrm{eff}(2)} = H_{nn}^{\mathrm{eff}(1)} + \epsilon^3 \left[-\frac{1}{2}\omega_{\mu\nu}\dot{x}^\mu \ddot{x}^\nu - \frac{1}{6}\gamma_{\lambda\mu\nu}\dot{x}^\lambda \dot{x}^\mu \dot{x}^\nu \right].$

3 new geometric objects on $\mathcal{M}$, each a nonadiabatic quantity sensitive to the energy gaps $\mathrm{E_n} - \mathrm{E_m}$.

Induced geometry on parameter space

$$\mathrm{M}_{2\mu\nu} = -2\,\mathrm{Re}\,\langle \mathrm{D}_\mu \mathrm{n}|(\mathrm{E_n} - \mathrm{H})^{-1}|\mathrm{D}_\nu \mathrm{n}\rangle \qquad \text{(mass correction)}$$

$$\omega_{\mu\nu} = -2\,\mathrm{Im}\,\langle \mathrm{D}_\mu \mathrm{n}|(\mathrm{E_n} - \mathrm{H})^{-2}|\mathrm{D}_\nu \mathrm{n}\rangle \qquad \text{(almost symplectic)}$$

$$\gamma_{\lambda\mu\nu} = -6\,\mathrm{Im}\,\langle \mathrm{D}_{(\lambda} \mathrm{n}|(\mathrm{E_n} - \mathrm{H})^{-2}|\mathrm{D}_\mu \mathrm{D}_{\nu)} \mathrm{n}\rangle$$
$$- 6\mathrm{Im}\langle \mathrm{D}_{(\lambda} \mathrm{n}|(\mathrm{E_n} - \mathrm{H})^{-1}\partial_\mu (\mathrm{E_n} - \mathrm{H})^{-1}|\mathrm{D}_{\nu)} \mathrm{n}\rangle\,. \qquad \text{(fully symmetric)}$$

- $\mathrm{M}_{2\mu\nu}$ is symmetric — it will renormalise the metric.
- $\omega_{\mu\nu}$ is antisymmetric — an almost symplectic 2-form. $\gamma_{\lambda\mu\nu}$ is not a tensor; under $\mathrm{x} \mapsto \tilde{\mathrm{x}}$:

$$\gamma_{\rho\mu\nu} \to \tilde{\gamma}_{\rho'\mu'\nu'} = \frac{\partial \mathrm{x}^\rho}{\partial \tilde{\mathrm{x}}^{\rho'}} \gamma_{\rho\mu\nu} \frac{\partial \mathrm{x}^\mu}{\partial \tilde{\mathrm{x}}^{\mu'}} \frac{\partial \mathrm{x}^\nu}{\partial \tilde{\mathrm{x}}^{\nu'}} + 3\,\frac{\partial \mathrm{x}^\rho}{\partial \tilde{\mathrm{x}}^{(\rho'}} \omega_{\rho\sigma} \frac{\partial^2 \mathrm{x}^\sigma}{\partial \tilde{\mathrm{x}}^{\mu'} \partial \tilde{\mathrm{x}}^{\nu')}}\,.$$

A hierarchy of effective forces

Key fact:

The (p+1)-th order effective action is obtained from the p-th order effective Hamiltonian as:

$$S^{\mathrm{eff(p+1)}}[x] = \int dt\ \langle \psi^{\mathrm{eff(p)}} | \left(i\epsilon \frac{d}{dt} - H^{\mathrm{eff(p)}} \right) | \psi^{\mathrm{eff(p)}} \rangle.$$

Variation w.r.t. x gives the effective equation of motion at each order. We will go up to order 3.

First-order effective action

$$\mathrm{S}^{\mathrm{eff}(1)} = \int \mathrm{dt}\, \left[\tfrac{1}{2} \mathrm{M}_{\mu\nu} \dot{\mathrm{x}}^{\mu} \dot{\mathrm{x}}^{\nu} - \mathrm{E}_{\mathrm{n}} + \epsilon \mathrm{A}_{\mu} \dot{\mathrm{x}}^{\mu} \right]$$

Euler–Lagrange equations:

$$\mathrm{M}_{\mu\nu}\, \mathrm{a}^{\nu}[\mathrm{M}] - \epsilon\, \mathrm{B}_{\mu\nu} \dot{\mathrm{x}}^{\nu} + \partial_{\mu} \mathrm{E}_{\mathrm{n}} = 0.$$

- ϵ^0: Born–Oppenheimer force $-\partial_{\mu} \mathrm{E}_{\mathrm{n}}$.
- ϵ^1: Berry–Lorentz force — $\mathrm{B}_{\mu\nu}$ as a generalised magnetic field ("geometric magnetism").

Relevant in many physical problems.

Second-order effective action

$$\mathrm{S}^{\mathrm{eff}(2)} = \mathrm{S}^{\mathrm{eff}(1)} + \epsilon^2 \int \mathrm{dt}\ \tfrac{1}{2}\mathrm{M}_{2\mu\nu}(\mathrm{x})\,\dot{\mathrm{x}}^{\mu}\dot{\mathrm{x}}^{\nu}$$

Euler–Lagrange equations:

$$\mathrm{M}^{\star}_{\mu\nu}\,\mathrm{a}^{\star\nu} - \epsilon \mathrm{B}_{\mu\nu}\dot{\mathrm{x}}^{\nu} + \partial_{\mu}\mathrm{E}_{\mathrm{n}} = 0, \qquad \boxed{\mathrm{M}^{\star}_{\mu\nu} = \mathrm{M}_{\mu\nu} + \epsilon^2 \mathrm{M}_{2\mu\nu}}$$

- Bare mass → effective mass tensor $\mathrm{M}^{\star}_{\mu\nu}$; $\mathrm{a}^{\star}$ uses the Levi-Civita $\mathring{\Gamma}[\mathrm{M}^{\star}]$.
- For a free particle this is the geodesic equation of $\mathrm{M}^{\star}$.
- A clean geometry–dynamics link: second order = Riemannian geometry (still).
- Known and used, see e.g. A. Goldhaber 2005 (“Newtonian adiabatics unified”.)

Third-order effective action — depends on acceleration

$$\mathrm{S}^{\mathrm{eff}(3)} = \mathrm{S}^{\mathrm{eff}(2)} + \epsilon^3 \int \mathrm{d}t \left[\tfrac{1}{2}\, \omega_{\mu\nu}(\mathrm{x})\, \dot{\mathrm{x}}^\mu \ddot{\mathrm{x}}^\nu + \tfrac{1}{6}\, \gamma_{\lambda\mu\nu}(\mathrm{x})\, \dot{\mathrm{x}}^\lambda \dot{\mathrm{x}}^\mu \dot{\mathrm{x}}^\nu \right]$$

An acceleration-dependent Lagrangian $\mathrm{L}(\mathrm{x}, \dot{\mathrm{x}}, \ddot{\mathrm{x}})$ obeys the Euler–Lagrange equation

$$\frac{\partial \mathrm{L}}{\partial \mathrm{x}^\mu} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathrm{L}}{\partial \dot{\mathrm{x}}^\mu} + \frac{\mathrm{d}^2}{\mathrm{d}t^2} \frac{\partial \mathrm{L}}{\partial \ddot{\mathrm{x}}^\mu} = 0.$$

Consequence: $\omega_{\mu\nu} \dot{\mathrm{x}}^\mu \ddot{\mathrm{x}}^\nu$ produces $\dddot{\mathrm{x}}$ — the jerk and the eom is now third order.

- cf. obstacle avoidance problems & control theory, robotic systems ⇒ only even-order eqs.
  [e.g. Bloch–Camarinha–Colombo 2021; Cabrera–Hatton 2023]
- cf. biological & biotechnological systems (arm movements, neural control &c.)
  [Todorov–Jordan 1998, Boulanger et al. 2024-26]

Direct computation of the equation of motion at third order yields the following:

$$\epsilon^3 \omega_{\mu\nu}\, \dddot{\mathrm{x}}^{\cdot\nu} + \epsilon^3 \zeta_{\mu\kappa\lambda} \dot{\mathrm{x}}^\kappa \ddot{\mathrm{x}}^\lambda + \epsilon^3 \xi_{\mu\kappa\lambda\rho} \dot{\mathrm{x}}^\kappa \dot{\mathrm{x}}^\lambda \dot{\mathrm{x}}^\rho + \mathrm{M}^\star_{\mu\nu} \mathrm{a}^{\star\nu} - \epsilon \mathrm{B}_{\mu\nu} \dot{\mathrm{x}}^\nu + \partial_\mu \mathrm{E}_\mathrm{n} = 0$$

with (defining $\mathrm{H} := \mathrm{d}\omega$)

$$\zeta_{\mu\kappa\lambda} = -\tfrac{1}{2}\mathrm{H}_{\mu\kappa\lambda} - 2\partial_{(\kappa}\omega_{\lambda)\mu} + \gamma_{\mu\kappa\lambda}, \qquad \xi_{\mu\kappa\lambda\rho} = -\tfrac{1}{6}\big(\partial_\mu \gamma_{\kappa\lambda\rho} - 3\,\partial_{(\rho}\gamma_{\kappa\lambda)\mu} + 3\,\partial_{(\kappa}\partial_\lambda \omega_{\rho)\mu}\big)\,.$$

- ζ, ξ are not tensors — covariance is not manifest.

Two questions

What geometry underlies this action? How do we define the jerk covariantly?

Effective Kawaguchi geometry

Consider the affine bundle $\mathrm{T}^2\mathcal{M} \subset \mathrm{TT}\mathcal{M}$, with $(\mathrm{x}^\mu, \mathrm{y}^\mu, \mathrm{z}^\mu) \sim (\mathrm{x}, \dot{\mathrm{x}}, \ddot{\mathrm{x}})$.

Positive second-order homogeneity

$\mathrm{K} : \mathrm{T}^2\mathcal{M} \to [0, \infty)$ with second-order homogeneity

$$\mathrm{K}(\mathrm{x}, \lambda \mathrm{y}, \lambda^2 \mathrm{z} + \mu \mathrm{y}) = \lambda\, \mathrm{K}(\mathrm{x}, \mathrm{y}, \mathrm{z}), \qquad \mu \in \mathbb{R}.$$

The homogeneity condition is tailored so the Zermelo conditions hold, [Zermelo's PhD thesis 1894!]

$$\mathrm{y}^\mu \frac{\partial \mathrm{K}}{\partial \mathrm{y}^\mu} + 2\mathrm{z}^\mu \frac{\partial \mathrm{K}}{\partial \mathrm{z}^\mu} = \mathrm{K}, \qquad \mathrm{y}^\mu \frac{\partial \mathrm{K}}{\partial \mathrm{z}^\mu} = 0,$$

making the "arc length" reparametrisation invariant:

$$\mathrm{S}_\mathrm{K} = \int_{\mathrm{t_i}}^{\mathrm{t_f}} \mathrm{dt}\ \mathrm{K}(\mathrm{x}^\mu, \dot{\mathrm{x}}^\mu, \ddot{\mathrm{x}}^\mu).$$

Such generalizations were first studied already a long time ago [Cartan 1936; Kawaguchi 1938].

We call the special class that gives ω and γ: Kawaguchi–Lemleyn–Losik (KL^2) manifolds. See [Losik 1960; Lemleyn 1957; Panzhenskii 2007].

NB: A non-degenerate 2-form ω is an almost symplectic structure. [NB: twisted Poisson.]

Consider a symmetric connection $\mathring{\nabla}$ with

$$\mathring{\nabla}_\mu \omega_{\nu\rho} = \tfrac{1}{3} \mathrm{H}_{\mu\nu\rho} \,.$$

- A symmetric connection cannot be strictly compatible with ω unless of course $\mathrm{H} = 0$ (then $\mathring{\nabla}\omega = 0$: a symplectic connection — not unique). [Bieliavsky et al. 2006]
- Any such $\mathring{\nabla}$ yields the fully symmetric object

$$\tfrac{1}{3}\gamma_{\mu\nu\rho} := \omega_{\nu\sigma}\mathring{\Gamma}^{\sigma}_{\mu\rho} + \tfrac{2}{3}\partial_{(\mu}\omega_{\rho)\nu}.$$

A reparametrization invariant action, the generalised arc length of a curve, is:

$$S_{\mathrm{KL}^2} = \int \mathrm{d}t \, \sqrt[3]{\tfrac{1}{2}\,\omega_{\mu\nu}(x)\,\dot{x}^\mu \ddot{x}^\nu + \tfrac{1}{6}\,\gamma_{\mu\nu\rho}(x)\,\dot{x}^\mu \dot{x}^\nu \dot{x}^\rho}$$

Because ω is non-degenerate, this can be written as

$$S_{\mathrm{KL}^2} = \int \mathrm{d}t \, \sqrt[3]{\tfrac{1}{2}\,\omega_{\mu\nu}\, v^\mu \mathring{a}^\nu}\,, \qquad v^\mu = \dot{x}^\mu, \quad \mathring{a} = \text{acceleration w.r.t. } \mathring{\nabla}.$$

- But the effective action $S^{\mathrm{eff}(3)}$ we found in APT has no cube root.
- Also it is not manifestly reparametrisation invariant.

The answer should be obvious to this audience

It is the "Nambu-Goto" action and there exists a gauge-fixed "Polyakov" one.

Start with the reparametrization invariant action,

$$\mathrm{S}_{\mathrm{KL}^2} = \mathrm{m}\int \mathrm{d}\tau \, \sqrt[3]{\tfrac{1}{2}\omega_{\mu\nu}\dot{\mathrm{x}}^\mu\ddot{\mathrm{x}}^\nu + \tfrac{1}{6}\gamma_{\mu\nu\rho}\dot{\mathrm{x}}^\mu\dot{\mathrm{x}}^\nu\dot{\mathrm{x}}^\rho}.$$

Introduce an einbein (density of weight 2):

$$\mathrm{S}'_{\mathrm{KL}^2} = \tfrac{1}{3}\int \mathrm{d}\tau \Big(\mathrm{e}^{-1}\,\tfrac{1}{2}\,\omega_{\mu\nu}\dot{\mathrm{x}}^\mu\mathring{\mathrm{a}}^\nu + 2\sqrt{\mathrm{e}}\,\mathrm{m}^{3/2}\Big).$$

- The EOM for e is algebraic; eliminating it recovers $\mathrm{S}_{\mathrm{KL}^2}$.
- Gauge-fix $\mathrm{e} = 1$, set $\mathrm{m} = 0 \Rightarrow$ the massless Kawaguchi particle:

$$\mathrm{S}'_{\mathrm{KL}^2,0} = \tfrac{1}{3}\int \mathrm{d}\tau \;\tfrac{1}{2}\,\omega_{\mu\nu}\dot{\mathrm{x}}^\mu\mathring{\mathrm{a}}^\nu = \tfrac{1}{3}\int \mathrm{d}\tau \Big(\tfrac{1}{2}\omega_{\mu\nu}\dot{\mathrm{x}}^\mu\ddot{\mathrm{x}}^\nu + \tfrac{1}{6}\gamma_{\mu\nu\rho}\dot{\mathrm{x}}^\mu\dot{\mathrm{x}}^\nu\dot{\mathrm{x}}^\rho\Big).$$

  This is precisely the ϵ^3 sector of the effective action!

Jerk & manifest covariance

Define the jerk as the covariant acceleration of the (covariant) acceleration:

$$\mathrm{j} := \nabla_{\mathrm{v}}\, \mathring{\mathrm{a}} = \nabla_{\mathrm{v}}\, \mathring{\nabla}_{\mathrm{v}} \mathrm{v},$$

using possibly two connections. In components, the jerk vector has the general form:

$$\boxed{\mathrm{j}^{\mu} = \dddot{\mathrm{x}}^{\mu} + \ddot{\mathrm{x}}^{\kappa}\dot{\mathrm{x}}^{\lambda}\big(2\mathring{\Gamma}^{\mu}_{\kappa\lambda} + \Gamma^{\mu}_{\lambda\kappa}\big) + \dot{\mathrm{x}}^{\rho}\dot{\mathrm{x}}^{\kappa}\dot{\mathrm{x}}^{\lambda}\big(\partial_{\rho}\mathring{\Gamma}^{\mu}_{\kappa\lambda} + \mathring{\Gamma}^{\nu}_{\kappa\lambda}\Gamma^{\mu}_{\rho\nu}\big).}$$

Solve $\mathring{\nabla}_\mu \omega_{\nu\rho} = \frac{1}{3} \mathrm{H}_{\mu\nu\rho}$ for the symmetric connection, then for the outer derivative pick

$$\Gamma^\mu_{\nu\rho} = \mathring{\Gamma}^\mu_{\nu\rho} - \tfrac{1}{2}\, \omega^{\mu\sigma} \mathrm{H}_{\sigma\nu\rho}\,.$$

Manifestly covariant equation of motion

$$\epsilon^3\, \omega_{\mu\nu}\, \dot{\mathrm{j}}^\nu - \tfrac{1}{2} \epsilon^3\, \omega_{\sigma\rho}\, \mathring{\mathrm{R}}^\sigma{}_{\kappa\lambda\mu} \dot{\mathrm{x}}^\kappa \dot{\mathrm{x}}^\lambda \dot{\mathrm{x}}^\rho + \mathrm{M}^\star_{\mu\nu} \mathrm{a}^{\star\nu} - \epsilon \mathrm{B}_{\mu\nu} \dot{\mathrm{x}}^\nu + \partial_\mu \mathrm{E_n} = 0\,.$$

At third order only two terms survive: the jerk vector and the Riemann curvature $\mathring{\mathrm{R}}$ of $\mathring{\nabla}$.
Of course the choice is not unique: $\nabla' = \nabla + \Phi$ shifts the jerk.

- Note that a choice $\Phi^\mu_{\nu\rho} = \frac{1}{3} \omega^{\mu\kappa} \mathrm{H}_{\kappa\nu\rho}$ even makes ∇' strictly compatible with ω.
- If a flat connection exists globally (KL^2 manifold flat), the cubic equation collapses to

$$\boxed{\mathrm{j}^\mu = 0} \qquad \text{(jerk-free motion)}.$$

Conclusions

Eliminating the quantum sector order by order yields a hierarchy of forces — new type of quantum geometry:

order	force	geometry
ϵ^0	Born–Oppenheimer	potential
ϵ^1	Berry–Lorentz	gauge curvature B
ϵ^2	mass renormalisation	Riemannian (forced geodesic)
ϵ^3	jerk	Kawaguchi KL^2 (generalised geodesic)

- KL^2 geometry = almost symplectic ω + symmetric $\gamma \Rightarrow$ a connection $\Rightarrow$ a covariant jerk.
- ω is the imaginary part of a higher quantum geometric tensor.

Why a tiny third-order force can matter

Third order in ϵ — yet it can dominate the long-time behaviour.

Foucault analogy

The weak Coriolis force has nonzero time average while the large restoring force averages out — so the swing plane visibly rotates over hours.

Likewise: if $M^{\star}_{\mu\nu}$ averages to a flat metric over a fast oscillation but the third-order jerk kicks do not average to 0, they accumulate into a qualitative effect on slow "drifting" nuclear motion.

Practically: implement reaction forces to capture higher-order nonadiabatic effects in molecular dynamics — without solving the electronic Schrödinger equation at every step.

- Odd-order equations of motion. Deserve more study (usually even-order are studied). Higher orders in $\epsilon \Rightarrow$ higher-order Kawaguchi structures ($\mathrm{T}^{\mathrm{k}}\mathcal{M}$). Snap, crackle, pop? Hamiltonian formalism?
- Consistency analysis. Constructing the effective eom directly gives a small discrepancy.
- Applications: in molecular dynamics simulations & beyond. E.g. jerk-driven systems.
- Relation to "general connections" (Otsuki, Wong, ... connection + endomorphism)?

Thank you!