# A simple mathematical description of Piezoelectricity

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**Piezoelectric effect:**

- Deformations of certain crystals cause a polarization of the probe
- Two contributions: Deformation of the *ionic structure* and deformation of the *electronic density*
- Naive definition of the polarization vector

$$P = \frac{1}{V}\left[-e\sum_{l} R_l Z_l + \int \mathrm{d}x\, x\rho(x)\right]$$

  does not define a bulk property and thus has no thermodynamic limit.
- The proper definition is is that of *relative polarization*

$$\Delta P = P_{\text{fin}} - P_{\text{in}} = \int_{T_{\text{in}}}^{T_{\text{fin}}} \mathrm{d}t\, \dot{P}(t)$$

  as the integral over the *Piezocurrent* $\dot{P}(t)$.

In the following we show how to derive mathematically the electronic contribution to the Piezocurrent in a *simple model*:

A single electron in a time-dependent crystalline background is described by the *Schrödinger equation with a slowly varying periodic potential*:

$$\mathrm{i}\frac{\partial}{\partial s}\tilde{\psi}^{\varepsilon}(s,x) = \left(-\frac{1}{2}\Delta_x + V_{\Gamma}(\varepsilon s, x)\right)\tilde{\psi}^{\varepsilon}(s,x)\,, \qquad \tilde{\psi}^{\varepsilon}(s,\cdot) \in L^2(\mathbb{R}^3)\,.$$

The time-dependent potential $V_{\Gamma}(t,x)$ is periodic with respect to a lattice

$$\Gamma = \left\{ x \in \mathbb{R}^3 \,|\, x = \sum_{j=1}^{3} \alpha_j \gamma_j \text{ for some } \alpha \in \mathbb{Z}^3 \right\},$$

spanned by a basis $(\gamma_1, \gamma_2, \gamma_3)$ of $\mathbb{R}^3$, i.e.

$$V_{\Gamma}(t, x+\gamma) = V_{\Gamma}(t,x) \quad \text{for all } \gamma \in \Gamma \text{ and } x \in \mathbb{R}^3\,.$$

In the following we show how to derive mathematically the electronic contribution to the Piezocurrent in a *simple model*:

A single electron in a time-dependent crystalline background is described by the *Schrödinger equation with a slowly varying periodic potential*:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}\tilde{\psi}^{\varepsilon}(s) = \left(-\frac{1}{2}\Delta + V_{\Gamma}(\varepsilon s)\right)\tilde{\psi}^{\varepsilon}(s)\,, \qquad \tilde{\psi}^{\varepsilon}(s) \in L^2(\mathbb{R}^3)\,.$$

Here $\varepsilon \ll 1$ is the *adiabatic parameter* and a change of variable to the *slow time-scale* $t = \varepsilon s$ yields

$$\mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\psi^{\varepsilon}(t) = \left(-\frac{1}{2}\Delta + V_{\Gamma}(t)\right)\psi^{\varepsilon}(t)\,, \qquad \psi^{\varepsilon}(t) \in L^2(\mathbb{R}^3)\,.$$

Our main result is that the macroscopic Wigner transform

$$w[\psi^\varepsilon(t)](q,k) = \frac{1}{(2\pi\varepsilon)^3}\int \mathrm{d}\xi\, \mathrm{e}^{\mathrm{i}\xi\cdot k}\,\bar{\psi}^\varepsilon(t,\frac{q}{\varepsilon}+\frac{\xi}{2})\,\psi^\varepsilon(t,\frac{q}{\varepsilon}-\frac{\xi}{2})$$

of the solution $\psi^\varepsilon(t,x)$ of the Schrödinger equation is approximately transported by the flow $\Phi^\varepsilon(t) : \mathbb{R}^6 \to \mathbb{R}^6$ of

$$\text{(CSCM)} \qquad \begin{cases} \dot{q} &=& \nabla_k E_n(k,t) - \varepsilon\,\Theta_n(k,t) \\ \dot{k} &=& 0\,, \end{cases}$$

whenever the initial state $\psi^\varepsilon(0)$ lies *in the $n$th Bloch subspace.* Here $E_n(k,t)$ is the $n$th Bloch eigenvalue for fixed lattice momentum $k$ and $\Theta_n(k,t)$ is a certain curvature term.

More precisely, for sufficiently smooth test functions $a(q,k)$ which are $\Gamma^*$-periodic in the second argument, we show that for $t \in I$

$$\left|\int_{\mathbb{R}^6} \mathrm{d}q\mathrm{d}k\, a(q,k)\left\{w[\psi^\varepsilon(t)] - w[\psi^\varepsilon(0)]\circ\Phi^\varepsilon(-t)\right\}(q,k)\right| \leq \varepsilon^2\, C_I\, \|\psi^\varepsilon(0)\|^2_{L^2}\,\|a\|\,.$$

Since the dynamical system (CSCM) naturally lives on the phase space $\mathbb{R}^3 \times \mathbb{T}^3_*$, one can alternatively define the reduced Wigner transform

$$w_{\mathrm{r}}[\psi^\varepsilon(t)](q,k) = \sum_{\gamma^* \in \Gamma^*} w[\psi^\varepsilon(t)](q, k + \gamma^*) \quad \text{for} \quad (q,k) \in \mathbb{R}^3 \times \mathbb{T}^3_*$$

Then the result reads that for $a \in C^\infty_{\mathrm{b}}(\mathbb{R}^3 \times \mathbb{T}^3_*)$ and $t \in I$

$$\left| \int_{\mathbb{R}^3} \mathrm{d}q \int_{\mathbb{T}^3_*} \mathrm{d}p \, a(q,k) \left\{ w_{\mathrm{r}}[\psi^\varepsilon(t)] - w_{\mathrm{r}}[\psi^\varepsilon(0)] \circ \Phi^\varepsilon(-t) \right\} (q,k) \right| \leq \varepsilon^2 \, C_I \, \|\psi^\varepsilon(0)\|^2_{L^2} \, \|a\| \, .$$

A straightforward computation now shows that an electron in the $n$th Bloch band contributes to the relative polarization per unit cell with

$$\begin{aligned} \Delta P_n \; &:= \; \frac{1}{\varepsilon} \int_0^T \mathrm{d}t \frac{\mathrm{d}}{\mathrm{d}t} \langle q \rangle_{\psi^\varepsilon(t)} = \frac{1}{\varepsilon} \int_0^T \mathrm{d}t \int_{\mathbb{T}^3_*} \mathrm{d}k \left( \nabla_k E_n(k,t) - \varepsilon \Theta_n(k,t) \right) |\widehat{\psi}^\varepsilon_{\mathrm{r}}(0,k)|^2 \\ &= \; - \int_0^T \mathrm{d}t \int_{\mathbb{T}^3_*} \mathrm{d}k \, \Theta_n(k,t) \, |\widehat{\psi}^\varepsilon_{\mathrm{r}}(0,k)|^2 \end{aligned}$$

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At zero temperature the relative polarization per unit cell of a semiconductor or insulator is therefore

$$\Delta P = \sum_{n=0}^{N} \Delta P_n = -\sum_{n=0}^{N} \int_0^T \mathrm{d}t \int_{\mathbb{T}^3_*} \mathrm{d}k\, \Theta_n(k,t)\,,$$

where $N$ the highest filled band.

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where $N$ the highest filled band.

We will show that

$$\Theta_n(k,t) = -\frac{\partial \mathcal{A}_n(k,t)}{\partial t} - \nabla_k \phi_n(k,t) \,,$$

with $\mathcal{A}_n(k,t)$ the connection coefficient of the Berry connection of the Bloch bundle and $\phi_n(k,t)$ a geometric scalar potential.

In summary we obtain the *King-Smith and Vanderbilt formula* for the relative polarization:

$$\Delta P = \sum_{n=0}^{N} \int_{\mathbb{T}^3_*} \mathrm{d}k \, \left( \mathcal{A}_n(k,T) - \mathcal{A}_n(k,0) \right) \,.$$

In the following I will explain how to prove the mathematical result for the effective transport of the Wigner function using the following steps:

1. Bloch-Floquet transformation $\Rightarrow$ fibration with respect to lattice momentum
2. Adiabatic approximation for each fixed lattice momentum up to $\mathcal{O}(\varepsilon^2)$ $\Rightarrow$ this requires use of *superadiabatic subspaces*
3. Egorov theorem up to $\mathcal{O}(\varepsilon^2)$ in the *superadiabatic representation*
4. Transformation to the original *physical representation*

The Bloch-Floquet transformation

$$\mathcal{B} : L^2(\mathbb{R}^3_x) \cong L^2(\Gamma \times \mathbb{T}^3_y) \cong \ell^2(\Gamma) \otimes L^2(\mathbb{T}^3_y) \to L^2(M^3_k) \otimes L^2(\mathbb{T}^3_y)$$

is just the regular Fourier transformation on the factor $\ell^2(\Gamma)$ followed by a multiplication with $\mathrm{e}^{-\mathrm{i}y\cdot k}$, i.e.

$$\mathcal{B}\,\psi(k,y) = \mathrm{e}^{-\mathrm{i}y\cdot k}\,(\mathcal{F}\otimes \mathbf{1}\,\psi)(k,y) = \sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}(y+\gamma)\cdot k}\,\psi(y+\gamma)\,.$$

Here $M^3_k$ is the centered fundamental domain of the dual lattice, called the Brillouin zone.

Thus $\mathcal{B}$ is unitary and one can check by direct computation that

$$\begin{aligned}\mathcal{B}\,(-\mathrm{i}\nabla_x)\,\mathcal{B}^{-1} &= \mathbf{1}\otimes(-\mathrm{i}\nabla_y) + k\otimes\mathbf{1}\\ \mathcal{B}\,x\,\mathcal{B}^{-1} &= \mathrm{i}\nabla^\tau_k\,,\end{aligned}$$

where $\nabla^\tau_k$ denotes the gradient with certain $y$-dependent boundary conditions.

Bloch-Floquet transformation of the Hamiltonian

$$H(t) = -\frac{1}{2}\Delta_x + V_\Gamma(x,t)$$

yields

$$\mathcal{B}\, H(t)\, \mathcal{B}^{-1} = -\frac{1}{2}(-\mathrm{i}\nabla_y + k)^2 + V_\Gamma(y,t) =: H(k,t)\,.$$

Thus $H(k,t)$ acts on

$$L^2(M_k^3) \otimes L^2(\mathbb{T}_y^3) \cong L^2(M_k^3; L^2(\mathbb{T}_y^3))$$

as an operator valued multiplication operator.

The Bloch bands $E_n(k,t)$ and Bloch projectors $P_n(k,t) \in \mathcal{L}(L^2(\mathbb{T}_y^3))$ are the eigenvalues and corresponding spectral projections of $H(k,t)$, i.e.

$$H(k,t)\, P_n(k,t) = E_n(k,t)\, P_n(k,t)\,,$$

enumerated according to $E_0(k,t) < E_1(k,t) < \ldots$

In Bloch-Floquet representation we are thus left to solve the Schrödinger equation

$$\text{(SE)} \qquad \mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\psi^\varepsilon(k,t) = H(k,t)\,\psi^\varepsilon(k,t)\,, \qquad \psi^\varepsilon(k,0) \in L^2(\mathbb{T}^3_y)\,,$$

for each $k \in M^d_k$.

*(Super)adiabatic theorem:* For each isolated Bloch band $E_n(k,t)$ there exists a projection $P^\varepsilon_n(k,t)$ and a unitary operator

$$T^\varepsilon_n(k,t) : P^\varepsilon_n(k,t)\,L^2(\mathbb{T}^3_y) \to \mathbb{C}$$

such that a solution $\psi^\varepsilon(k,t)$ of (SE) with $\psi^\varepsilon(k,0) \in P^\varepsilon_n(k,0)\,L^2(\mathbb{T}^3_y)$ satisfies

$$\|\,(\mathbf{1} - P^\varepsilon_n(k,t))\,\psi^\varepsilon(k,t)\,\| = \mathcal{O}(|t|\varepsilon^\infty)\,,$$

and $T^\varepsilon_n(k,t)P^\varepsilon_n(k,t)\,\psi^\varepsilon(k,t) \in \mathbb{C}$ is $\mathcal{O}(|t|\varepsilon^\infty)$ close to the solution of the effective $n$th band Schrödinger equation

$$\mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\varphi^\varepsilon(k,t) = H^{\text{eff}}_n(k,t)\,\varphi^\varepsilon(k,t) \quad \text{with} \quad \varphi^\varepsilon(k,0) = T^\varepsilon_n(k,0)P^\varepsilon_n(k,0)\,\psi^\varepsilon(k,0)\,.$$

*(Super)adiabatic theorem:* For each isolated Bloch band $E_n(k,t)$ there exists a projection $P_n^\varepsilon(k,t)$ and a unitary operator

$$T_n^\varepsilon(k,t) : P_n^\varepsilon(k,t)\, L^2(\mathbb{T}_y^3) \to \mathbb{C}$$

such that a solution $\psi^\varepsilon(k,t)$ of (SE) with $\psi^\varepsilon(k,0) \in P_n^\varepsilon(k,0)\, L^2(\mathbb{T}_y^3)$ satisfies

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$$\mathrm{i}\,\varepsilon \frac{\mathrm{d}}{\mathrm{d}t}\varphi^\varepsilon(k,t) = H_n^{\mathrm{eff}}(k,t)\,\varphi^\varepsilon(k,t) \quad \text{with} \quad \varphi^\varepsilon(k,0) = T_n^\varepsilon(k,0)P_n^\varepsilon(k,0)\,\psi^\varepsilon(k,0)$$

and

$$H_n^{\mathrm{eff}}(k,t) = E_n(k,t) + \mathcal{O}(\varepsilon^2)\,.$$

All estimates are uniform for $k \in M_k^3$ and $t$ in a finite interval.
$P_n^\varepsilon$ and $T_n^\varepsilon$ are smooth functions of $k$ and $t$ provided that $V_\Gamma(t)$ is smooth.

*Proof:* $P_n^\varepsilon(k,t)$ is obtained from truncating the unique asymptotic series expansion of the solution to

$$[\,P_n^\varepsilon(k,t),\,(\mathrm{i}\varepsilon\partial_t - H(k,t))\,] = 0 \quad \text{and} \quad P_n^\varepsilon(k,t)^2 = P_n^\varepsilon(k,t)$$

starting with

$$\begin{aligned} P_n^\varepsilon(k,t) &= P_n(k,t) \\ &\quad + \mathrm{i}\,\varepsilon\left(P_n(k,t)\dot{P}_n(k,t)(H(k,t)-E_n(k,t))^{-1}P_n(k,t)^\perp + \text{adj.}\right) \\ &\quad + \mathcal{O}(\varepsilon^2)\,. \end{aligned}$$

The unitary $T_n^\varepsilon(k,t) : P_n^\varepsilon(k,t)L^2(\mathbb{T}^3) \to \mathbb{C}$ is not unique. We construct it from a normalized eigenfunction $\chi_n(k,t)$ in the eigenspace $P_n(k,t)\,L^2(\mathbb{T}^3)$ of $H(k,t)$ satisfying

$$\phi_n(k,t) = -\mathrm{i}\,\langle \chi_n(k,t), \partial_t\,\chi_n(k,t)\rangle_{L^2(\mathbb{T}^3)} = 0$$

and at leading order simply reads

$$T_n^\varepsilon(k,t) = \langle \chi_n(k,t)| + \mathcal{O}(\varepsilon^2)\,.$$

We can now easily solve the effective Schrödinger equation

$$\mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\varphi^\varepsilon(t) = H_n^{\mathrm{eff}}(t)\,\varphi^\varepsilon(t)\,,\quad \text{for}\quad \varphi^\varepsilon(t)\in L^2(\mathbb{T}^3_*;\mathbb{C})\,,$$

or directly for the propagator

$$\mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}U_n^\varepsilon(t,0) = H_n^{\mathrm{eff}}(t)\,U_n^\varepsilon(t,0)\quad \text{with}\quad U_n^\varepsilon(0,0) = \mathbf{1}_{L^2(\mathbb{T}^3_*)}$$

by

$$\varphi^\varepsilon(k,t) = U_n^\varepsilon(t,0)\varphi^\varepsilon(k,0) = \mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}\int_0^t \mathrm{d}s\, H_n^{\mathrm{eff}}(k,s)}\,\varphi^\varepsilon(k,0)\,.$$

However, in order to compute $U_n^\varepsilon(t,0)$ up to errors of order $\mathcal{O}(\varepsilon^2)$ we would need to know $H_n^{\mathrm{eff}}(k,t)$ up to terms of order $\mathcal{O}(\varepsilon^3)$!

Since we are lazy and only interested in the evolution of the Wigner function $w[\varphi^\varepsilon(t)](r,k)$ tested against "classical observables" $a(r,k)$, we use the duality

$$\begin{aligned}\langle a, w[\varphi^\varepsilon(t)]\rangle_W &:= \int_{\mathbb{R}^3} \mathrm{d}r \int_{\mathbb{T}^3_*} \mathrm{d}k\, a(r,k)\, w[\varphi^\varepsilon(t)](r,k)\\ &= \langle \varphi^\varepsilon(t), a(\mathrm{i}\nabla_k, k)\, \varphi^\varepsilon(t)\rangle_{L^2(\mathbb{T}^3_*)}\\ &= \langle \varphi^\varepsilon(0), U^\varepsilon_n(t)^{-1}\, a(\mathrm{i}\nabla_k, k)\, U^\varepsilon_n(t)\, \varphi^\varepsilon(0)\rangle_{L^2(\mathbb{T}^3_*)}\end{aligned}$$

and instead determine the time evolution of semiclassical observables

$$U^\varepsilon_n(t)^{-1}\, \widehat{a}\, U^\varepsilon_n(t)\,.$$

*Egorov theorem:* Let $\Phi^0(t) : \mathbb{R}^3 \times \mathbb{T}^3_* \to: \mathbb{R}^3 \times \mathbb{T}^3_*$ be the flow of

$$\text{(SCM)} \qquad \begin{cases} \dot{r} &= \nabla_k E_n(k,t) \\ \dot{k} &= 0 \end{cases}$$

starting at time 0.

Then for each finite time interval $0 \in I \subset \mathbb{R}$ there is a constant $C_I$ such that for all sufficiently smooth test function $a(r,k)$

$$\left\| U_n^\varepsilon(t)^{-1}\, \hat{a}\, U_n^\varepsilon(t) \;-\; a \circ \widehat{\Phi^0(t)} \right\| \leq \varepsilon^2 C_I \, \|a\| \, .$$

*Proof:* The approximation is exact for position operator $a(r,k) = r$:

$$\frac{\mathrm{d}}{\mathrm{d}t} U_n^\varepsilon(t)^{-1}\, (\mathrm{i}\varepsilon\nabla_k)\, U_n^\varepsilon(t) = U_n^\varepsilon(t)^{-1}\, [\nabla_k, H^\varepsilon_{\mathrm{eff}}(t)]\, U_n^\varepsilon(t) = \nabla_k E_n(k,t)$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \left( \mathrm{i}\varepsilon\nabla_k + \int_0^t \mathrm{d}s\, \nabla_k E_n(k,s) \right) = \nabla_k E_n(k,t)$$

For general observables the usual pseudodifferential calculus does the job.

Now we understand the time-evolution of observables in the reference space, but we still have to map everything back to physical space. That is we have to undo the transformation $T_n^\varepsilon(t)$ and the Bloch-Floquet transformation $\mathcal{B}$:

We observed before that the macroscopic position operator $\widehat{q} = \varepsilon x$ on $L^2(\mathbb{R}^3_x)$ is mapped by $\mathcal{B}$ to

$$\mathcal{B}\,\widehat{q}\,\mathcal{B}^{-1} = \mathrm{i}\varepsilon\nabla_k^\tau\,.$$

With

$$T_n^\varepsilon(k,t) = \langle\chi_n(k,t)| + \mathrm{i}\,\varepsilon\langle(H(k,t) - E_n(k,t))^{-1}P_n^\varepsilon(k,t)^\perp\partial_t\chi_n(k,t)| + \mathcal{O}(\varepsilon^2)$$

we thus have

$$\begin{aligned} T_n^\varepsilon(k,t)\,\mathcal{B}\,\widehat{q}\,\mathcal{B}^{-1}\,T_n^\varepsilon(k,t)^{-1} &= \mathrm{i}\varepsilon\nabla_k + \varepsilon\,\mathrm{i}\,\langle\chi_n(k,t),\nabla_k\chi_n(k,t)\rangle + \mathcal{O}(\varepsilon^2) \\ &= \widehat{r} + \varepsilon\,\mathcal{A}_n(k,t)\,. \end{aligned}$$

## 5. Transformation to physical representation

With $\dot{r} = \nabla_k E_n(k,t)$ and $q = r + \varepsilon \mathcal{A}_n(k,t)$ we thus find

$$\dot{q} = \nabla_k E_n(k,t) + \varepsilon \frac{\partial \mathcal{A}_n(k,t)}{\partial t}$$

i.e. the corrected semiclassical equations of motion

$$\text{(CSCM)} \qquad \begin{cases} \dot{q} &= \nabla_k \, E_n(k,t) - \varepsilon \, \Theta_n(k,t) \\ \dot{k} &= 0 \end{cases}$$

with

$$\Theta_n(k,t) = -\frac{\partial \mathcal{A}_n(k,t)}{\partial t} - \nabla_k \phi_n(k,t)\,.$$

$\Theta_n(k,t)$ is gauge invariant, i.e. independent of the choice of $\chi_n(k,t)$, as can be seen from the identity

$$\Theta_n(k,t) = \mathrm{Tr}\;(\,P_n(k,t)\;[\,\partial_t P_n(k,t), \nabla_k P_n(k,t)]\,)\;.$$

The *Bloch bundle* is the subbundle of the *trivial bundle*

$$\underbrace{(\mathbb{T}^3_{*\,k} \times \mathbb{R}_t)}_{\text{basis}} \times \underbrace{L^2(\mathbb{T}^3_y)}_{\text{fibre}}$$

defined by the eigenprojections $P_n(k,t)$. It carries a natural connection, the Berry connection, induced by the trivial connection on the trivial bundle.

The connection coefficients

$$\begin{aligned} \mathcal{A}(k,t)_0 &:= \phi(k,t) = -\mathrm{i}\langle \chi(k,t), \partial_t \chi(k,t)\rangle \\ \mathcal{A}(k,t)_j &= \mathrm{i}\langle \chi(k,t), \partial_{k_j} \chi(k,t)\rangle \end{aligned}$$

depend on the gauge, i.e. the local trivialization $\chi(k,t)$.

The associated curvature two form

$$R(k,t)_{\mu\nu} = \mathrm{d}\mathcal{A}(k,t)_{\mu\nu} = \partial_\mu \mathcal{A}(k,n)_\nu - \partial_\nu \mathcal{A}(k,n)_\mu$$

is gauge independent.

The associated curvature two form

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is gauge independent. It contains the

- the "electric field" $\Theta(k,t)_j = R(k,t)_{j0}$ which gives rise to the Piezo current
- the "magnetic field" $\Omega(k,t) = \nabla_k \times \mathcal{A}(k,t)$ which gives rise to the quantum Hall effect in the presence of nonperiodic perturbations: The (CSCM) for

$$\mathrm{i}\,\varepsilon \frac{\partial}{\partial t}\psi^\varepsilon(t,x) = \Big(-\frac{1}{2}\,(\mathrm{i}\nabla_x + A(\varepsilon x))^2 + V_\Gamma(x) + V(\varepsilon x)\Big)\,\psi^\varepsilon(t,x)$$

is

$$(\text{CSCM}) \qquad \begin{cases} \dot q &= \nabla_p \left(E_n(p) - \varepsilon B(q)\cdot M_n(p)\right) - \varepsilon\,\dot p \times \Omega_n(p) \\ \dot p &= -\nabla_q \left(V(q) - \varepsilon B(q)\cdot M_n(p)\right) + \dot q \times B(q) \end{cases}$$

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