Berry curvature, symplectic stuff, and Chern insulators

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We will label coordinates on our phase space by ζ^i, e.g. $\zeta = (q_1, \ldots, q_n, p_1, \ldots, p_n)$. Let $|\psi(\zeta)\rangle$ denote the complete set of single-particle states that we use to form the resolutions of the identity that we insert into the trotterization of e^{-iHT}. The partition function is then (keeping ∂ conds implicit)

$$Z = \int \prod_i \mathcal{D}\zeta^i \exp\left(\int dt \left[\langle\psi(\zeta)|\frac{d}{dt}|\psi(\zeta)\rangle - iH(\zeta)\right]\right), \tag{1}$$

with $H(\zeta) = \langle\psi(\zeta)|H|\psi(\zeta)\rangle$. We write the time derivative as

$$\langle\psi(\zeta)|\frac{d}{dt}|\psi(\zeta)\rangle = \dot{\zeta}^j\langle\psi(\zeta)|\partial_{\zeta^j}|\psi(\zeta)\rangle + \langle\psi(\zeta)|\partial_t|\psi(\zeta)\rangle = i(\dot{\zeta}^j\mathcal{A}_j + \mathcal{A}_0), \tag{2}$$

where $\mathcal{A}_j = -i\langle\psi(\zeta)|\partial_{\zeta^j}|\psi(\zeta)\rangle$ is the Berry connection, and the temporal part is $\mathcal{A}_0 = -i\langle\psi(\zeta)|\partial_t|\psi(\zeta)\rangle$. The factor of $-i$ is to make it real, since $\partial^\dagger_{\zeta^j} = -\partial_{\zeta^j}, \partial^\dagger_t = -\partial_t$. We then can write the action concisely as

$$S = \int (\mathcal{A}_j d\zeta^j - [H(\zeta) - \mathcal{A}_0]dt). \tag{3}$$

We now take a variation with respect to the phase space variables ζ^j. This gives us a term $-\delta\zeta^j(d\mathcal{A}_j/dt)$, which is $-\delta\zeta^j\dot{\zeta}^k\partial_{\zeta_k}\mathcal{A}_j - \delta\zeta^j\partial_t\mathcal{A}_j$. Thus

$$\delta S = \int \left(\mathcal{F}_{ij}d\zeta^j - [\partial_{\zeta^i}H(\zeta) + \partial_t\mathcal{A}_i - \partial_{\zeta^i}\mathcal{A}_0]dt\right)\delta\zeta^i, \tag{4}$$

where we have defined the Berry curvature $\mathcal{F} = d\mathcal{A}$, with the exterior derivative being taken in the ζ^i coordintes. This shows us why the Berry curvature is intimately related to the symplectic structure of phase space: the Berry curvature is the symplectic form, since the symplectic form ω_{ij} appears in δS via[1]

$$\delta S \ni \int \delta\zeta^i\omega_{ij}d\zeta^j. \tag{6}$$

[1] Another way to see this is to write the boundary term obtained in the course of finding the eom as $\mathcal{A}_j\delta\zeta^j|_{t_i}^{t_f}$. Taking a second variation gives

$$\delta(\mathcal{A}_j\delta\zeta^j) = \delta\mathcal{A}_j \wedge \delta\zeta^j = \partial_{\zeta^i}\mathcal{A}_j\delta\zeta^i \wedge \delta\zeta^j = \frac{1}{2}\mathcal{F}_{ij}\delta\zeta^i \wedge \delta\zeta^j, \tag{5}$$

where the wedge product is in variational space. Now we know that the above is $\omega = \frac{1}{2}\omega_{ij}\delta\zeta^i \wedge \delta\zeta^j$ where ω is the symplectic form, and so $\omega = d\mathcal{A}$: the symplectic form and Berry curvature are one and the same.

To elaborate on the indentification between $\mathcal{A}$ and the sympletic structure, we can write quite generally the action as

$$S = \int d\zeta^i \theta_i - \int dt\, H, \tag{7}$$

which describes motion of a trajectory in phase space (θ is the symplectic potential). The condition that H generate time evolution is $\partial_{\zeta_i} H = \omega_{ij} V_H^j$, where $V_H = \dot{\zeta}^j \partial_{\zeta_j}$ is the Hamiltonian vector field (therefore $\int d\zeta^i \theta_i = \int dt\, \theta(V_H)$). This equation is obtained as the equation of motion of the above action provided that $d\theta = \omega$, where the d is in $d\zeta^i$ space. Comparing this to the action derived above via the usual Trotterization procedure, we see that $\mathcal{A}_i = \theta_i$: thus the Berry connection is the essentially the symplectic potential, while the Berry curvature is essentially the symplectic form.

Anyway, the equations of motion are

$$\frac{d\zeta^j}{dt} = [\mathcal{F}^{-1}]^{ji}(\partial_{\zeta^i} H(\zeta) + \partial_t \mathcal{A}_i - \partial_{\zeta^i} \mathcal{A}_0). \tag{8}$$

Now in classical mechanics we know that the time evolution of ζ^j is generated by taking the Poisson bracket of ζ^j with $H(\zeta)$. Since $\{\zeta^j, H(\zeta)\} = \{\zeta^j, \zeta^i\}\partial_{\zeta^i} H(\zeta)$, we can classically identify $[\mathcal{F}^{-1}]^{ij} = \{\zeta^i, \zeta^j\}$. In the quantum theory then, since the Poisson bracket goes to $-i$ times the commutator, the commutation relations in the time-independent case when $\partial_t \mathcal{A}_i = \partial_{\zeta^i} \mathcal{A}_0 = 0$ are determined from the Berry curvature via

$$[\zeta^i, \zeta^j] = i[\mathcal{F}^{-1}]^{ij}. \tag{9}$$

When canonical coordinates $\zeta = (q_1, \dots, q_n, p_1, \dots, p_n)$ are chosen, $\mathcal{F}$ has the canonical structure of a symplectic form, namely

$$\mathcal{F}_{ij} = \begin{pmatrix} 0 & -\mathbf{1}_{n\times n} \\ \mathbf{1}_{n\times n} & 0 \end{pmatrix}_{ij}. \tag{10}$$

In geometric terms, this means that the $U(1)$ bundles over the q and p subspaces are trivial, while the bundle is twisted in the pq plane. The inverse is $\mathcal{F}^{-1} = -\mathcal{F}$, and we of course get $[q^i, p^j] = i\delta^{ij}$.

To be concrete for a second, consider the simple example of a particle coupled to a background electromagnetic field. The action is

$$S = \int \left((p_i + A_i)dq^i - (H(p,q) - A_0)dt\right). \tag{11}$$

Working in the basis $(q_1, \dots, q_d, p_1, \dots, p_d)$, we see that the Berry curvature is given by (here $F = dA$ is the coordinate part of the Berry curvature)

$$\mathcal{F}_{ij} = \begin{pmatrix} F & -\mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix}_{ij}. \tag{12}$$

Thus the coordinate part of the Berry curvature is equal to the magnetic field. This of course tells us that the curvature in the coordinate part of phase space is nontrivial: translations in different directions in coordinate space don't commute. This in turn means that the momenta p_i will not commute with one another, which we can see formally by computing $\mathcal{F}^{-1} = (X \otimes \mathbf{1}_{d\times d})\mathcal{F}(X \otimes \mathbf{1}_{d\times d})$, which tells us that $[p_i, p_j] = iF_{ij}$. Of course, the symplectic form can be recast in as the canonical $J \otimes \mathbf{1}_{d\times d}$ form by changing basis: a glance at the action tells us that the right way to do this is to define the canonical momenta $\pi_j = p_i + A_i$: in the basis $(q_1, \ldots, q_d, \pi_1, \ldots, \pi_d)$, we have $\mathcal{F}_{ij} = J \otimes \mathbf{1}_{d\times d}$. In the non-canonical basis, the equations of motion are the familiar

$$\dot{p}^i = -F^{ij}\partial_{p^j} H - \partial_{q^i} H - \partial_{q^i} A_0 + \partial_t A_i, \qquad \dot{q}^i = \partial_{p^i} H, \tag{13}$$

which, assuming $\partial_{p^i} H(\zeta) = \dot{q}^i$ with $H(\zeta) = p^2/2m + V(q)$, we can re-write as

$$\dot{p}^i = \epsilon^{ijk}\dot{q}^j B^k + E^i - \partial_{q^i} V(q), \qquad \dot{q}^i = p^i/m. \tag{14}$$

Now consider an analogous situation in which the magnetic field is zero, but the momentum part of the Berry curvature is non-vanishing, so that the action contains the term $\mathscr{A}_i dp^i$ (our notation is such that the total Berry connection / curvature are written with mathcal, with the coordinate part written in roman and the momentum part written in script). Proceeding in the same way, we get the equations of motion

$$\dot{q}^i = \mathscr{F}^{ij}\partial_{q^i} H(\zeta) + \partial_{p^i} H(\zeta) + \partial_t \mathscr{A}_{p^i} - \partial_{p^i}\mathscr{A}_0, \qquad \dot{p}^i = -\partial_{q^i} H(\zeta). \tag{15}$$

Taking $H(\zeta) = p^2/2m + V(q)$ again, we can write this as

$$\dot{q}^i = \epsilon^{ijk}\mathscr{B}^j \partial_{q^k} V(q) + \mathscr{E}^i + p^i/m, \qquad \dot{p}^i = -\partial_{q^i} V(q), \tag{16}$$

where $\mathscr{E}_i = \partial_{p^i}\mathcal{A}_0 - \partial_t \mathscr{A}_i$ and $\mathscr{B}$ are momentum-space electric and magnetic fields, which are responsible for an "anomalous velocity".

Finally, consider the general case where both F and $\mathscr{F}$ are nonzero. To analyze this we will work semiclassically, to first order in $\hbar$. Restoring $\hbar$ momentarily, the action is

$$S = \int \left((p_i + A_i)dx^i + \hbar \mathscr{A}_i dp^i - [H(\zeta) - \mathcal{A}_0]dt \right). \tag{17}$$

The $\hbar$ in front of $\mathscr{A}_i dp^i$ is due to the fact that $\mathscr{A}_i$ has dimensions of inverse momentum, so that $\mathscr{A}_i dp^i$ is dimensionless, and needs to be multiplied by $\hbar$ in order to have dimensions of action (on the other hand, A_i has dimensions of momentum so $A_i dx^i$ already has dimensions of action). This means that the semiclassical limit can be taken by working to first order in $\mathscr{A}$ and $\mathscr{F}$.

Now the full Berry curvature is (going back to $\hbar = 1$)

$$\mathcal{F}_{ij} = \begin{pmatrix} F & -\mathbf{1} \\ \mathbf{1} & \mathscr{F} \end{pmatrix}_{ij} \implies [\mathcal{F}^{-1}]^{ij} = \frac{1}{1 + F\mathscr{F}} \begin{pmatrix} \mathscr{F} & \mathbf{1} \\ -\mathbf{1} & F \end{pmatrix}^{ij}, \tag{18}$$

where e.g. $F\mathscr{F}$ denotes matrix multiplication. In the semiclassical approximation then,

$$\mathcal{F}^{-1} = \begin{pmatrix} \mathscr{F} & \mathbf{1} - F\mathscr{F} \\ -\mathbf{1} + F\mathscr{F} & F - F\mathscr{F}F \end{pmatrix}. \tag{19}$$

Now we can get the equations of motion. We will consider the case when $\partial_{p^i}\mathcal{A}_0 = \partial_t \mathscr{A}_i = 0$ for simplicity. We then have

$$\begin{aligned}\dot{q}^j &= \mathscr{F}^{ji}(\partial_{q^i}H - E_i) + \partial_{p^j}H - F^{jk}\mathscr{F}^{ki}\partial_{p^i}H,\\ \dot{p}^j &= (F^{ji} - F^{jk}\mathscr{F}^{kl}F^{li})\partial_{p^i}H + (-\delta^{ji} + F^{jk}\mathscr{F}^{ki})(\partial_{q^i}H - E_i).\end{aligned} \tag{20}$$

We can rewrite these in a simpler form as

$$\begin{aligned}\dot{q}^j &= \partial_{p^j}H + \epsilon^{jik}(\partial_{q^i}H - E_i)\mathscr{B}^k - \epsilon^{jkl}\epsilon^{kim}\partial_{p^i}HB^l\mathscr{B}^m\\ \dot{p}^j &= -\partial_{q^j}H + E^j + \epsilon^{jik}\dot{q}^iB^k.\end{aligned} \tag{21}$$

For example, suppose $\partial_{q^i}H = 0$ and $B = 0, \mathscr{B} \neq 0$, with q^i denoting the position of an electron in some Bloch band (this is the context of a Chern insulator). Then, supposing that the $\mathscr{B}$ and $\mathscr{E}$ fields live in three dimensions, we have

$$\dot{\mathbf{q}} = \vec{\nabla}H(p) + \mathscr{B}\times\mathbf{e}, \qquad \dot{\mathbf{p}} = \mathbf{e}. \tag{22}$$

The consequences of the $\mathscr{B}\times\mathbf{e}$ term are seen by computing the current density (restoring the electric charge e momentarily):

$$\mathbf{j} = -e\int_{BZ}\frac{d^dp}{(2\pi)^d}f(H(p))(\vec{\nabla}H(p) + \mathscr{B}\times e\mathbf{e}), \tag{23}$$

where $f(H(p))$ is the Fermi function. Suppose we are in a filled band, so that $f(H(p)) = 1$ for all $p \in BZ$. The first term then vanishes upon integration, which tells us that in the absense of momentum-space Berry curvature, filled bands don't contribute to the current (duh).

Now consider the case where the electrons live in a $d = 2$ plane, with the $\mathscr{B}$ and $\mathbf{e}$ fields living in three dimensions. Further suppose that $\mathbf{e}$ is uniform and in the plane, and $\mathscr{B}$ is orthogonal to the plane.[2] Then we get

$$\mathbf{j}^i = \epsilon^{ij}E^j\frac{e^2}{2\pi}\int_{BZ}\frac{\mathscr{B}}{2\pi} = \epsilon^{ij}E^j\frac{e^2}{2\pi}C, \tag{24}$$

where C is the Chern number. Thus we can get a (quantized!) Hall conductance without a real space magnetic field—a momentum space one will do the job as well. A consequence of having a nonzero Chern number for the Berry connection in coordinate space is that the single-particle wavefunctions $|\psi(\zeta)\rangle$ cannot be chosen to be localized in momentum space. This is because a function localized in momentum space is smooth in real space, which $|\psi(\zeta)\rangle$ cannot be due to the fact that the $U(1)$ bundle over X admits no global section.

As a more basic example showing where the usual off-diagonal Berry curvature (which sets up the usual q and p commutation relations) comes from, suppose our single-particle

[2] if the problem is really two-dimensional then $\mathscr{B}$ is a scalar and we should just be writing $\mathscr{B}\times\mathbf{e} \to \mathscr{B}(-E_y, E_x)$. But we haven't done this since eh, cross products are nice-looking.

states are the wavepackets[3]

$$|\psi(q,p)\rangle = \frac{1}{(\sigma^2\pi)^{1/4}} \int dx\, e^{ipx} e^{-(x-q)^2/2\sigma^2} |x\rangle. \tag{26}$$

Then $\mathcal{A}_q = 0$, while $\mathcal{A}_p = q$, so that $\mathcal{F}_{qp} = 1$. This of course gives the equations of motion $\dot{q} = \partial_q H$ and $\dot{p} = -\partial_q H$. The fact that $\mathcal{F}_{qp} = 1$ is just telling us that the symplectic volume of the pq plane is non-zero: translations in the q and p directions (implemented by p and q, respectively) do not commute, and the failure of their commutativity is measured by $\mathcal{F}_{qp}$.

[3]These of course are not orthogonal; setting $\sigma^2 = 1/2$ for simplicity gives an overlap like

$$\langle\psi(p,q)|\psi(p',q')\rangle \propto \exp\left(-(p-p')^2 - (q-q')^2 + i(q+q')(p'-p)\right). \tag{25}$$