Problem sheet 3: Berry curvature and Berry phase **27.10.2026**

3.1. Change in the Berry phase

Consider a 1D crystal, which is translated to the right by a distance x_0. The new Bloch functions are given by $\tilde{\psi}_{n\mathbf{k}} = \psi_{n\mathbf{k}}(x - x_0)$. Find the relation between $\tilde{u}_{n\mathbf{k}}$ and $u_{n\mathbf{k}}$ and use this to show that the Berry phase changes as $\tilde{\gamma}_n = \gamma_n + 2\pi x_0/a$.

3.2. Gauge invariance

(a) Consider the Schrödinger equation for the periodic part of the Bloch function,

$$\mathcal{H}_{\mathbf{k}}\, u_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k})\, u_{n\mathbf{k}}(\mathbf{r}),$$

Show that this equation remains valid under the gauge transformation

$$u_{n\mathbf{k}}(\mathbf{r}) \quad \longrightarrow \quad \tilde{u}_{n\mathbf{k}}(\mathbf{r}) = e^{i\varphi_n(\mathbf{k})}\, u_{n\mathbf{k}}(\mathbf{r}),$$

where $\varphi_n(\mathbf{k})$ is an arbitrary and sufficiently differentiable real function. Explain why the periodic part of the Bloch function is not uniquely defined.

(b) Show that the Berry connection $\mathbf{A}_n(\mathbf{k})$ is not invariant under this gauge transformation, whereas the corresponding Berry curvature $\mathbf{\Omega}_n(\mathbf{k})$ is invariant.

3.3. Wannier center and electric polarization

Consider a one-dimensional crystal with lattice constant a and Bloch eigenstates $\psi_{nk}(x) = e^{ikx}u_{nk}(x)$, where $u_{nk}(x + a) = u_{nk}(x)$ is the periodic part of the Bloch function. The Wannier function associated with band n and unit cell R is defined as

$$W_{nR}(x) = \frac{a}{2\pi}\int_{\mathrm{BZ}} dk\, e^{-ikR}\, \psi_{nk}(x).$$

(a) By differentiating $\psi_{nk}(x)$ with respect to k, show that

$$x\psi_{nk}(x) = -i\partial_k\psi_{nk}(x) + ie^{ikx}\partial_k u_{nk}(x).$$

(b) Consider the Wannier function in the home unit cell, $W_{n0}(x)$. Using the result of (a), express $xW_{n0}(x)$ in terms of the derivative $\partial_k u_{nk}(x)$.

(c) Calculate the expectation value of the position operator, $\bar{x}_n = \langle W_{n0}|\hat{x}|W_{n0}\rangle$, and obtain the Wannier center

$$\bar{x}_n = \frac{a}{2\pi}\int_{\mathrm{BZ}} dk\, A_n(k),$$

where $A_n(k)$ is the Berry connection.

(d) For a fully filled band, the electronic charge density associated with a Wannier function is $\rho_{nR}(x) = -e\,|W_{nR}(x)|^2$. Use this expression to obtain the dipole moment,

$$p_{n0} = \int dx\, x\, \rho_{n0}(x)$$

and evaluate electric polarization P_{el} (dipole moment per unit of length) via the Berry phase.

(e) Consider an adiabatic cyclic evolution of the crystal, such that $\mathcal{H}(T) = \mathcal{H}(0)$. Using $j(t) = dP_{\mathrm{el}}/dt$, demonstrate quantization of charge in the Thouless pump.