All equations one going to be derived for non-interacting Hamiltonian
\[ H_N = \sum_i \gamma_i, \] where \( \langle \gamma_i \gamma_j \rangle = \gamma_i(\hat{\gamma}) \) is wave function for a single particle.
All final equations translate to multi-particle system with "trivial" modifications, i.e. \( M_2(\hat{\gamma}, \hat{\gamma}) = M_2(\hat{\gamma}_1, \hat{\gamma}_2, \ldots, \hat{\gamma}_N) \).

However, the MTP is defined only through the wave function and its phase, i.e., Berry phase. No formulation of polarization in terms of response functions exists. Knowing \( G(\hat{\gamma}, \hat{\gamma}) \) seems not sufficient. Probably \( \gamma(\hat{\gamma}, \hat{\gamma}_1, \hat{\gamma}_2, \ldots, \hat{\gamma}_N) \) not enough either? Open problem!

Short intro to problems in defining polarization

Naive expectation: \( P_{\text{naive}} = \frac{1}{V_{\text{cell}}} \int d^2 \vec{r} \frac{\partial}{\partial t} \hat{\rho}(n) \)

Minimally fails:
1) Answer depends on the choice of the unit cell
2) For solids it is diverging

1) Non-uniqueness of polarization.

Consider NaCl 1D analog but with completely localized charges.

For completely localized charges we can use \( P_{\text{Loc}} \).

\[
P = \frac{2}{V_{\text{cell}}} \left( -\frac{e}{4} + \frac{3e}{4} \right) = \frac{e}{V_{\text{cell}}} \quad \text{vs.} \quad P = \frac{2}{V_{\text{cell}}} \left( \frac{e}{4} - \frac{3e}{4} \right) = \frac{3}{V_{\text{cell}}} \left( -\frac{e}{2} \right)
\]

Which one is correct? It turns out \( P_{\text{Loc}} \) is defined up to \( P \pm \frac{eE}{V_{\text{cell}}} \).

Given a system, we can not define it more precisely than up to \( \pm \frac{eE}{V_{\text{cell}}} \). David calls such quantity "lattice valued vector," which can take values

\[
P = \left( p_0 - \frac{\text{latt} e}{V_{\text{cell}}} | p_0 - \frac{\text{latt} e}{V_{\text{cell}}} | ... | p_0 + \frac{\text{latt} e}{V_{\text{cell}}} \right)
\]

\( M \to \infty \)
This is not a problem, because in experiment we always care about the change of polarization and not the absolute value.

The change $\frac{dP}{dt} = J$ is current that flows through a unit cell.

Imagine we take our original system of charges and transport one unit of charge from atom: $1 \rightarrow 2 \rightarrow 3 \rightarrow \ldots$

After that operation, the charges of the system are the same, hence the same polarization. But we transported an entire quantum of polarization, hence large current. Polarization actually changed from

$$P_1 = (p_0 - \frac{\epsilon_0 E_0}{V_{cell}} | p_0 - \frac{(m-1)\epsilon_0}{V_{cell}} | \ldots | p_0 + \frac{\epsilon_0}{V_{cell}} | \ldots ) \quad \text{m} → ∞$$

$$P \rightarrow (p_0 + \frac{\epsilon_0}{V_{cell}} - \frac{\epsilon_0 E_0}{V_{cell}}) p_0 + \frac{\epsilon_0}{V_{cell}} - \frac{(m-1)\epsilon_0}{V_{cell}}) \quad \text{m} → ∞$$

but $P_1 = P$, hence we see no change of the system.

Hence to calculate polarization, we need to follow the evolution of the system with external field.

Theoretical calculation should give

$$E = -E_0$$

$$E = +E_0$$

Extrapolated $P(E = 0^+)$ for infinite domain.

If we take the wrong branch, the result is wrong. Need to follow the evolution!
Now we know that the change with displacement should be measurable. Let's calculate it.

\[
\begin{align*}
P_2 &= \frac{e}{V_{\text{cell}}} \left( -\frac{3\alpha}{4} + \frac{3\alpha}{4} + d \right) \quad P_2 &= \frac{e}{V_{\text{cell}}} \left( \frac{3\alpha}{4} + d - \frac{3\alpha}{4} \right) \\
&= P_1 + \frac{e}{V_{\text{cell}}} \cdot d \quad P_2 = P_1 + \frac{e}{V_{\text{cell}}} \cdot d
\end{align*}
\]

Then:\[ P_2 - P_1 = \frac{e}{V_{\text{cell}}} \cdot d \] as expected and is unique.

Why is \( P \) not zero when there is no displacement? If the system has inversion symmetry, then \( P \) has to commute with inversion \( I \cdot P = P \)

- If \( P = \frac{e}{V_{\text{cell}}} (-M, -M + 1, \ldots, 1, 0, 1, \ldots, M-1, M) \) then \( I \cdot P = P \)
- If \( P = \frac{e}{V_{\text{cell}}} (-M + \frac{1}{2}, -M + \frac{3}{2}, \ldots, \frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \ldots, M - \frac{3}{2}, M - \frac{1}{2}) \) then \( I \cdot P = P \)

These are the only two possibilities. Either integer or half-integer function.

More realistic system would look like that Fig below, because electronic cloud is not point-like, but it moves and spreads.

It turns out that the details of the Wannier function do not matter. Only its center of mass plays the role of displacement. If we calculate \( \langle r \rangle = \int \psi^* \psi \, dx \) we get \( \langle r \rangle = \frac{\alpha}{4} - \Delta \)

Then:\[ P_2 = \frac{e}{V_{\text{cell}}} \left( \frac{\alpha}{4} - 2 \left( \frac{\alpha}{4} - \Delta \right) + \frac{3\alpha}{4} + d \right) = P_1 + \frac{e}{V_{\text{cell}}} \left( d + 2\Delta \right) \]

extra change due to movement of Wannier functions.
What if we do not want to construct Monnier functions. Can we compute $P^2$? Yes, there is formula in terms of Bloch states, which can be used:

$$\langle \hat{P} \rangle = \sum_{m} \int d^3r \; M_m(\mathbf{r}) \cdot \hat{r} \; M_m(\mathbf{r}) = \frac{V_{\text{vol}}}{(2\pi)^3} \sum_{m} \int d^3r \; \langle M_m | \frac{\partial M_m}{\partial \hat{r}} \rangle$$

(1)

$$\Gamma_{m}(\mathbf{r}) = e^{i \mathbf{k} \cdot \mathbf{r}} M_m(\mathbf{r})$$

Bloch \text{ wave function } M_m(\mathbf{r} + \mathbf{K}) = e^{i \mathbf{k} \cdot \mathbf{r}} M_m(\mathbf{r})

Solution of S.E. periodic point

We will first prove this identity (1), and later introduce more rigorously the polarization operator in Q.M. formulation.

Proof of (1):

Monnier function for an isolated band $M_m(\mathbf{r} - \mathbf{b}) = \frac{V_{\text{vol}}}{(2\pi)^3} \int d^3r \; e^{i \mathbf{k} \cdot \mathbf{r}} \; \gamma_m(\mathbf{r})$

Note also that

$$\int_{BZ} d^3r \; e^{i \mathbf{k} \cdot \mathbf{r}} = \frac{k}{V_{\text{vol}}} \text{ reciprocal}$$

$$\sum_{BZ} e^{-i \mathbf{k} \cdot \mathbf{b}} = \frac{1}{V_{\text{vol}}} \delta^3(\mathbf{k} - \mathbf{b})$$

Let's check:

- $\langle M_m \frac{\partial}{\partial \hat{r}} | M_n \frac{\partial}{\partial \hat{r}} \rangle = \int d^3r \; \langle M_m | \frac{\partial M_n}{\partial \hat{r}} \rangle \gamma_n(\mathbf{r}) = \int d^3r \; \gamma_m(\mathbf{r}) \gamma_n(\mathbf{r})$

- $M_m(\mathbf{r} - \mathbf{b}) = \frac{V_{\text{vol}}}{(2\pi)^3} \sum_{BZ} e^{i \mathbf{k} \cdot \mathbf{r}} \gamma_m(\mathbf{r}) = \sum_{BZ} M_m(\mathbf{r} - \mathbf{b}) e^{i \mathbf{k} \cdot \mathbf{r}} = \gamma_m(\mathbf{r})$

- $\langle M_m | M_n \frac{\partial}{\partial \hat{r}} \rangle = \int d^3r \; e^{i \mathbf{k} \cdot \mathbf{r}} \sum_{BZ} e^{-i \mathbf{k} \cdot \mathbf{b}} M_m^{*}(\mathbf{r} - \mathbf{b}) \frac{\partial}{\partial \hat{r}} M_n(\mathbf{r} - \mathbf{b})$

  depends only on $\frac{\mathbf{r} - \mathbf{b}}{\mathbf{k}}$, hence we can set $\mathbf{b} = 0$ and cancel $\mathbf{k}$.

  $$\langle M_m | M_n \frac{\partial}{\partial \hat{r}} \rangle = \sum_{BZ} e^{i \mathbf{k} \cdot \mathbf{r}} \sum_{BZ} e^{-i \mathbf{k} \cdot \mathbf{b}} M_m^{*}(\mathbf{r} - \mathbf{b}) \frac{\partial}{\partial \hat{r}} M_n(\mathbf{r} - \mathbf{b}) = \sum_{BZ} e^{i \mathbf{k} \cdot \mathbf{r}} \sum_{BZ} \left( \int d^3r \; M_m^{*}(\mathbf{r} - \mathbf{b}) \frac{\partial}{\partial \hat{r}} M_n(\mathbf{r} - \mathbf{b}) \right)$$

  $$\langle M_m | M_n \frac{\partial}{\partial \hat{r}} \rangle = \int d^3r \; M_m^{*}(\mathbf{r}) \frac{\partial}{\partial \hat{r}} M_n(\mathbf{r})$$

- Expand both sides for small $\mathbf{b}$:

  $$\langle M_m | M_n \frac{\partial}{\partial \hat{r}} + \mathbf{b} \cdot \frac{\partial}{\partial \hat{r}} M_n+ \frac{1}{2} (\frac{\partial}{\partial \hat{r}} M_n) \rangle = \sum_{BZ} e^{i \mathbf{k} \cdot \mathbf{r}} \langle M_m | M_n \frac{\partial}{\partial \hat{r}} + \mathbf{b} \cdot \frac{\partial}{\partial \hat{r}} M_n+ \frac{1}{2} (\frac{\partial}{\partial \hat{r}} M_n) \rangle$$

  $$\langle M_m | M_n \hat{r} \rangle = \int d^3r \; M_m^{*}(\mathbf{r}) M_n(\mathbf{r})$$

  $$\langle M_m | M_n \hat{r} \rangle = \int d^3r \; M_m^{*}(\mathbf{r}) M_n(\mathbf{r})$$
Previous equation is valid for any \( I \), hence

\[
\langle M_{\alpha} | M_{\beta} \rangle = \sum_i e^{i \frac{\pi}{2} \hat{r}} \langle M_{\alpha} | \hat{r} | M_{\beta} \rangle = 1
\]

\[
\frac{i}{\hbar} \langle M_{\alpha} | \frac{\partial}{\partial \hat{r}} M_{\beta} \rangle = \sum_i e^{i \frac{\pi}{2} \hat{r}} \langle M_{\alpha} | \frac{\partial}{\partial \hat{r}} | M_{\beta} \rangle \Rightarrow \frac{\hbar}{2 \pi} \int \hat{r} \langle M_{\alpha} | \frac{\partial}{\partial \hat{r}} M_{\beta} \rangle d^2 \hat{r} = \langle M_{\alpha} | \hat{r} | M_{\beta} \rangle
\]

\[
-\langle M_{\alpha} | \frac{\partial}{\partial \hat{r}} M_{\beta} \rangle = \sum_i e^{i \frac{\pi}{2} \hat{r}} \langle M_{\alpha} | \frac{\partial}{\partial \hat{r}} | M_{\beta} \rangle \Rightarrow -\frac{\hbar}{2 \pi} \int \hat{r} \langle M_{\alpha} | \frac{\partial}{\partial \hat{r}} M_{\beta} \rangle d^2 \hat{r} = \langle M_{\alpha} | \frac{\partial}{\partial \hat{r}} | M_{\beta} \rangle
\]

Finally for the home cell \( \vec{r} = \langle M_{\alpha} | \hat{r} | M_{\beta} \rangle = \frac{\hbar}{2 \pi} \int d^2 \hat{r} \langle M_{\alpha} | \hat{r} | M_{\beta} \rangle \) is a promised.

This is well defined only for impurities

\[
\langle \vec{r} | \langle M_{\alpha} | \hat{r} | M_{\beta} \rangle = \frac{\hbar}{2 \pi} \int d^2 \hat{r} \langle M_{\alpha} | \hat{r} | M_{\beta} \rangle
\]

Fluctuations of the magnetic centers.

We have a recipe to compute \( P \), and we know that only AP makes sense, which is:

\[
\langle \vec{r} \rangle_{\text{final}} - \langle \vec{r} \rangle_{\text{initial}} = \frac{\hbar}{2 \pi} \int d^2 \hat{r} [\langle M_{\alpha} | \frac{\partial}{\partial \hat{r}} M_{\beta} \rangle - \langle M_{\alpha} | \frac{\partial}{\partial \hat{r}} M_{\beta} \rangle]
\]

But we do not have real understanding of why \( P \) is not uniquely defined and how this is connected to the Berry phase.

How this follow from general laws of QM?

Back to the question of why \( P \) is not a simple correlation function.

We expect: \( P = \frac{\hbar}{2 \pi} \int d^2 \hat{r} \hat{P}(\hat{r}) \) and for

\[
\text{current we know:} \quad j(\hat{r}) = \frac{\hbar}{2 \pi} \int d^2 \hat{r} \hat{j}(\hat{r}, \hat{r} + \hat{r})(\hat{r}, \hat{r} + \hat{r})\]

where we have in mind slow adiabatic change with time, so that we are always in quasi equilibrium.

When we slowly move on voltage, the positive ion slowly moves to new positions, which allows the current to flow.
Than: \[ \mathbf{\hat{P}} = J \mathbf{\hat{f}} \text{ should be obeyed} \]

\[
\mathbf{\hat{P}}(t) = \frac{1}{V_{\text{tot}}} \int d^3r \mathbf{r} \frac{\delta \mathbf{P}}{\delta \mathbf{r}} \mathbf{f} \]

\[ = -\frac{1}{V_{\text{tot}}} \int d^3r \mathbf{r} \cdot \nabla (\mathbf{\hat{P}}) \mathbf{f} \]

\[
\nabla \cdot (\mathbf{\hat{P}} \mathbf{f}) = \frac{\partial}{\partial t} \int d^3r \mathbf{r} \mathbf{f} + \int d^3r \mathbf{r} \cdot \nabla \mathbf{\hat{P}} \mathbf{f} \]

\[
\nabla \cdot (\mathbf{\hat{P}} \mathbf{f}) = \int d^3r \nabla \cdot (\mathbf{\hat{P}} \mathbf{f}) = \int d^3r \mathbf{r} \cdot \nabla \mathbf{\hat{P}} \mathbf{f}
\]

\[
\mathbf{\hat{P}}(t) = -\frac{1}{V_{\text{tot}}} \int d^3r \mathbf{r} \cdot \nabla \mathbf{\hat{P}} \mathbf{f} + \frac{1}{V_{\text{tot}}} \int d^3r \mathbf{r} \frac{\delta \mathbf{P}}{\delta \mathbf{r}} \mathbf{f} \]

The true current we observe in experiment

The unit point is the \( \mathbf{P} \) formula will ill defined \( \hat{\mathbf{r}} \) in the equation heat grows and diverges, it not cell periodic.

In treating isolated molecules, when boundary is insulating, we can use

\[ \mathbf{P} = \int d^3r \mathbf{r} \mathbf{f}(\mathbf{r}) \] because the surface term vanishes. But in solids it would have the form

\[ \mathbf{P} = \sum_{\text{occupied}} \int d^3 \mathbf{r} \mathbf{f}(\mathbf{r}) \mathbf{\hat{r}} \mathbf{k}_s = \sum_{\text{occupied}} \mathbf{k}_s \cdot \mathbf{P}(\mathbf{r}) \] which is ill defined for infinite solid.

Conclusion: We need to start from observables we know how to handle, the current \( \mathbf{f} \) and derive \( \mathbf{\hat{P}} \) to satify

\[ \mathbf{I} = \frac{\delta \mathbf{P}}{\delta t} \]
\[ \dot{\mathbf{r}} = \frac{\partial \mathbf{P}}{\partial t} = \frac{\partial \mathbf{P}}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial t} = \mathbf{\dot{x}} = \mathbf{\lambda} \frac{\partial \mathbf{P}}{\partial \mathbf{x}} = \mathbf{\lambda} \sum V_{nm} \frac{d\langle \mathbf{r} \rangle}{d\mathbf{x}} \]  

Need \( \frac{d\langle \mathbf{r} \rangle}{d\mathbf{x}} \).

\[ \dot{N} = \frac{d}{dt} e^{i\mathbf{H}t} \mathbf{\hat{r}} e^{-i\mathbf{H}t} = i [H, \mathbf{\hat{r}}] \]

Hermitian operators

\[ \langle \mathbf{\tilde{r}}_{m_1} | \mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} \rangle = i \langle \mathbf{\tilde{r}}_{m_1} | H \mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} \rangle - \langle \mathbf{\tilde{r}}_{m_1} | \mathbf{\tilde{r}}_1 H \mathbf{\tilde{r}}_{m_2} \rangle \]

\[ = i (E_m - E_n) \langle \mathbf{\tilde{r}}_{m_1} | \mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} \rangle \]

Hence: \( \langle \mathbf{\tilde{r}}_{m_1} | \mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} \rangle = -i \frac{1}{E_m - E_n} \langle \mathbf{\tilde{r}}_{m_1} | \mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} \rangle \) well defined object because \( \mathbf{\tilde{r}} = \mathbf{\tilde{r}}_1 = -i \frac{\partial}{\partial \mathbf{x}} \)

Use Bloch's theorem \( \psi_{m_0}(t) = e^{it\mathbf{\tilde{r}}_1} \psi(x, t) \) where \( \psi(x, t) \) is all periodic. Then

\[ \langle \mathbf{\tilde{r}}_{m_1} | \mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} \rangle = \int \mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t) e^{i\mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t)} \]

Idea: Replace \( \mathbf{\tilde{r}}_1 \) by \( \frac{\partial}{\partial \mathbf{x}} \).

Check: \( \frac{\partial}{\partial \mathbf{x}} (e^{i\mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t)}) = -i e^{i\mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t)} \mathbf{\tilde{r}}_1 = i e^{-i\mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t)} \mathbf{\tilde{r}}_1 = e^{i\mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t)} \mathbf{\tilde{r}}_1 \]

There is no term \( \frac{\partial}{\partial \mathbf{x}} \) because in this representation \( H = \sum (U)^2 + V_{nm} \Psi_n (t) + \sum U_n (\mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t)) \)

Note that \( e^{i\mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t)} \) is all periodic.

Therefore: \( \langle \mathbf{\tilde{r}}_{m_1} | \mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} \rangle = \int \mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t) \frac{\partial}{\partial \mathbf{x}} (e^{i\mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t)}) e^{i\mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t)} \mathbf{\tilde{r}}_1 = \langle \mathbf{\tilde{r}}_{m_1} | \frac{\partial}{\partial \mathbf{x}} (e^{i\mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t)}) \mathbf{\tilde{r}}_{m_2} \rangle \)

\[ \langle \mathbf{\tilde{r}}_{m_1} | \mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} \rangle = -i \frac{1}{E_m - E_n} \langle \mathbf{\tilde{r}}_{m_1} | \frac{\partial}{\partial \mathbf{x}} (e^{i\mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} (t)}) \mathbf{\tilde{r}}_{m_2} \rangle \]  \( m \neq n \)

For polarization \( P = \frac{\partial}{\partial \mathbf{x}} \langle \mathbf{\tilde{r}}_1 \mathbf{\tilde{r}}_{m_2} \rangle \) we would need \( \langle \mathbf{\tilde{r}}_1 | \mathbf{\tilde{r}}_{m_2} \rangle \) which we do not have.

However, for the change of \( P \) (\( \frac{\partial P}{\partial \mathbf{x}} \)) only off-diagonal matrix elements contribute, and we can definitely compute \( \frac{\partial P}{\partial \mathbf{x}} \) due to movement of atoms. To do that, we need to repeat perturbation theory, i.e., how to compute the change of the W.F. under adiabatic change: \( \frac{\partial}{\partial \mathbf{x}} | M(\mathbf{x}) \rangle \)
Linear response through ordinary perturbation theory

We have a variable $x$, which changes the system adiabatically (like electric field moves atoms in the unit cell, or momentum changes unit).

How do eigenvectors change as a function of $x$?

$|M(x)\rangle$ eigenvectors for current value of $x$

$$H(x)|M(x)\rangle = E_m(x)|M(x)\rangle$$

depend on $x$ smoothly

First order derivative:

$$\frac{\partial H}{\partial x}|M\rangle + H\frac{\partial M}{\partial x} = \frac{\partial E_m}{\partial x}|M\rangle + E_m\frac{\partial M}{\partial x}$$

$$\frac{\partial E_m}{\partial x} = \frac{\partial}{\partial x}\langle M|H|M\rangle = \langle M|\frac{\partial H}{\partial x}|M\rangle + \langle M|\frac{\partial M}{\partial x}|H|M\rangle + \langle M|H\frac{\partial M}{\partial x}|M\rangle$$

$$(E_m - H)\frac{\partial M}{\partial x} = (\frac{\partial H}{\partial x} - \langle M|\frac{\partial H}{\partial x}|M\rangle) |M\rangle$$

$$\sum_{m+M} |m\rangle \langle m|\frac{\partial H}{\partial x}|m\rangle = \sum_{m+M} |m\rangle \langle m|\frac{\partial H}{\partial x}|m\rangle$$

$$\sum_{m+M} |m\rangle \langle m|\frac{\partial H}{\partial x}|m\rangle - \sum_{m+M} |m\rangle \langle m|\frac{\partial H}{\partial x}|m\rangle$$

$$(E_m - H)\frac{\partial M}{\partial x} = \sum_{m+M} |m\rangle \langle m|\frac{\partial H}{\partial x}|m\rangle$$

if $m \neq m$ then:

$$|\frac{\partial M}{\partial x}\rangle = (E_m - H)^{-1} \sum_{m+M} |m\rangle \langle m|\frac{\partial H}{\partial x}|m\rangle = \sum_{m+M} \frac{1}{E_m - E_m} |m\rangle \langle m|\frac{\partial H}{\partial x}|m\rangle$$

but there must be a term also in the direction of $|M\rangle$.

It is an arbitrary value, denoted by $iA_m$

$$|\frac{\partial M}{\partial x}\rangle = -iA_m |M\rangle + \sum_{m+M} \frac{1}{E_m - E_m} |m\rangle \langle m|\frac{\partial H}{\partial x}|m\rangle$$

We can check the correctness by plugging it back to Eq. (1).
Recall: \[ |\Omega^M_{\alpha}\rangle = -i A_m |m\rangle + \sum_{m' \neq m} \frac{1}{E_m - E_{m'}} |m\rangle <m| \frac{\partial H}{\partial \alpha} |m\rangle \] (2)

Check that if \( H \) does not depend on \( \alpha \) we get:

\[ |\Omega^M_{\alpha}\rangle = -i A_m |m\rangle \Rightarrow |M(\alpha)\rangle = e^{-i A_m} |M(0)\rangle \]

When \( H \) does not depend on \( \alpha \), we do not expect eigenfunctions to change, hence \( A_m \in \mathbb{R} \)

charge of "irrelevant" phase. Most often this term is dropped because of "irrelevant phase".

But note that this is a Berry phase, because multiplying by \( |m\rangle \) we get:

\[ <M| \Omega^M_{\alpha} |M(0)\rangle = -i A_m \]

For now we will avoid this term and write:

\[ \hat{Q}_m |\Omega^M_{\alpha}\rangle = \sum_{m' \neq m} \frac{1}{E_m - E_{m'}} |m\rangle <m| \frac{\partial H}{\partial \alpha} |m\rangle \] (3)

where \( \hat{Q}_m = 1 - |m\rangle <m| \) is projector to the rest of the Hilbert space.

How do observables change with \( \alpha \)? \[ <M| \hat{O} |M(\alpha)\rangle = \frac{\partial}{\partial \alpha} <M| \hat{O} |M(0)\rangle \]

We knew in mind an operator \( \hat{O} \) that does not depend on \( \alpha \) explicitly:

\[ \hat{O} \neq \hat{O} |\Omega^M_{\alpha}\rangle = \hat{O} |\Omega^M_{\alpha}\rangle \]

\[ \hat{O} \text{ Hermitian, then } \langle \Omega^M_{\alpha} | \hat{O} |\Omega^M_{\alpha}\rangle = \langle M(\alpha) | \hat{O} |M(0)\rangle = <M| \hat{O} |M(0)\rangle \]

\[ \frac{\partial}{\partial \alpha} <M| \hat{O} |M(\alpha)\rangle = 2 \text{Re} \left( \langle \Omega^M_{\alpha} | \hat{O} |\Omega^M_{\alpha}\rangle \right) \]
We can also insert identity

\[
2 \text{Re} \left( \frac{\partial}{\partial \alpha} \langle m | 01 \rangle \right) = 2 \text{Re} \left( \sum_{m \neq \alpha} \frac{\partial}{\partial \alpha} \langle m | 01 \rangle \right) + \left( \frac{\partial}{\partial \alpha} \langle m | 01 \rangle \right)
\]

We get:

\[
\frac{\partial}{\partial \alpha} \langle m | 01 \rangle = 2 \text{Re} \left( \frac{\partial}{\partial \alpha} \langle m | 01 \rangle \right)
\]

Next if \( |m\rangle \) is an occupied state, we would to replace \( \Phi_m \) by more convenient

\[
\Phi = \sum_{m \text{ occupied}} |m\rangle - |\Phi\rangle
\]

which is independent of \( m \).

\[
\sum_{m \text{ occupied}} \frac{\partial}{\partial \alpha} \langle m | 01 \rangle = \sum_{m \text{ occupied}} 2 \text{Re} \left( \frac{\partial}{\partial \alpha} \langle m | 01 \rangle \right)
\]

We will prove that the difference \((4)-(5)\) vanishes when summing over all occupied states.

\[
X_m = \text{Re} \left( \frac{\partial}{\partial \alpha} \langle m | 01 \rangle \right) = \text{Re} \left( \sum_{m \neq \alpha} \frac{\partial}{\partial \alpha} \langle m | 01 \rangle \right) + \left( \frac{\partial}{\partial \alpha} \langle m | 01 \rangle \right)
\]

Then \( \frac{\partial}{\partial \alpha} \langle m | 01 \rangle = 0 \) therefore

\[
\langle m | 01 \rangle + \langle m | 01 \rangle = 0
\]

\[
X_m = \sum_{m \neq \alpha} \langle m | 01 \rangle + \langle m | 01 \rangle
\]

\[
\sum_{m \text{ occupied}} X_m = \sum_{m \text{ occupied}} \langle m | 01 \rangle + \langle m | 01 \rangle - \langle m | 01 \rangle = 0
\]

\[
\text{dummy variable}
\]
We derived before:

\[
\langle \gamma_{\mathbf{m}_1} | \hat{\gamma} | \gamma_{\mathbf{m}_2} \rangle = -i \frac{1}{E_m - E_n} \langle \mathbf{m}_1 | \frac{\partial}{\partial \gamma} (e^{i \mathbf{H} \gamma} \mathbf{1}) | \mathbf{m}_2 \rangle \quad m \neq m
\]

Multiply by \(| \mathbf{m}_2 \rangle \) and sum over \(m\):

\[
\sum_{m \neq m} | \mathbf{m}_2 \rangle \langle \mathbf{m}_1 | \frac{\partial}{\partial \gamma} (e^{i \mathbf{H} \gamma} \mathbf{1}) | \mathbf{m}_2 \rangle = -i \sum_{m \neq m} \frac{1}{E_m - E_n} | \mathbf{m}_2 \rangle \langle \mathbf{m}_1 | \frac{\partial}{\partial \gamma} \mathbf{H} | \mathbf{m}_2 \rangle
\]

We derived by perturbation theory

\[
\hat{Q}_\lambda \frac{\partial M}{\partial \lambda} = \sum_{m_1, m_2} \frac{1}{E_m - E_n} |m_1 \rangle \langle m_2 | \frac{\partial M}{\partial \lambda} |m_2 \rangle \quad \text{valid for any } m_2 \neq m
\]

Then:

\[
| \mathbf{m}_1 \rangle \sum_{m \neq m} | \mathbf{m}_2 \rangle \langle \mathbf{m}_1 | \frac{\partial}{\partial \gamma} | \mathbf{m}_2 \rangle = +i \hat{Q}_\lambda \frac{\partial M}{\partial \gamma}
\]

\[
\langle \mathbf{m}_1 | \frac{\partial}{\partial \gamma} | \mathbf{m}_2 \rangle = +i \langle \mathbf{m}_1 | \hat{Q}_\lambda \frac{\partial M}{\partial \gamma} | \mathbf{m}_2 \rangle \quad \text{valid for any } m_2 \neq m
\]

Then:

\[
\hat{Q}_\lambda | \mathbf{m}_2 \rangle = +i \hat{Q}_\lambda \frac{\partial M}{\partial \gamma} | \mathbf{m}_2 \rangle
\]

hence it looks like we can replace \( \frac{\partial}{\partial \gamma} \) in matrix element of \( | \mathbf{m}_2 \rangle \)

\[ \frac{\partial}{\partial \gamma} \rightarrow i \hat{Q}_\lambda \]

\( \quad \) Matrix elements of \( \hat{\gamma} \) operator are:

\[ \langle \mathbf{m}_1 | \hat{\gamma} | \mathbf{m}_2 \rangle = \langle \mathbf{m}_1 | (i \frac{\partial}{\partial \gamma}) | \mathbf{m}_2 \rangle \]

\[ \quad \text{as long as } m \neq m! \]

We previously derived:

\[
\sum_{\mathbf{m} \in \text{occ}} \frac{\partial M}{\partial \lambda} \langle \mathbf{m} | 1 | \mathbf{m} \rangle = \sum_{\mathbf{m} \in \text{occ}} 2 \text{Re} \left( \langle \mathbf{m} | \hat{Q}_\lambda | \mathbf{m} \rangle \right) \quad (5)
\]

To calculate the change of \( \frac{\partial M}{\partial \lambda} \) for occupied states we need matrix elements of \( \hat{Q}_\lambda \) only between occupied and unoccupied states, i.e.,

\[ \frac{\partial}{\partial \lambda} \]

needs only matrix elements: \( \langle \mathbf{m}_1 | \hat{\gamma} | \mathbf{m}_2 \rangle \) hence \( m \neq m! \)

which is simply given by: \( \hat{\gamma} = (i \frac{\partial}{\partial \gamma}) \)
Repeat:

\[ \sum_{\text{meac}} \frac{2}{\alpha} \langle M_{101M} \rangle = \sum_{\text{meac}} 2 \Re \left( \frac{\Omega M}{\alpha} \mid Q \uparrow 0 \downarrow M \right) \] (5)

Next:

\[ \langle \hat{\mathcal{H}} \rangle = \sum_{\text{meac}} \frac{2}{\alpha} \langle M_{01} \rangle \]

Finally:

\[ \frac{d}{d\lambda} P = \frac{2}{\alpha} \sum_{\text{meac}} \int d^{2}\mathbf{r} \left( \sum_{\text{occupied}} \text{Im} \left( \frac{\Omega M}{\alpha} \right) \right) \]

Finally:

\[ \frac{dP}{d\lambda} = \frac{2}{\alpha} \sum_{\text{meac}} \int d^{2}\mathbf{r} \left( \sum_{\text{occupied}} \text{Im} \left( \frac{\Omega M}{\alpha} \right) \right) \]

Next we want to compute \( P \) for each state of the crystal, i.e., we need two point formula for change of \( \Delta P = P_{\text{final}} - P_{\text{initial}} \). Formally we just write

\[ \Delta P = \int \frac{dP}{d\lambda} d\lambda = \int \frac{dP}{d\lambda} d\lambda \]
(33) Let's see what thin means for 1D crystal life we discussed in the intro:

\[ \Delta P = \frac{2e}{2\pi} \sum_{n=0}^{\infty} \int_{\lambda_0}^{\infty} \int_{\lambda_0}^{\infty} \gamma_{\text{in}} \left( \frac{\partial \mu_n}{\partial \lambda} \right) \left( \frac{\partial \mu_n}{\partial \omega} \right) \, d\lambda \, d\omega \]

2D space

Define a vector quantity

\[ \vec{A} = \begin{pmatrix} A_1(x) \\ A_2(x) \end{pmatrix} = \begin{pmatrix} i \left\langle \mu_n \right| \frac{\partial \mu_n}{\partial \lambda} \right\rangle \\ i \left\langle \mu_n \right| \frac{\partial \mu_n}{\partial \omega} \right\rangle \]

Then

\[ (\nabla \times \vec{A}) = \frac{\partial}{\partial x} A_2(x) - \frac{\partial}{\partial y} A_1(x) = i \left\langle \mu_n \right| \frac{\partial \mu_n}{\partial \lambda} \right\rangle + i \left\langle \mu_n \right| \frac{\partial \mu_n}{\partial \omega} \right\rangle 
- i \left\langle \mu_n \right| \frac{\partial \mu_n}{\partial \lambda} \right\rangle - i \left\langle \mu_n \right| \frac{\partial \mu_n}{\partial \omega} \right\rangle 
= i \left( \left\langle \mu_n \right| \frac{\partial \mu_n}{\partial \lambda} \right\rangle - \left\langle \mu_n \right| \frac{\partial \mu_n}{\partial \omega} \right\rangle \right) 
= -2 \gamma_{\text{in}} \left( \frac{\partial \mu_n}{\partial \lambda} \right) \left( \frac{\partial \mu_n}{\partial \omega} \right) \right) \]

Stokes theorem:

\[ \oint_{\text{shape}} \vec{A} \cdot d\vec{A} = \int_{\text{area}} \nabla \times \vec{A} \cdot dA \]

Here \( dA = dx \cdot dy \)

Define 2D space

\[ \begin{array}{cccc}
\lambda = 0 & 1 & \text{contrib} & \text{canal} \\
\text{A} & \text{B} & \text{C} & \text{D} \\
2 = 0 & 2 = \frac{2\pi}{2} \end{array} \]

Crucial point \( \mu_{n_0} |_{\xi = 0} = \mu_{n_0} |_{\xi = \frac{2\pi}{2}} \) because this is the same point.

Hence B and D segments cancel

\[ \int_{\lambda=0}^{\lambda=1} \left( \frac{\partial \mu_n}{\partial \lambda} \right) \left( \frac{\partial \mu_n}{\partial \omega} \right) d\lambda = 0 \]
Then \[ \Delta P = \frac{\hbar}{2\pi} \sum_{\text{momo}} \int d\xi \left[ A^{(1)}(\lambda=1) - A^{(3)}(\lambda=0) \right] = \frac{\hbar}{2\pi} \sum_{\text{momo}} \int d\xi \left[ \left\langle M_{n=2} \left( \frac{\partial}{\partial N} \right) \right\rangle - \left\langle M_{n=2} \left( \frac{\partial}{\partial N} \right) \right\rangle \right]. \]

Important: We need to subtract value at \( \lambda = 1 \) and \( \lambda = 0 \). Hence \( P \) is a property of the state (up to \( \hbar \) quantum).

Finally we can generalized this to 3D (straightforward) to get:

\[ \Delta P^k = \frac{\hbar}{2\pi} \sum_{\text{momo}} \int d^2\xi (i) \left[ \left\langle M_{n=1} \left( \frac{\partial}{\partial N} \right) \right\rangle - \left\langle M_{n=1} \left( \frac{\partial}{\partial N} \right) \right\rangle \right] = \frac{\hbar}{2\pi} \int d^2\beta \sum_{\text{momo}} \Phi^k_m(\beta) - \Phi^k_{m'}(\beta) \]

Here we introduce Berry connection:

\[ \hat{A}^m_x = i \left\langle M_{n=1} \left( \frac{\partial}{\partial N} \right) \right\rangle \]

Berry phase:

\[ \Phi^k_m(\beta) = \oint A^x_m d^2\xi \]

Berry curvature:

\[ \gamma^{k}_{m}= -2\text{Tr} \left( \frac{\partial}{\partial N} \right) \left\langle M_{n=1} \left( \frac{\partial}{\partial N} \right) \right\rangle \]

Some of these quantities are not gauge invariant \( \Rightarrow \) \( P \) is lattice vector quantity (defined up to \( \hbar \) quantum of \( P = \frac{\hbar}{2\pi} \) \text{V.m} \))

Let's redefine \( \tilde{M}_m^{(\xi)} = e^{i\beta(\xi)} \left( M_{n=1}^{(\xi)} \right) \)

\( e^{i\beta(\xi)} \) periodic function of \( \xi \) in \( B^2 \), hence \( \Phi(\xi=0) = \Phi(\xi=2\pi B) = 2\pi m \)

\[ \hat{A}^x_m = i \left\langle M_{n=1} \left( \frac{\partial}{\partial N} \right) \right\rangle \left[ \frac{\partial}{\partial x^k} \right] e^{-i\beta(\xi)} \left| M_{n=1} \right\rangle. \]

Conclusion: \( \hat{A}^x_m \) is not gauge invariant (like vector potential \( \hat{A} \) for \( B \) field \( B = \nabla \times A \))

What about Berry phase?

\[ \Phi^k_m = \int d^2\xi \left( \frac{\partial}{\partial x^k} \hat{A}^x_m \right) = \Phi^k_m + \left[ \frac{\partial}{\partial x^k} \left( \hat{A}^x_m \right) \right] = \Phi^k_m + \int d^2\xi \hat{A}^x_m \]

Conclusion: Berry phase unique up to \( 2\pi m \) quantum.

If \( \Phi^k_m = \Phi^k_m + 2\pi m \) then \( \Delta P^k = \Delta P^k - \frac{\hbar}{2\pi} \left( \frac{\partial}{\partial x^k} \hat{A}^x_m \right) \]

\( 2\pi m = \Delta P^k - \frac{\hbar}{2\pi} \text{V.m} \)

P quantum