Introduction to Geometric phases

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OUTLINE

1. Geometric phases

    - Quantum Systems
    - Generalization of geometric phases
    - Methods of calculation

2. Electronic polarization as geometric phase of Bloch electrons

3. Wannier functions

Geometric (Berry) Phases in Quantum Mechanics

Dependence on parameter ξ: H(ξ)

$$i\frac{d}{dt}\Psi(t) = H(\xi(t))\Psi(t) \qquad (1)$$

At t=0: $\Psi(0) = |n, \xi(0) >$, and ξ(t) is changed asdiabatically:

$$H(\xi(t))|n, \xi(t) >= E_n(\xi(t))|n, \xi(t) >$$

$$\Psi(t) = exp\left(i\gamma_n(t) - i\int_0^t E_n(\xi(s))ds\right)|n, \xi(t) >$$

$\Psi(t)$ satisfies Schrodinger equation if:

$$\gamma_n = i\int_0^{\xi(t)} < n, \xi|\frac{d}{d\xi}|n, \xi > d\xi$$

γ_n is real, topological, non-dynamical phase independent of the rate of change in ξ with time.

Information in the phases
Consider closed paths: $H(t = 0) = H(t = T)$
$\rightarrow$ Berry phase.

- Dynamical Phase (dependent on energy):
  "How long did your trip take?"

- Geometric Phase (dependent on path and geometry):
  "Where have you been?"
  sort of like *memory*.

Geometric phase

Quantum Hamiltonian $H(\xi)$ parametrized by a scalar field ξ.
Relative phase between eigenstates u_n at ξ and ξ':

$$\begin{aligned} e^{-i\Delta\gamma_n} &= \frac{\langle u_n(\xi)|u_n(\xi')\rangle}{|\langle u_n(\xi)|u_n(\xi')\rangle|} \\ \Rightarrow \Delta\gamma_n &= -\ \mathrm{Im}\ \ln\ \langle u_n(\xi)|u_n(\xi')\rangle \end{aligned} \quad (2)$$

For $\xi' = \xi + \Delta\xi$ with $\Delta\xi \to 0$. The leading order in $\Delta\xi \Rightarrow$

$$\Delta\gamma_n = i\langle u_n(\xi)|\frac{\partial}{\partial\xi}u_n(\xi)\rangle\Delta\xi$$

For an evolving $H(\xi)$ from ξ_1 to ξ_2 the total geometric phase picked up by the system:

$$\gamma_n = i\int_{\xi_1}^{\xi_2}\langle u_n(\xi)|\frac{\partial}{\partial\xi}u_n(\xi)\rangle d\xi \quad (3)$$

Berry phase

Consider a closed path in parameter space:

$$\xi_1 \rightarrow \xi_2 \rightarrow \xi_3 \rightarrow \xi_1$$

Adiabaticity: system evolves slowly such that it is always in the same eigen state (labelled by n) of the instantaneous Hamiltonian.
Total geometric phase:

$$\gamma_n = \gamma_n^{12} + \gamma_n^{23} + \gamma_n^{31}$$

$$= - \text{ Im ln } \langle u_n(\xi_1)|u_n(\xi_2)\rangle\langle u_n(\xi_2)|u_n(\xi_3)\rangle\langle u_n(\xi_3)|u_n(\xi_1)\rangle \quad (4)$$

Note : All arbitrary phases cancel out.
Continuum limit:

$$\gamma_n^{Berry} = \oint \chi_n(\xi) d\xi, \quad (5)$$

where $\chi_n(\xi) = i\langle u_n(\xi)|\frac{\partial}{\partial \xi} u_n(\xi)\rangle$ is the Berry connection.

Generalization of geometric phase

- Aharonov and Anandan (1987):

  Adiabatic evolution is not necessary.
  Any closed loop parametric evolution of Hamiltonian yields geometric phase γ.
  γ becomes γ^{Berry} in the adiabatic limit.

- Samuel and Bhandari (1988):

  Closed loop not a necessary condition for defining γ.
  Pancharatnam connection β between eigenstates at ξ and ξ' gives the phase:

$$\beta = - \text{ Im ln } \langle u_n(\xi) | u_n(\xi') \rangle$$

  .

Open path geometric phase

Consider an open path in parameter space :

$$\xi_1 \rightarrow \xi_2 \rightarrow \xi_3 \rightarrow \xi_4$$

Hamiltonian at ξ_1 and ξ_4 are related by a symmetry:

$$H(\xi_4) = W^{-1} H(\xi_1) W \Rightarrow u_n(\xi_4) = W^{-1} u_n(\xi_1)$$

$$\Rightarrow \gamma_n = - \text{ Im ln (}$$

$$\langle u_n(\xi_1)|u_n(\xi_2)\rangle\langle u_n(\xi_2)|u_n(\xi_3)\rangle\langle u_n(\xi_3)|W^{-1}|u_n(\xi_1)\rangle)$$

Example : Bloch electrons in an isolated band n

For a direction α :
$k_\alpha^i = \frac{(i-1)}{M} b_\alpha, i = 1$ to M
b_α: a reciprocal space lattice vector

$$H(k_\alpha + b_\alpha) = \exp(-i b_\alpha \cdot r) H(k_\alpha) \exp(i b_\alpha \cdot r)$$

$H(k)$: Hamiltonian for the cell periodic part of Bloch functions

$u_{n(k_\alpha + b_\alpha)} = \exp(-i b_\alpha \cdot r) u_{n k_\alpha} \rightarrow$ Periodic gauge

$$\gamma_n^\alpha = -\ \text{Im ln}\ \langle u_{nk_\alpha^1}|u_{nk_\alpha^2}\rangle\langle u_{nk_\alpha^2}|u_{nk_\alpha^3}\rangle$$

$$...\langle u_{nk_\alpha^{(M-1)}}|e^{(-ib_\alpha r_\alpha)}|u_{nk_\alpha^1}\rangle \qquad (7)$$

In the continuum limit:

$$\gamma_n^\alpha = i\int_0^{b_\alpha}\langle u_{nk_\alpha}|\frac{\partial}{\partial k_\alpha}u_{nk_\alpha}\rangle dk_\alpha \qquad (8)$$

Non Abelian geometric phase

N-electron single Slater determinant state from independent electronic wavefunctions:
$|\Psi(\xi)\rangle = \frac{1}{\sqrt{N!}}|u_1(\xi)u_2(\xi)...u_N(\xi)|$

From (2): $\Delta\gamma = -$ Im ln $\langle\Psi(\xi)|\Psi(\xi')\rangle$

$$= - \text{ Im ln } \det S(\xi,\xi'), \qquad (9)$$

$S_{ij}(\xi,\xi') = \langle u_i(\xi)|u_j(\xi')\rangle \rightarrow (N\times N)$ matrix
For a closed path made of M contiguous discreet points in ξ space the Berry phase [(3)] generalizes to $(N\times N)$ matrix Γ given by:

$$e^{i\Gamma} = \Pi_{s=1}^{M} S(\xi_s,\xi_{s+1})$$

In the continuum limit:

$$\exp -i\Gamma = P\exp -i\oint \chi(\xi)d\xi, \qquad (10)$$

P is path ordering operator.

$\chi_{ij}(\xi) = i\langle u_i(\xi)|\frac{\partial}{\partial\xi}u_j(\xi)\rangle$: Non Abelian connection

$$\begin{aligned}\gamma &= - \text{ Im ln } \Pi_{s=1}^{M}\langle\Psi(\xi_s)|\Psi(\xi_{s+1})\rangle \\ &= - \text{ Im ln det } e^{-i\Gamma} = \text{ Re tr } \Gamma \qquad (11)\end{aligned}$$

(11) implies :

$$\gamma = \text{ Re tr } \Gamma = \sum_{j=1}^{N} \gamma_j \qquad (12)$$

$\left\{\gamma_j\right\}$, the eigenvalues of gauge invariant Γ, are potential physical observable.
Within parallel transport gauge the open path geometric phase [(6)] if obtained as:

$$|u_n^{||}(\xi_4)\rangle = e^{i\gamma_n} W^{-1} |u_n^{||}(\xi_1)\rangle \qquad (13)$$

Similarly the geometric phase matrix Γ is obtained as:

$$\left[e^{i\Gamma}\right]_{ij} = \langle u_i^{||}(\xi_1)|W|u_j^{||}(\xi_4)\rangle \qquad (14)$$

For Bloch electrons along k_α in the Brillouin zone :

$$\left[e^{i\Gamma_\alpha}\right]_{ij} = \langle u^{||}_{\mathbf{k},\mathbf{i}}|e^{b_\alpha \cdot r}|u^{||}_{\mathbf{k}+\vec{\mathbf{e}}_\alpha \mathbf{b}_\alpha,\mathbf{j}}\rangle \qquad (15)$$

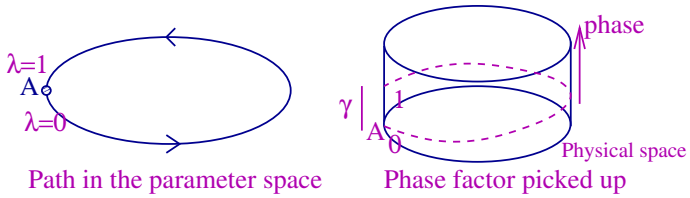
where $b_\alpha = 2\pi/a$, a being the lattice constant in the α direction.

Parallel Transported Wavefunctions and Geometric Phase

- Parallel Transport:

$$< n, \xi | \frac{d}{d\xi} | n, \xi >= 0$$

- Geometric phase: $|n, \xi + \Delta\xi >_{||} = |n, \xi >_{||} + \Delta\xi \frac{d}{d\xi} |n, \xi >_{||}$



γ recoverd once the loop is closed!

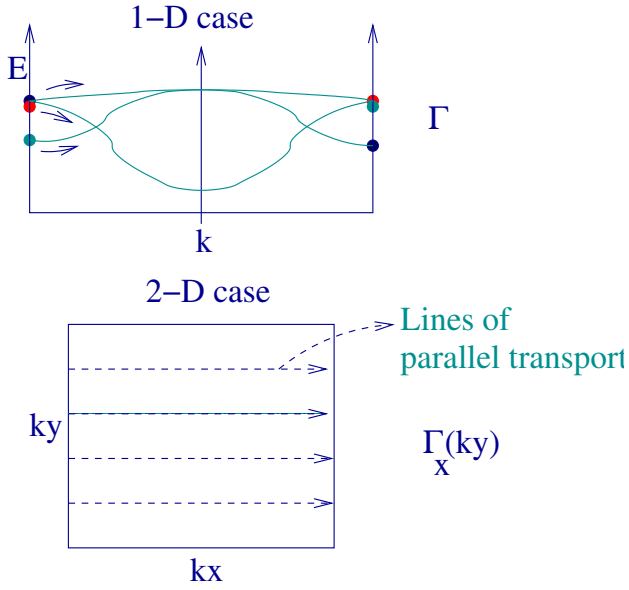
$$\gamma = Im(Log(< n, \xi = 0 | n, \xi = 1 >))$$

- No random phases if:
  $\psi(\xi_1)$ and $\psi(\xi_2)$ are related to each other by parallel transport

Calculation of Γ phase matrix (DFT)

- Parallel Transport(PT) Bloch functions from $k = -\frac{\pi}{a}$ to $k = \frac{\pi}{a}$
  - Obtain $\frac{d}{dk}|u_{kn}>$ using DFT linear response s.t. $< u_{km}|\frac{d}{dk}|u_{kn}>= 0$
  - $|u_{k+\Delta kn}>= |u_{kn}> + \Delta k \frac{d}{dk}|u_{kn}>$: Runge-Kutta integrate from k to $k + \delta k$
  - Obtain $\Gamma = ImLog < u_{k+\frac{2\pi}{a}m}|W|u_{kn}>$
- Discretized parallel transport:
  - Obtain overlap matrix: $S(k, k + \Delta k)$
  - Singular Value Decomposition $S = U\Sigma V^\dagger$
  - Rotate wavefunctions at $k+\Delta k$ by $T = (UV^\dagger)^\star$
  - Obtain $\Gamma = ImLog < u_{k+\frac{2\pi}{a}m}|W|u_{kn}>$

Geometric Phases in 1-d and 2-d



- Eigenvalues of Γ: Centre of Wannier function ("Bond")

- Eigenvectors of Γ: which bands make up the "Bond"

Electronic polarization: geometric phase

For electrons in a crystal: conventional definition of electronic polarization in terms of Bloch functions :

$$P_\alpha = \frac{f q_e}{N\Omega} \sum_{k_\alpha} \sum_{m}^{M} \langle \psi^\lambda_{\mathbf{k},\mathbf{m}} | r_\alpha | \psi^\lambda_{\mathbf{k},\mathbf{m}} \rangle$$

is ill defined.

Rather, the change of polarization $\triangle P_\alpha = \int d\lambda \left(\frac{\partial P_\alpha}{\partial \lambda} \right)$ in an evolving system (λ being the evolving parameter) is a meaningful physical quantity.

In the derivative of P_α(as given above) w.r.t. λ, substituting perturbation expansion for the wavefunction derivatives and using the identity $\frac{i}{\hbar} \left[H\widehat{(\lambda)}, \widehat{r} \right] = \frac{1}{m_e} \widehat{p}$ we obtain :

$$\frac{\partial P^\lambda_\alpha}{\partial \lambda} =$$

$$\frac{-ie\hbar}{\Omega m_e}\sum_{k_\alpha}\sum_{m}^{occ}\sum_{n}^{empty}\frac{\langle\psi^\lambda_{\mathbf{k,m}}|\widehat{p_\alpha}|\psi^\lambda_{\mathbf{k,n}}\rangle\langle\psi^\lambda_{\mathbf{k,n}}|\frac{\partial V^\lambda_{KS}}{\partial\lambda}|\psi^\lambda_{\mathbf{k,m}}\rangle}{(E_{k_\alpha,m}-E_{k_\alpha,n})^2}+cc \quad (16)$$

With identities: $\widehat{p_\alpha}=\frac{m_e}{\hbar}[\frac{\partial}{\partial k_\alpha},H(\lambda)]$; $[\frac{\partial}{\partial\lambda},H^\lambda_{k_\alpha}]=\frac{\partial V^\lambda}{\partial\lambda}$ and $[\frac{\partial}{\partial\lambda},\frac{\partial}{\partial k_\alpha}]=0$, followed by algebraic manipulation eqn.(16) yields:

$$\triangle P_\alpha=\frac{ifq_e}{8\pi^3}\sum_m^M\int_{BZ}dk_\alpha\langle u^\lambda_{\mathbf{k,m}}|\frac{\partial}{\partial k_\alpha}|u^\lambda_{\mathbf{k,m}}\rangle|_0^1$$

$$-\frac{ifq_e}{8\pi^3}\sum_m^M\int_{BZ}dk_\alpha\left[\int_0^1 d\lambda\frac{\partial}{\partial k_\alpha}\langle u^\lambda_{\mathbf{k,m}}|\frac{\partial}{\partial\lambda}|u^\lambda_{\mathbf{k,m}}\rangle\right] \quad (17)$$

where $u^\lambda_{\mathbf{k,m}}=e^{-i\mathbf{k.r}}\psi^\lambda_{\mathbf{k,m}}$

Periodic gauge: $\psi^\lambda_{\mathbf{k,m}}(\mathbf{r})=\psi^\lambda_{\mathbf{k}+\vec{\mathbf{e}}_\alpha\mathbf{b}_\alpha,\mathbf{m}}(\mathbf{r})$ eliminates the second term and gives:

$$P^\lambda_\alpha=\frac{ifq_e}{8\pi^3}\sum_m^M\int_{BZ}dk_\alpha\langle u^\lambda_{\mathbf{k,m}}|\frac{\partial}{\partial k_\alpha}|u^\lambda_{\mathbf{k,m}}\rangle \quad (18)$$

Same as the Zak phase expression [(8)] for single band.

In the discreet $\mathbf{k}$ mesh in Brillouin zone P_α is

obtained by integrating Eqn.(9) :

$$P_x = -\frac{f q_e}{8\pi^3} \int_{b_y, b_z} dk_y dk_z$$

$$\left\{ \text{Im ln } \Pi_{s=1}^{M} \text{ det } (\langle u^{\lambda}_{k_{X_s}, m} | u^{\lambda}_{k_{X_{s+1}}, n} \rangle) \right\} \quad (19)$$

where k_{X_s} forms a regular grid of M k_X points for each (k_y, k_z).

Eqn (19) is used in the Berry phase calculation of polarization:

M: # of k-points along the direction of P.

N: # of bands (size of the subspace).

Wannier function

Definition: Fourier transform of cell periodic wave functions.

$$W_n(\mathbf{r},\mathbf{R}) = \sqrt{N}\Omega/(2\pi)^3 \int_{\mathbf{BZ}} \mathbf{e}^{\mathbf{ik.(r-R)}} \mathbf{u_{k,n}}(\mathbf{r})\mathbf{dk} \tag{20}$$

$\mathbf{R} \rightarrow$ real space lattice vector.
Orthogonality relation:

$$\int_\Omega d\mathbf{r}\mathbf{W}^*_{\mathbf{n}}(\mathbf{r},\mathbf{R})\mathbf{W}_{\mathbf{n'}}(\mathbf{r},\mathbf{R'}) = \delta_{\mathbf{nn'}}\delta_{\mathbf{RR'}}$$

Orthonormal set of Wannier function(WF) as basis:

$$u_{n\mathbf{k}}(\mathbf{r}) = 1/\sqrt{N}\sum_{\mathbf{R}} \mathbf{e}^{\mathbf{ik(R-r)}}\mathbf{W_n}(\mathbf{r},\mathbf{R}) \tag{21}$$

$u_{\mathbf{k,n}}$ can have two types of phases:
1. Random phase due to diagonalization.
2. Gauge dependent phase of geometric origin.
$\Rightarrow$ WFs are non-unique.

Localized WFs are obtained from wave functions which are cell periodic and differentiable through out the BZ.

Substituting (21) in (18) we get:

$$P_\alpha = \frac{f q_e}{\Omega} \sum_{n=1}^{M} \int r_\alpha |W_n(\mathbf{r})|^{\mathbf{2}} \mathbf{dr} \qquad (22)$$

For any arbitrary direction α in real space, a unique set of gauge exist that diagonalize $e^{i\Gamma_\alpha}$ [(15)].

The resultant WFs are perfectly localized in α direction. They are eigen states of projected position operator:

$$\hat{P}\hat{r}_\alpha\hat{P} \qquad (23)$$

where $\hat{P}$ is the projection operator onto the group of bands under consideration.

Centroid of these WFs:

$\frac{1}{\Omega}\int r_\alpha |W_n(\mathbf{r})|^{\mathbf{2}} \mathbf{dr} = \mathbf{a}\gamma_\mathbf{n}/\mathbf{2}\pi$

a is lattice constant and γ_n are eigen values of Γ_α.

In terms of parallel transported wave functions $\left\{v_{\mathbf{k},\mathbf{n}}\right\}$ obtained from the energy eigen states $\left\{u_{\mathbf{k},\mathbf{n}}\right\}$ for multibands in 1D (chosen to be α) the desired unique gauge at each k_α :

$$U_{nm,k_\alpha} = \exp\left\{-ik_\alpha\left(\frac{\gamma_n a}{2\pi}\right)\right\} M^{\star}_{mn} \qquad (24)$$

M diagonalizes Γ_α.

Generalized expression for WF for insulator as well as metals at temperature T:

$$|W_n^T(r_\alpha, R)\rangle = \int dk_\alpha \sum_m e^{ik_\alpha(r_\alpha - R)}$$

$$C^{k_\alpha}_{nm}\left[f(E_{mk_\alpha}, T)\right]^{\frac{1}{2}} |u_{\mathbf{k},\mathbf{m}}\rangle \qquad (25)$$

$f(E_{mk}, T)$ is FD distribution and

$$C^{k_\alpha} = U^{k_\alpha} R^{k_\alpha},$$

R: unitary transformation from energy eigen states to parallel transported states.

For 3-D crystal systems : three projected position operators or Γ matrices do not commute.

$\Rightarrow$ No unique gauge that gives WFs perfectly localized in all directions.

Maximally localized Wannier function(MLWF):

A conceptual extension of Foster-Boys localization scheme to periodic systems.

MLWFs obtained through variational minimization of second moment (cumulant) of squared WFs w.r.t. evolving unitary transformation matrix at each $\mathbf{k}$

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