

# Berry Phase, Polarization, Persistent Current (1)

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## Berry phase:

- Pancharatnam (classical optics)  
precursor of Berry phase
- Hamiltonian of some system:  $H(\vec{\xi})$   
 $\vec{\xi}$  - parameter (can be many dimensional)

$$H(\vec{\xi}) |\Psi(\vec{\xi})\rangle = E(\vec{\xi}) |\Psi(\vec{\xi})\rangle$$

example: electronic Hamiltonian depends  
parametrically on nuclear coordinates  
(nuclear coordinates:  $\vec{\xi}$ )

- for this example: assume non-degenerate  
ground state

$$~~H(\vec{\xi}) = E~~ \quad H(\vec{\xi}) |\Psi_0(\vec{\xi})\rangle = E_0(\vec{\xi}) |\Psi_0(\vec{\xi})\rangle$$

- if we take two different points in parameter space  
 $\vec{\xi}_1$  and  $\vec{\xi}_2$ , we can define quantity

$$-i \frac{\Delta\varphi_{12}}{e} = \frac{\langle \Psi(\vec{\xi}_1) | \hat{U}(\vec{\xi}_1, \vec{\xi}_2) | \Psi(\vec{\xi}_2) \rangle}{|\langle \Psi(\vec{\xi}_1) | \Psi(\vec{\xi}_2) \rangle|}$$

$$\text{phase: } \Delta\varphi_{12} = -\text{Im} \log \langle \Psi(\vec{\xi}_1) | \hat{U}(\vec{\xi}_1, \vec{\xi}_2) | \Psi(\vec{\xi}_2) \rangle$$

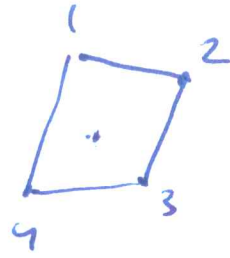
$\Delta\varphi_{12}$  - defined up to  $2\pi m$ , unless  $\langle \Psi(\vec{\xi}_1) | \hat{U}(\vec{\xi}_1, \vec{\xi}_2) | \Psi(\vec{\xi}_2) \rangle = 0$   
orthogonal states)

- phase usually has no physical meaning:  
wave functions are undetermined up to  
a phase  $\Rightarrow$  phase is a "choice"  
gauge

- consider a finite number of points in  $\vec{\xi}$ -space

(2)

$$\gamma = \Delta\varphi_{12} + \Delta\varphi_{23} + \Delta\varphi_{34} + \Delta\varphi_{41} \rightarrow$$



$$= -\text{Im} \log \left[ \langle \bar{\Psi}(\vec{\xi}_1) | \Psi(\vec{\xi}_1) \rangle \langle \bar{\Psi}(\vec{\xi}_2) | \Psi(\vec{\xi}_2) \rangle \right. \\ \left. \langle \bar{\Psi}(\vec{\xi}_3) | \Psi(\vec{\xi}_3) \rangle \langle \bar{\Psi}(\vec{\xi}_4) | \Psi(\vec{\xi}_4) \rangle \right]$$

$\gamma$ -gauge invariant! each  $|\Psi(\vec{\xi}_i)\rangle$  has a  $\langle \bar{\Psi}(\vec{\xi}_i) |$   
"pair"  $\Rightarrow$  arbitrary phase is cancelled

$\Downarrow$   $\Downarrow$   
 $\gamma$ -well-defined physical quantity  $\rightarrow$  depends on  
path in  $\vec{\xi}$ -space

new aspect of  $\gamma$ : usually in quantum mechanics  
physically well-defined quantities correspond  
to Hermitian operators

- Berry argued for the physical significance  
of  $\gamma$

- initial assumption: Hamiltonian is parametric

$\Rightarrow$  follows that isolated systems do  
not exhibit a Berry phase

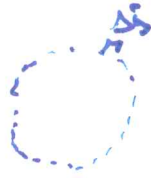
$\Downarrow$   $\Downarrow$   
system + surroundings (rest of universe)  
gives rise to Berry phase

# The continuum limit

(3)

$$e^{-i\Delta\phi} = \frac{\langle \Psi(\vec{s}) | \Psi(\vec{s} + \Delta\vec{s}) \rangle}{|\langle \Psi(\vec{s}) | \Psi(\vec{s} + \Delta\vec{s}) \rangle|}$$

- consider case when  $\Delta\vec{s} \rightarrow 0$ , moreover construct circular path which is closed



$$-i\Delta\phi = \log \langle \Psi(\vec{s}) | \Psi(\vec{s} + \Delta\vec{s}) \rangle - \log |\langle \Psi(\vec{s}) | \Psi(\vec{s} + \Delta\vec{s}) \rangle|$$
$$= \log [ \langle \Psi(\vec{s}) | \Psi(\vec{s}) \rangle + \langle \Psi(\vec{s}) | \nabla_{\vec{s}} | \Psi(\vec{s}) \rangle \cdot \Delta\vec{s} ] - \log |\langle \Psi(\vec{s}) | \Psi(\vec{s}) \rangle|$$

$$\text{Im} \left[ \Delta\phi = -\text{Im} \log \langle \Psi(\vec{s}) | \Psi(\vec{s} + \Delta\vec{s}) \rangle \right]$$

$$= -\text{Im} \log [ \langle \Psi(\vec{s}) | \Psi(\vec{s}) \rangle + \langle \Psi(\vec{s}) | \nabla_{\vec{s}} | \Psi(\vec{s}) \rangle \cdot \Delta\vec{s} ] \quad \text{for small } \Delta\vec{s}$$

$$= -\text{Im} \langle \Psi(\vec{s}) | \nabla_{\vec{s}} | \Psi(\vec{s}) \rangle \cdot \Delta\vec{s}$$

~~the~~ the circuit integral  $\oint d\phi$  around closed path given by  $\rightarrow \gamma = \oint d\phi = -\text{Im} \oint \langle \Psi(\vec{s}) | \nabla_{\vec{s}} | \Psi(\vec{s}) \rangle \cdot d\vec{s}$

$$\text{or equivalently: } \gamma = i \oint \langle \Psi(\vec{s}) | \nabla_{\vec{s}} | \Psi(\vec{s}) \rangle \cdot d\vec{s}$$

- this limit can be carried out only if  $|\Psi(\vec{s})\rangle$  is differentiable, but the discrete Berry phase is always well-defined



# Connection and Curvature

(4)

$$\gamma = \oint_C db = i \oint_C \langle \Psi(\hat{\xi}) | \nabla_{\hat{\xi}} \Psi(\hat{\xi}) \rangle \cdot d\hat{\xi}$$

relation to magnetism

vector potential:  $\vec{A}(\hat{\xi})$

magnetic field:  $\vec{B}(\hat{\xi}) = \nabla_{\hat{\xi}} \times \vec{A}(\hat{\xi})$

Stokes theorem:  $\oint_C \vec{A}(\hat{\xi}) \cdot d\hat{\xi} = \iint_{\text{surface}} \vec{B}(\hat{\xi}) \cdot \vec{n} da$   
 line integral                      surface integral

- Berry connection:  $i \langle \bar{\Psi}(\hat{\xi}) | \nabla_{\hat{\xi}} \Psi(\hat{\xi}) \rangle = \vec{V}(\hat{\xi})$

- Berry curvature:  ~~$\gamma_{\alpha\beta} = - \left( \frac{\partial \gamma_{\beta\alpha}(\hat{\xi})}{\partial \xi_{\alpha}} - \frac{\partial \gamma_{\alpha\beta}(\hat{\xi})}{\partial \xi_{\beta}} \right)$~~

$$\gamma_{\alpha\beta} = - \left( \frac{\partial \gamma_{\beta\alpha}(\hat{\xi})}{\partial \xi_{\alpha}} - \frac{\partial \gamma_{\alpha\beta}(\hat{\xi})}{\partial \xi_{\beta}} \right)$$

consider one component of ~~curvature~~ connection

$$\gamma_{\alpha}(\hat{\xi}) = i \langle \bar{\Psi}(\hat{\xi}) | \frac{\partial \Psi(\hat{\xi})}{\partial \xi_{\alpha}} \rangle$$

$$\frac{\partial \gamma_{\alpha}(\hat{\xi})}{\partial \xi_{\beta}} = i \left\langle \frac{\partial \bar{\Psi}(\hat{\xi})}{\partial \xi_{\beta}} \left| \frac{\partial \Psi(\hat{\xi})}{\partial \xi_{\alpha}} \right. \right\rangle$$

$$+ i \langle \bar{\Psi}(\hat{\xi}) | \frac{\partial^2 \Psi(\hat{\xi})}{\partial \xi_{\beta} \partial \xi_{\alpha}} \rangle$$

$$\gamma_{\alpha\beta} = -i \left( \left\langle \frac{\partial \bar{\Psi}(\hat{\xi})}{\partial \xi_{\beta}} \left| \frac{\partial \Psi(\hat{\xi})}{\partial \xi_{\alpha}} \right. \right\rangle - \left\langle \frac{\partial \bar{\Psi}(\hat{\xi})}{\partial \xi_{\alpha}} \left| \frac{\partial \Psi(\hat{\xi})}{\partial \xi_{\beta}} \right. \right\rangle \right)$$

$$= 2 \text{Im} \left\langle \frac{\partial \bar{\Psi}(\hat{\xi})}{\partial \xi_{\alpha}} \left| \frac{\partial \Psi(\hat{\xi})}{\partial \xi_{\beta}} \right. \right\rangle$$

- real wavefunctions:  $\gamma_{\alpha\beta} = 0$

(5)

- nontrivial Berry phase occurs if domain  $\vec{s}$  is not simply connected

- complex wavefunctions: nontrivial Berry phase can occur

### Perturbation expression for curvature

$$\nabla_{\vec{s}} |\Psi_0(\vec{s})\rangle \approx \sum_n \frac{|\Psi_n(\vec{s})\rangle \langle \Psi_n(\vec{s}) | \nabla_{\vec{s}} H(\vec{s}) | \Psi_0(\vec{s}) \rangle}{E_n(\vec{s}) - E_0(\vec{s})}$$

(expression can be derived from first-order perturbation theory)

$\Downarrow$

$\Downarrow$

$$\gamma_{\alpha\beta} = 2 \operatorname{Im} \sum_{n \neq 0} \frac{\langle \Psi_0(\vec{s}) | \frac{\partial H(\vec{s})}{\partial \vec{z}_\alpha} | \Psi_n(\vec{s}) \rangle \langle \Psi_n(\vec{s}) | \frac{\partial H(\vec{s})}{\partial \vec{z}_\beta} | \Psi_0(\vec{s}) \rangle}{(E_0(\vec{s}) - E_n(\vec{s}))^2}$$

curvature diverges at degeneracies

for real  $\Psi$  non-trivial Berry phase obtained if singularities present

complex wavefunctions can always give a non-trivial Berry phase

# Physical Example of Berry Phase: Crystalline (6)

## Polarization

Definition:  $\vec{P} = -e \int d\vec{r} \vec{r} n(\vec{r}) \rightarrow$  valid for  
finite systems (molecules)

for crystals: definition is not valid due to  
absence of a valid position operator for periodic  
systems

- constructing one is easier if we switch to  
 $k$ -space: assume system is periodic in  $L$

$$\langle \psi | \hat{X} | \psi \rangle = \langle \psi | \sum_i x_i | \psi \rangle$$

$$\text{in } k\text{-space: } i \langle \psi | \sum_i \frac{\partial}{\partial k_i} | \psi \rangle$$

$$= i \int dk_1, \dots, dk_n \psi^*(k_1, \dots, k_n) \left( \sum_i \frac{\partial}{\partial k_i} \right) \psi(k_1, \dots, k_n)$$

- write wave function as

$$\psi(k_1 + K, \dots, k_n + K)$$

$$\sum_i \frac{\partial}{\partial k_i} \psi(k_1 + K, \dots, k_n + K)$$

$$= \frac{\partial}{\partial K} \psi(k_1 + K, \dots, k_n + K)$$

- in crystalline system:  $K$  - crystalline momentum

has to be sampled (integrated over)

$$\rightarrow \frac{1}{L^n} \int_{-\pi}^{\pi} dK \dots$$

thus: polarization becomes  $\frac{iL}{2\pi} \int_{-\pi}^{\pi} dk \langle \Psi | \partial_{\epsilon} | \Psi \rangle$  (7)

- of interest is the discretized version:

$\frac{iL}{2\pi} \int_{-\pi}^{\pi} dk \langle \Psi | \partial_{\epsilon} | \Psi \rangle$  is a Berry phase since  $k$  can be viewed as a parameter

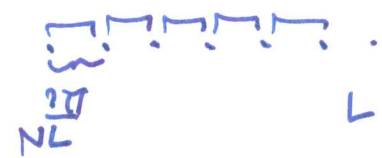
- we have shown in the beginning that a discretized Berry phase is related to a continuous one as

$$i \oint \langle \Psi | \partial_{\epsilon} | \Psi \rangle d\epsilon = \text{Im} \log \prod_{i=1}^N \langle \Psi(\epsilon_i) | \Psi(\epsilon_{i+1}) \rangle$$

$$\Downarrow$$

$$\langle X \rangle = \frac{iL}{2\pi} \int dk \langle \Psi | \partial_k | \Psi \rangle = \frac{L}{2\pi} \text{Im} \log \prod_{i=0}^{N-1} \langle \Psi(k_i) | \Psi(k_{i+1}) \rangle$$

where  $k_i$  defines a set of grid points



$L$  - length of system (periodicity)

- suppose there exists an operator which shifts the total momentum of the system by  $\frac{2\pi}{NL}$

let's denote it as  $\hat{U}(\frac{2\pi}{NL})$

$$\hat{U}(\frac{2\pi}{NL}) | \Psi(k_1, \dots, k_N) \rangle = | \Psi(k_1 + \frac{2\pi}{NL}, \dots, k_N + \frac{2\pi}{NL}) \rangle$$

$\Downarrow$

$$\hat{U}(\frac{2\pi}{NL}) | \Psi(k_i) \rangle = | \Psi(k_{i+1}) \rangle$$



$$\hat{U}\left(\frac{2\pi}{NL}n\right)|\Psi(k_0)\rangle = |\Psi(k_m)\rangle \quad (8)$$

- if we are lucky this operator will also have the property

~~$$\langle \Psi(k_0) | \hat{U}\left(-\frac{2\pi}{NL}m\right) = \langle \Psi(k_m) |$$~~

$$\langle \Psi(k_0) | \hat{U}\left(-\frac{2\pi}{NL}m\right) = \langle \Psi(k_m) |$$

and most likely it will since it must be unitary (but we'll see that when we construct it)

- For any "i" I can write

$$\begin{aligned} \langle \Psi(k_i) | \Psi(k_{i+1}) \rangle &= \langle \Psi(k_i) | \hat{U}\left(\frac{2\pi}{NL}\right) | \Psi(k_i) \rangle \\ &= \langle \Psi(k_0) | \hat{U}\left(-\frac{2\pi}{NL}i\right) \hat{U}\left(\frac{2\pi}{NL}\right) \hat{U}\left(\frac{2\pi}{NL}i\right) | \Psi(k_0) \rangle \\ &= \langle \Psi(k_0) | \hat{U}\left(\frac{2\pi}{NL}\right) | \Psi(k_0) \rangle \end{aligned}$$

$$\begin{aligned} \Rightarrow \text{polarization: } \langle \chi \rangle &= \frac{1}{2\pi} \text{Im} \log \left[ \langle \Psi | \hat{U}\left(\frac{2\pi}{NL}\right) | \Psi \rangle \right]^N \\ &= \frac{NL}{2\pi} \text{Im} \log \left[ \langle \Psi | \hat{U}\left(\frac{2\pi}{NL}\right) | \Psi \rangle \right] \end{aligned}$$

where  $|\Psi\rangle$  is the wavefunction at any of the points  $k_i$

(choose  $k_i = 0$ )



- remaining task construct total momentum shift

(9)

- second quantized formalism: fermions

$$[c_i^\dagger, c_j^\dagger] = [c_i, c_j] = 0$$

$$[c_i, c_j^\dagger] = \delta_{ij}$$

permutation operator:  $P_{ij} = 1 - (c_i^\dagger - c_j^\dagger)(c_i - c_j)$

$$P_{ij} = P_{ij}^\dagger$$

$$P_{ij} = P_{ji}$$

$$P_{ij} c_j = c_i P_{ij}$$

$$P_{ij} c_i^\dagger = c_j^\dagger P_{ij}$$

$$P_{ij} c_j^\dagger = c_i^\dagger P_{ij}$$

~~Proof of~~

Proof of

$$\rightarrow [1 - (c_i^\dagger - c_j^\dagger)(c_i - c_j)] c_j$$

$$= c_j - c_i^\dagger c_i c_j + c_j^\dagger c_i c_j$$

$$= c_j - (1 - c_i c_i^\dagger) c_j - c_i c_j^\dagger c_j$$

$$= c_i c_i^\dagger c_j - c_j^\dagger c_j$$

$$= c_i [c_i^\dagger c_j - c_j^\dagger c_j]$$

$$= c_i [(c_i^\dagger - c_j^\dagger) c_j] \leftarrow c_j$$

not quite  $P_{ij}$

missing:  $1 - (c_i^\dagger - c_j^\dagger) c_i$

$$c_i [1 - (c_i^\dagger - c_j^\dagger) c_i] =$$

$$= c_i - c_i c_i^\dagger c_i + c_i c_j^\dagger c_i$$

$$= c_i (1 - c_i^\dagger c_i) + c_i c_j^\dagger c_i$$

$$= c_i c_i c_i^\dagger - c_i c_i c_i^\dagger = 0 \checkmark$$

QED

$$P_{ij} P_{jk} = P_{in} P_{ij} = P_{jk} P_{in}$$

$$P_{ij} P_{ij} = 1$$

$$[P_{ij}, P_{kl}] = 0 \quad (\text{commutator})$$

these properties can be shown using the rules at second quantization (anti-commutator)

~~spin-dependent generalization also possible~~

- define:

$$\hat{U}_n = P_{n-1, n} \dots P_{23} P_{12} \quad n = 2, \dots, L$$

$$\hat{U}_L \text{ satisfies: } \hat{U}_L c_j = \begin{cases} c_{j+1} \hat{U}_L & j=2, \dots, L \\ c_L \hat{U}_L & j=1 \end{cases}$$

$$\hat{U}_L^\dagger = P_{12} \dots P_{n-1, n} \Rightarrow \hat{U}_L^\dagger \hat{U}_L = 1$$

$\hat{U}_L = \text{unitary}$

suppose now that the states  $c_j$  are momentum eigenstates: ~~lets denote them as  $\tilde{c}_j$~~

$c_j$  - momentum eigenstates  $\rightarrow \tilde{c}_j$   $k_j = \frac{2\pi j}{NL}$

$\tilde{c}_j$  - position eigenstates

if I have a state:  $|\bar{\Psi}\rangle = c_{j_1}^\dagger \dots c_{j_n}^\dagger |0\rangle$

$$\hat{U}_L |\bar{\Psi}\rangle = c_{j_1+1}^\dagger \dots c_{j_n+1}^\dagger |0\rangle$$

the shift is to the negative direction with modulo  $(\frac{2\pi}{L})$

the operator constructed is indeed the momentum shift operator which gives the polarization

- Here is another interesting way to express it: (derived by very different means first by Resta, PRL (1998)) consider a one-particle system:

$$|\Psi\rangle = \tilde{c}_{x_1} |0\rangle$$

~~c~~  $\tilde{c}_{x_1}$  - position basis

$$\tilde{c}_{x_1} = \frac{1}{\sqrt{N}} \sum_n e^{i\frac{2\pi}{NL} k x_1} c_n$$

$$\hat{U} \tilde{c}_{x_1} |0\rangle = \hat{U} \frac{1}{\sqrt{N}} \sum_k e^{i\frac{2\pi}{NL} k x_1} c_k |0\rangle$$

$$= \frac{1}{\sqrt{N}} \sum_n e^{i\frac{2\pi}{NL} k x_1} \hat{U} c_n |0\rangle$$

$$= \frac{1}{\sqrt{N}} \sum_n e^{i\frac{2\pi}{NL} k x_1} c_{n-1} |0\rangle$$

sum over k runs over all points in the Brillouin zone, so we can shift the sum

$$= \frac{1}{\sqrt{N}} \sum_n e^{i\frac{2\pi}{NL} (k+1) x_1} c_n |0\rangle$$

$$= e^{i\frac{2\pi}{NL} x_1} \tilde{c}_{x_1} |0\rangle$$



we can then also write the momentum shift operator as (12)

$$\hat{U} c_{x_1}^+ \dots c_{x_N}^+ |0\rangle = e^{\frac{i\omega}{NL} (x_1 + x_2 + \dots + x_N)} c_{x_1}^+ \dots c_{x_N}^+ |0\rangle$$

and the polarization as

$$\langle X \rangle = \frac{NL}{2\omega} \text{Im} \log \langle \Psi | e^{i\frac{2\omega}{NL} \hat{X}} | \bar{\Psi} \rangle$$

$$\hat{X} = \sum_i x_i$$

the same formalism, with appropriate modifications can be used to develop a Berry phase theory for the persistent current

~~the~~ definition of persistent current:

$$J(\bar{\Phi}) = \frac{\partial E(\bar{\Phi})}{\partial \bar{\Phi}}$$

$\bar{\Phi}$  - perturbation

(momentum shift, or vector potential)

$$E(\bar{\Phi}) = \langle \Psi(\bar{\Phi}) | H(\bar{\Phi}) | \Psi(\bar{\Phi}) \rangle$$

$|\Psi(\bar{\Phi})\rangle$  = ground state energy

$H(\bar{\Phi})$  = Hamiltonian

both under the perturbation

$$H(\bar{\phi}) = \sum_i \frac{(p_i + \bar{\phi})^2}{2m} + \hat{V}$$

(13)

$\hat{V}$  - some potential

current: 
$$\frac{\partial \langle \Psi(\bar{\phi}) | H(\bar{\phi}) | \bar{\Psi}(\bar{\phi}) \rangle}{\partial \bar{\phi}} = \langle \Psi(\bar{\phi}) | \frac{\partial H(\bar{\phi})}{\partial \bar{\phi}} | \bar{\Psi}(\bar{\phi}) \rangle$$

$$\frac{\partial H(\bar{\phi})}{\partial \bar{\phi}} = \sum_i \frac{(p_i + \bar{\phi})}{m} = \frac{N}{m} \bar{\phi} + \sum_i \frac{p_i}{m}$$

$$\begin{aligned} \sigma(\bar{\phi}) &= \cancel{\frac{N}{m} \bar{\phi}} + \langle \Psi(\bar{\phi}) | \sum_i \frac{p_i}{m} | \bar{\Psi}(\bar{\phi}) \rangle \\ &= \frac{N}{m} \bar{\phi} + \frac{i}{m} \langle \Psi(\bar{\phi}) | \sum_i \partial_{x_i} | \bar{\Psi}(\bar{\phi}) \rangle \end{aligned}$$

we can write wavefunction as

$$\begin{aligned} \sum_i \partial_{x_i} \Psi(x_1 + x, \dots, x_N + x; \bar{\phi}) \\ = \partial_x \Psi(x_1 + x, \dots, x_N + x; \bar{\phi}) \end{aligned}$$

and average over  $x$

$$\begin{aligned} \sigma(\bar{\phi}) &= \frac{N}{m} \bar{\phi} + \frac{i}{m} \frac{1}{L} \int_0^L dx \Psi^*(x_1 + x, \dots, x_N + x) \partial_x \Psi(x_1 + x, \dots, x_N + x; \bar{\phi}) \\ &+ \frac{i}{m} \frac{1}{L} \int_0^L dx \langle \Psi^*(x; \bar{\phi}) | \partial_x | \bar{\Psi}(x; \bar{\phi}) \rangle \\ &= \underbrace{\hspace{10em}}_{\text{Berry phase}} \end{aligned}$$

$$\langle x_1, \dots, x_N | \bar{\Psi}(x; \bar{\phi}) \rangle = \Psi(x_1 + x, \dots, x_N + x; \bar{\phi})$$

- One can apply the same analysis as before to obtain

(14)

$$\frac{1}{L} \int dx \langle \Psi(x, \theta) | \partial_x | \Psi(x, \theta) \rangle$$

$$\approx \frac{1}{L} \sum_{i=0}^{N-1} \text{Im} \ln \langle \Psi(x_i) | \Psi(x_{i+1}) \rangle$$

$$= \frac{1}{L} \sum_{i=0}^{N-1} \text{Im} \ln \langle \Psi(0) | U(\Delta x) | \Psi(0) \rangle$$

$U(\Delta x)$  is the total position shift

rather than the total momentum shift

it also holds that

$$U(\Delta x) = e^{i \Delta x (\hat{h}_+ - \hat{h}_-)} = e^{i \Delta x \hat{k}}$$

total momentum

- current response for some variational wave functions for the Hubbard model

Gutzwiller wavefunction:  $|\Psi_G\rangle = e^{-\gamma \sum_i n_{i\uparrow} n_{i\downarrow}} |\text{FS}\rangle$

Baeriswyl wavefunction:  $|\Psi_B\rangle = e^{-\alpha \hat{T}} |\Psi_\infty\rangle$

mixed wave functions:

$$|\Psi_{BG}\rangle = e^{-\alpha \hat{T}} e^{-\gamma \sum_i n_{i\uparrow} n_{i\downarrow}} |\text{FS}\rangle$$

$$|\Psi_{GB}\rangle = e^{-\gamma \sum_i n_{i\uparrow} n_{i\downarrow}} e^{-\alpha \hat{T}} |\Psi_\infty\rangle$$

$\hat{T}$  - kinetic energy operator  $n_{i\uparrow} n_{i\downarrow}$  - double occupation



the projector operators  $e^{-\delta \sum_i n_{i\sigma} n_{i\downarrow}}$  and  $e^{-2\hat{T}}$  both commute with  $\hat{U}(\Delta x)$  (15)

- to see this:  $\hat{U}(\Delta x) e^{-\delta \sum_i n_{i\sigma} n_{i\downarrow}}$

$\hat{U}(\Delta x)$  shifts the positions of all particles  $\Rightarrow$  the number of double occupations cannot change

$$\hat{U}(\Delta x) e^{-2\hat{T}} = e^{i\Delta x \hat{K}} e^{-2\hat{T}}$$

Both  $\hat{K}$  and  $\hat{T}$  are diagonal in momentum space

- we can say that the function on which the projector acts determines the current response for these wavefunctions

example Gutzwiller

$$\text{phase: } \frac{1}{\Delta x} \text{Im} \ln \frac{\langle \Psi_G | e^{i\Delta x \hat{K}} | \Psi_G \rangle}{\langle \Psi_G | \Psi_G \rangle}$$

$$= \frac{1}{\Delta x} \text{Im} \ln \frac{\langle \text{FS} | e^{-\delta \sum_i n_{i\sigma} n_{i\downarrow}} e^{i\Delta x \hat{K}} | \text{FS} \rangle}{\langle \text{FS} | e^{-\delta \sum_i n_{i\sigma} n_{i\downarrow}} | \text{FS} \rangle}$$

$$= \frac{1}{\Delta x} \text{Im} \ln e^{i\Delta x K_{\text{FS}}} = K_{\text{FS}}$$

$$\hat{K} | \text{FS} \rangle = K_{\text{FS}} | \text{FS} \rangle$$

- for the Baeriswyl wavefunctions the function  $|\Psi_0\rangle$  is not an eigenfunction of  $\hat{U}(x)$

### Sources:

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