Current Response as a Geometric Phase: Interpretation of Conductivity in Variational Wavefunctions

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Background

- Kohn (PR, 1964) derived an expression for the DC conductivity in crystalline systems, by taking the zero frequency limit of the frequency dependent conductivity

$$D = \frac{\pi}{L}\frac{\partial^2 E(\Phi=0)}{\partial \Phi^2}$$

- Drude (D_c) and superfluid (D_s) weights have "identical" expressions
- Scalapino, White, and Zhang (PRL,1991)
  D_c derivative is adiabatic (perturbed system remains in the same state)
  D_s derivative is "envelope" (perturbed system remains in the lowest energy state)

D_c and D_s in variational theory

- Dc and Ds for a finite temperature system can be defined (Zotos, Castella, and Prelovsek, 1996) as

$$D_c = \frac{\pi}{L}\sum_i P_i \frac{\partial^2 E_i(\Phi=0)}{\partial \Phi^2} \qquad P_i = e^{-\beta E_i}$$

$$D_s = \frac{\pi}{L}\frac{\partial^2 \sum_i P_i(\Phi=0)E_i(\Phi=0)}{\partial \Phi^2} \qquad P_i(\Phi) = e^{-\beta E_i(\Phi)}$$

- In variational theory the Boltzmann weights are replaced by

$$P_i = |\langle \tilde{\Psi}|\Psi_i\rangle|^2$$

where $\tilde{\Psi}$ denotes the variational wavefunction, Ψ_i denotes the eigenstates of the system Hamiltonian
- Difficulty with D_c: need perturbed eigenstates

Current response as a phase

- The persistent current can be expressed as a geometric phase
- Definition of current

$$J(\Phi) = \partial_\Phi E(\Phi) = \langle \Psi(\Phi)|\partial_\Phi \hat{H}(\Phi)|\Psi(\Phi)\rangle.$$

Since

$$\hat{H}(\Phi) = \sum_{i=1}^{N}\frac{(\hat{p}_i+\Phi)^2}{2m} + V(x_1,...,x_N).$$

$$\partial_\Phi \hat{H}(\Phi) = \sum_{i=1}^{N}\frac{(\hat{p}_i+\Phi)}{m}$$

The current can be rewritten as

$$J(\Phi) = \frac{N\Phi}{m} - \frac{i}{m}\sum_{i=1}^{N}\langle \Psi(\Phi)|\frac{\partial}{\partial x_i}|\Psi(\Phi)\rangle$$

The wavefunction can be written in terms of the total position as

$$\langle x_1,...x_N|\Psi(\Phi;X)\rangle = \Psi(x_1+X,...,x_N+X;\Phi).$$

Using X we can write

$$\sum_{i=1}^{N}\frac{\partial}{\partial x_i}\Psi(x_1+X,...,x_N+X;\Phi) = \partial_X \Psi(x_1+X,...,x_N+X;\Phi).$$

The current response can thus be written as

$$J(\Phi) = \frac{N\Phi}{m} - \frac{i}{mL}\int_0^L \mathrm{d}X\,\langle \Psi(\Phi;X)|\partial_X|\Psi(\Phi;X)\rangle.$$

The second term in the expression for the current is a Berry phase. The variable X can be viewed as an external parameter, the adabatic cycle arises by taking the system across the periodic cell.

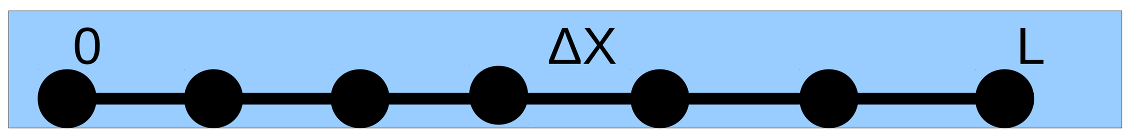
Connection to Polarization Theory

- Due to the ill-defined nature of the position in periodic systems polarization can not be written as a simple average over the dipole moment
- Modern theory of polarization (Resta,RMP 1996): $P = \frac{ie}{2\pi}\int \mathrm{d}K\langle \Psi(K)|\partial_K|\Psi(K)\rangle$
- The variable K in polarization plays a similar role to the variable X for the current response
- The discrete analog of P can be written:

$$P = \frac{eL}{2\pi}\mathrm{Im}\ln\langle \Psi|e^{i2\pi X/L}|\Psi\rangle$$

The Discrete Case

- The discrete analog for the phase corresponding to the current $J(\Phi)$ can be obtained by discretizing the integral over X:



$$J(0) = \lim_{\Delta X\to 0}\frac{1}{mL}\mathrm{Im}\ln\prod_{s=0}^{M-1}\langle \Psi(s\Delta X)|\Psi((s+1)\Delta X)\rangle.$$

(Φ was taken to be zero without loss of generality)

- Can be rewritten with the help of the **total position shift operator**
  Definition: $\hat{U}(\Delta X)|\Psi(X)\rangle = |\Psi(X+\Delta X)\rangle$
- Using $\hat{U}(\Delta X)$ the current can be written

$$J(0) = \lim_{\Delta X\to 0}\frac{1}{m}\frac{1}{\Delta X}\mathrm{Im}\ln\langle \Psi(0)|\hat{U}(\Delta X)|\Psi(0)\rangle.$$

Construction of Shift Operators

- For discrete systems shift operators can be constructed via the **permutation operator**:

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

- The permutation operator satisfies identities

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

- To construct $\hat{U}(\Delta X)$ one can take a product of lattice site permutation operators as:

$$\hat{U}(\Delta X) = P_{12}P_{23}...P_{L-1L}$$

for which it holds that

$$\hat{U}(\Delta X)c_i = \begin{cases} c_{i-1}\hat{U}(\Delta X), & i=2,...,L \\ c_L\hat{U}(\Delta X), & i=1. \end{cases}$$

in other words it shifts the position of particles module L.
- On momentum states the action of $\hat{U}(\Delta X)$ is:

$$\hat{U}(\Delta X)\tilde{c}_k = e^{i\Delta X k}\tilde{c}_k\hat{U}(\Delta X)$$

- As a result the current can also be written as

$$J(0) = \lim_{\Delta X\to 0}\frac{1}{m}\frac{1}{\Delta X}\mathrm{Im}\ln\langle \Psi(0)|e^{i\Delta X\hat{K}}|\Psi(0)\rangle.$$

where $\hat{K} = \sum \hat{k}_i$ the total momentum. This expression is analogous to the one for the polarization with the roles of X and K reversed.

Projected wavefunctions

Gutzwiller wavefunction

- Form of Gutzwiller wavefunction:

$$|\Psi_G(\gamma)\rangle = e^{-\Gamma\hat{D}}|FS\rangle$$

double occupations D are projected out of the Fermi sea ($|FS>$).

- **Normalized spread:** $\frac{\langle X^2\rangle - \langle X\rangle^2}{L^2}$.

where the total position operator X is defined as a sawtooth wave:

$$X = \sum_{\substack{m=-L/2 \\ m\neq 0}}^{L/2-1}\left(\frac{1}{2} + \frac{\hat{W}^m}{\exp\left(i\frac{2\pi m}{L}\right)-1}\right)$$

with $\hat{W} = e^{i2\pi\hat{X}/L}$.
- For the Fermi Sea the normalized spread approaches 1/12 as L->∞.

Size L	Fermi sea	Γ=1.0	Γ=2.0
12	0.08275	0.079(1)	0.0412(9)
24	0.08312	0.0830(6)	0.0682(6)
36	0.08327	0.0831(5)	0.0797(5)
48	0.08330	0.0833(4)	0.0824(4)
60	0.08331	0.0829(3)	0.0830(3)
∞	1/12		

Table I. Fermi sea and Gutzwiller results (variational Monte Carlo, Yokoyama and Shiba (JP3J, 1987)).

- For large L the normalized spread converges to 1/12 for the Fermi sea and both Gutzwiller wavefunctions.
- **Current response**: it holds that

$$[\hat{U}(\Delta X), e^{-\Gamma D}] = 0$$

- since shifting the positions of all particles will not change the number of doubly occupied sites

$$\hat{U}(\Delta X)|\Psi(\gamma)\rangle = e^{-\gamma\sum_i n_{i\uparrow}n_{i\downarrow}}\hat{U}(\Delta X)|FS\rangle = e^{i\Delta X\sum_i k_i}|\Psi(\gamma)\rangle,$$

Current response for the Gutzwiller wavefunction is identical to that of the Fermi sea.

- Conclusion can be generalized to simple Jastrow-type projections diagonal in coordinate space.

Other projected wavefunctions

- Baeriswyl-Gutzwiller wavefunction

$$|\Psi_{BG}(\alpha,\gamma)\rangle = e^{-\alpha\hat{T}}e^{-\gamma\hat{D}}|FS\rangle.$$

Since $\hat{U}(\Delta X)$ commutes with both projectors, the current response will again be that of the Fermi sea.
- Baeriswyl wavefunction, Gutzwiller-Baeriswyl wavefunction:

$$|\Psi_B(\alpha,\gamma)\rangle = e^{-\alpha\hat{T}}|\Psi_\infty\rangle,\ |\Psi_{GB}(\alpha,\gamma)\rangle = e^{-\gamma\hat{D}}e^{-\alpha\hat{T}}|\Psi_\infty\rangle.$$

current response determined by $|\Psi_\infty\rangle$.
- Non-trivial behavior: non-centrosymmetric or phase-dependent projectors.

References:
[1] B. Hetényi, accepted (see also arXiv.org:1208.0671), *J. Phys. Soc. Japan* **82** 023701 (2012).