A comprehensive theory of transport: distinguishing insulators, conductors, superconductors, and bosonic superfluids

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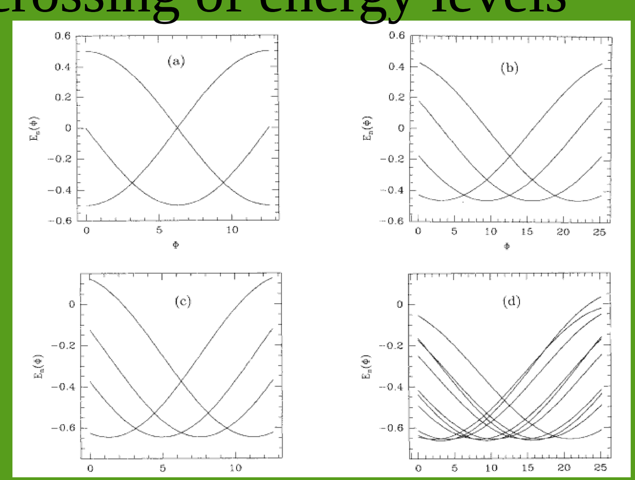
Transport coefficients

- **Drude weight:** $$D = \frac{1}{V}\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}$$
  - Perturbation is of the form: $\Phi(\omega) = \frac{E e^{i\omega t}}{i\omega}$
  - D obtained by taking the zero frequency limit of $\omega\sigma''(\omega)$
  - D is the strength of the conductivity at zero frequency
  - Sensitive to ballistic conduction
- **Meissner weight:** $$n^{(s)} = \frac{1}{V}\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}$$
  - Perfect conductor: $\mathbf{E} = \frac{1}{n^{(s)}}\frac{\partial \mathbf{j}}{\partial t}$.
  - Maxwell equation: $\frac{\partial}{\partial t}(\nabla\times\mathbf{j} + n^{(s)}\mathbf{B}) = 0$.
  - London equation: $\mathbf{j} = n^{(s)}\mathbf{A}$.
  - Sensitive to the density of superconducting charge carriers
- **Non-classical rotational inertia:** $$I^{(s)} = \left[\frac{\partial^2 E^{(s)}(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}$$
  - Liquid helium, rotating bucket experiment (Andronikashvili, Hess and Fairbank experiments)
    - Work to rotate above Tc: $\Delta W_{T>T_c} = \frac{I}{2}\Phi^2$.
    - Work to rotate below Tc: $\Delta W_{T<T_c} = \frac{I^{(n)}}{2}\Phi^2$.

Question: How can transport coefficients be distinguished?

Adiabatic vs. envelope derivative

- Scalapino, White, Zhang (PRL 1993, PRB 1992): The derivative with respect to is Φ ambiguous due to the crossing of energy levels
  - Adiabatic derivative: D
  - Envelope derivative: $n^{(s)}$
  - Crossing point occurs at: $\Phi_c \approx A/L^{d-1}$
    d – dimensionality



- Problems with this approach:
  - Distinguishes only two categories
  - Does not distinguish in one dimension
  - Application to variational theory is problematic

D at finite temperature and in variational theory

- Zotos, Castella, and Prelovšek (PRL, 1992) generalized the Drude weight to finite temperature
$$D = \frac{1}{V}\sum_{i=1}\frac{\exp(-\beta E_i(0))}{Q(0)}\left[\frac{\partial^2 E_i(\Phi)}{\partial\Phi^2}\right]_{\Phi=0}.$$
  - The Boltzmann weights are independent of Φ
  - This way the adiabatic derivative is reproduced at zero temperature
- In variational theory the ground state energy is also a weighted average:
$$E_{\mathrm{var}} = \sum_i P_i E_i$$
where $P_i = |\langle\Psi_{\mathrm{var}}|\Phi_i\rangle|^2$ are the weights instead of the Boltzmann weights
- In variational calculations of the Drude weight the weights P_i are assumed to vary as a function of Φ
  - Example: Millis and Coppersmith proof that the Gutzwiller wavefunction is metallic (PRB, 1991)

Defining current

- Definition of current: $J(\Phi) = \frac{\partial E(\Phi)}{\partial \Phi}$
- Ground state energy: $E(\Phi) = \langle\Psi(\Phi)|H(\Phi)|\Psi(\Phi)\rangle$
- Hamiltonian: $H(\Phi) = \sum_{i=1}^{N}\frac{(\hat{p}_i+\Phi)^2}{2m} + \hat{V}$
- Current expectation value:
$$J(\Phi) = \langle\Psi(\Phi)|\left[\sum_i \frac{(\hat{p}_i+\Phi)}{m}\right]|\Psi(\Phi)\rangle$$

Center of mass momentum

- Diamagnetic current: $J_D(\Phi) = \langle\Psi(\Phi)|\left[\sum_i \frac{\hat{p}_i}{m}\right]|\Psi(\Phi)\rangle$
- Diamagnetic current can be written in terms of the center of mass (COM) momentum:
  - Momentum operator is the generator of translations
  $$\hat{p} = -i\frac{\partial}{\partial x}. \qquad |\Psi(x+\delta x)\rangle = \exp(i\hat{p}\delta x)|\Psi(x)\rangle.$$
  - COM momentum operator is the generator of COM translations: $\hat{P}_{cm} = -i\frac{\partial}{\partial x_{cm}} = \sum_{i=1}^{N}\hat{p}_i$
$$|\Psi(x_1+x_{cm}+\delta x,...,x_N+x_{cm}+\delta x)\rangle =$$
$$\exp(i\hat{P}_{cm}\delta x)|\Psi(x_1+x_{cm},...,x_N+x_{cm})\rangle$$

A wavefunction describing identical particles which is an eigenstate of the single-particle momentum is also an eigenstate of the center of mass momentum, but the converse is not necessarily true.

Many-body current as a geometric phase

- With the help of the COM momentum the current can be written as:
$$J(\Phi) = \frac{N\Phi}{m} - \frac{i}{mL}\int_0^L \mathrm{d}X_{cm}\langle\Psi(X_{cm})|\frac{\partial}{\partial X_{cm}}|\Psi(X_{cm})\rangle.$$
or in the discrete case (lattice)
$$J(\Phi) = \frac{N\Phi}{m} - \lim_{\Delta X\to 0}\frac{1}{m\Delta X}\mathrm{Im}\ln\langle\Psi|e^{i\Delta X\hat{P}_cm}|\Psi\rangle.$$
  - The second term (diamagnetic term) is a geometric phase
- Compare to the results of the modern theory of polarization (King-Smith and Vanderbilt, PRB 1992; Resta, RMP 1993)
$$\langle X\rangle = \frac{i}{2\pi}\int_{BZ}\mathrm{d}\Phi\langle\Psi(\Phi)|\frac{\partial}{\partial_\Phi}|\Psi(\Phi)\rangle.$$
$$\langle X\rangle = \lim_{\Delta\Phi\to 0}\frac{1}{\Delta\Phi}\mathrm{Im}\ln\langle\Psi|e^{i\Delta\Phi\hat{X}}|\Psi\rangle$$

Drude weight as a topological invariant

- Taking the derivative of the current with respect to Φ corresponds to the Drude weight:
$$D = \frac{N}{m} - \frac{i}{2\pi m}\int_{BZ}\int_0^L \mathrm{d}\Phi\mathrm{d}X\left(\left\langle\frac{\partial}{\partial\Phi}\Psi\middle|\frac{\partial}{\partial X}\Psi\right\rangle - \left\langle\frac{\partial}{\partial X}\Psi\middle|\frac{\partial}{\partial\Phi}\Psi\right\rangle\right)$$
  - second term is a topological invariant
- Compare to TKNN invariant which describes Hall conductance (Thouless, Kohmoto, Nightingale, den Nijs, PRL 1983):
$$\sigma_H = \frac{ie^2}{2\pi h}\sum\int d^2k\int d^2r\left(\frac{\partial u^*}{\partial k_1}\frac{\partial u}{\partial k_2} - \frac{\partial u^*}{\partial k_2}\frac{\partial u}{\partial k_1}\right)$$
$$= \frac{ie^2}{4\pi h}\sum\oint dk_j\int d^2r\left(u^*\frac{\partial u}{\partial k_j} - \frac{\partial u^*}{\partial k_j}u\right), \qquad (5)$$
- Also related to expression for adiabatic charge pumping by Thouless (PRB 1983)
$$C = \frac{i}{2\pi}\int_0^T \mathrm{d}t\int_{BZ}\mathrm{d}\Phi\left(\left\langle\frac{\partial}{\partial\Phi}\Psi\middle|\frac{\partial}{\partial t}\Psi\right\rangle - \left\langle\frac{\partial}{\partial t}\Psi\middle|\frac{\partial}{\partial\Phi}\Psi\right\rangle\right)$$
- Discrete analog of D: $D = \frac{N}{m} + \frac{\gamma}{m}$
$$\gamma = -\lim_{\Delta X,\Delta\Phi\to 0}\frac{1}{\Delta X\Delta\Phi}\left[\mathrm{Im}\frac{\langle\Psi|e^{i\Delta\Phi\hat{X}}e^{i\Delta X\hat{P}}|\Psi\rangle}{\langle\Psi|e^{i\Delta X\hat{P}}|\Psi\rangle} + \mathrm{Im}\frac{\langle\Psi|e^{i\Delta X\hat{P}}e^{-i\Delta\Phi\hat{X}}|\Psi\rangle}{\langle\Psi|e^{i\Delta X\hat{P}}|\Psi\rangle}\right]$$

Can be shown that (see Refs.):

- **if a state is an eigenstate of the COM momentum, the Drude weight is finite, and the state is delocalized.**
- **If a state is NOT an eigenstate of the COM momentum, the Drude weight is zero, and the state is localized.**

Different types of current

- "Two" textbook expressions for the current:
$$J(\Phi) = \frac{N}{m}\Phi + \langle\Psi|\left[\sum_i\hat{p}_i\right]|\Psi\rangle \qquad J(\Phi) = \frac{N}{m}\Phi + \sum_i\langle\Psi|\hat{p}_i|\Psi\rangle$$
  - Are they equivalent?
- Using two discrete expressions for the current in a system of identical particles we can write
$$J(\Phi) = \frac{N}{m}\Phi + \lim_{\Delta X\to 0}\frac{1}{m\Delta X}\mathrm{Im}\ln\langle\Psi|\exp\left(i\Delta X\sum_j\hat{p}_j\right)|\Psi\rangle$$
$$J(\Phi) = \frac{N}{m}\Phi + \lim_{\Delta X\to 0}\frac{N}{m\Delta X}\mathrm{Im}\ln\langle\Psi|\exp(i\Delta X\hat{p})|\Psi\rangle$$
  - Taking the limit $\Delta X\to 0$ appears to lead to the same quantity, however, the first expression can be written in terms of the full density matrix, whereas the second one in terms of the reduced density matrix (RDM) of order one.
- Define a general p-particle current
$$J_p(\Phi) = \frac{N}{m}\Phi + \lim_{\Delta X\to 0}\frac{(N/p)}{m\Delta X}\mathrm{Im}\ln\mathrm{Tr}\left\{\hat{\rho}_p\exp\left(i\Delta X\sum_{j=1}^{p}\hat{k}_j\right)\right\}$$
- And its associated transport coefficient:
$$D_p = \left[\frac{\partial J_p(\Phi)}{\partial\Phi}\right]_{\Phi=0}$$

Off-diagonal long-range order

- Definition of the reduced density matrix:
$$\rho_p(x_1,...x_p;x'_1,...,x'_p) = \int...\int dx_{p+1}...dx_N$$
$$\Psi(x_1,...,x_p,x_{p+1},...,x_N)\Psi(x'_1,...,x'_p,x_{p+1},...,x_N)$$
- The RDM provides a measure of condensation in the form of **off-diagonal long-range order (ODLRO)** (Penrose and Onsager, PR 1959):
  - For the first order RDM ODLRO is defined as:
  $$\lim_{|x_1-x'_1|\to\infty}\rho_1(x_1;x'_1) = \mathrm{finite}$$
- Yang (RMP 1962) has shown that
  - **If ODLRO occurs in the RDM of order p then it also occurs for RDMs of order higher than p.**

Can be shown that (see Refs.):

- If an eigenstate of the RDM of order p is also an eigenstate of the p-particle momentum, then it will contribute to the transport coefficient or order p (D_p)
- Otherwise the contribution is zero

Comprehensive theory of transport coefficients

- To determine whether a model exhibits superfluidity, superconductivity or conduction
  - Determine the minimum p for which D_p is finite
  - If p is a microscopically small number then the model exhibits superfluidity *(p=1)* or superconduction *(p=2)*
  - If p is microscopically large then the model exhibits ballistic conduction
- Associated flux quantization rule for minimum p: $\Phi_B = nhc/(pe)$, where n is an integer
  - As $p\to\infty$ the flux is no longer quantized

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