A comprehensive theory of conductivity

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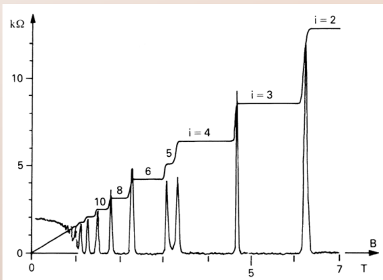
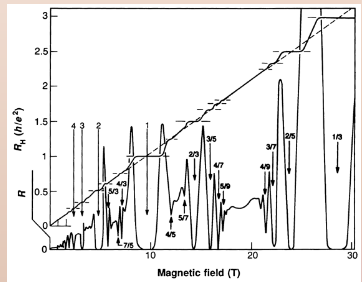
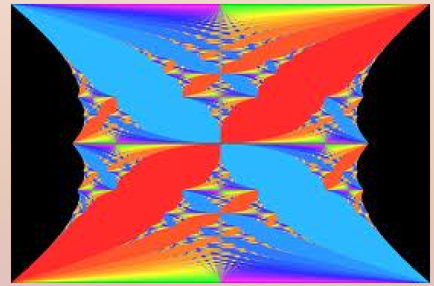
Topology and physics

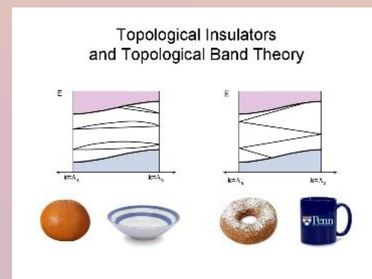


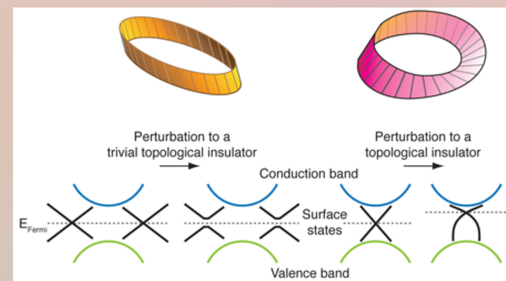




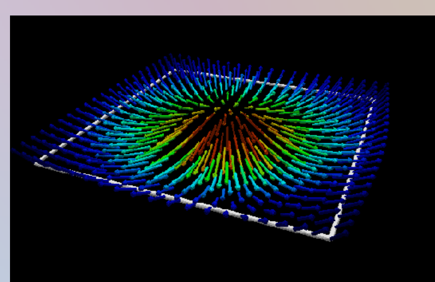
Quantum Hall effect (integer & fractional)

Topological insulators





Skyrmions



These are “exotic effects”, but even the criterion for <u>normal insulation</u> can be cast in terms of a <u>topological invariant</u>

BEC, ODLRO, NCRI

- P. W. Anderson: “Theory of Supersolidity” (JLTP, **169** 124 (2012))

1967 that finite concentrations of vacancy defects would superflow.) But it has never been demonstrated that ODLRO, superfluidity, and NCRI are synonymous, and the indirect nature of these arguments leaves one, at best, unsatisfied.

- Understand connection between off-diagonal long-range order and non-classical rotational inertia in bosonic superfluids.
- Open question: difference between superfluid and BEC

Current vs. total current

- Expression for current:

$$J_N(A) = \frac{\partial E(A)}{\partial A} = -\frac{Ne}{mc}A + \frac{e}{mc}\langle\Psi(A)|\left[\sum_{i=1}^{N}\hat{p}_i\right]|\Psi(A)\rangle.$$

- Generator of one-body translations: one-body momentum

$$|\Psi(x+\delta x)\rangle = \exp(i\hat{p}\delta x)|\Psi(x)\rangle. \qquad \hat{p} = -i\frac{\partial}{\partial x}.$$

- Generator of center of mass translations: total momentum

$$|\Psi(x_1 + x_{cm} + \delta x, \ldots, x_N + x_{cm} + \delta x)\rangle = \exp(i\hat{P}_{cm}\delta x)|\Psi(x_1 + x_{cm}, \ldots, x_N + x_{cm})\rangle$$

$$\hat{P}_{cm} = -i\frac{\partial}{\partial x_{cm}} = \sum_{i=1}^{N}\hat{p}_i$$

OUTLINE

- Drude weight as a geometric phase: proof of Kohn's hypothesis
    - Modern theory of polarization (Resta, King-smith, Vanderbilt)
    - Current as a geometric phase
    - Drude weight as a topological invariant
- Transport quantities: Drude weight, Meissner weight, rotational inertia of bosonic superfluids
    - How can they be distinguished?

Part I

Why do some materials conduct and others insulate?

- Is it possible to give a **comprehensive** answer?

Theory of the Insulating State*

Walter Kohn
University of California, San Diego, La Jolla, California
(Received 30 August 1963)

In this paper a new and more comprehensive characterization of the insulating state of matter is developed. This characterization includes the conventional insulators with energy gap as well as systems discussed by Mott which, in band theory, would be metals. The essential property is this: Every low-lying wave function Φ of an insulating ring breaks up into a sum of functions, $\Phi = \Sigma_{-\infty}^{\infty} \Phi_M$, which are localized in disconnected regions of the many-particle configuration space and have essentially vanishing overlap. This property is the analog of localization for a single particle and leads directly to the electrical properties characteristic of insulators. An Appendix deals with a soluble model exhibiting a transition between an insulating and a conducting state.

Physical Review **133** A171 (1964).

- **Insulation** results from **localization** in the **many-body** configuration space

DC conductivity/Drude weight

- Introduce **electric field** as a **momentum shift** into the Hamiltonian. In the DC limit (zero frequency) it will be a constant shift in the momenta (Kohn, 1964)
  - Hamiltonian: $$H = \sum_i \frac{(p_i + K)^2}{2m} + \hat{V}$$
  - Current: $$J(K) = \frac{\partial E_0(K)}{\partial K}$$
  - Drude weight: $$D^{(c)} = \frac{1}{V}\left[\frac{\partial^2 E_0(K)}{\partial K^2}\right]_{K=0}$$

Problem: position is ill-defined

- Ill-defined nature of the position operator gives rise to **difficulties** in calculating **physical quantities: polarization,** quantifying **localization,** and even **conductivity**
- As emphasized by Resta (RMP, 1994), this issue **invalidates** the **Clausius-Mosotti** picture of dielectrics, where a unique boundary for the periodic unit cell is assumed. It also invalidates the polarization expressions given in a number of textbooks.
- **Modern theory of polarization**: **total position** corresponds to a **geometric phase**

Polarization theory

- We are after $\langle X \rangle = \langle \Psi_0 | \hat{X} | \Psi_0 \rangle$ where $\hat{X} = \sum_{i=1}^{N} \hat{x}_i$.
- Write the position operators in reciprocal space as $\hat{X} = i \sum_{j=1}^{N} \frac{\partial}{\partial k_j}$
- For a wavefuntion in reciprocal space it holds that

$$\hat{X}\Psi_0(k_1 + K, ..., k_N + K)\rangle = i\frac{\partial}{\partial K}\Psi_0(k_1 + K, .., k_N + K)$$

Polarization theory

- Averaging over K results in

$$\langle X \rangle = \frac{i}{2\pi} \int_{BZ} \mathrm{d}K \langle \Psi_0(K) | \frac{\partial}{\partial_K} | \Psi_0(K) \rangle$$

- To arrive at a practical scheme: discretize the variable K which results in $\Delta K = \frac{2\pi}{L}$

$$\langle X \rangle = \lim_{\Delta K \to 0} \frac{1}{\Delta K} \operatorname{Im} \ln \langle \Psi_0 | e^{i \Delta K \hat{X}} | \Psi_0 \rangle$$

Quantifying localization

- Expression for the spread

$$\sigma_X^2 = -\lim_{\Delta K \to 0} \frac{2}{\Delta K^2} \mathrm{Re} \ln \langle \Psi_0 | e^{i\Delta K \hat{X}} | \Psi_0 \rangle$$

can be used to quantify localization

- Divergent spread: conductor
- Finite spread: insulator
- It has been applied in a large number of cases, band structure calculations, srtongly correlated systems, Anderson localized systems, etc. and the **results are always in agreement with Kohn's hypothesis regarding localization**

Can we prove Kohn's hypothesis?

- **Question:** Can we show that localization and insulation are in a one-to-one relationship starting from the Drude weight and investigating its connection to localization?
- **Answer:** We can express the Drude weight using shift operators, and obtain a “modern theory of conductivity”. With some refinements Kohn's hypothesis can be demonstrated.

Current as a geometric phase

- Similarly to the theory of polarization the current can also be expressed as a geometric phase
  - Hamiltonian: $$H = \sum_i \frac{(p_i + K)^2}{2m} + V$$
  - Current: $$J(K) = \frac{\partial E_0(K)}{\partial K}$$

$$J(K) = \frac{NK}{m} - \frac{i}{mL} \int_0^L \mathrm{d}X \langle \Psi(X) | \frac{\partial}{\partial X} | \Psi(X) \rangle$$

BH, *J. Phys. Soc. Japan*, (2012)

Current as a geometric phase

- Discretizing in X results in

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

- Persistent current at zero field:

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

Drude weight as a geometric phase

- Starting with the current

$$J(K) = \frac{NK}{m} - \frac{i}{mL}\int_0^L \mathrm{d}X \langle \Psi(X)| \frac{\partial}{\partial X} |\Psi(X)\rangle$$

and taking the derivative with respect to K and averaging over the Brillouin zone results in

$$D = \frac{N}{m} - \frac{i}{2\pi m}\int_{BZ}\int_0^L \mathrm{d}K\mathrm{d}X \left(\left\langle \frac{\partial}{\partial K}\Psi \middle| \frac{\partial}{\partial X}\Psi \right\rangle - \left\langle \frac{\partial}{\partial X}\Psi \middle| \frac{\partial}{\partial K}\Psi \right\rangle \right)$$

BH, *Phys. Rev. B* **87** 235123 (2013).

Drude weight as a geometric phase

$$D = \frac{N}{m} - \frac{i}{2\pi m}\int_{BZ}\int_0^L \mathrm{d}K\mathrm{d}X \left(\left\langle \frac{\partial}{\partial K}\Psi \middle| \frac{\partial}{\partial X}\Psi \right\rangle - \left\langle \frac{\partial}{\partial X}\Psi \middle| \frac{\partial}{\partial K}\Psi \right\rangle\right)$$

Expression for the Hall conductance:

$$\sigma_{\mathrm{H}} = \frac{ie^2}{2\pi h}\sum\int d^2k\int d^2r\left(\frac{\partial u^*}{\partial k_1}\frac{\partial u}{\partial k_2} - \frac{\partial u^*}{\partial k_2}\frac{\partial u}{\partial k_1}\right)$$
$$= \frac{ie^2}{4\pi h}\sum\oint dk_j\int d^2r\left(u^*\frac{\partial u}{\partial k_j} - \frac{\partial u^*}{\partial k_j}u\right), \qquad (5)$$

- Thouless, Kohmoto, Nightingale, and den Nijs, *Phys. Rev. Lett.* **49** 405 (1982).

- Drude weight consists of a TKNN-like topological invariant

Drude weight as a geometric phase

$$D = \frac{N}{m} - \frac{i}{2\pi m}\int_{BZ}\int_0^L \mathrm{d}K\,\mathrm{d}X \left(\left\langle \frac{\partial}{\partial K}\Psi \middle| \frac{\partial}{\partial X}\Psi \right\rangle - \left\langle \frac{\partial}{\partial X}\Psi \middle| \frac{\partial}{\partial K}\Psi \right\rangle \right)$$

- The TKNN term consists of the commutator of two "heuristic" many-body operators $i\frac{\partial}{\partial K}$ $i\frac{\partial}{\partial X}$
- First term can also be written as $\frac{i}{m}\sum_{j=1}^{N}\langle\Psi|[\partial_{k_j},\partial_{x_j}]|\Psi\rangle$
- Drude weight is the difference of commutator of single body momenta and positions and commutator of total momentum and position

Drude weight as a geometric phase

- Can also start with the discretized expression

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

and taking the derivative with respect to K
and averaging over the Brillouin zone results in

BH, *Phys. Rev. B* **87** 235123 (2013).

Drude weight as a geometric phase

- In this case the Drude weight becomes

$$D_c = \frac{N}{m} + \frac{\gamma}{m}$$

$$\gamma = - \lim_{\Delta X, \Delta K \rightarrow 0} \frac{1}{\Delta X \Delta K} \left[\mathrm{Im} \ln \frac{\langle \Psi | e^{i\Delta K \hat{X}} e^{i\Delta X \hat{K}} | \Psi \rangle}{\langle \Psi | e^{i\Delta X \hat{K}} | \Psi \rangle} + \mathrm{Im} \ln \frac{\langle \Psi | e^{i\Delta X \hat{K}} e^{-i\Delta K \hat{X}} | \Psi \rangle}{\langle \Psi | e^{i\Delta X \hat{K}} | \Psi \rangle} \right]$$

- Taking the limits one can expand the exponentials and the result is that $D_c = 0$

BH, *Phys. Rev. B* **87** 235123 (2013).

Drude weight as a geometric phase

- In this case the Drude weight becomes

$$D_c = \frac{N}{m} + \frac{\gamma}{m}$$

$$\gamma = -\lim_{\Delta X, \Delta K \rightarrow 0} \frac{1}{\Delta X \Delta K} \left[\mathrm{Im} \ln \frac{\langle \Psi | e^{i\Delta K \hat{X}} e^{i \Delta X \hat{K}} | \Psi \rangle}{\langle \Psi | e^{i \Delta X \hat{K}} | \Psi \rangle} + \mathrm{Im} \ln \frac{\langle \Psi | e^{i \Delta X \hat{K}} e^{-i \Delta K \hat{X}} | \Psi \rangle}{\langle \Psi | e^{i \Delta X \hat{K}} | \Psi \rangle} \right]$$

- Such an expansion is not always valid. If the wavefunction is an eigenstate of the total current (and has eigenvalue zero, eigenvalue of an unpeturbed system) then $D_c = \frac{N}{m}$

Summary

- If wavefunction is an eigenstate of the current: Drude weight is finite and equals N/m (maximum it can be) the system is conductor.
- If wavefunction is a smooth function of the momenta, the Drude weight is zero, the system is an insulator.
- In between case, see later

Connection to localization

- Recall that the spread is given by

$$\sigma_X^2 = -\lim_{\Delta K \to 0} \frac{2}{\Delta K^2} \mathrm{Re} \ln \langle \Psi_0 | e^{i\Delta K \hat{X}} | \Psi_0 \rangle$$

an expectation value of the total momentum shift.

- If the wavefunction is an eigenstate of the total current than the scalar product

$$\langle \Psi_0 | e^{i\Delta K \hat{X}} | \Psi_0 \rangle = 0$$

since the shifted wavefunction will necessarily be orthogonal to the unshifted one. Q.E.D.

Example: Anderson localization

- Hamiltonian: $$H = -t\sum_i c_i^\dagger c_{i+1} + \mathrm{H.\,c.} + U\sum_i \xi_i n_i$$
    - ξ_i Drawn from a Gaussian distribution
- Well known insulator for finite U.
- Exactly diagonalize for system with 1024 lattice sites and 512 particles
- Quantities calculated: DC conductivity, spread in position, spread in current ,kinetic energy,

Example: Anderson localization

- Spread in current:

$$\sigma_K^2 = -\lim_{\Delta X \to 0} \frac{2}{\Delta X^2} \mathrm{Re} \ln \langle \Psi_0 | e^{i \Delta X \hat{K}} | \Psi_0 \rangle$$

  - Zero for eigenstate of the current.

U	$D^{(c)}$	-½ Kinetic energy	Spread in current	Spread in position
0	327.95	327.95	0	----------
1	0.01154(4)	297(7)	5.8(2)	38(4)
2	0.0087(1)	233(3)	9.8(2)	17.8(9)
3	0.0066(2)	175(5)	12.8(2)	11.7(5)
4	0.0051(2)	136(5)	15.1(2)	8.4(4)
5	0.0041(2)	110(5)	16.7(3)	6.5(3)

Part II

Drude weight

- Drude weight: $$D = \frac{1}{V}\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}$$
- Form of the perturbation: $$\Phi(\omega) = \frac{Ee^{i\omega t}}{i\omega}$$
- Drude weight is obtained by calculating the zero frequency limit of $\omega\sigma''(\omega)$, i.e. it is the peak of the zero frequency component of the conductivity

Meissner weight

- Perfect conductor: $\mathbf{E} = \frac{1}{n^{(s)}} \frac{\partial \mathbf{j}}{\partial t}$
- Maxwell equation for curl of electric field leads to: $$\frac{\partial}{\partial t}\left(\nabla \times \mathbf{j} + n^{(s)}\mathbf{B}\right) = 0$$
- London equation: $\mathbf{j} = n^{(s)}\mathbf{A}$
- Associating the vector potential $\mathbf{A}$ with Φ we obtain $$n^{(s)} = \frac{1}{\mathrm{V}}\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}$$

Non-classical rotational inertia

- Liquid helium, rotating bucket experiment: below the critical point rotational inertia of rotating He^4 is reduced (Andronikashvili, Hess & Fairbank experiments)
- Work to rotate above T_c: $\Delta W = \frac{I}{2}\Phi^2$
- Work to rotate below T_c: $\Delta W = \frac{I^{(n)}}{2}\Phi^2$
- Rotational inertia associated with the superfluid fraction: $I^{(s)} = \frac{\partial^2 E^{(s)}(\Phi)}{\partial \Phi^2}$ (Φ angular velocity)

Drude weight, Meissner weight, NCRI of superfluids

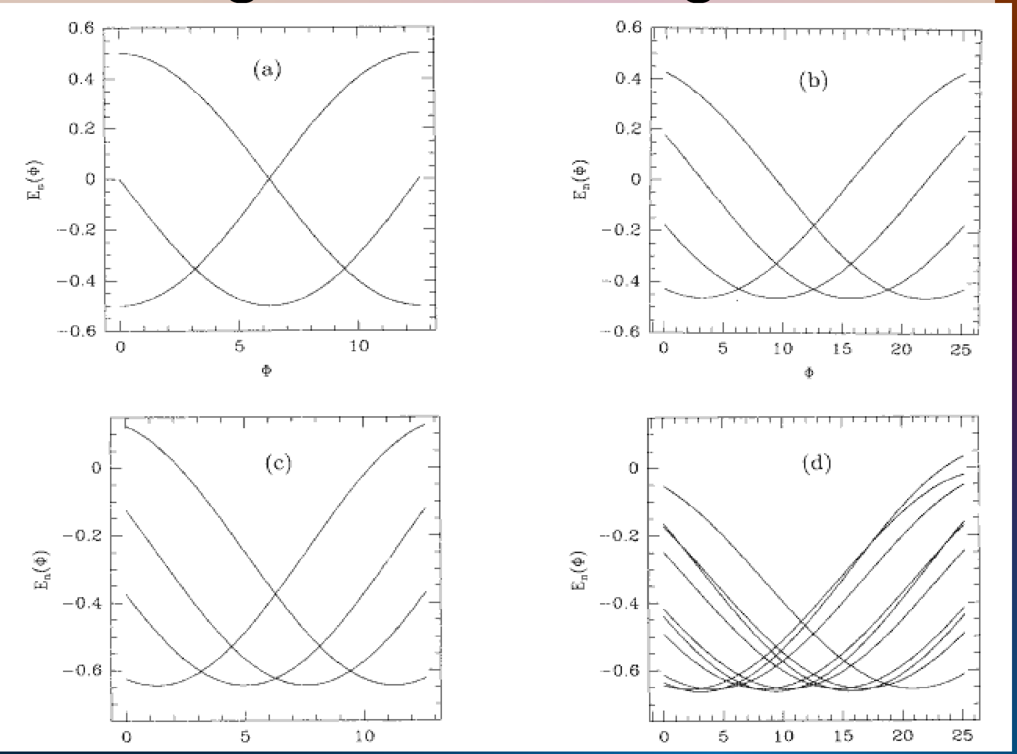
- Drude weight: $$D = \frac{1}{V}\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}$$
- Meissner weight: $$n^{(s)} = \frac{1}{V}\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}$$
- Reduction in rotational inertia of bosonic superfluid: $$I^{(s)} = \left[\frac{\partial^2 E^{(s)}(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}$$
- **Question: how can these quantities be distinguished?**

Adiabatic vs. envelope derivative

- Scalapino, White and Zhang (PRL, 1992, PRB 1993)
  - For the Drude weight the second derivative with respect to the perturbing field is ambiguous
  - Energy levels can cross !!!

Adiabatic derivative: Drude weight

„Envelope“ derivative: Meissner weight



Finite temperature generalization

- Zotos, Castella, and Prelovšek (PRL, 1992, PRB 1993): Drude weight

$$D_c(T) = \frac{\pi}{\mathrm{V}} \sum_n \frac{\exp(-\beta E_n)}{Q} \left[\frac{\partial^2 E_n(\Phi)}{\partial \Phi^2} \right]_{\Phi=0}.$$

  - Weighted adiabatic derivatives

- Meissner weight based on this idea could possibly be of the form:

$$n^{(s)}(T) = \frac{\pi}{\mathrm{V}} \left[\frac{\partial^2}{\partial \Phi^2} \sum_n \frac{\exp(-\beta E_n(\Phi))}{Q} E_n(\Phi) \right]_{\Phi=0}.$$

Variational theory

- A variational ground state energy is a weighted average over exact eigenstates:

$$E(\gamma) = \sum_n \langle \Psi(\gamma) | \tilde{\Psi}_n \rangle E_n \langle \tilde{\Psi}_n | \Psi(\gamma) \rangle = \sum_n P_n(\gamma) E_n.$$

which suggests that the Drude weight should be of the form (weighted adiabatic derivatives)

$$D_c = \frac{\pi}{V} \sum_n P_n(\gamma) \left[\frac{\partial^2 E_n(\Phi)}{\partial \Phi^2} \right]_{\Phi=0}.$$

and the Meissner weight of the form (one envelope derivative)

$$n^{(s)} = \frac{\pi}{V} \left[\frac{\partial^2}{\partial \Phi^2} \sum_n P_n(\gamma(\Phi)) E_n(\Phi) \right]_{\Phi=0}.$$

Variational theory

- In general the working assumption is that the variational ground state energy is a good approximation to the exact ground state, and $n^{(s)}$ is taken to be the Drude weight.
    - Example: for the Gutzwiller projected Fermi sea

$$\frac{\pi}{V}\left[\frac{\partial^2}{\partial\Phi^2}\sum_n P_n(\gamma(\Phi))E_n(\Phi)\right]_{\Phi=0} = \text{finite}.$$

Millis and Coppersmith, (PRB, 1991)

Expressions for the current

- Textbook expression for the current:

$$J(\Phi) = \frac{N}{m}\Phi + \langle\Psi(\Phi)|\left(\sum_i \hat{k}_i\right)|\Psi(\Phi)\rangle$$

- Alternatively,

$$J(\Phi) = \frac{N}{m}\Phi + \sum_i \langle\Psi(\Phi)|\hat{k}_i|\Psi(\Phi)\rangle$$

- <u>**Are these two expressions the same?**</u>

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Expressions for the current

- Berry phase expression for the current (BH, JPSJ, 2012):

$$J(\Phi) = \frac{N}{m}\Phi + \lim_{\Delta X \to 0} \frac{1}{m\Delta X} \mathrm{Im} \ln \langle \Psi(\Phi) | \exp\left(i\Delta X \sum_j \hat{k}_j \right) | \Psi(\Phi) \rangle$$

- Alternatively,

$$J(\Phi) = \frac{N}{m}\Phi + \lim_{\Delta X \to 0} \frac{N}{m\Delta X} \mathrm{Im} \ln \langle \Psi(\Phi) | \exp\left(i\Delta X \hat{k} \right) | \Psi(\Phi) \rangle$$

- <u>**Are these two expressions the same?**</u>

Expressions for the current

- Reduced density matrix of order m:

$$\rho_m(x_1, ...x_m; x'_1, ..., x'_m) = \int ... \int dx_{m+1}...dx_N$$

$$\Psi(x_1, ..., x_m, x_{m+1}, ..., x_N)\Psi(x'_1, ..., x'_m, x_{m+1}, ..., x_N)$$

Current expressions become:

$$J(\Phi) = \frac{N}{m}\Phi + \lim_{\Delta X \to 0} \frac{1}{m\Delta X} \mathrm{Im} \ln \mathrm{Tr} \left\{ \hat{\rho}_N \exp\left(i\Delta X \sum_j \hat{k}_j \right) \right\}$$

$$J(\Phi) = \frac{N}{m}\Phi + \lim_{\Delta X \to 0} \frac{N}{m\Delta X} \mathrm{Im} \ln \mathrm{Tr} \left\{ \hat{\rho}_1 \exp\left(i\Delta X \hat{k} \right) \right\}$$

- **Two expressions are not the same!!!**

Reduced density matrix/ODLRO

- Ordering in the reduced density matrix, known as off-diagonal long range order (ODLRO)

$$\lim_{|x_1 - x_1'| \to \infty} \rho_1(x_1; x_1') = \text{finite}$$

Penrose and Onsager (PRB, 1956)

- ODLRO in $\hat{\rho}_1$: condensation of single particles (example: superfluidity in He^4)
- ODLRO in $\hat{\rho}_2$: condensation of pairs of particles (example: Cooper pairs in superconductors)

Yang (RMP, 1959)

- ODLRO in $\hat{\rho}_N$: standard conductor

BH (PRB, 2013; arXiv:1310.4144)

Different kinds of currents

- General expression for the current:

$$J_p(\Phi) = \frac{N}{m}\Phi + \lim_{\Delta X \to 0} \frac{(N/p)}{m\Delta X} \mathrm{Im}\ln\mathrm{Tr}\left\{\hat{\rho}_p \exp\left(i\Delta X \sum_{j=1}^{p} \hat{k}_j\right)\right\}$$

- General expression for transport quantities:

$$D_p = \left[\frac{\partial J_p(\Phi)}{\partial \Phi}\right]_{\Phi=0}$$

- Eigenstates of *p*-momenta contribute to *p*-transport coefficients

Transport quantities

- D_1 : $I^{(s)}$ non-classical rotational inertia
- D_2 : $n^{(s)}$ Meissner weight
- D_N : $D^{(c)}$ Drude weight

Associated flux quantization:

- D_p: $\Phi_B = nhc/(pe)$ as $p \rightarrow \infty$ flux is no longer quantized
- Hubbard model phase transition: between a quantized flux vs. continuous flux state

Transport quantities

- Yang (RMP, 1959): if ODLRO found in $\hat{\rho}_p$ it will also be found in $\hat{\rho}_m$ for all $m > p.$
- **Comprehensive theory of conductivity:**
  - If D_p is finite, so is D_m for all $m>p$.
  - If the minimum p for which D_p is finite is a microscopic number ($p<<N$), then superconduction
  - If $p\sim N$ normal conduction
  - If all D_p are zero, then material is insulating

BEC, ODLRO, NCRI

- P. W. Anderson: “Theory of Supersolidity” (JLTP, **169** 124 (2012))

> 1967 that finite concentrations of vacancy defects would superflow.) But it has never been demonstrated that ODLRO, superfluidity, and NCRI are synonymous, and the indirect nature of these arguments leaves one, at best, unsatisfied.

- ...but D_1 (or $I^{(s)}$) is the non-classical rotational inertia (superfluid weight): measures contributions from momentum eigenstates of the reduced one-body density matrix
- ODLRO measures contributions from zero momentum eigenstates of the reduced one-body density matrix

Conclusions

- Total Current can be expressed in terms of a Berry phase
- DC conductivity can be expressed in terms of a topological invariant (similar to TKNN invariant)
- Berry phase theory of current allows to distinguish supercurrents from normal current
- Transport quantities (Drude weight, Meissner weight, non-classical rotational inertia) can be distinguished
- BEC vs. superfluid can be distinguished

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Thank you for your attention!