Title: Diamagnetic response and phase stiffness for interacting isolated narrow bands

Speakers: Dan Mao

Series: Quantum Matter

Date: September 30, 2022 - 11:00 AM

URL: https://pirsa.org/22090086

Abstract: Superconductivity in electronic systems, where the non-interacting bandwidth for a set of isolated bands is small compared to the scale of the interactions, is a non-perturbative problem. Here we present a theoretical framework for computing the electromagnetic response in the limit of zero frequency and vanishing wavenumber for the interacting problem, which controls the superconducting phase stiffness, without resorting to any mean-field approximation. Importantly, the contribution to the phase stiffness arises from (i) ``integrating-out'' the remote bands that couple to the microscopic current operator, and (ii) the density-density interactions projected on to the isolated bands. We also obtain the electromagnetic response directly in the limit of an infinite gap to the remote bands, using the appropriate ``projected'' gauge-transformations. These results can be used to obtain a conservative upper bound on the phase stiffness, and relatedly the superconducting transition temperature, with a few assumptions. In a companion article, we apply this formalism to a host of topologically (non-)trivial ``flat-band'' systems, including twisted bilayer graphene.

Zoom link: https://pitp.zoom.us/j/99631762791?pwd=dU4yaU1wKzJNTisrazJjaUF2ODlXUT09

Diamagnetic response and phase stiffness for interacting isolated narrow bands

Dan Mao (Cornell)

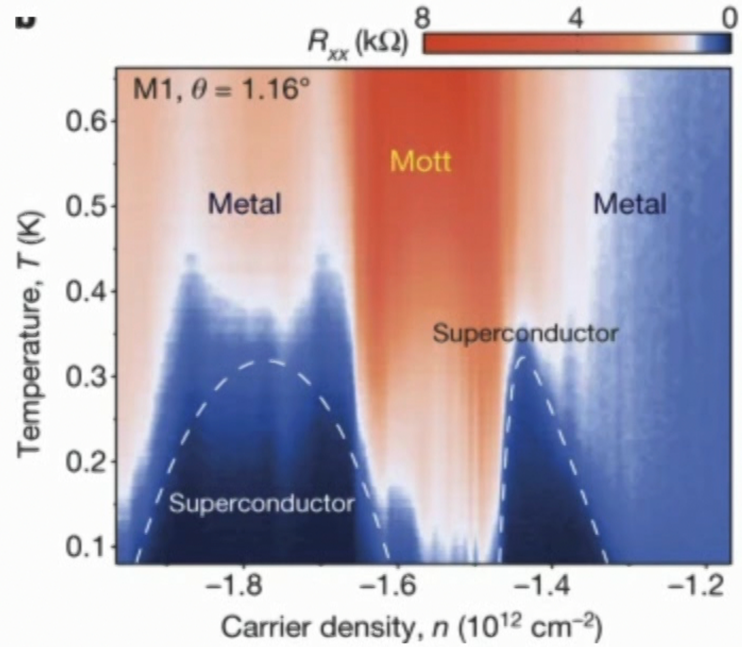
2022.9.30

DM, D.Chowdhury, arXiv:2209.06817 & to appear

Superconductivity in moiré materials

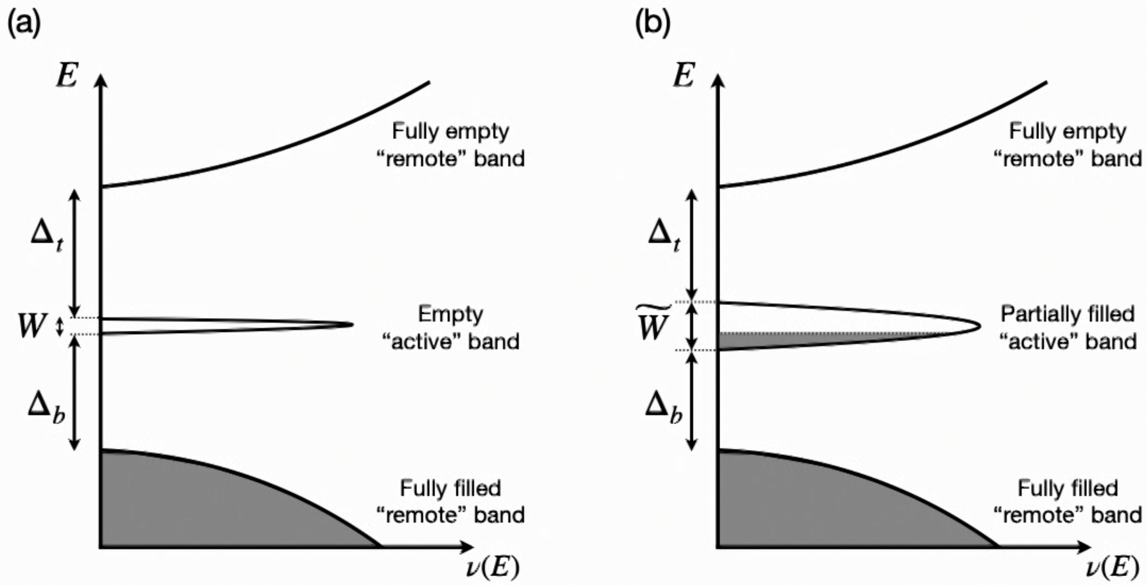
- **Twisted bilayer graphene** (Cao, Y., Fatemi, V., Fang, S. *et al.,* Nature, 2018 ; Lu, X., Stepanov, P., Yang, W. *et al.,* Nature, 2019*;* M. Yankowitz, S. Chen, H. Polshyn, *et al.,* Science, 2019; Arora, H.S., Polski, R., Zhang, Y. *et al.,* Nature, 2020)
- **Alternating twist magic angle graphene** (Hao, Z., Zimmerman, A.M. *et al.,* Science, 2020)
- **Twisted trilayer graphene** (Park, J.M., Cao, Y., Watanabe, K. *et al.,* Nature, 2021)

……



(From Cao, Y., Fatemi, V., Fang, S. *et al.,* Nature, 2018)

Superconductivity in narrow bands



$$\Delta \gg W, V$$

Attempts in addressing the superfluid stiffness:

- mean-field (S. Poetta, P. Törmä, 15'; X. Hu, *et al.* 19'; A.Julku, *et al*., 20'; F. Xie *et al*., 20'; P. Törmä, et al., 21'…)
- exact soluble models (K. Huhtinen, et al. 21'; J. Herzog-Arbeitman, *et al.,* 22'…)

Challenge: strong coupling regime, BCS mean-field does not apply, lack of general formalism

More general question: effective response

Say we would like to some properties of the superconductor, for example phase stiffness, which can be related to the response function to external electromagnetic field.

Question: how to couple an effective theory to probe gauge field?

Why is this a non-trivial question?

- Conventionally, would like to perform Peierls' substitution but for interacting topological bands, there is no tight-binding model to begin with.
- Even for trivial bands, the definition of Wannier orbitals has gauge ambiguity but the physical observables should be gauge independent.

In this work: obtain the effective gauge coupling in the long wave length, static limit without relying on tight-binding Hamiltonians.

Outline

- Superfluid stiffness in terms of response functions
- Warm-up: multi-band free electron systems
- Result for interacting narrow band systems
- Example: trivial bands, LLL, TBG

Superfluid stiffness D_s

- Superfluid stiffness can be related to transverse current response in the following way:

$$\frac{D_s}{\pi e^2} = \langle K_{xx} \rangle - \chi_{xx}(q_x = 0, q_y \to 0, \omega = 0)$$ (Scalapino, White, Zhang, PRB 93')

$$K_{\mu\nu} = \frac{\delta^2 H[A]}{\delta A_\mu \delta A_\nu}$$: diamagnetic term

$\chi_{xx}(q, \omega)$: current-current correlator

Since $\chi_{xx}(q, \omega) \geq 0$,

$$D_s \leq \pi e^2 \langle K_{xx} \rangle$$

Bound on superfluid stiffness

$$\frac{D_s}{\pi e^2} \leq \langle K_{xx} \rangle \sim \frac{n}{m}$$, for Galilean-invariant systems

Electron mass (not a very useful bound for narrow band systems)

On the other hand, since the gap is large, we expect effectively,

$$\frac{D_s}{\pi e^2} = \langle K_{xx}^{\text{eff}} \rangle - \chi_{xx}^{\text{eff}}(\omega = q_x = 0, q_y \to 0)$$ and $$\frac{D_s}{\pi e^2} \leq \langle K_{xx}^{\text{eff}} \rangle$$

$+O(\frac{W}{\Delta})$ terms

only involves d.o.f. within the narrow bands.

How to get the effective response functions?

Two approaches:

1. Start with a UV Hamiltonian including all the remote bands, couple to a probing gauge field, then take band gap to infinity and keep the O(1) terms.

2. Start with the *effective* Hamiltonian, then couple to a probing gauge field.

Benchmark:

For band electrons (ignore interaction), one should expect,

$$\langle K_{xx}^{\text{eff}} \rangle \sim \frac{n}{m_*}$$

m_* : effective mass , gives Drude weight.

Warm-up: multi-band free electron systems

Hamiltonian: $H_{\text{kin}} = \sum_{k,n} \epsilon_{k,n} c^{\dagger}_{k,n} c_{k,n}$ n: band index

By definition, H[A] is obtained by letting

$$c_{k,m} \to \sum_n c_{k+A,n} \langle u_{k,m} | u_{k+A,n} \rangle$$

- If we start with the *effective* Hamiltonian, for simplicity only one active band,

$$\langle \bar{K}_{xx} \rangle = \sum_k f(\epsilon_k) \langle u_k | \partial^2_{k_x} \bar{h}_k | u_k \rangle = \sum_k f(\epsilon_k) \left[\partial^2_{k_x} \epsilon_k - 2\epsilon_k g_{xx}(k) \right]$$

Drude weight ???

(If we start with the full Hamiltonian, we get the Drude weight as expected.)

$g_{xx}(k)$: quantum metric

Warm-up: multi-band free electron systems

Why an extra piece proportional to quantum metric? **Symptom of violation of unitarity.**

Since the gauge transformation is *not* diagonal in the band basis, an infinitesimal gauge transformation restricted to the active ands gives,

$$c_k \to \mathcal{P} U_\alpha^\dagger c_k U_\alpha \mathcal{P} = c_{k+\alpha} \langle u_k | u_{k+\alpha} \rangle$$

Not a phase, $$|\langle u_k | u_{k+\alpha} \rangle|^2 \approx 1 - \alpha^2 g_{xx}(k)$$

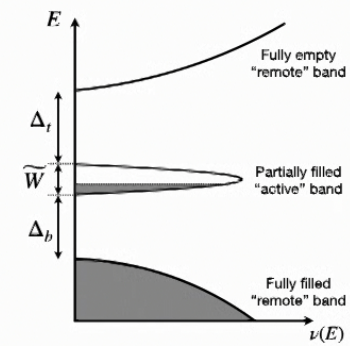
Q: What should one do to ``couple effective theory to a probing gauge field"?

Q: What should one do to ``couple effective theory to a probing gauge field”?

Let us take a step back, and ask the following question:

Suppose we start with a UV Hamiltonian and calculate the superfluid stiffness, what should we get if we let the band gap go to infinity at the end of the day?

By performing a perturbative expansion in terms of W/Δ , the terms that are *independent* of the band gap should give the effective diamagnetic and paramagnetic terms, namely K_{xx}^{eff} and χ_{xx}^{eff} .



Setup

Let us consider a microscopic Hamiltonian of the system with density-density interaction,

$$H = H_{\text{kin}} + H_{\text{int}}$$

$$H_{\text{kin}} = \sum_{r,r',\alpha,\alpha'} t_{\alpha\alpha'}(r-r') c^{\dagger}_{r\alpha} c_{r'\alpha'} - \mu N$$

$$H_{\text{int}} = \sum_{r,r'} V(r-r')\, n_r n_{r'}$$

Let us resolve the Hamiltonian into its ``diagonal" and ``off-diagonal" pieces, respectively,

$$\begin{aligned} H =& H_d + H_o, \\ H_d =& \mathbb{P}H\mathbb{P} + \mathbb{Q}H\mathbb{Q}, \\ H_o =& \mathbb{P}H\mathbb{Q} + \mathbb{Q}H\mathbb{P}, \end{aligned}$$

$\mathbb{P}$ is the projection operator to the sub-Hilbert space $\mathbb{H}$, spanned by the many-body states with partially occupied active bands and fully occupied (empty) lower energy (higher energy) remote bands.

Schrieffer-Wolff (SW) transformation

$$\begin{aligned} H &= H_d + H_o, \\ H_d &= \mathbb{P}H\mathbb{P} + \mathbb{Q}H\mathbb{Q}, \\ H_o &= \mathbb{P}H\mathbb{Q} + \mathbb{Q}H\mathbb{P}, \end{aligned}$$

- Without coupling to probing gauge field, the correction to H_d by H_o is $\sim V^2/\Delta$

  And the effective Hamiltonian is therefore $H_{\text{eff}} = \mathbb{P}H\mathbb{P}$

- Now let us consider $H[A]$, for a small A, we expand

$$H[A] = H[0] + J_\mu A_\mu + \frac{1}{2} K_{\mu\nu} A_\mu A_\nu + ... \equiv H_d[A] + H_o[A].$$

By performing a unitary transformation, that is SW transformation, we can block diagonalize H[A]

$$\widetilde{H}[A] = e^{T[A]} H[A] e^{-T[A]} \quad , \quad \langle m|T[A]|n\rangle = \langle m|H_o[A]|n\rangle / \underbrace{(E_m - E_n)}_{\sim \Delta}$$

- Why is this different from A = 0?

$$J_\mu(q_\mu \to 0) = -i\left[\hat{X}_\mu, H\right] \quad \text{, so} \quad \langle m|J_\mu(q_\mu \to 0)|n\rangle = -i(E_n - E_m)\langle m|\hat{X}_\mu|n\rangle \sim \Delta$$

T[A] has pieces that are *independent* of Δ !

Our results

- The effective Hamiltonian coupled to gauge field should be defined as,

$$H_{\mathrm{eff}}[A] \equiv \mathbb{P}\widetilde{H}[A]\mathbb{P} = \mathbb{P}e^{T[A]}H[A]e^{-T[A]}\mathbb{P}$$

$$= H_{\mathrm{eff}} + J_{\mu}^{\mathrm{eff}}A_{\mu} + \frac{1}{2}K_{\mu\nu}^{\mathrm{eff}}A_{\mu}A_{\nu}$$ + higher order terms in Δ

with

$$J_{\mu}^{\mathrm{eff}}(q \to 0) = \mathbb{P}J_{\mu}(q \to 0)\mathbb{P} + i\left[\mathbb{P}\hat{X}_{\mu}\mathbb{P}, \mathbb{P}H_{\mathrm{int}}\mathbb{P}\right]$$ (S. Sondhi and S. Kivelson, 92')

$$K_{xx}^{\mathrm{eff}} = -\left[\mathbb{P}\hat{X}\mathbb{P}, \left[\mathbb{P}\hat{X}\mathbb{P}, H_{\mathrm{eff}}\right]\right]$$

Diamagnetic term K_{xx}^{eff}

$$\langle K_{xx}^{\mathrm{eff}} \rangle = \lim_{\alpha\to 0} \partial_\alpha^2 \langle e^{i\alpha \mathbb{P}\hat{X}\mathbb{P}} H_d e^{-i\alpha \mathbb{P}\hat{X}\mathbb{P}} \rangle$$

$$= \langle K_{xx}^{\mathrm{naive}} \rangle + \langle \hat{X}\mathbb{Q}\hat{X}\mathbb{P}H_d\mathbb{P} \rangle + \langle \mathbb{P}H_d\mathbb{P}\hat{X}\mathbb{Q}\hat{X} \rangle,$$

$$\text{where } \langle K_{xx}^{\mathrm{naive}} \rangle \equiv \lim_{\alpha\to 0} \partial_\alpha^2 \langle e^{i\alpha \hat{X}} \mathbb{P}H_d\mathbb{P} e^{-i\alpha \hat{X}} \rangle.$$

what we would get starting with the projected Hamiltonian

Sanity check: free fermion with one active band, we get

$$\mathbb{P}\hat{X}\mathbb{Q}\hat{X}\mathbb{P} = 2\sum_k f(\epsilon_k) g_{xx}(k) \quad \text{and} \quad \langle K_{xx}^{\mathrm{eff}} \rangle = \sum_k f(\epsilon_k) \partial_{k_x}^2 \epsilon_k$$

Diamagnetic term K_{xx}^{eff}

To be concrete, we can also write K_{xx}^{eff} in terms of the fermion creation/annihilation operators for generic Hamiltonian.

For simplicity, let us only write the formula for one active band.
The contribution from interacting term is,

$$\langle K_{xx}^{\text{eff}}\rangle|_{\text{int}} = \sum_{q,k_1,k_2} V(q)\langle c^\dagger_{k_1,\alpha}c_{k_1-q,\alpha}c^\dagger_{k_2,\beta}c_{k_2+q,\beta}\rangle\left[\mathcal{D}_{k_{1,x}}+\mathcal{D}_{k_{2,x}}\right]^2\left[\langle u_{k_1}|u_{k_1-q}\rangle\langle u_{k_2}|u_{k_2+q}\rangle\right]$$

$$\mathcal{D}_{k_x}\left[\langle u_k|u_{k-q}\rangle\right] \equiv \partial_{k_x}\left[\langle u_k|u_{k-q}\rangle\right] + i(\mathcal{A}_{k,x}-\mathcal{A}_{k-q,x})\langle u_k|u_{k-q}\rangle$$

Berry connection

$\mathcal{D}_{k_x}$: ``covariant" derivative to keep the gauge invariance under $|u_k\rangle \rightarrow e^{i\theta_k}|u_k\rangle$

Examples: trivial band

When Peierls' substitution holds?

For the case of one active band, if it is trivial, we can always choose a gauge such that the Berry connection is zero. This is equivalent to Wannier orbitals being maximally localized.

Then we can simply perform the usual Peierls' substitution in the tight-binding Hamiltonian $d_{i,\alpha} \to d_{i,\alpha} e^{i\vec{A}\cdot\vec{r}_i}$ to get the effective gauge coupling.

Note that the projected interaction also couples to the gauge field due to the spreading of the Wannier function, for example,

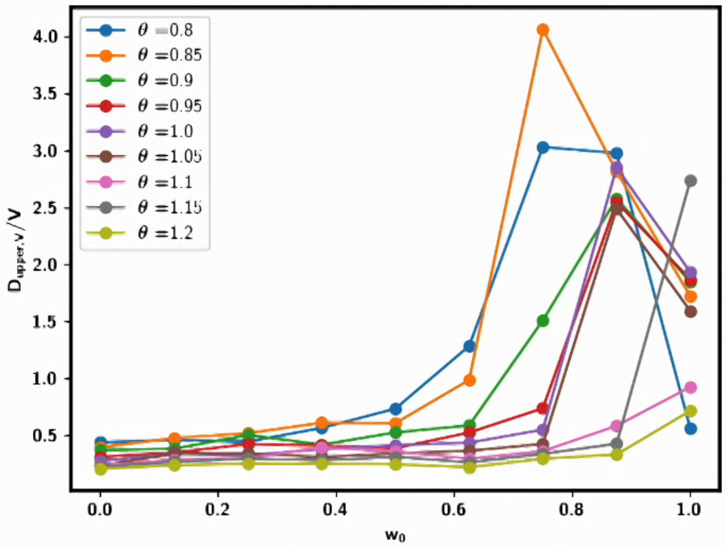
$$d^\dagger_{i,\alpha} d^\dagger_{i,\beta} d_{j,\beta} d_{j,\alpha} \to d^\dagger_{i,\alpha} d^\dagger_{i,\beta} d_{j,\beta} d_{j,\alpha} e^{i2\vec{A}\cdot(\vec{r}_j - \vec{r}_i)} \qquad \text{(pair hopping)}$$

Intuition: spreading of Wannier orbitals can enhance the coherence between pairs.

More Examples:

Lowest Landau level: $K_{\mathrm{xx}}^{\mathrm{eff}} = 0$

Twisted bilayer graphene:



A bonus: partial f-sum rule

K^{eff}_{xx} is also related to integration of optical spectrum weight.

At temperature much smaller than band gap, we have,

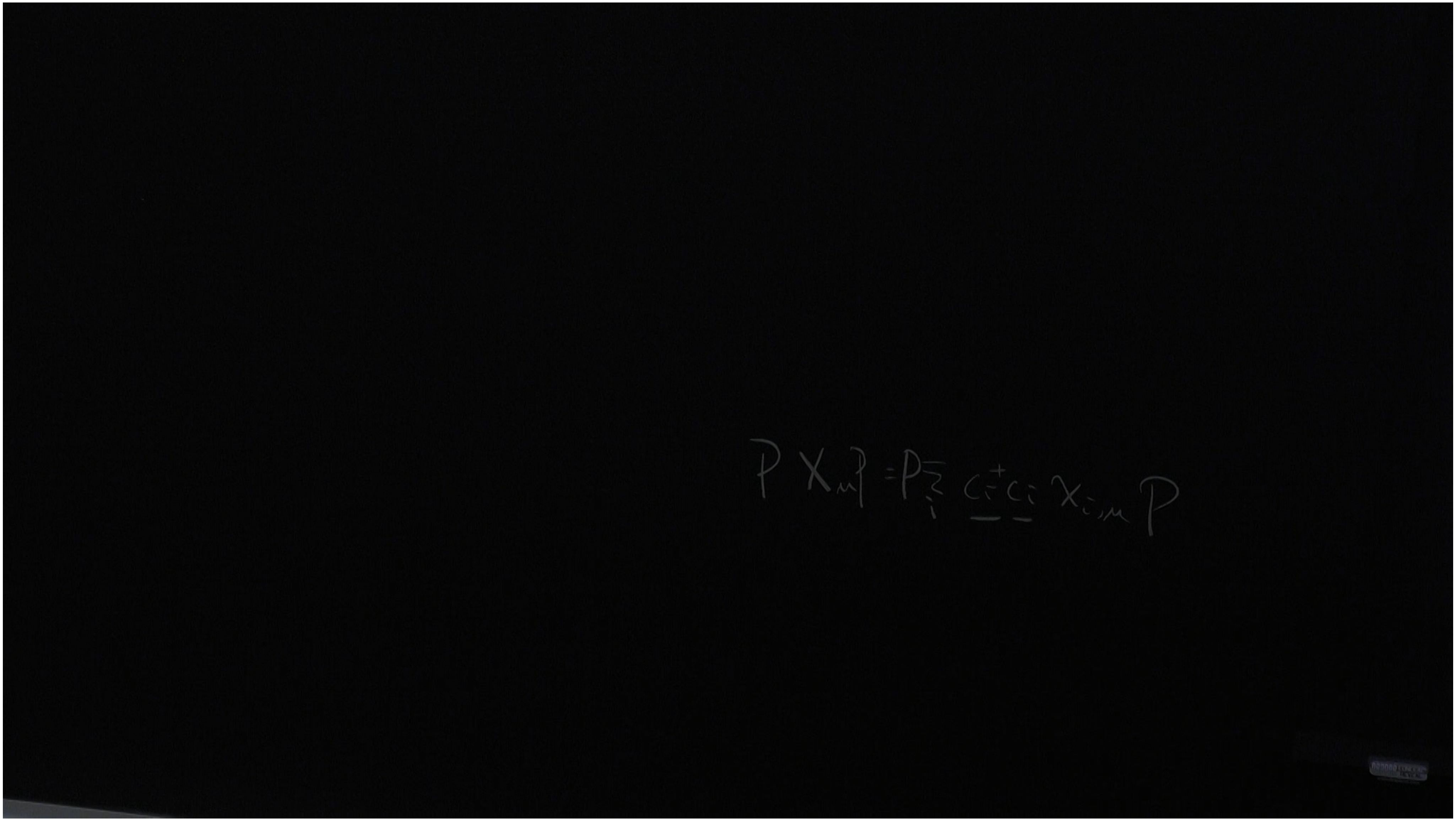
$$\int_0^{\Lambda} d\omega \ \mathrm{Re}[\sigma_{\mathrm{xx}}(q_x \to 0, \omega)] = \frac{\pi e^2}{2} \langle K^{\text{eff}}_{xx} \rangle$$

This is a manifestation of an emergent U(1) symmetry of the system, that is the particle number conservation of the active bands.

Outlook

- We obtained a general formula for effective diamagnetic term. Still need to know the ground state to determine the value of superfluid stiffness.

- The effective formula for superfluid stiffness is equivalent to viewing the gauge field A as couple to the matter fields via $e^{iA_\mu \mathbb{P}\hat{X}_\mu \mathbb{P}}$ instead of the usual gauge transformation $e^{iA_\mu \hat{X}_\mu}$. From the symmetry perspective, the charge of the emergent symmetry is $\bar{Q} = \int_x \bar{\rho}(x)$. $e^{iA_\mu \mathbb{P}\hat{X}_\mu \mathbb{P}}$ can also be thought of as a gauge transformation if we are to gauge the emergent U(1). We need to consider general space-time dependent gauge field and we can get other response functions.


$P X_\mu P = P \sum_i c_i^\dagger c_i x_{i,\mu} P$