# A Field Theory Approach to Orbital Magnetic Responses in Interacting Multi-Band Systems

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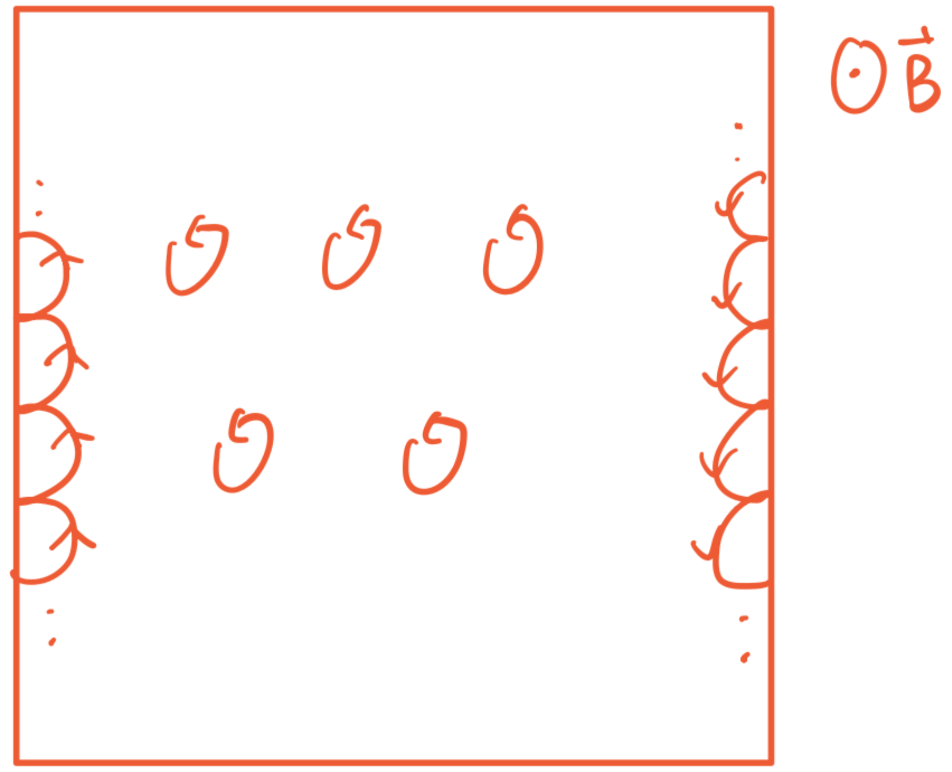
University of Utah

Dec. 8th, 2023, ICTP workshop: Fractionalization and Emergent Gauge Fields in Quantum Matter

# Orbital magnetic responses

Orbital motion of electrons in 2D

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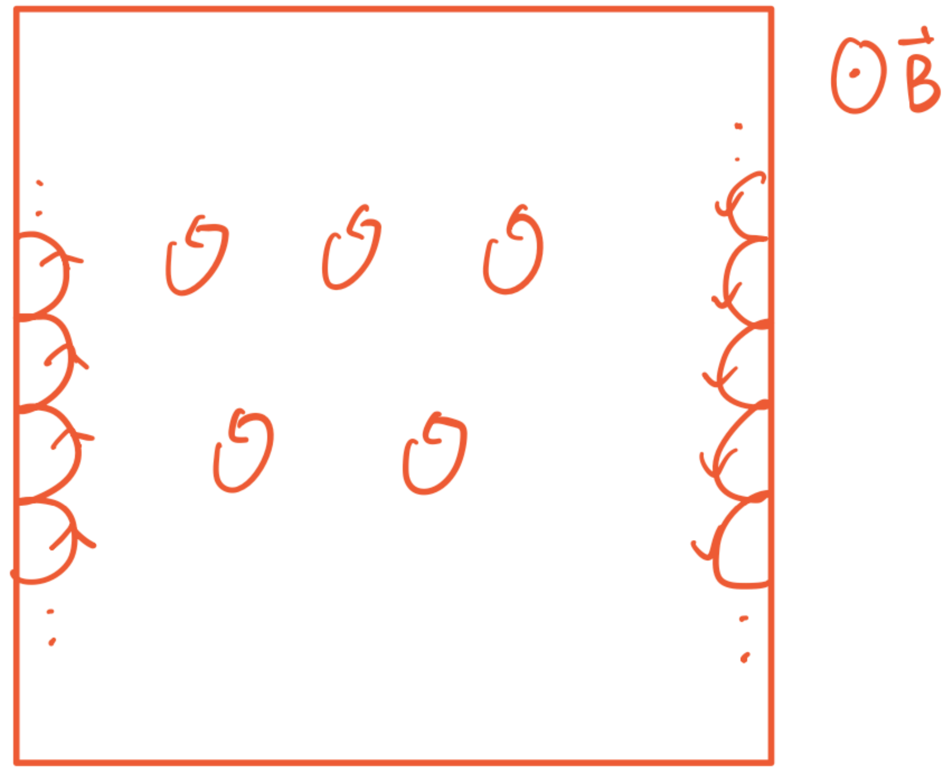


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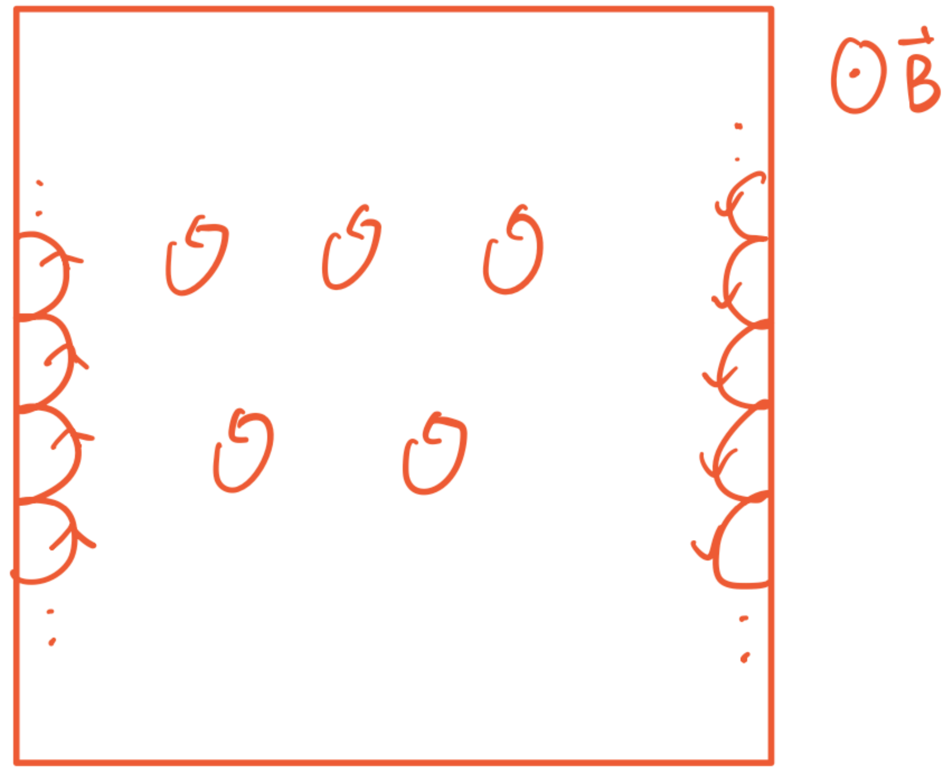

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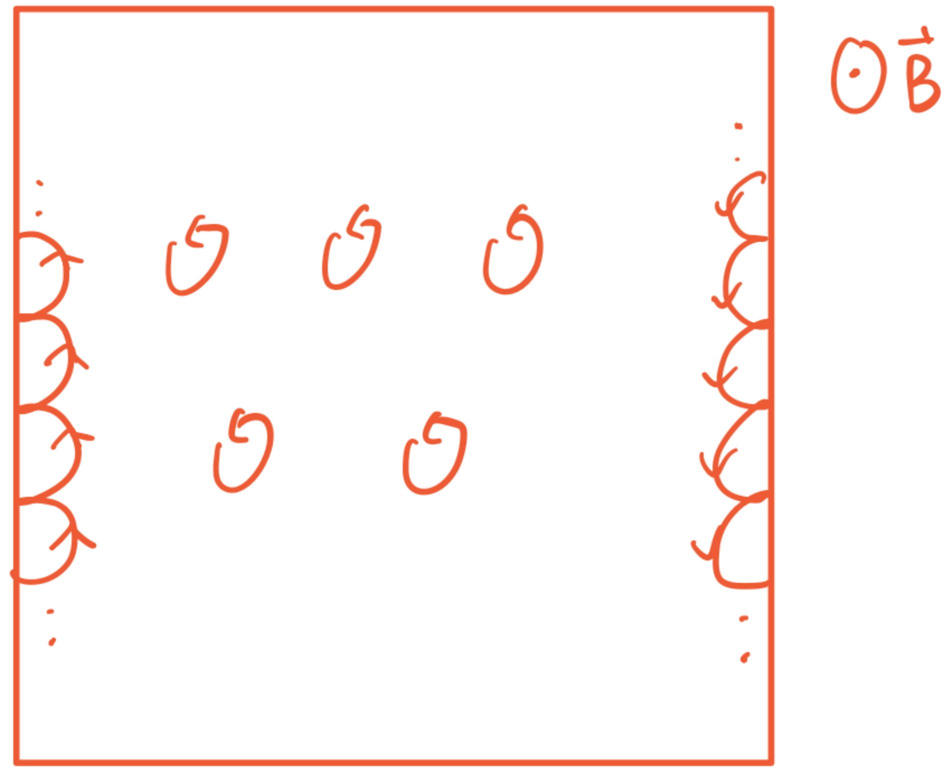

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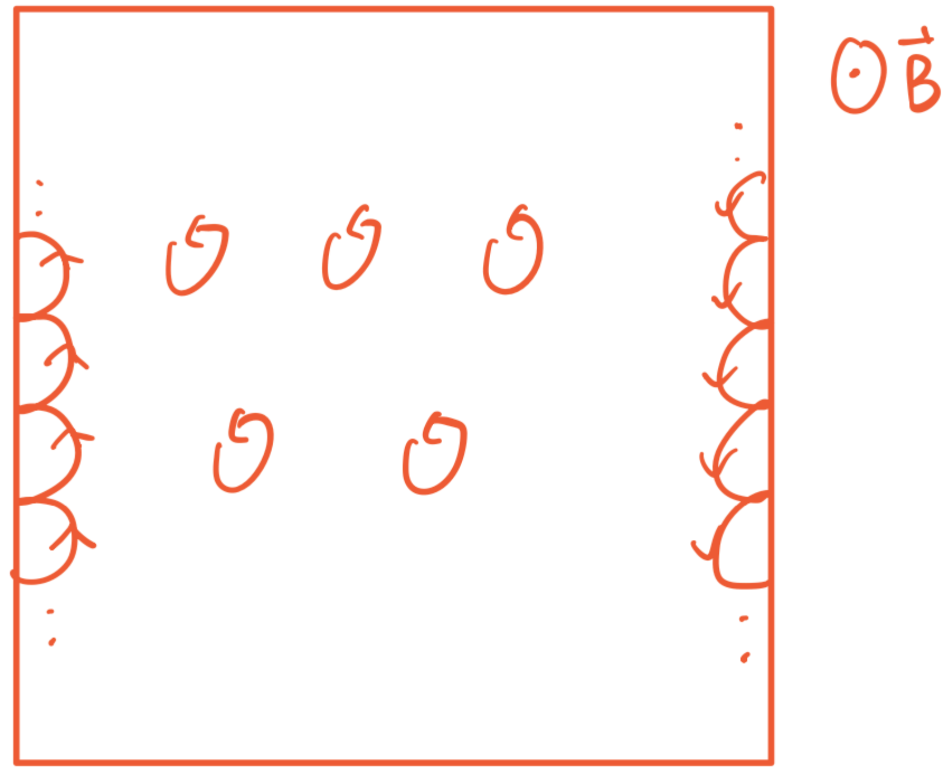

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Scope of this talk.

$\omega_c \ll T \ll \mu$ ✓ Based on: MY, *to appear*

$T \lesssim \omega_c \ll \mu$ ?

# Spontaneous orbital magnetization

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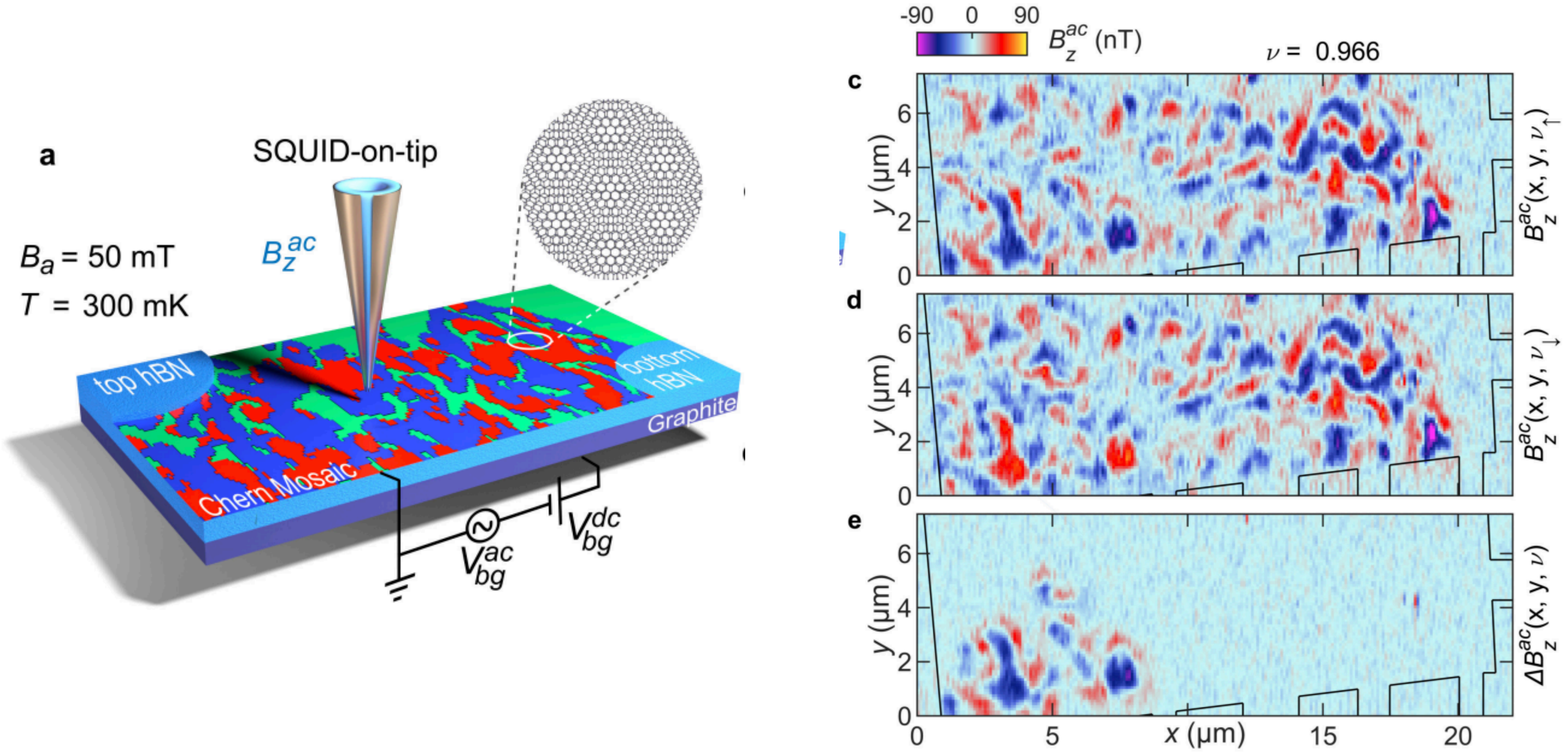
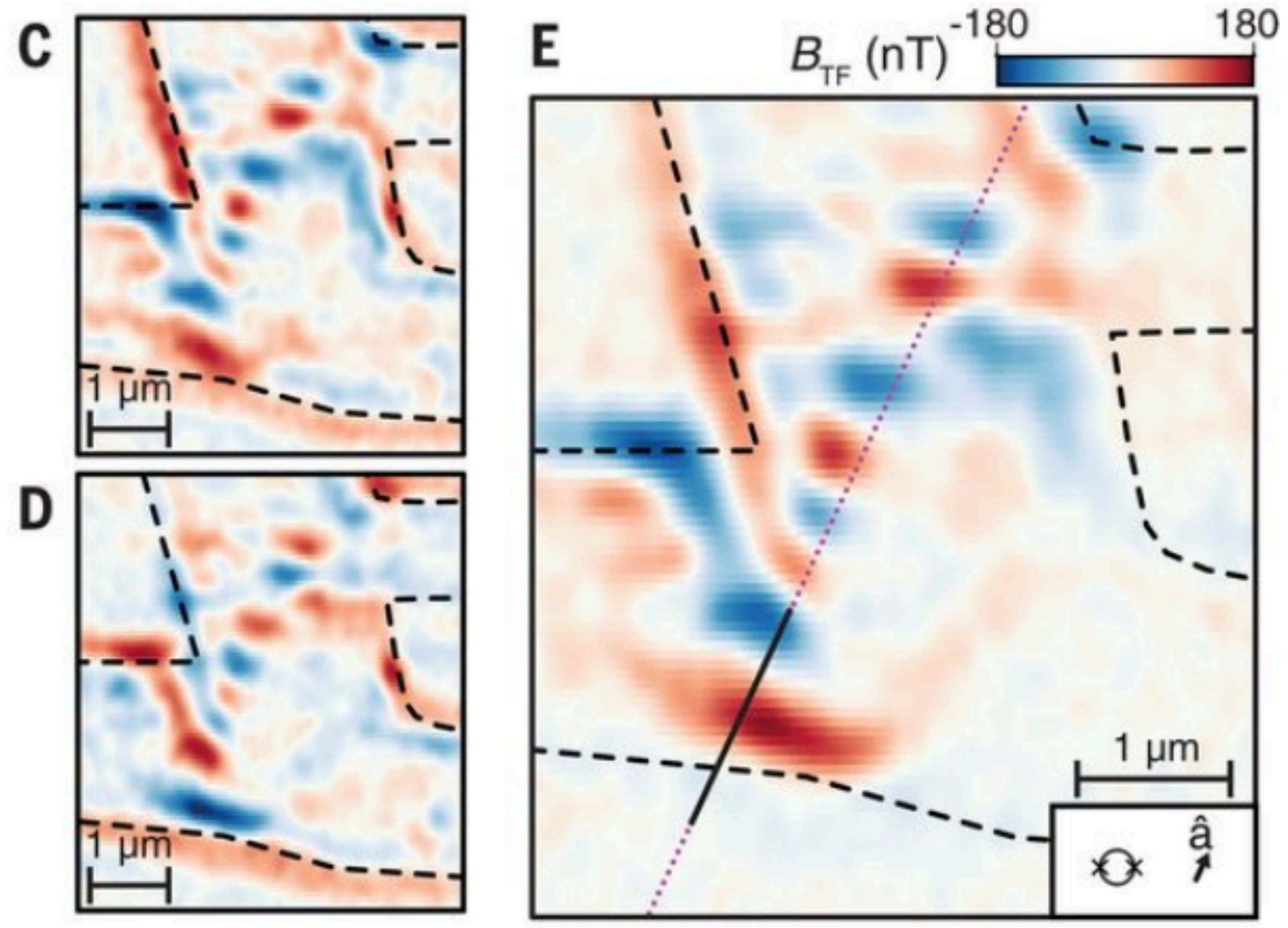



E. Zeldov, et al, Nat. Phys. (2022)




A. Young, et al, Science (2021)

# Orbital magnetization

- Classical definition: $M_{orb} = \int d^2\mathbf{r}\ \left(\mathbf{r} \times \mathbf{J}(\mathbf{r})\right)$
- Subtleties to define and compute $M_{orb}$ in a periodic crystal quantum mechanically:
  - $\mathbf{M}_{\text{orb}} = \frac{\mathbf{m}_{\text{orb}}}{V} = -\frac{e}{2cV}\sum_n f_n \langle\psi_n|\mathbf{r}\times\mathbf{v}|\psi_n\rangle \qquad \mathbf{v} = -\frac{i}{\hbar}[\mathbf{r}, H]$
  - $M_{orb}$ can not be uniquely determined from local current density:

$$c\nabla \times M_{orb} = J(\mathbf{r}) \Rightarrow\Rightarrow\Rightarrow M'_{orb} = M_{orb} + M_{const} + \nabla\xi$$

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    Periodic crystal ⇘ $\psi_n \rightarrow \psi_{n,\mathbf{k}}$

    $\mathbf{r}$ ill-defined for extended Bloch wave function

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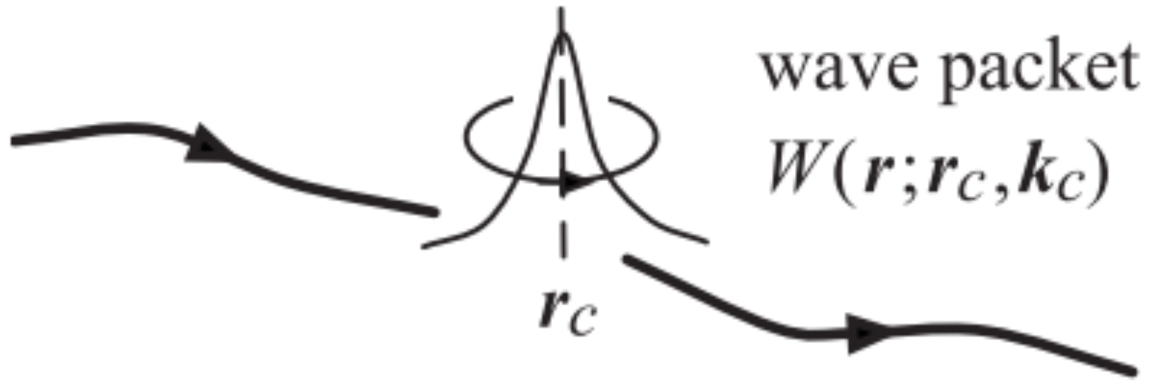
# “Modern” theories of spontaneous orbital magnetization

- Semiclassical derivation of $M_{orb}^{(0)}$ D. Xiao, J. Shi, Q. Niu, PRL (2005)




- Matrix element of $\mathbf{r} \times \mathbf{J}$ on Wannier orbitals T. Thonhauser, D. Ceresoli, D. Vanderbilt, and R. Resta, PRL (2005, 2006)
- Quantum mechanical: $B \rightarrow B(\mathbf{q}) = \mathbf{q} \times \mathbf{A}(\mathbf{q})$ J. Shi, G. Vignale, D. Xiao, and Q. Niu, PRL (2007)

$$\lim_{\mathbf{q}\to 0}\lim_{V\to\infty} \quad \text{v.s.} \quad \lim_{V\to\infty}\lim_{\mathbf{q}\to 0}$$

Interacting case:
R. Nourafkan, G. Kotliar, and A.-M.S. Tremblay, PRB (2014)

- More recent developments for non-interacting systems: gauge invariant formulation

K. T. Chen and P. A. Lee, PRB (2011)
D. Haldane, Journal of Mathematical Physics (2021)

# Our Goal

How to compute thermodynamic quantities for multi-band systems in a magnetic field?

A theory that we want to develop:

- Orbital magnetic response derived from the thermodynamic potential, e.g. $M_{orb}^{(0)} = -\frac{\partial \Omega}{\partial B}|_{B=0,\mu,T}$
  - Can be generalized to interacting systems.
  - Define $M_{orb}^{(0)}$ un-ambiguously. c.f. $c\nabla \times M_{orb} = J(\mathbf{r})$
- Obtained from an infinite system with periodic boundary condition.
- Make it clear the meaning of momentum $\mathbf{k}$ in a magnetic field.
- Do not have to consider inhomogeneous magnetic field, i.e. take the limit " $\lim_{\mathbf{q}\to 0} \lim_{V\to\infty}$ " in the calculation.

# Review of thermodynamic potential

$$\Omega = -T\,\mathrm{Tr}\ln(\mathrm{e}^{-(\beta\hat{H}-\mu\hat{N})})$$

$$= -\lim_{\eta\to 0^+} T\sum_n \mathrm{e}^{i\omega_n\eta}\left(\mathrm{Tr}\ln G_n^{-1} - T\,\mathrm{Tr}\Sigma_n\circ G_n\right) + \Phi(G)$$

Definition:

$G_n(x_1,x_2), \Sigma_n(x_1,x_2)$ are bi-local fields with Matsubara frequency $\omega_n$ ➩➩➩ $G_{12}, \Sigma_{12}$ i.e. $1 \equiv x_1$

$$(f\circ g)_{11'} = \int \mathrm{d}2\, f_{12}\, g_{21'}$$

$$\mathrm{Tr}(f\circ g) = \mathrm{tr}\int \mathrm{d}1\ \mathrm{d}1'\,\delta_{11'}(f\circ g)_{11'};$$

Satisfy:

$$\begin{cases}\text{Dyson equation:} & \left(G_0^{-1}-\Sigma\right)_{12} = G^{-1}{}_{12} \leftrightarrow \left(\left(G_0^{-1}-\Sigma\right)\circ G\right)_{11'} = \delta_{11'} \\ \text{Self-energy definition for 2PI diagrams:} & \frac{\delta\Phi(G)}{\delta G_{12}} = \Sigma_{21}\end{cases}$$

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With translation symmetry: $G_{1,2} = G(1-2), \Sigma_{1,2} = \Sigma(1-2)$

Fourier transform <—> Unitary transformation $U(\mathbf{k}) = \sum_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}x}|x><\mathbf{k}|$

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tr over internal d.o.f.

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N-band model: $\Psi = (\psi_1, \psi_2, \ldots, \psi_N)^T$

Homogeneous magnetic field: $\hat{H}_{non-int} = \int d\mathbf{r} \bar{\Psi}_{\mathbf{r}} \sum_{<ij>} (-\underline{t}_{ij}\, \mathrm{e}^{iq \int_{r-\delta}^{r} A \cdot \delta_{ij}}) \Psi_{\mathbf{r}-\delta_{ij}}$

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Plane wave is not the proper basis to use, for any $B \neq 0$ !

## Technical goal:

Find a proper and physical basis that allows for diagonalization in “momentum” space order by order in $B$.

# New basis functions and Fourier transform

"Fourier transform" of local fields $\Psi(x)$, $\bar{\Psi}(x)$, or generally $\mathcal{O}(x)$:

Define $\hat{\tau}_x = e^{i\hat{\pi}\cdot x}$ $\quad [\hat{\pi}_i, \hat{\pi}_j] = i\epsilon_{ij} qB = i\epsilon_{ij} l_B^{-2} = i\theta_{ij}$ $\qquad \hat{\pi}_i = -i\partial_i - qA_i$

Fuzziness in momentum space ➾ ➾ ➾ Coherent state basis:

$$\hat{a} = \frac{1}{\sqrt{2}\ell_B^{-1}}(\pi_x + \mathrm{i}\pi_y) = -\mathrm{i}\sqrt{2}(\ell_B \partial_{\bar{z}} + \frac{1}{4\ell_B} z), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}\ell_B^{-1}}(\pi_x - \mathrm{i}\pi_y) = -\mathrm{i}\sqrt{2}(\ell_B \partial_z - \frac{1}{4\ell_B}\bar{z})$$

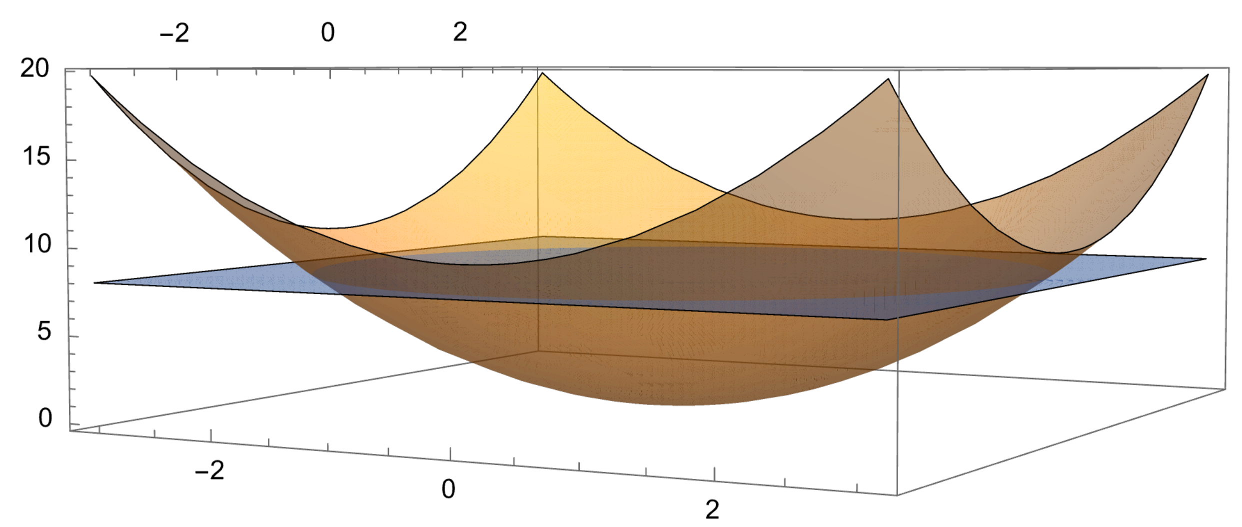
$$|\eta) = e^{\frac{\eta a^\dagger}{\sqrt{2} l_B^{-1}}}|0), \ (\xi| = (0|e^{\frac{\xi a}{\sqrt{2} l_B^{-1}}}$$

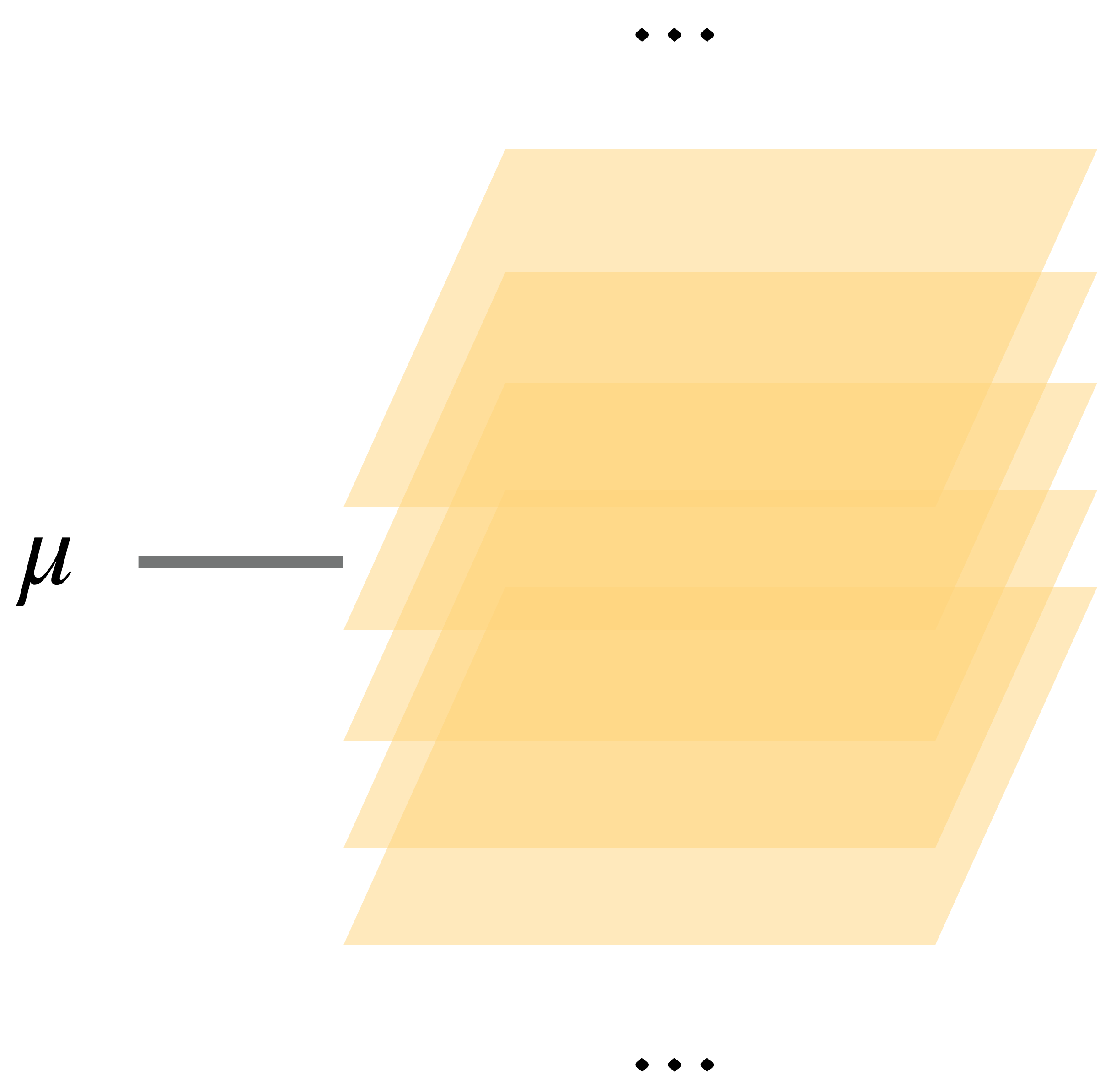
Define an invertible transformation: $\hat{\mathcal{O}}_{\hat{\pi}} = \int \frac{d^2x}{2\pi l_B^2} \mathcal{O}(x)\hat{\tau}_{-x}$ $\qquad \mathcal{O}(x) = \tilde{\mathrm{tr}}(\hat{\mathcal{O}}_{\hat{\pi}}\, \hat{\tau}_x)$

$\tilde{\mathrm{tr}}(\,.\,) = \int_{\eta,\xi} (\xi|\,.\,|\eta)$, i.e. tracing over the basis functions.

# Physical intuitions:

$B = 0$

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Landau levels

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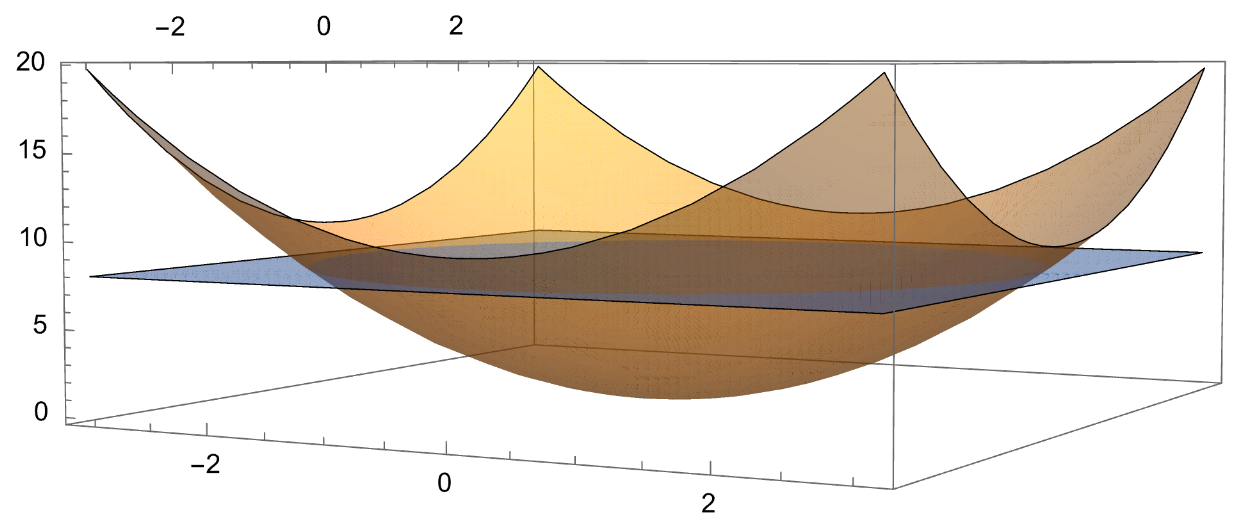


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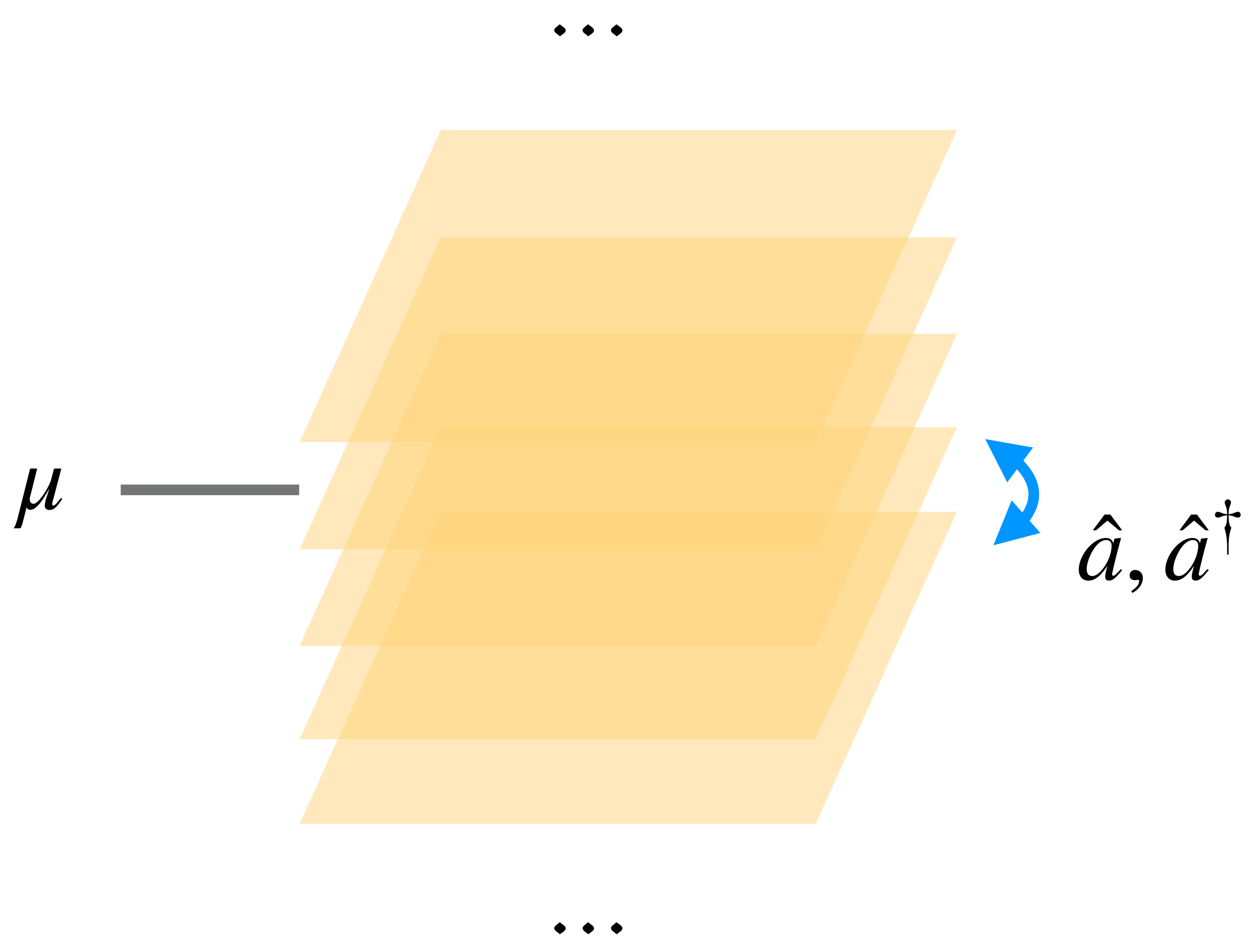

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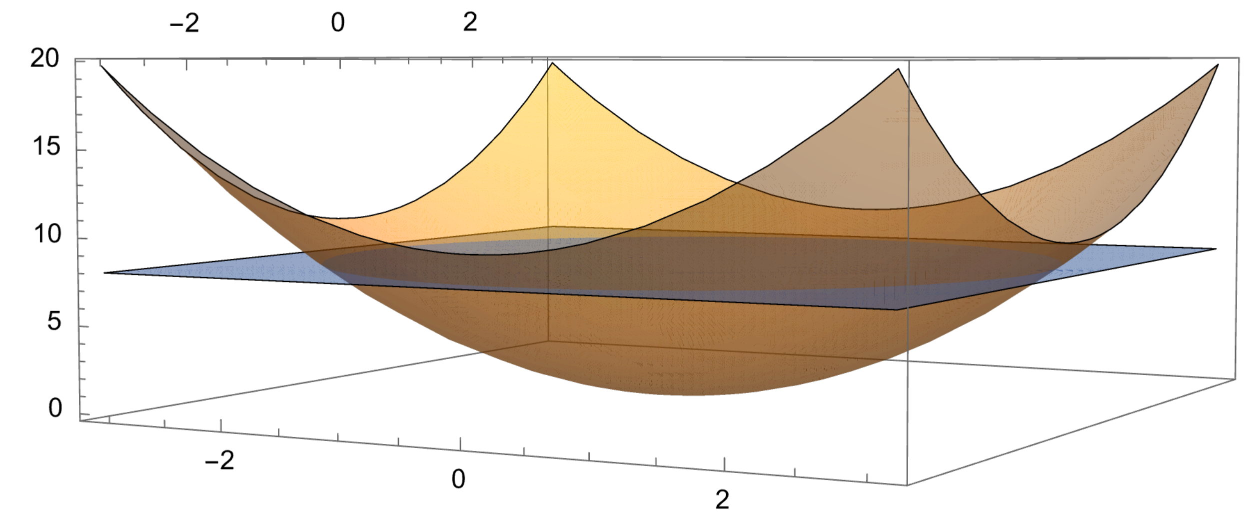


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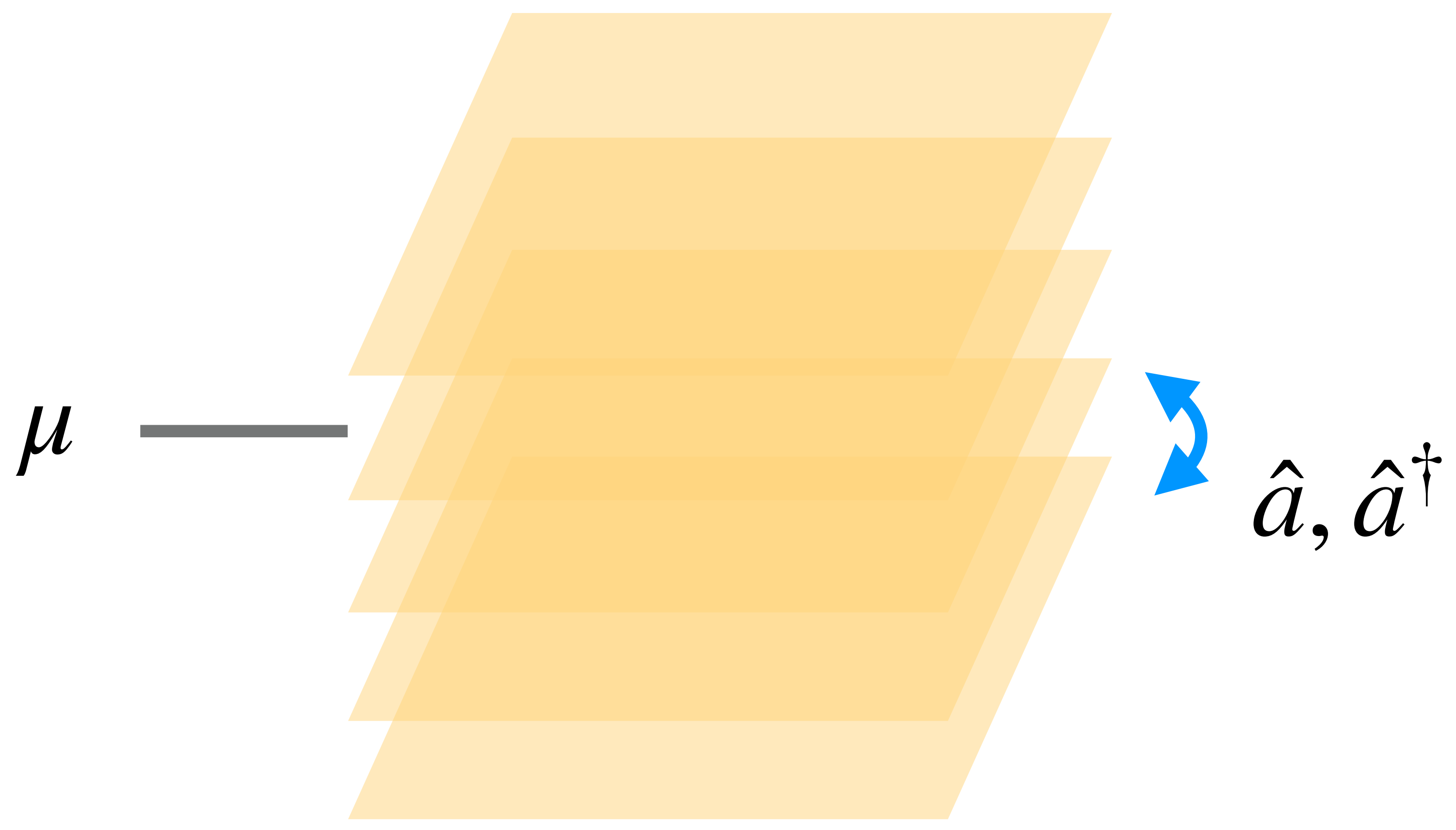


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Coherent state basis: Superposition of LLs $|\eta) = \mathrm{e}^{\frac{\eta a^\dagger}{\sqrt{2} l_B^{-1}}}|0), \ (\xi| = (0|\mathrm{e}^{\frac{\xi a}{\sqrt{2} l_B^{-1}}}$

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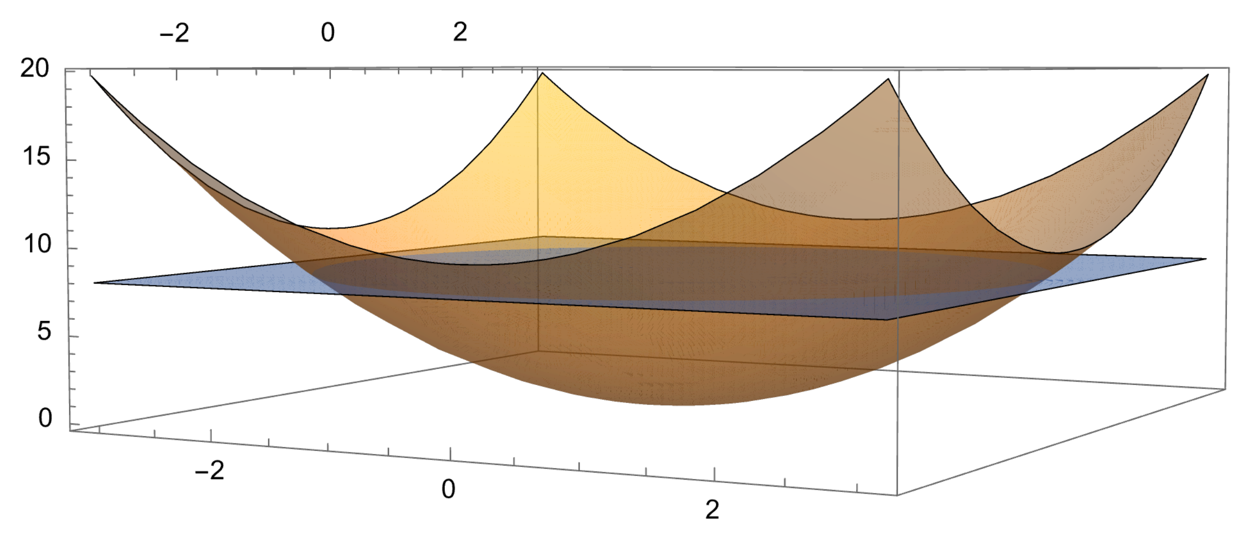


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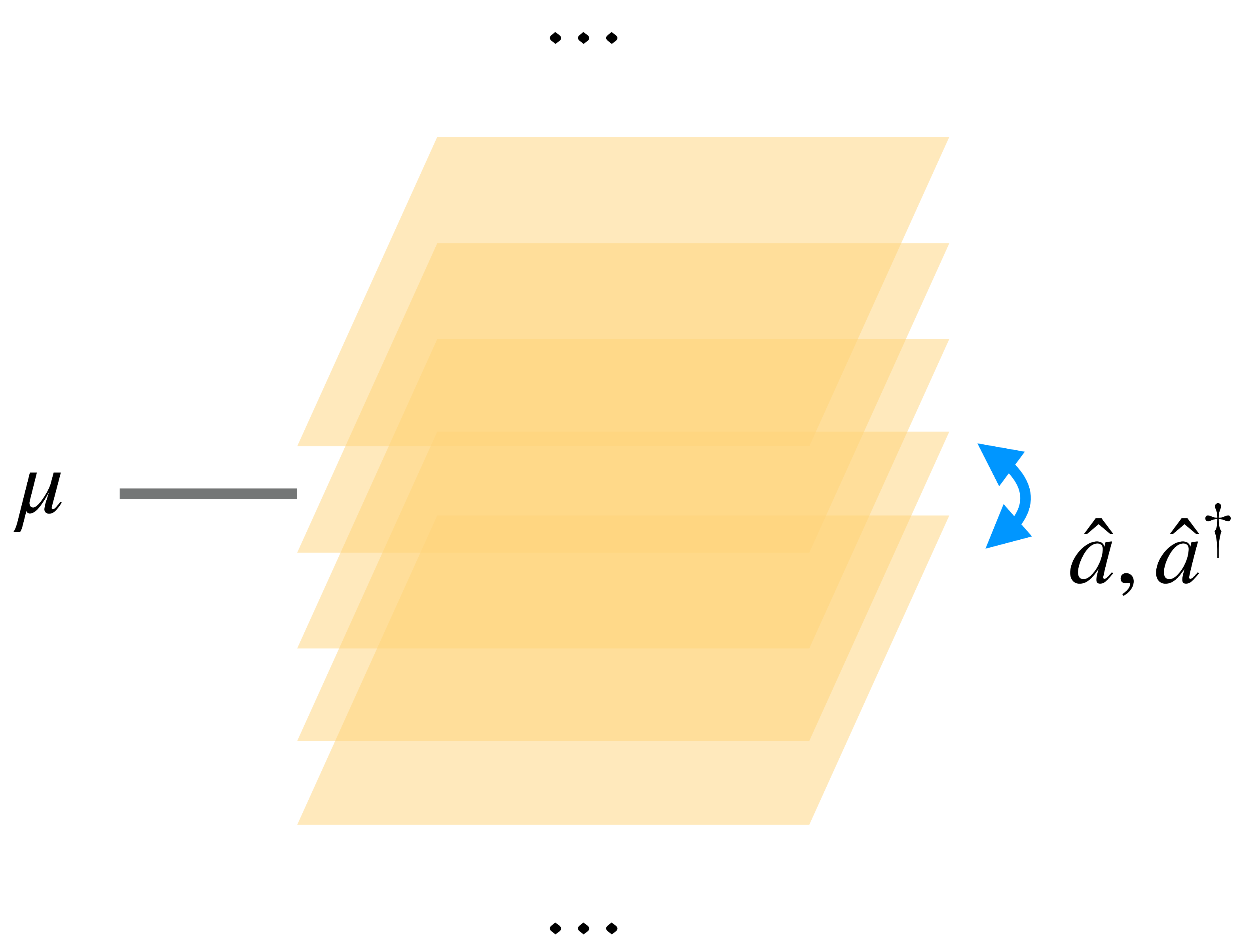


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$(\xi|\hat{\tau}_x|\eta)$

B=0

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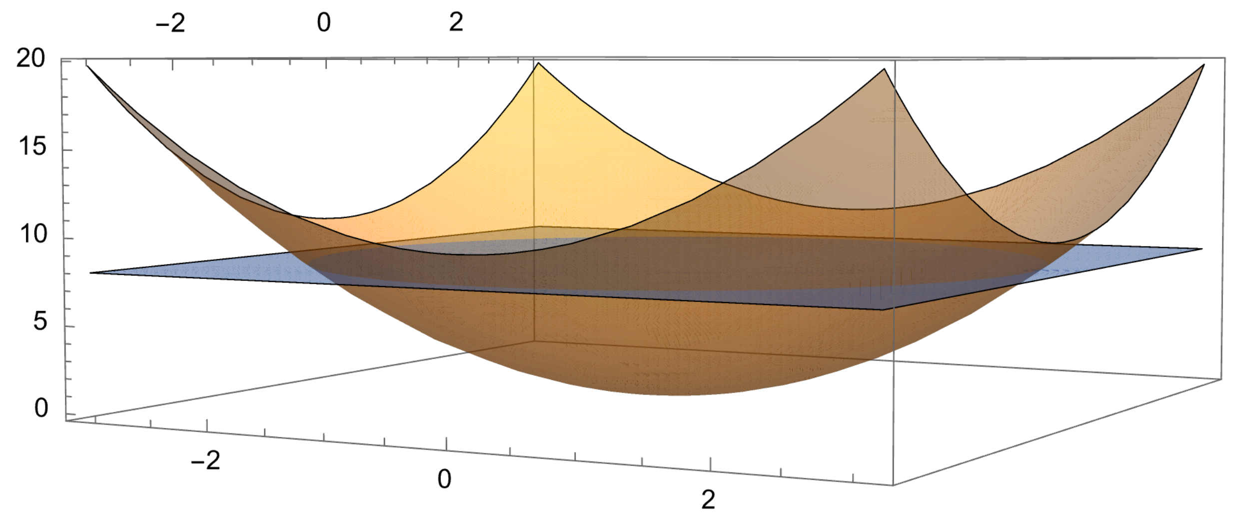


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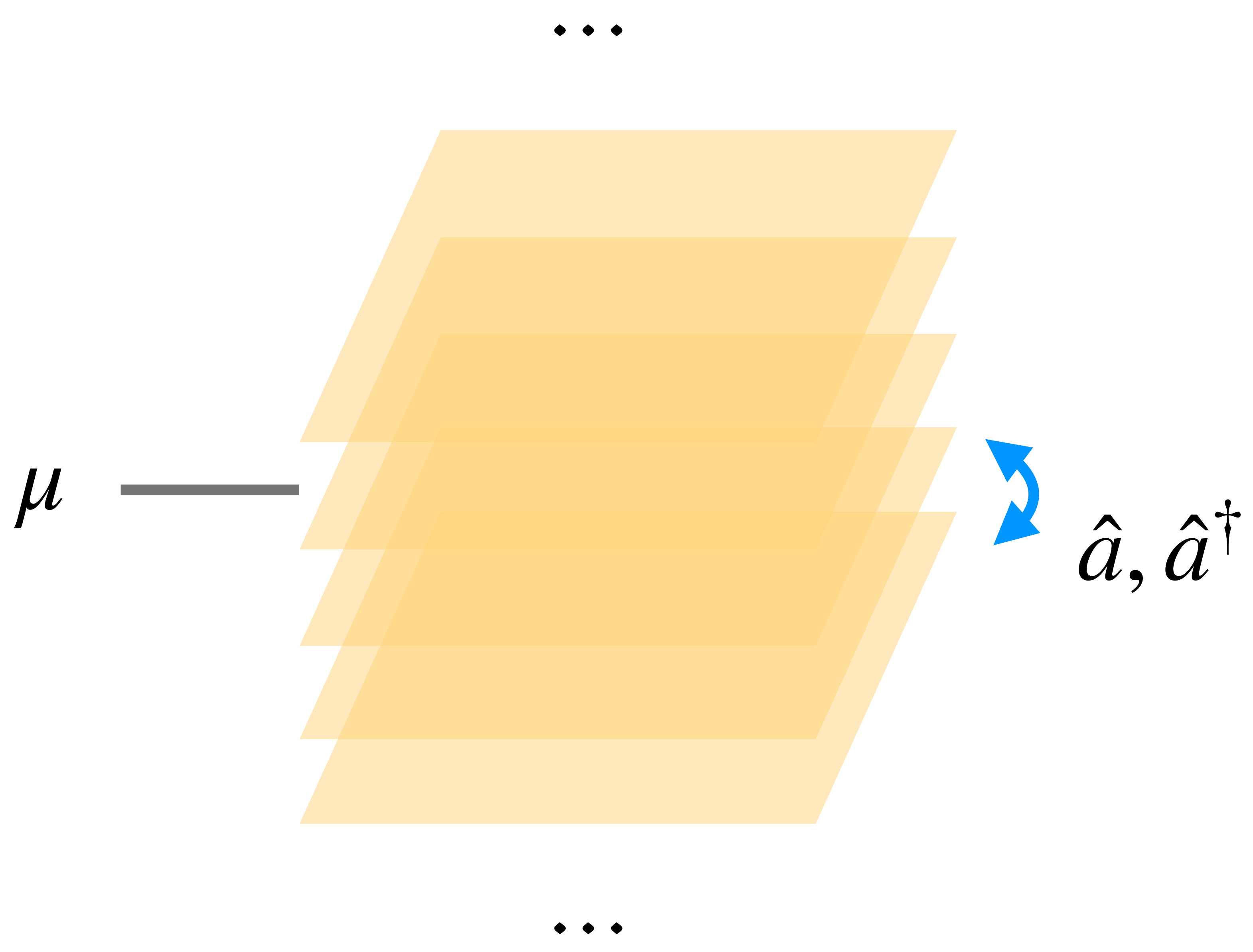
Landau levels




Coherent state basis: Superposition of LLs $|\eta) = \mathrm{e}^{\frac{\eta a^\dagger}{\sqrt{2} l_B^{-1}}} |0), \ (\xi| = (0| \mathrm{e}^{\frac{\xi a}{\sqrt{2} l_B^{-1}}}$

$(k|\mathrm{e}^{i\hat{k}x}|k') = \mathrm{e}^{ikx}\delta_{k,k'}$ ⟵ $(\xi|\hat{\tau}_x|\eta)$

B=0

# Thermodynamic Potential when $B \neq 0$

$$\Omega = -T\,\mathrm{Tr}\ln(\mathrm{e}^{-(\beta\hat{H}-\mu\hat{N})}) \quad = -\lim_{\eta\to 0^+} T\sum_n \mathrm{e}^{i\omega_n\eta}\left(\mathrm{Tr}\ln G_n^{-1} - T\,\mathrm{Tr}\Sigma_n\circ G_n\right) + \Phi(G)$$

$$\mathrm{Tr}\ln G^{-1} = \int \mathscr{D}\bar{\Psi}\mathscr{D}\Psi\,\mathrm{e}^{\int dx_1 dx_2 \bar{\Psi}(x_1)G^{-1}(x_1,x_2)\Psi(x_2)}$$

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Fourier transform of $H_0(x_1 - x_2), \tilde{\Sigma}(x_1 - x_2)$

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Non-commutative field theory

S. Onoda, N. Sugimoto, and N. Nagaosa, 2006

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Non-commutative field theory

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Jacobian

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$$f(\pi)\star g(\pi) = f(\pi)g(\pi) + \sum_{m=1}^{\infty}(i/2)^n f(\pi)\overleftarrow{\partial}_{i_1 i_2 .. i_m}\theta^{i_1 j_1}\theta^{i_2 j_2}..\theta^{i_m j_m}\overrightarrow{\partial}_{j_1 j_2 .. j_m} g(\pi)$$

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Dyson equation: $\left(i\omega_n - H_0(\pi) - \tilde{\Sigma}_n(\pi)\right) \star G_n(\pi) = 1$

$\tilde{\Sigma}(\pi)$ can be determined from the functional $\Phi(G)$ and $G(\pi)$ self-consistently order by order in B.

# Results

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Where $\tilde{\Sigma}, G$ satisfies

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# Application: spontaneous orbital magnetization

Linear in B contribution to Ω:

$$\Omega = -\lim_{\eta\to 0^+} T \sum_n \mathrm{e}^{i\omega_n \eta} \left( \int \mathscr{D}\bar{\Psi}_\pi \mathscr{D}\Psi_\pi \, \mathscr{J}^2 \, \mathrm{e}^{\int_\pi \left( \bar{\Psi}_\pi \star \left( i\omega_n - H_0(\pi) - \tilde{\Sigma}_n(\pi) \right) \star \Psi_\pi \right)} + \tilde{\Sigma}_n(\pi) G_n(\pi) \right) + \Phi(G)$$

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$\Sigma^{(0)} \equiv \tilde{\Sigma}^{(0)}$

Reproduce the expression of $M^{(0)}_{orb}$ in non-interacting case

found in the early literatures.

# Comments on higher order responses

Higher order responses from perturbative expansions in B:

$$\Omega = -\lim_{\eta\to 0^+} T\sum_n \mathrm{e}^{i\omega_n\eta}\left(\int \mathscr{D}\bar{\Psi}_\pi \mathscr{D}\Psi_\pi\, \mathrm{e}^{\int_\pi \left(\bar{\Psi}_\pi \star \left(i\omega_n - H_0(\pi) - \tilde{\Sigma}_n(\pi)\right) \star \Psi_\pi\right)} + \tilde{\Sigma}_n(\pi) G_n(\pi)\right) + \Phi(G)$$

In the earlier days to study orbital magnetic responses, e.g. Landau diamagnetism:

$$F \sim \sum_n \frac{\Phi_B}{\Phi_q} \ln(1 + \mathrm{e}^{-\beta\omega_c(n+1/2)})$$

Euler–Maclaurin formula

$$\sum_n h(n+1/2) = \int dx h(x) - \frac{1}{24} h'(0) + \frac{7}{5760} h'''(0) + \ldots$$

$B^2$ $\qquad$ $B^4$

Generalization to interacting multi-band systems

# Outlook

- Compute orbital magnetic susceptibility

Controversy between semiclassical and finite q method.

M. Ogata, H. Fukuyama, PRB (2003),
Y. Gao, S. Yang, Q. Niu et al, PRB (2015)

- Projection to narrow band systems
- Add other ingredients:
  - Spacial inhomogeneity
  - Magneto-electric response in multi-band systems
  - Compute quantum oscillation ($\Omega_{osc}$) without explicit projection to Landau levels.

Thanks!

Thank to many colleagues for helpful discussions, in particular, Leon Balents, Xiao-Chuan Wu, Zhihuan Dong, Sri Raghu, Yuxuan Wang, Duncan Haldane, …