Projective Construction of FCI Wave functions

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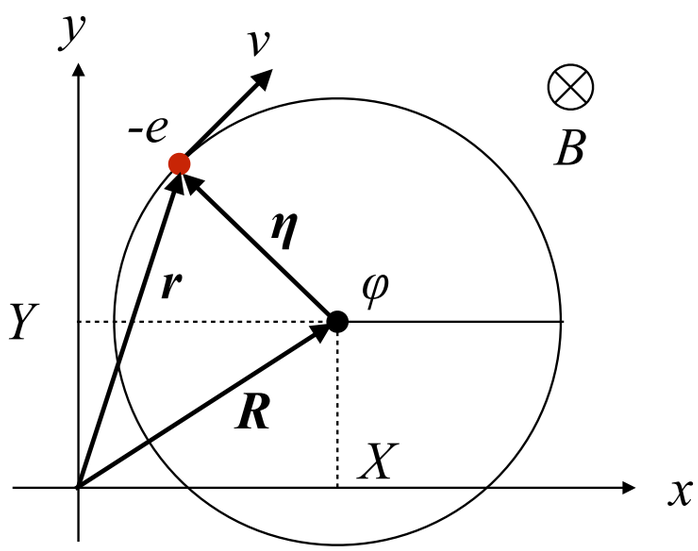
Motivation

- We would like to have some reasonable understanding at the Hartree-Fock level
- We would also like a way to construct the FCI wave function on the lattice

Landau Level Basics

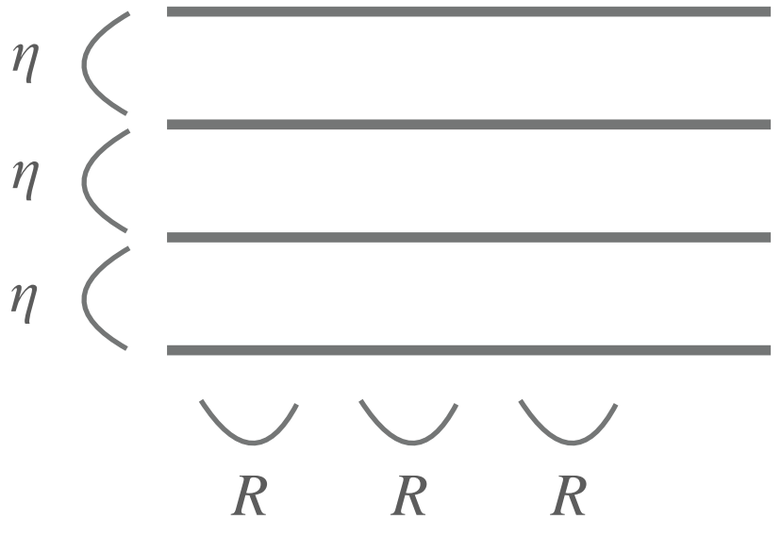


The position operator can be decomposed into a guiding center "coordinate" and a cyclotron "coordinate"

$$r = R + \eta \qquad \eta = \frac{\ell^2}{\hbar}\Pi \times \hat{z}$$

$$[\eta_x, \eta_y] = i\ell^2 \qquad [R_x, R_y] = -i\ell^2 \qquad \ell = \sqrt{\frac{\hbar}{eB}}$$

The Landau level degeneracy is given by $N_s = \dfrac{A}{2\pi\ell^2} = \dfrac{eBA}{h}$



From R and η we can introduce two sets of ladder operators

$$(\eta_x, \eta_y) \to (a^\dagger, a) \qquad (R_x, R_y) \to (b^\dagger, b)$$

$$H = \frac{\hbar^2\eta^2}{2m\ell^4} = \hbar\omega_c(a^\dagger a + \frac{1}{2})$$

If we project into a single Landau level, only the guiding center part of the position operator survives

Landau Level Wave Functions

- Under the symmetric gauge $A = -\frac{1}{2} r \times B$, the LLL wave function is given by

$$\psi_m(z, \bar{z}) = z^m e^{-|z|^2/4\ell^2} \qquad z = x + iy$$

- A generic LLL wave function can be written as an analytic function of z multiplied by the gaussian factor. We can introduce the Bargmann space of analytic functions

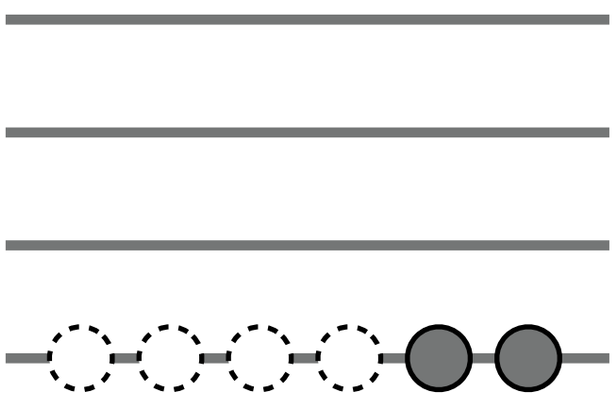
$$\langle \psi_1 | \psi_2 \rangle = \int d\mu_B \, \psi_1^*(z) \psi_2(z) \qquad d\mu_B = \frac{d^2 z}{2\pi\ell^2} e^{-|z|^2/2\ell^2}$$

$$\hat{P}_{\mathrm{LLL}} f(z', \bar{z}') = \int d\mu_B(z') \, e^{z\bar{z}'/2\ell^2} f(z', \bar{z}')$$

- For filling factor $\nu = 1$, the many-body wave function is a Slater determinant

$$\Psi_{\nu=1} = \prod_{i<j} (z_i - z_j) e^{-\sum_i |z_i|^2/4\ell^2}$$

The Hamiltonian

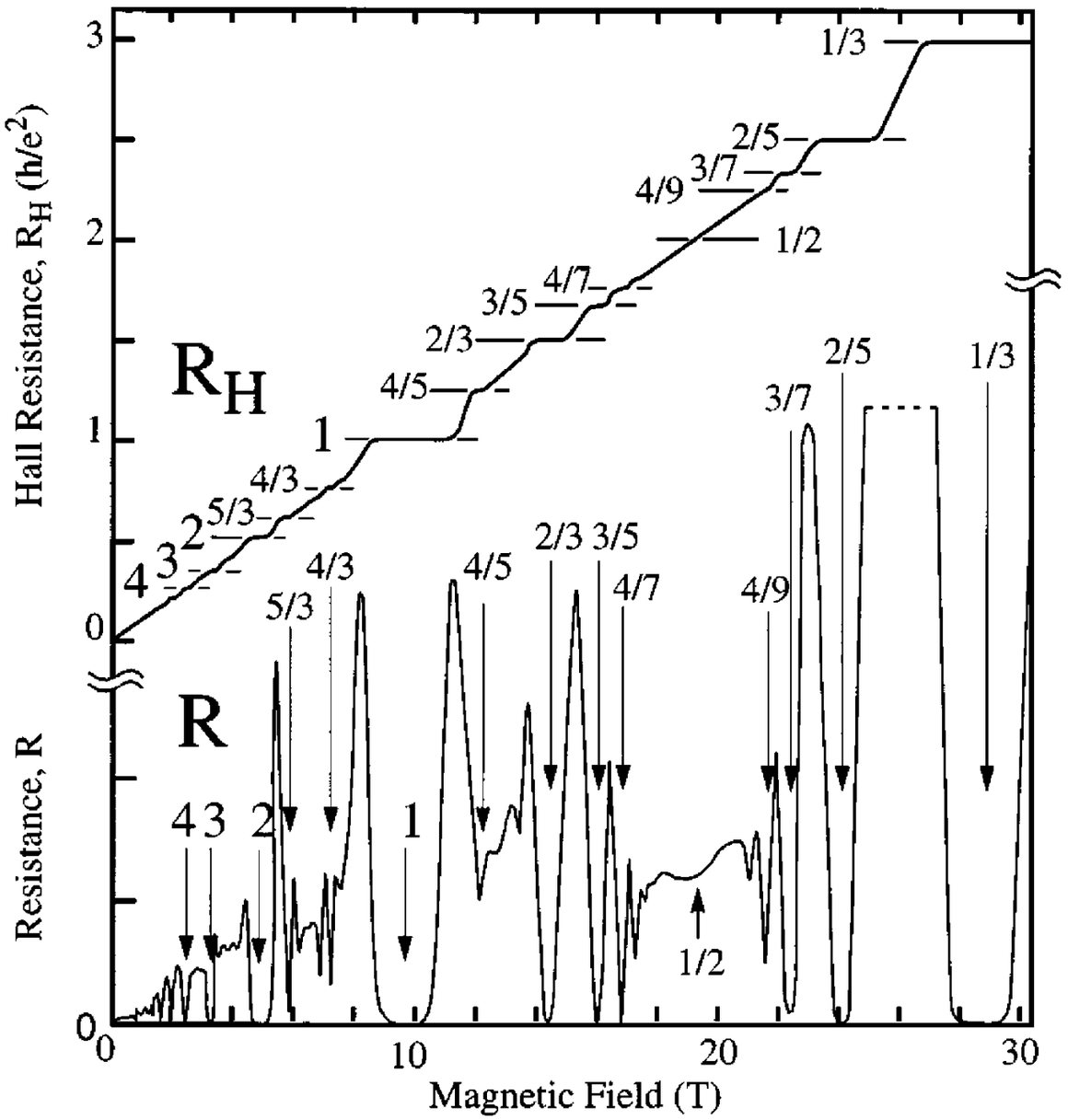


$$H_{\mathrm{LLL}} = \frac{1}{2}\sum_{q} v(q) e^{-q^2\ell^2/2} : \rho(q)\rho(-q) :$$

$$\rho(q) = \sum_{j} e^{-iq\cdot R_j} \qquad [R_{j,x}, R_{j,y}] = -i\ell^2$$

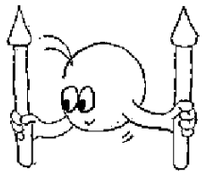
Guiding center

- Kinetic energy is completely quenched
- Huge degeneracy due to the Landau level degeneracy, perturbative calculations are hopeless
- Hartree-Fock doesn’t work either; it yields a topologically trivial Wigner crystal



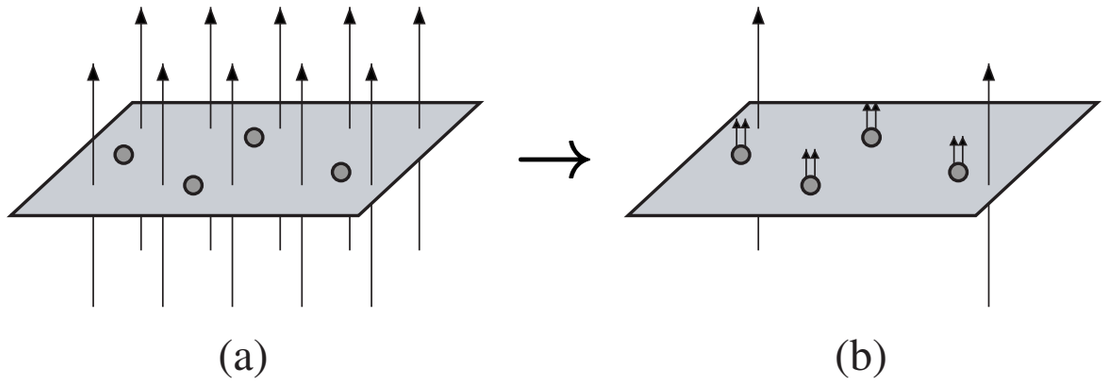
If we remove the labeling of the fillings, there is no difference between integer and fractional fillings, so it is reasonable to hope that FQHE can be explained by some type of weakly interacting quasiparticles

Composite Fermions



A composite fermion is an electron attached by two flux quanta

J. K Jain



$$\nu = \frac{nh}{eB} = \frac{1}{3}$$

$$B^* = B - 2n\frac{h}{e} = \frac{1}{3}B$$

By grabbing two flux quanta, the effective field felt by the CF is reduced

$$\nu^* = \frac{nh}{eB^*} = 1$$

More generally, if $\nu = \dfrac{p}{2ps+1}$, by attaching $2s$ flux quanta to each electron, the resulting CF will have an integer filling $\nu^* = p$

Composite Fermions

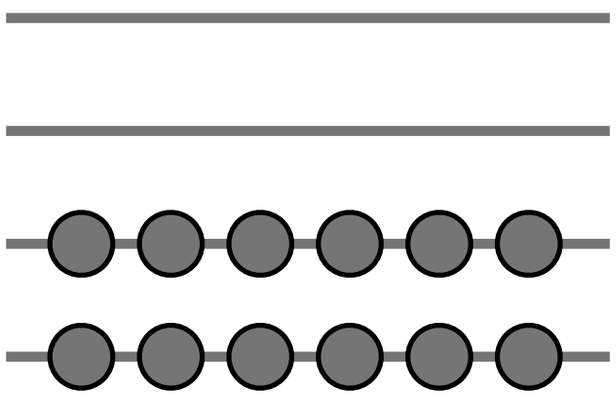
$$\Psi_{\text{Jain}} = \hat{P}_{\text{LLL}} \prod_{i<j} (z_i - z_j)^2 \Psi_{\text{CF}}(z, \bar{z})$$

Example: let us look at $\nu = 1/3$. The CFs is in the $\nu^* = 1$ state, so

$$\Psi_{\frac{1}{3}} = \prod_{i<j} (z_i - z_j)^2 \prod_{i<j} (z_i - z_j) e^{-\sum_i |z_i|^2/4\ell^2} = \prod_{i<j} (z_i - z_j)^3 e^{-\sum_i |z_i|^2/4\ell^2}$$

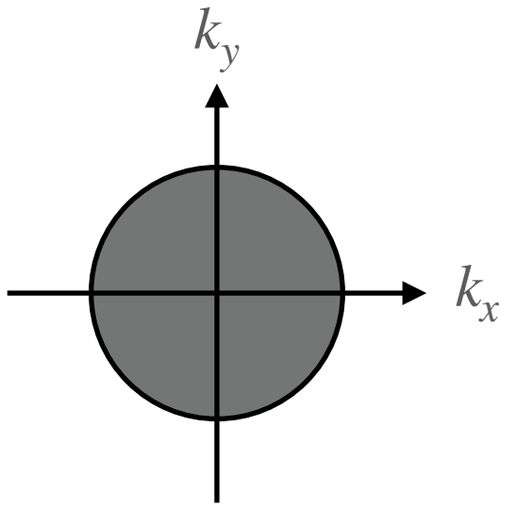
Flux attachment $\nu = 1$ CF state Laughlin wave function

Jain's sequence



$$\nu = \frac{p}{2ps + 1}$$

Halperin-Lee-Read CF liquid

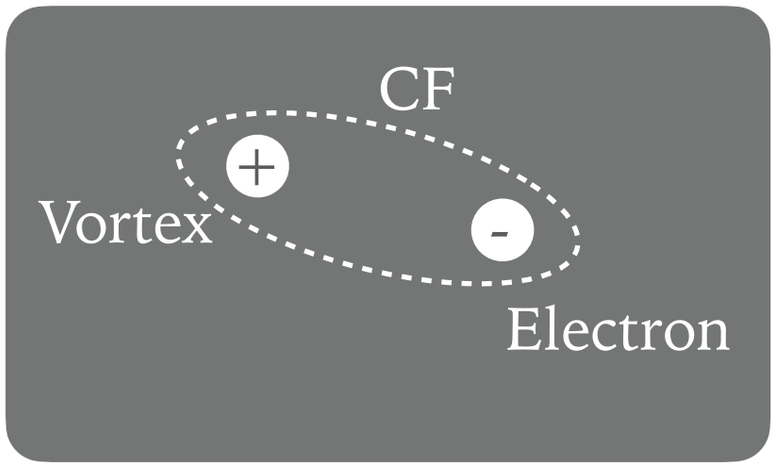


$$\nu = \frac{1}{2} \quad (B^* = 0)$$

Dipole Picture of Composite Fermions

A vortex located at ζ carries a positive charge of νe.

$$\prod_i (z_i - \zeta)\, \Psi_{\mathrm{LLL}}(z_i)$$



Read, Semicond. Sci. Technol. (1994)

The ground state of the FQHE can be regarded as a collection of the CF dipoles

The CF dipoles have the right filling factor

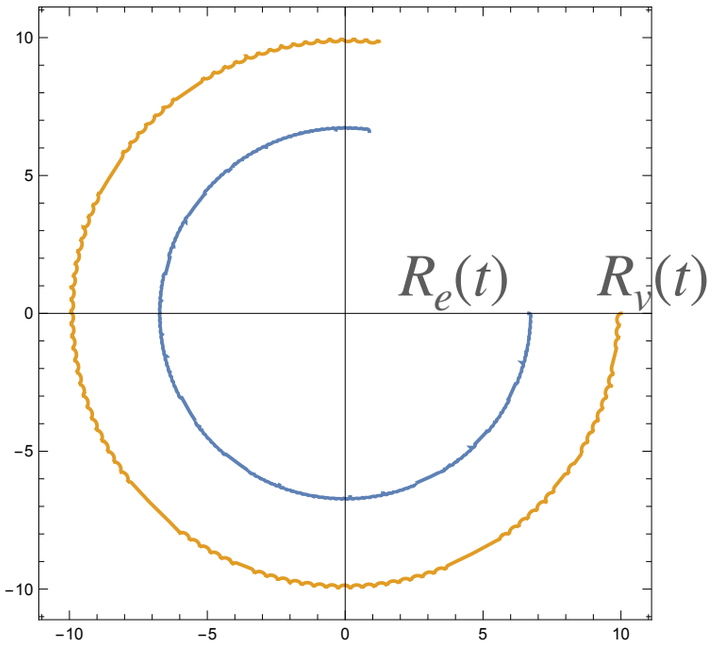
$$q_e = -e \qquad q_v = 2s\nu e \qquad q^* = q_e + q_v$$

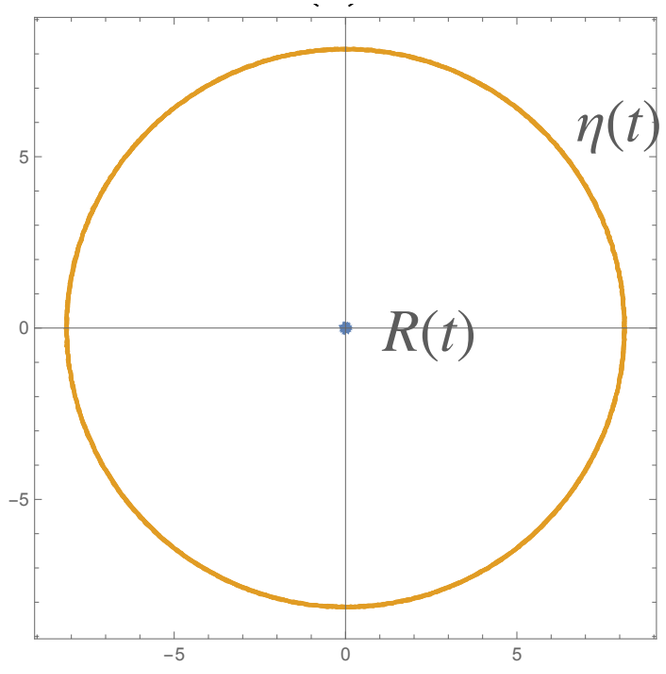
$$\nu_v = \frac{1}{2s} \qquad \nu^* = \frac{nh}{q^* B} = \frac{nh}{(1-2s\nu)eB} = \frac{\nu}{1-2s\nu} = p$$

Two-Particle Problem in the LLL

$$\mathscr{L} = q_e \dot{R}_e \cdot A(R_e) + q_v \dot{R}_v \cdot A(R_v) - V(R_e - R_v)$$

- We have set both the electron and vortex mass to zero, effectively confining their dynamics to the LLL
- Classical solution shows that we can introduce a center-of-charge coordinate and a relative coordinate to describe the two-particle motion





Guiding center

$$R = \frac{q_e R_e + q_v R_v}{q_e + q_v}$$

Cyclotron coordinate

$$\eta = \frac{\sqrt{q_e q_v}}{|q_e + q_v|}(R_e - R_v)$$

Two-Particle Problem in the LLL

- Now, we look at the this problem quantum mechanically. The commutators are (recall that $\ell = \sqrt{\hbar/qB}$)

$$[R_{e,x}, R_{e,y}] = -i\ell_e^2 \qquad [R_{v,x}, R_{v,y}] = i\ell_v^2$$
$$[R_x, R_y] = -i\ell^{*2} \qquad [\eta_x, \eta_y] = i\ell^{*2}$$

- The projected Hamiltonian reads

$$H = V(\eta)$$

- If $V(\eta)$ is quadratic in η, i.e., $H = \dfrac{\hbar^2\eta^2}{2m^*\ell^{*4}}$, then we will have Landau levels for composite fermions
- The LLL wave function of composite fermion is given by (ignoring the Gaussian factor)

$$\psi_m = z^m e^{z\bar{\xi}/2\ell_v^2}$$

The two-particle bound state problem in the LLL can be equally described by the electron and vortex guiding centers (R_e, R_v) or the CF guiding-center (R) and cyclotron coordinate (η)

$$R = \frac{R_e - c^2 R_v}{1 - c^2} \qquad \eta = \frac{c}{1 - c^2}(R_e - R_v)$$

$$R_e = R + c\eta \qquad R_v = R + \frac{1}{c}\eta$$

$c^2 = q_v = 2s\nu$ is the vortex charge in unites of the electron charge e

Composite Fermion Substitution

$$H_{\mathrm{LLL}} = \frac{1}{2}\sum_{q} v(q) e^{-q^2\ell_e^2/2} : \rho_e(q)\rho_e(-q) : \qquad \rho_e(q) = \sum_j e^{-iq\cdot R_{e,j}} \qquad [R_{ej,x}, R_{ej,y}] = -i\ell_e^2$$

How to introduce CFs into our problem? $\qquad R_e \to R + c\eta$

$$H_{\mathrm{CF}} = \frac{1}{2}\sum_{i,j,q} v(q) e^{-q^2\ell_e^2/2} \exp\{iq\cdot[(R_i - R_j) + c(\eta_i - \eta_j)]\}$$

Great news! The p-filled CF LL state is the Hartree-Fock ground state of H_{CF}

$$(R_e, R_v) \quad \leftrightarrow \quad (R, \eta)$$

By introducing the CF coordinates, we have enlarged our Hilbert space!

Murthy & Shankar, RMP (2003)

Spin Liquid: An Example of Enlarged Hilbert space

- In the field of quantum spin liquids in Mott insulators, enlarged Hilbert space is common
- Starting from the quantum Heisenberg Hamiltonian, to capture the bond correlation in a spin liquid, one usually introduce the spinon operator

$$\boldsymbol{S} = \frac{1}{2} f^\dagger \boldsymbol{\sigma} f$$

- However, the local basis went from $|\uparrow\rangle, |\downarrow\rangle$ to $|00\rangle, |10\rangle, |01\rangle, |11\rangle$. To stay in the physical Hilbert space, we impose the constraint $f_\uparrow^\dagger f_\uparrow + f_\downarrow^\dagger f_\downarrow = 1$
- The mean-field theory is obtained by minimizing

$$\langle \Psi_{\mathrm{MF}} | H | \Psi_{\mathrm{MF}} \rangle + \sum_i \lambda_i \langle \Psi_{\mathrm{MF}} | f_{i,\uparrow}^\dagger f_{i,\uparrow} + f_{i,\downarrow}^\dagger f_{i,\downarrow} - 1 | \Psi_{\mathrm{MF}} \rangle$$

- The physical wave function is obtained by using the Gutzwiller projector

$$|\Psi_{\mathrm{phys}}\rangle = P_G |\Psi_{\mathrm{MF}}\rangle$$

Enlarged Hilbert Space of Composite Fermions

- The CF Hamiltonian lives in the enlarged Hilbert space. However, it does not depend on the vortex coordinates, so the eigenstates can be written as $\psi_e \otimes \psi_v$, where ψ_v can be arbitrary
- The vortex function ψ_v represents a gauge symmetry because physical quantities also do not depend on ψ_v
- How do we deal with this gauge symmetry? Just like how we deal with the gauge potential in EMs, we just need to commit to a gauge choice $\psi_{\text{phys}} = \psi_e \otimes \psi_v^G$
- We can define a projector $P_G = |\psi_v^G\rangle\langle\psi_v^G|$, then

$$Z = \text{Tr}\, e^{-\beta H_e} = \text{Tr}\, e^{-\beta H_{CF}} P_G$$

- Finally, for an arbitrary CF state, we can extract a physical state from it:

$$|\psi_{\text{phys}}\rangle \otimes |\psi_v^G\rangle = P_G |\psi_{CF}\rangle$$

How To Implement Constraint?

- In a mean-field treatment, constraints are usually implemented as Lagrangian multipliers applied to some expectation values
- However, we don't have an operator form of the constraint. Our constraint is basically the wave function must be in the direct product form
- What can we do? We shall do our best!

$$\langle \psi_{CF} | \rho_v(q) | \psi_{CF} \rangle = \langle \psi_v^G | \rho_v(q) | \psi_v^G \rangle \quad \forall q$$

  Note that the vortex density operator $\rho_v(q)$ form a complete basis for all one-body vortex operators, so we are doing the best we can for a Hartree-Fock calculation
- Which ψ_v^G shall we use? Choose a ψ_v^G, perform HF calculation to obtain ψ_{CF}, then use the projector P_G to obtain the physical wave function ψ_{phys}. We should use whichever ψ_v^G that gives us the lowest energy for ψ_{phys}.
- This sounds fun, but almost impossible to do. Let's take a guess. The vortices are bosons with a filling factor of $\nu_v = \dfrac{1}{2s}$, so we take $\psi_v^G = \psi_{\text{Laughlin}}^{\nu=1/2} = \prod_{i<j} (\zeta_i - \zeta_j)^2$

How To Implement Constraint?

- "Justification" of the choice of the bosonic $\nu = 1/2$ Laughlin state as ψ_ν^G: The physical wave function $\psi_{\text{phys}} = \langle \psi_{\text{Laughlin}}^{\nu=1/2} | \psi_{\text{CF}} \rangle$ is equivalent to Jain's wave function ansatz
- For a Laughlin state, there is no charge fluctuation:

$$\langle \psi_{\text{Laughlin}} | \rho_\nu(q) | \psi_{\text{Laughlin}} \rangle = 0 \text{ for } q \neq 0$$

Summary: The unconstrained electron problem is mapped to a constrained CF problem, with the mean field constraint given by $\langle \psi_{CF} | \rho_\nu(q) | \psi_{CF} \rangle = 0$ for $q \neq 0$. The electron wave function is then given by $\psi_{\text{phys}} = \langle \psi_{\text{Laughlin}}^{\nu=1/2} | \psi_{\text{CF}} \rangle$

Example

- Let's consider the $\nu = 1/3$ filling. This corresponds to a CF filling of $\nu^* = 1$
- The single-particle CF LLL wave function is given by $\psi_m = z^m e^{z\bar{\xi}/2\ell_v^2}$
- The $\nu^* = 1$ CF state is a Slater determinant

$$\Psi_{\text{CF}} = \prod_{i<j} (z_i - z_j) e^{\sum_i z_i \bar{\xi}_i / 2\ell_v^2}$$

- The physical, electronic wave function is obtained by projected onto the vortex state

$$\begin{aligned}
\Psi_{\text{phys}} &= \langle \Psi_v^G \,|\, \Psi_{\text{CF}} \rangle \\
&= \int d\mu_B(\zeta) \prod_{i<j} (\zeta_i - \zeta_j)^2 \prod_{i<j} (z_i - z_j) e^{\sum_i z_i \bar{\zeta}_i / 2\ell_v^2} \\
&= \prod_{i<j} (z_i - z_j)^3
\end{aligned}$$

Also see Junren Shi, PRR (2024)

Summary So Far

- The extended Hamiltonian theory by Murthy and Shankar provides an operator-based approach to the fractional quantum Hall effect
- They've shown that by the CF substitution, one can obtain the CF Hamiltonian that amendable to Hartree-Fock calculations, but with the constraint

$$\langle \psi_{CF} | \rho_v(q) | \psi_{CF} \rangle = \langle \psi_v^G | \rho_v(q) | \psi_v^G \rangle \quad \forall q$$

- We showed that by using the same projective construction technique from QSL, we can construct the physical wave function from the mean-field solution. In particular, if we choose $|\Psi_v^G\rangle = |\Psi_{\text{Laughlin}}^{\nu=1/2}\rangle$, the wave function is equivalent to Jain's wave function ansatz

How to apply this theory to Fractional Chern Insulators?

Map a Chern Band to the LLL

- Let's look at the LLL Hamiltonian again

$$H_{\mathrm{LLL}} = \frac{1}{2}\sum_{q} v(q) e^{-q^2\ell^2/2} : \rho_{\mathrm{GMP}}(q)\rho_{\mathrm{GMP}}(-q) :$$

- Previously, we have stated that the projected density operator is given in terms of the guiding center operators. Equivalently, we can also demand ρ_{GMP} satisfies the Girvin-MacDonald-Platzman (GMP)algebra

$$[\rho_{\mathrm{GMP}}(q_1), \rho_{\mathrm{GMP}}(q_2)] = 2i \sin(\frac{q_1 \times q_2}{2}\ell^2)\rho_{\mathrm{GMP}}(q_1 + q_2)$$

- Murthy and Shankar ('12) made the observation that since $\rho_{\mathrm{GMP}}(q)$ form a complete basis for one-body operators, the band-projected density operator can be expanded using ρ_{GMP}

$$\rho_B(q) = \sum_{G} c(q, G)\rho_{\mathrm{GMP}}(q + G)$$

- This way, we can write a band-projected Hamiltonian in terms of ρ_{GMP}, then apply the same projective construction procedure outlined earlier

The Projected Wave Function is a Hyperdeterminant

- What is a hyperdeterminant?

$$\text{Hyperdet}(T) = \sum_{P,Q,R \in S_N} (-1)^P (-1)^Q (-1)^R \, T_{1,P(1),Q(1),R(1)} \cdots T_{N,P(N),Q(N),R(N)}$$

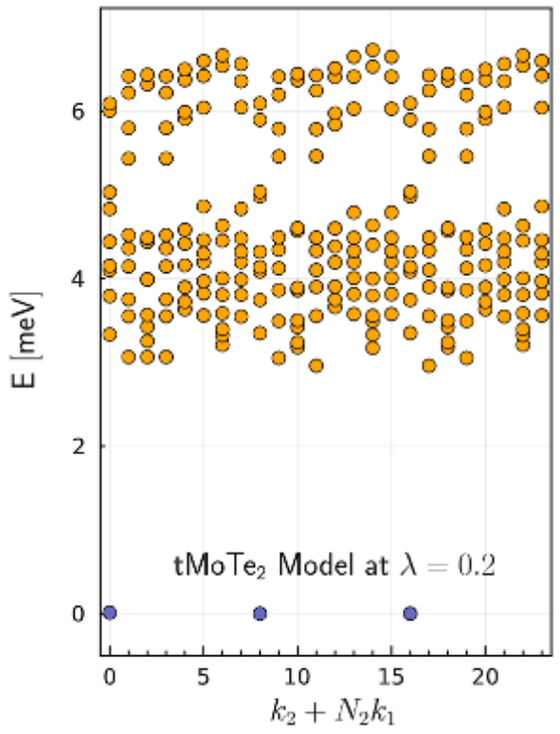
- If T is a rank-2 tensor, then $\text{Hyperdet}(T)$ is the standard determinant
- If $T_{ijkl} = A_{ij} B_{ik} C_{il}$, then $\text{Hyperdet}(T) = \det(A)\det(B)\det(C)$. So the Laughlin state is a hyperdeterminant.
- The projected wave function is a hyperdeterminant of a rank-4 tensor.
  - The Slater determinant is a hyperdeterminant of a rank-2 tensor
  - The bosonic Laughlin state is a hyperdeterminant of a rank-3 tensor
  - The fermionic Laughlin state is a hyperdeterminant of a rank-4 tensor

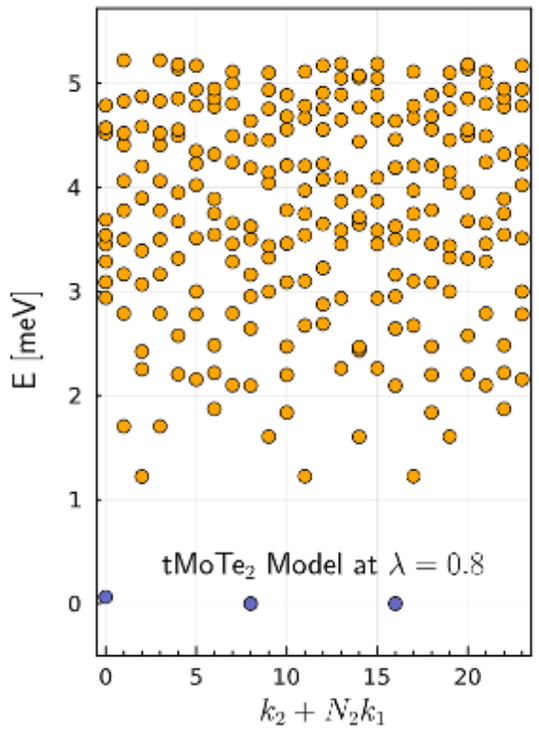
Result

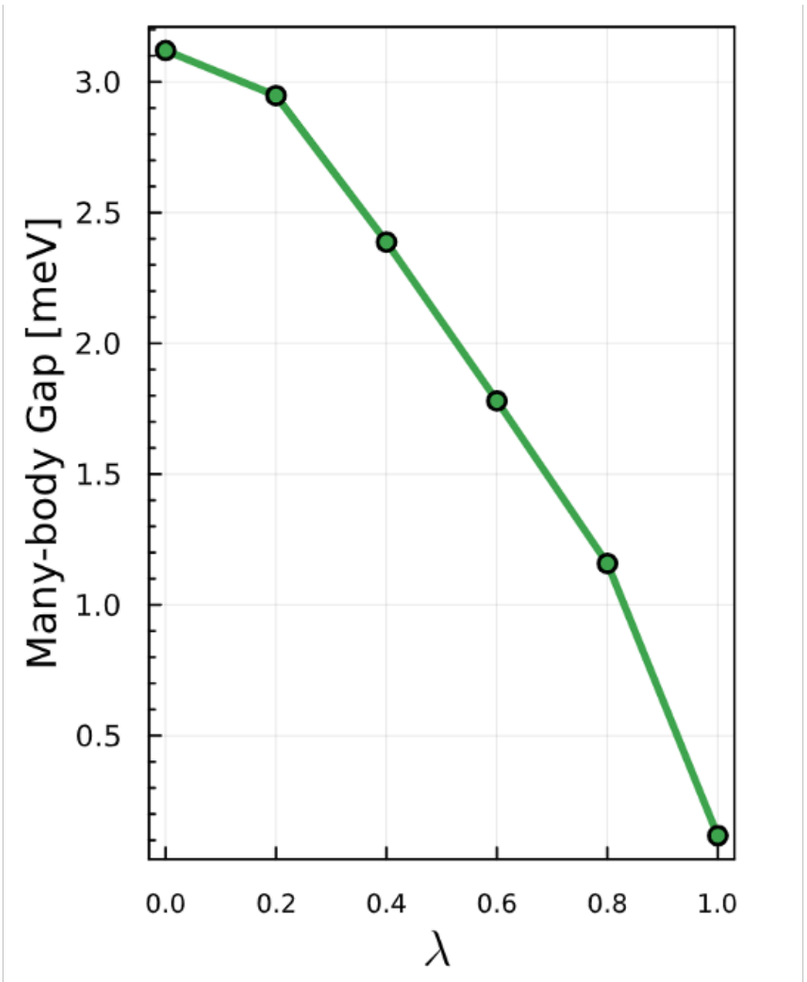
- Starting Hamiltonian

$$H = \hat{P}(\lambda H_K + H_U)\hat{P}$$

- By varying λ we can kill the FCI state

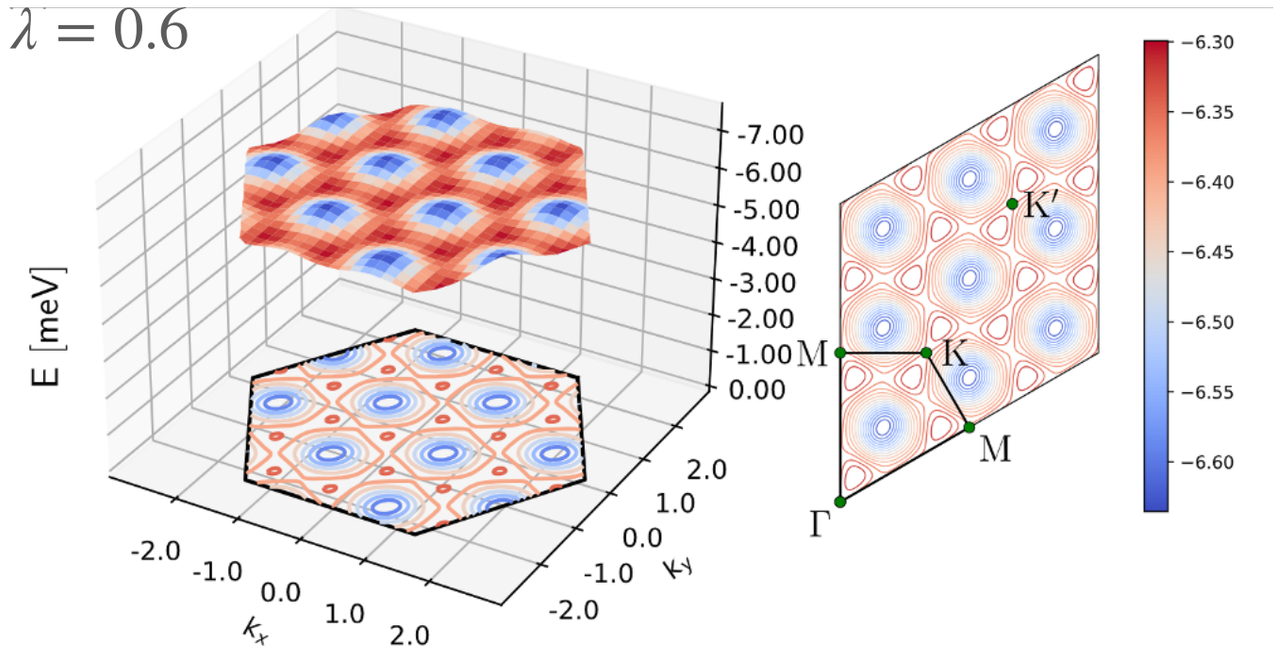




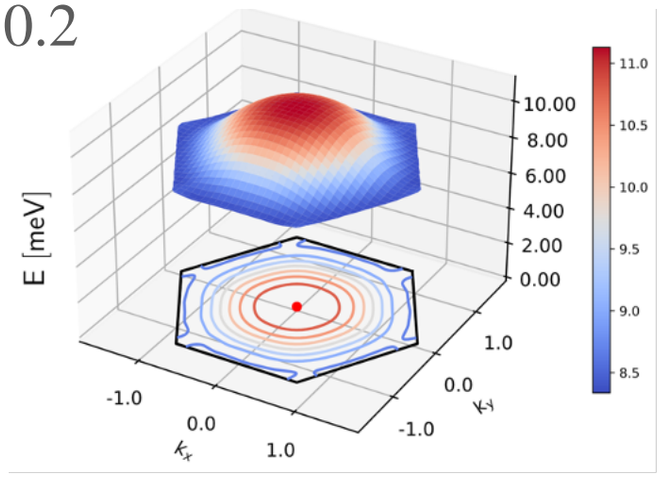


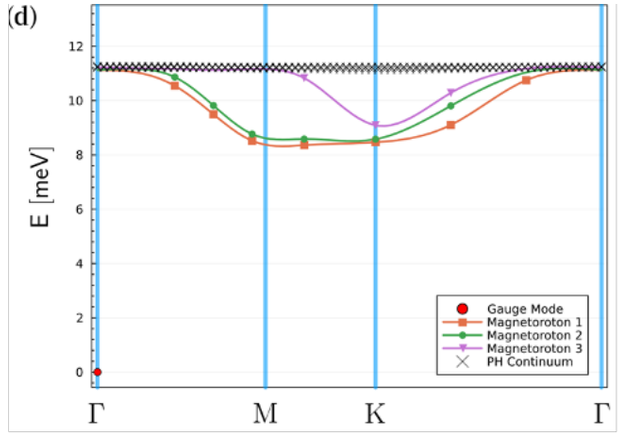
Result: Mean-Field Calculation

CF band structure from constrained HF



Magnetoroton band from constrained TDHF

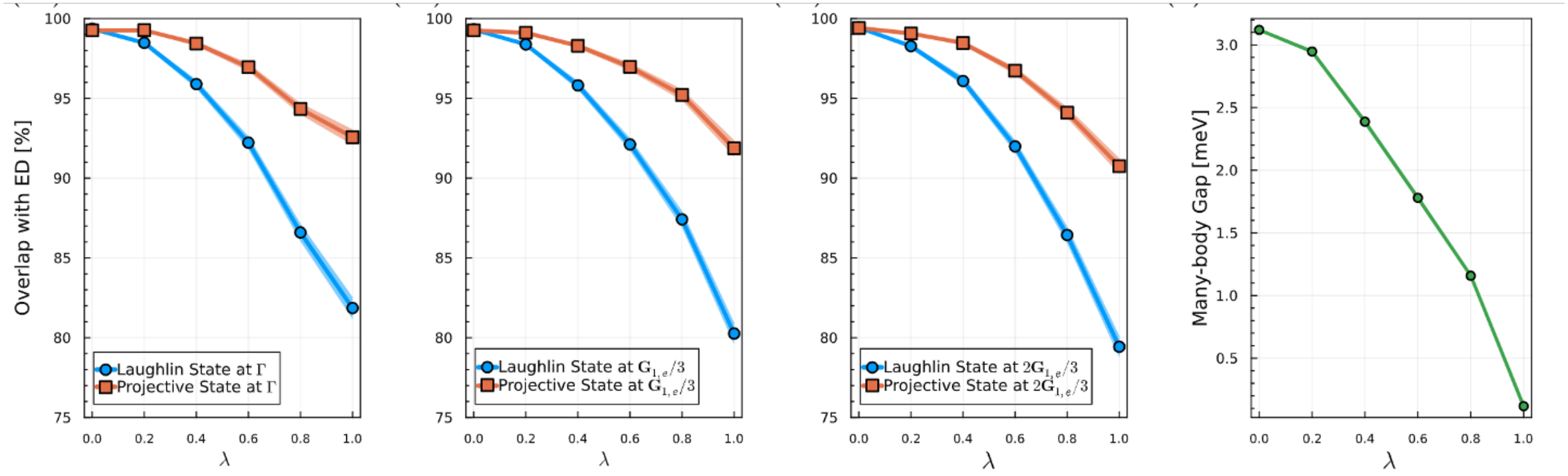




band #	Γ	K	K′
1		1	1
2		$e^{-i2\pi/3}$	$e^{-i2\pi/3}$
3		$e^{i2\pi/3}$	$e^{i2\pi/3}$

Result: Projected Wave Function

Beyond mean-field: $|\Psi_{\text{phys}}\rangle = P_G |\Psi_{\text{CF}}\rangle$



What's Next?

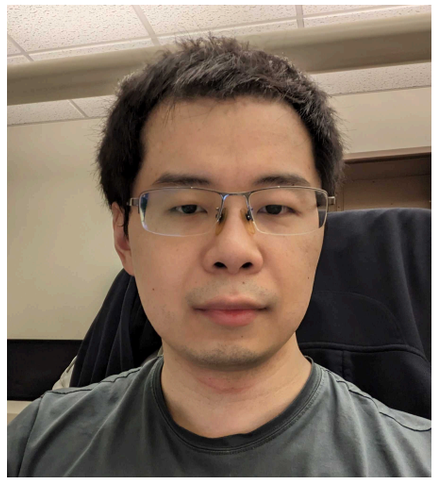
- Can we generalize this to paired CF states to enable the description of non-Abelian states (Hyperphaffian?)

- In the Landau level setting, it is reasonable to assume the vortex state ψ_v^G is the $\nu = 1/2$ bosonic Laughlin state. In FCI, there is no reason to believe this is still true.

- In our approach, ψ_v^G is essentially a variational parameter. Optimizing ψ_v^G will both leads to improved mean-field theory and projected wave functions

Summary

- We have developed a projective construction of the composite fermion state in a partially filled Chern band with $C = \pm 1$
- At the mean-field level, the wave functions of the ground state and excited states are found self-consistently in an enlarged Hilbert space
- Beyond the mean field, these wave functions can be projected back to the physical Hilbert space to construct the electronic wave functions



Xiaodong Hu

Ying Ran

Hu, DX and Ran, PRB, 109, 245125 (2024)