Numerical Study of Fractional Quantum Hall Effect via Parallel Exact Diagonalization

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Exact diagonalization

Wikipedia

In linear algebra, a square matrix *M* is called diagonalizable if it is similar to a diagonal matrix.

$$P^{-1}MP = \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \lambda_n \end{pmatrix} \longrightarrow MP = P \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \lambda_n \end{pmatrix}$$

Writing *P* as a block matrix of its column vector $P = (\vec{\alpha}_1 \quad \vec{\alpha}_2 \quad \cdots \quad \vec{\alpha}_n)$

$$M\vec{\alpha}_i = \lambda_i \vec{\alpha}_i \quad (i = 1, 2, \cdots, n)$$
$$|M - \lambda_i I| = 0$$

In general, no analytic solution can be found for n > 4 → Numerical method !!!

- LAPACK, GSL
- Mathematica, Matlab

Exact diagonalization

When, $n = 10^4 \sim 10^9$

However, for finding several (<10) low-energy eigenvalues & eigenvectors of a sparse matrix *M*, the Lanczos method allows much faster computations.

- **Lanczos method**
  - Matrix-vector multiplications are implemented iteratively until eigenvalues converge to the desired accuracy.

$$\begin{pmatrix} \cdots & \cdots & \cdots & \cdots \\ \cdots & \text{Sparse} & M & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \cdots \\ a_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \cdots \\ b_n \end{pmatrix}$$

- Memory or speed problem for $n \geq 10^6$ → Parallel Lanczos method.

Exact diagonalization in Quantum Physics

A common theme in all branches of quantum physics is to identify the eigenenergy & eigenstates of Hamiltonian.

- Schrödinger Equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle \quad \longrightarrow \quad |\psi(t)\rangle = \exp\left[\frac{-iH(t-t_0)}{\hbar}\right]|\psi(t_0)\rangle$$

$$H = T + V$$

$$H|\phi_i\rangle = E_i|\phi_i\rangle$$

1) Construct *H* matrix.
2) Diagonalize *H* matrix.

- In many-body condensed matter systems,

$$H = \sum_j \frac{1}{2m_b}\left[\frac{\hbar}{i}\nabla_j + \frac{e}{c}\mathbf{A}(\mathbf{r}_j)\right]^2 + \frac{e^2}{\epsilon}\sum_{j<k}\frac{1}{|\mathbf{r}_j - \mathbf{r}_k|} + \sum_j U(\mathbf{r}_j) + g\mu\mathbf{B}\cdot\mathbf{S}$$

$$\mathbf{B} = \nabla \times \mathbf{A}$$

Exact diagonalization in Condensed Matter : Present Day Limits

- Fractional Quantum Hall Effect

  up to 16-20 electrons : 100 million basis states

- Spin S=1/2 models

  40 spins square lattice : 1000 million basis states

- t-J models

  32 sites square lattice with 4 holes : 2000 million basis states

- Hubbard models

  20 sites square lattice at half filling : 10 billion basis states

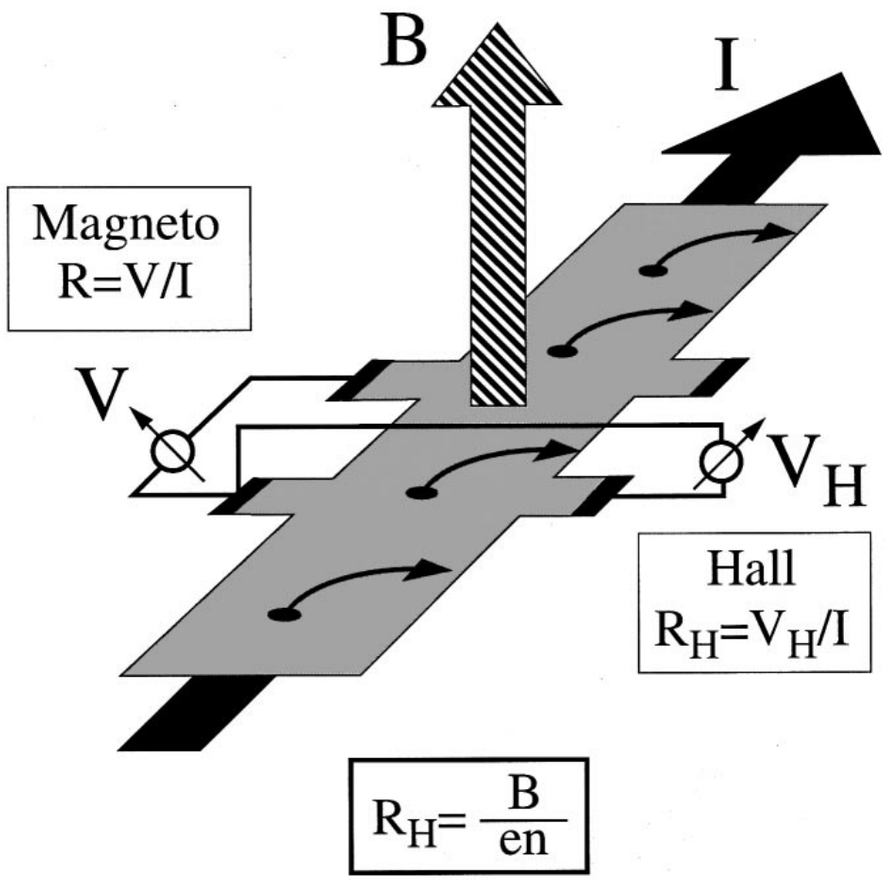
Why we are interested in "large" system ?

- We want to know the physics of the many-body system with N ~ 10^{23} exactly not approximately, which is not possible by using "classical" computer.

- If we reveal unknown many-body physics in finite system with N ~ 10 via exact diagonalization, and further, it remains with increasing the number of particle (finite size scaling), then, we can argue that the uncovered many-body physics would emerge in thermodynamic limit with N ~ 10^{23}.

Hall effect (classical) (Edwin Hall, 1879)

- In a normal conductor the **Hall resistance** is linearly proportional to the strength B of the magnetic field.
- The origin is from the classical electrodynamics.



H. L. Stormer, RMP (1999)

$$F = \frac{e}{c}(\mathbf{v} \times \mathbf{B}) \text{ : Lorentz force}$$

$$\frac{evB}{c} = eE_x$$

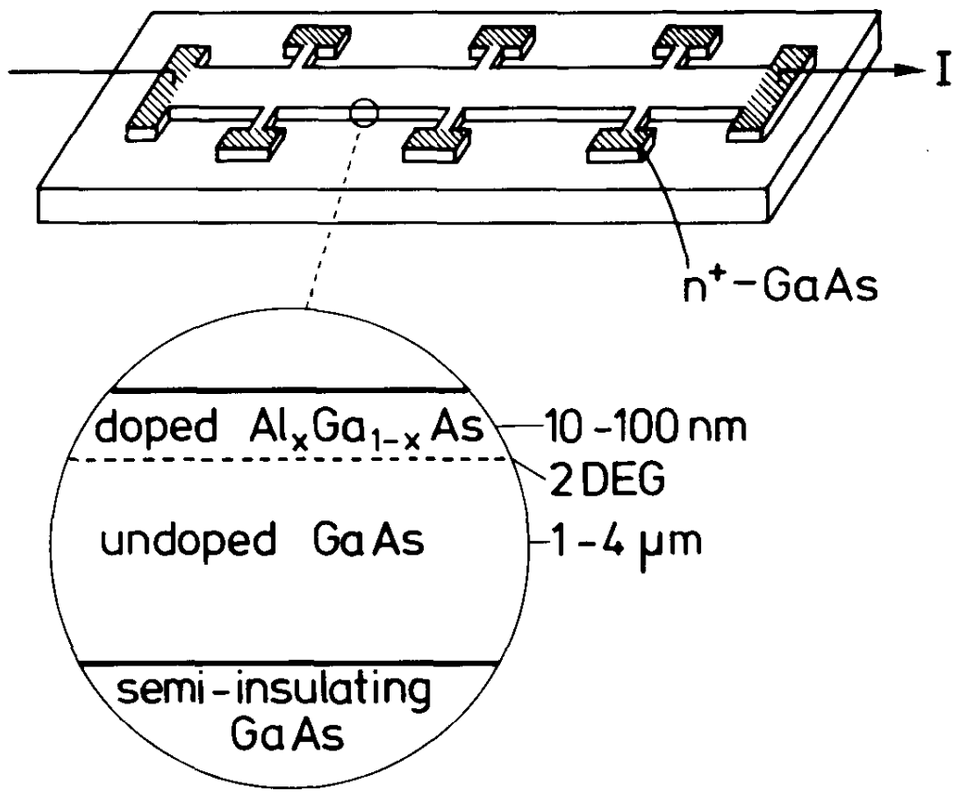
$$nevB = nceE_x$$

$$B \int dx\ nev = nce \int dx\ E_x$$

$$BI = -nceV_H$$

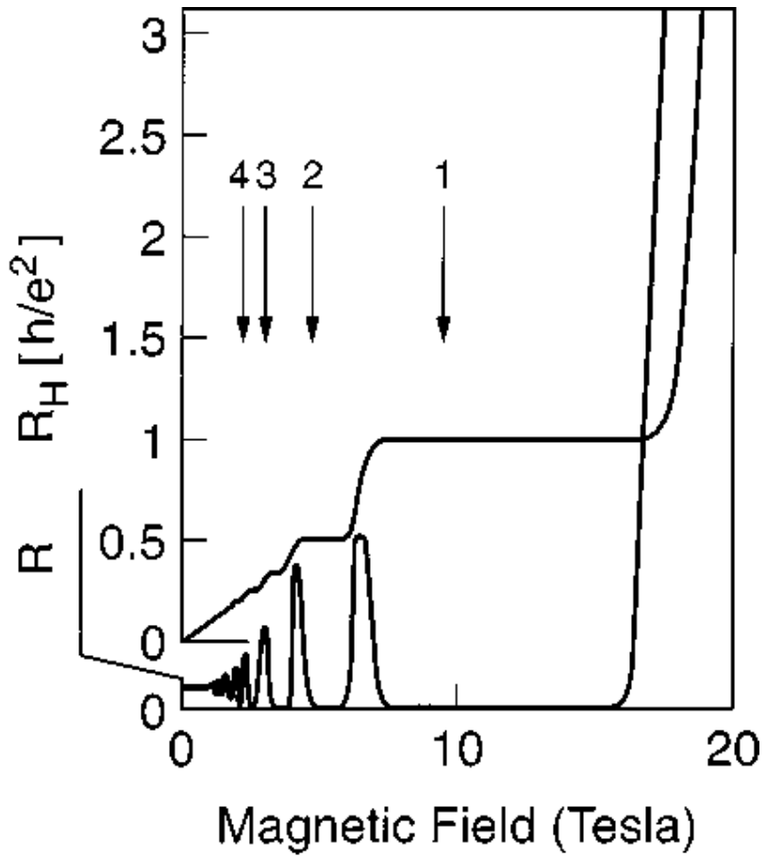
$$R_H = \frac{V_H}{I} = -\frac{B}{nec}$$

Integer quantum Hall effect (IQHE) (Klaus von Klitzing, 1980)



K. v. Klitzing (1985)

H. L. Stormer, RMP (1999)



T = 4K

- In two-dimensional electron system, R_H is quantized to $R_H = \frac{h}{ie^2}$.

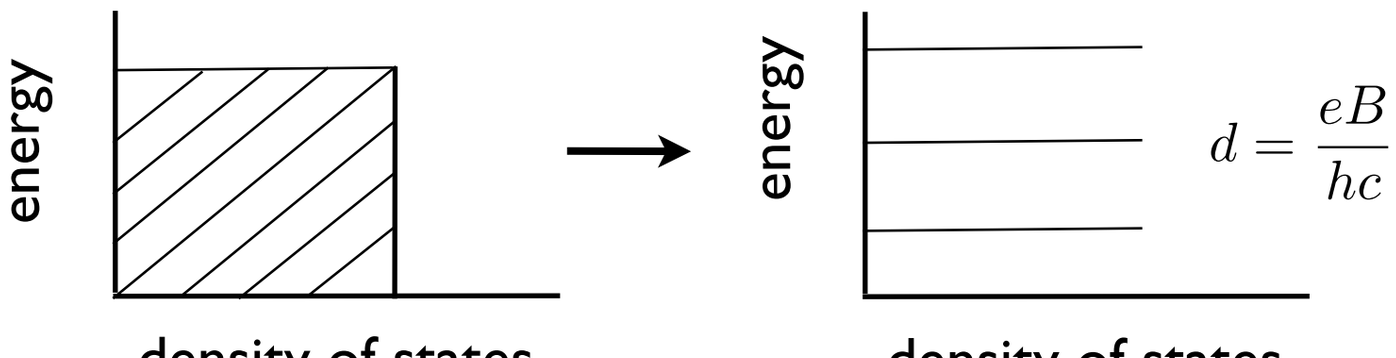
- Simultaneously the *R* drops to vanishingly small values.

IQHE : single-particle physics

$$H = \frac{1}{2m_b}\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)$$

Landau levels :

$$E_n = \hbar\omega_c\left(n + \frac{1}{2}\right), \quad n = 0, 1, \ldots$$



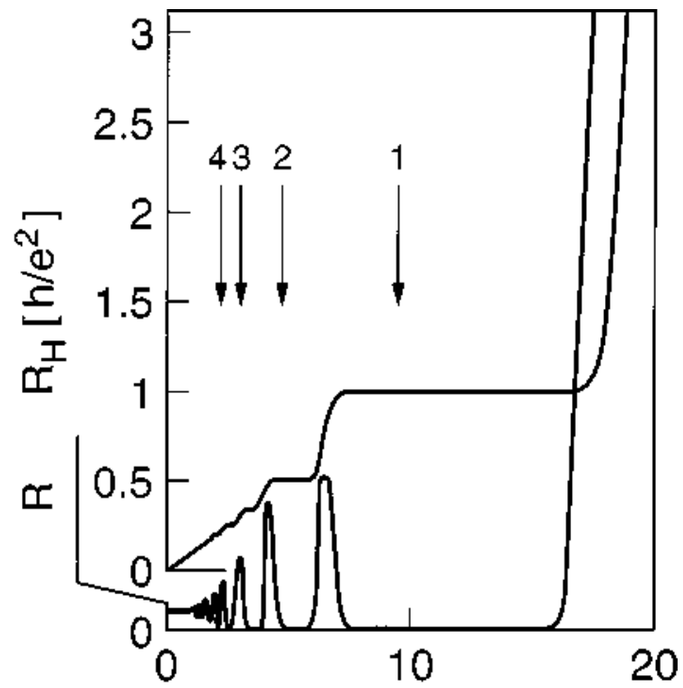
$$d = \frac{eB}{hc}$$

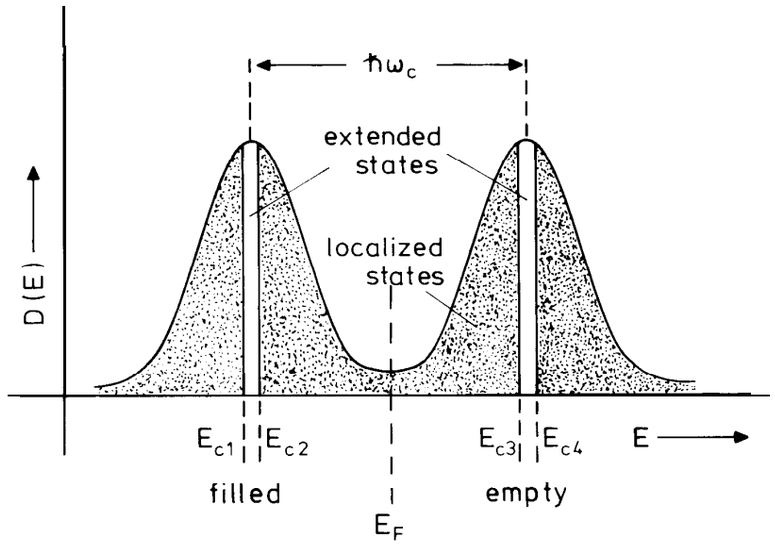
$$\mathbf{A} = 0 \qquad \mathbf{A} = (-yB, 0, 0)$$

$$B_1 = \frac{nhc}{e} \quad B_2 = \frac{nhc}{2e} \quad \cdots \quad B_i = \frac{nhc}{ie}$$

$$R_H = \frac{B_i}{nec} = \frac{h}{ie^2}$$

H. L. Stormer, RMP (1999)

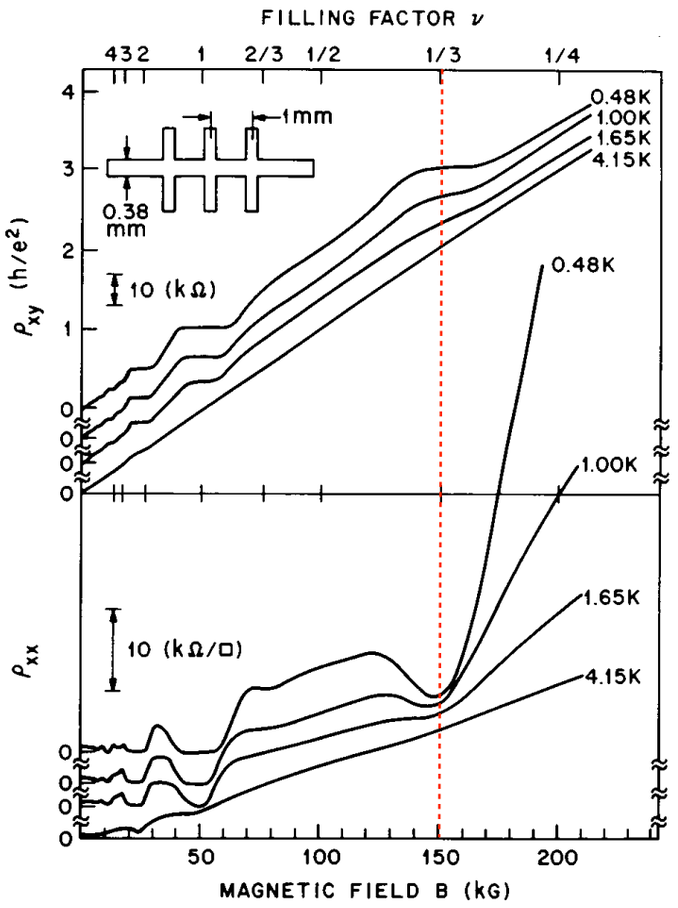


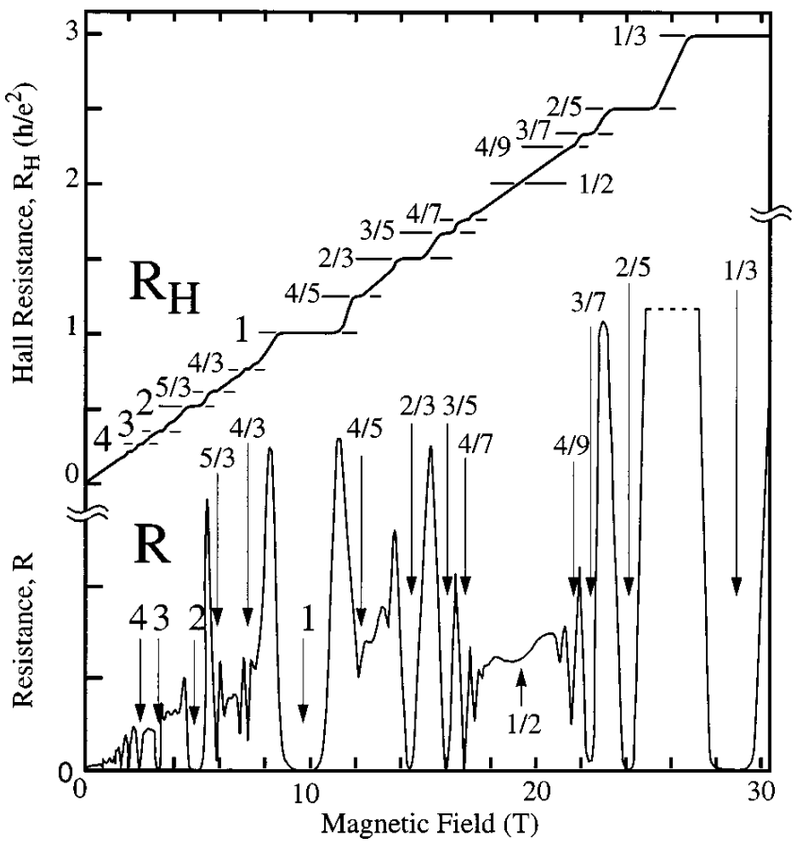


K. v. Klitzing (1985)

electron localization

Fractional quantum Hall effect (FQHE) (D.Tsui & H. L. Stormer, 1982)





$$R_H = \frac{h}{fe^2}$$

f : rational fraction

μ=90,000cm²/Vs, T=1.5K

H. L. Stormer, RMP (1999)

H. L. Stormer, RMP (1999)

The FQHE can no longer be understood on the basis of the behavior of individual electrons.

- All magnetic-field-induced energy gaps emerged as integral quantization of the R_H .

Other energy gaps, at fractional filling of a "Landau" level, must be of a different origin.

→ Many-particle effects : electronic correlation

FQHE : Many-body physics

- Many-particle correlation sometimes becomes the essence of a physical effect

  → emergence : superconductivity, superfluidity & FQHE

- Many-Body Hamiltonian in the presence of the magnetic field

$$H = \sum_j \frac{1}{2m_b}\left[\frac{\hbar}{i}\nabla_j + \frac{e}{c}\mathbf{A}(\mathbf{r}_j)\right]^2 + \frac{e^2}{\epsilon}\sum_{j<k}\frac{1}{|\mathbf{r}_j - \mathbf{r}_k|} + \sum_j U(\mathbf{r}_j) + g\mu\mathbf{B}\cdot\mathbf{S}$$

$$\hbar\omega_c = \hbar\frac{eB}{m_b c} \approx 20B[T]\mathrm{K} \qquad V_C \equiv \frac{e^2}{\epsilon l} \approx 50\sqrt{B[T]}\mathrm{K} \qquad E_Z = 2g\mu B\cdot S = \frac{g}{2}\frac{m_b}{m_e}\hbar\omega_c \approx 0.3B[\mathrm{T}]\mathrm{K}$$

$$H = \sum_j \frac{1}{2m_b}\left[\frac{\hbar}{i}\nabla_j + \frac{e}{c}\mathbf{A}(\mathbf{r}_j)\right]^2 + \frac{e^2}{\epsilon}\sum_{j<k}\frac{1}{|\mathbf{r}_j - \mathbf{r}_k|}$$

$$H = \sum_j \frac{1}{2m_b}\left[\frac{\hbar}{i}\nabla_j + \frac{e}{c}\mathbf{A}(\mathbf{r}_j)\right]^2 + \frac{e^2}{\epsilon}\sum_{j<k}\frac{1}{|\mathbf{r}_j - \mathbf{r}_k|}$$

Laughlin's ansatz

R. B. Laughlin, PRL (1983)

For $\nu = \frac{1}{3}$, $\Psi_{\frac{1}{3}} = \prod_{j<k}(z_j - z_k)^3 \exp\left[-\frac{1}{4}\sum_i |z_i|^2\right]$

$$\mathbf{A} = \frac{B}{2}(-y, x, 0)$$
$$z = x - iy$$

Composite Fermion (CF)

J. K. Jain, PRL (1989)

Principle : Strongly interacting electrons in the presence of the magnetic field turn into weakly interacting composite fermions, where a composite fermions is a bound state of an electron and an even number of quantized vortices.

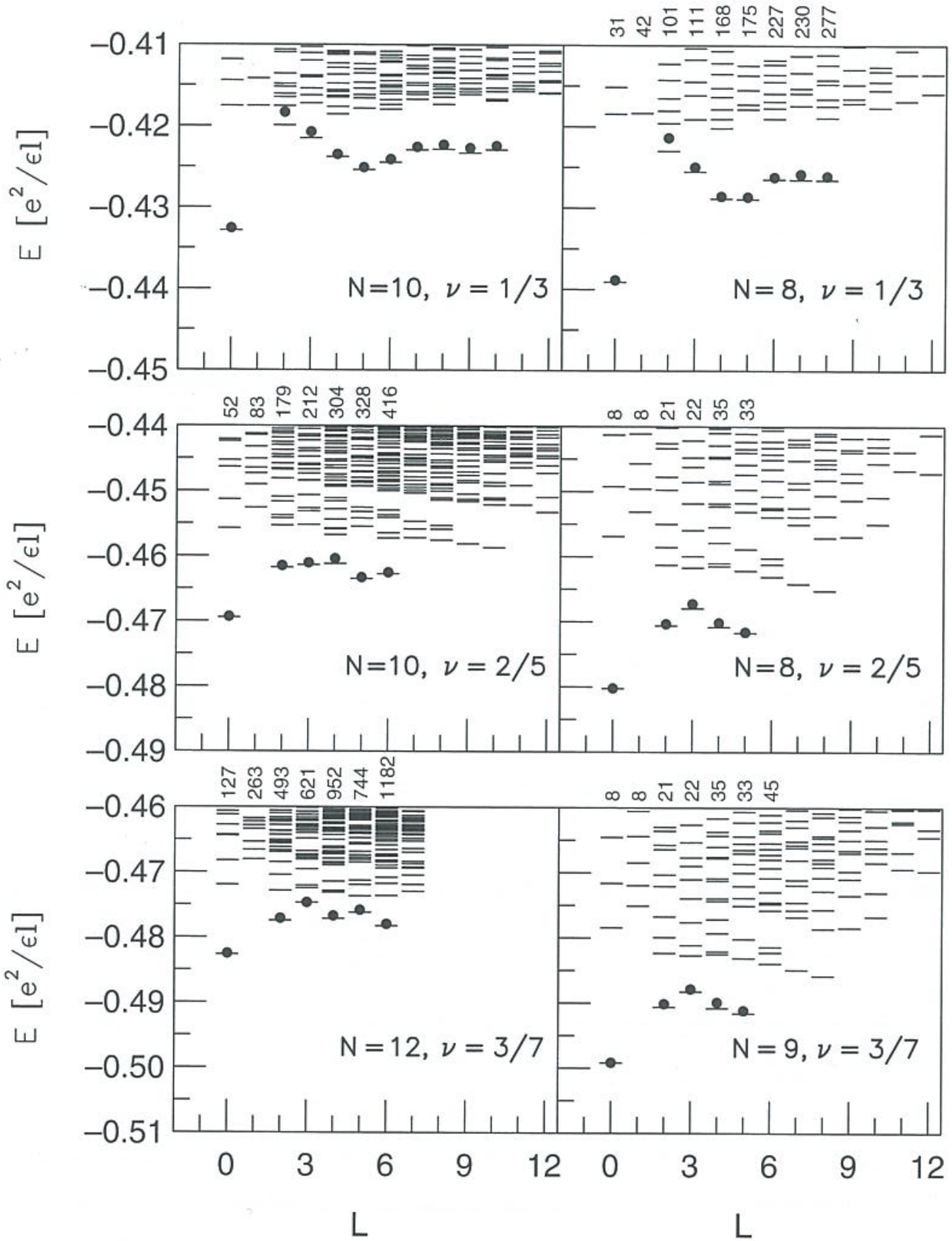
$\Psi_\nu = \Phi_{\nu^*}\prod_{j<k}(z_j - z_k)^{2p}$ Φ_{ν^*} : many body wave function for electrons (w/o Coulomb)

$$\nu = \frac{N}{N\nu^{*-1} + 2p(N-1)} = \frac{\nu^*}{2p\nu^* + 1} \quad (N \to \infty)$$

For $\nu = \frac{1}{3}$, 2*p*=2, & $\nu^* = 1$, CF wavefunction reproduces Laughlin wavefunction.

$$\Psi_{\frac{1}{3}} = \prod_{j<k}(z_j - z_k)^2\Phi_1 \qquad \Phi_1 = \prod_{j<k}(z_j - z_k)\exp\left[-\frac{1}{4}\sum_i |z_i|^2\right]$$

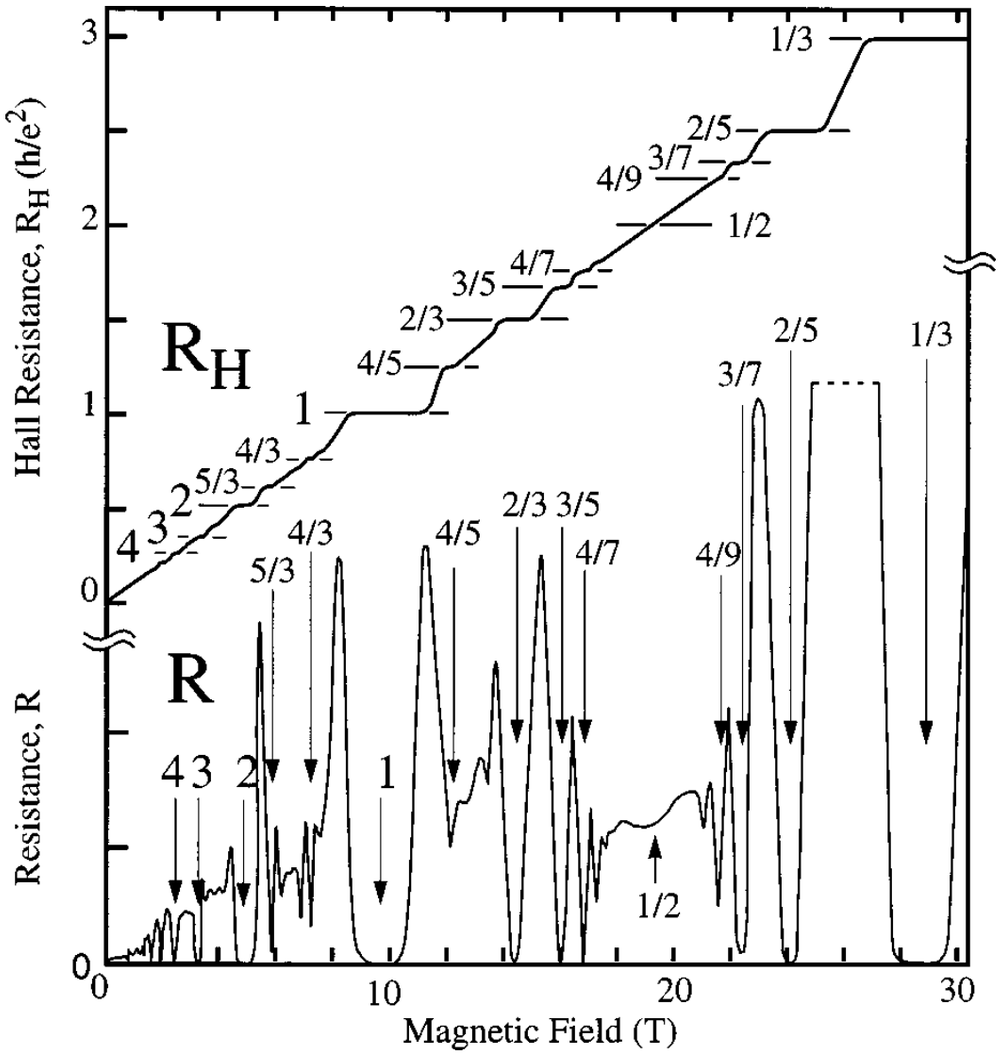
Numerical verification - Exact diagonalization



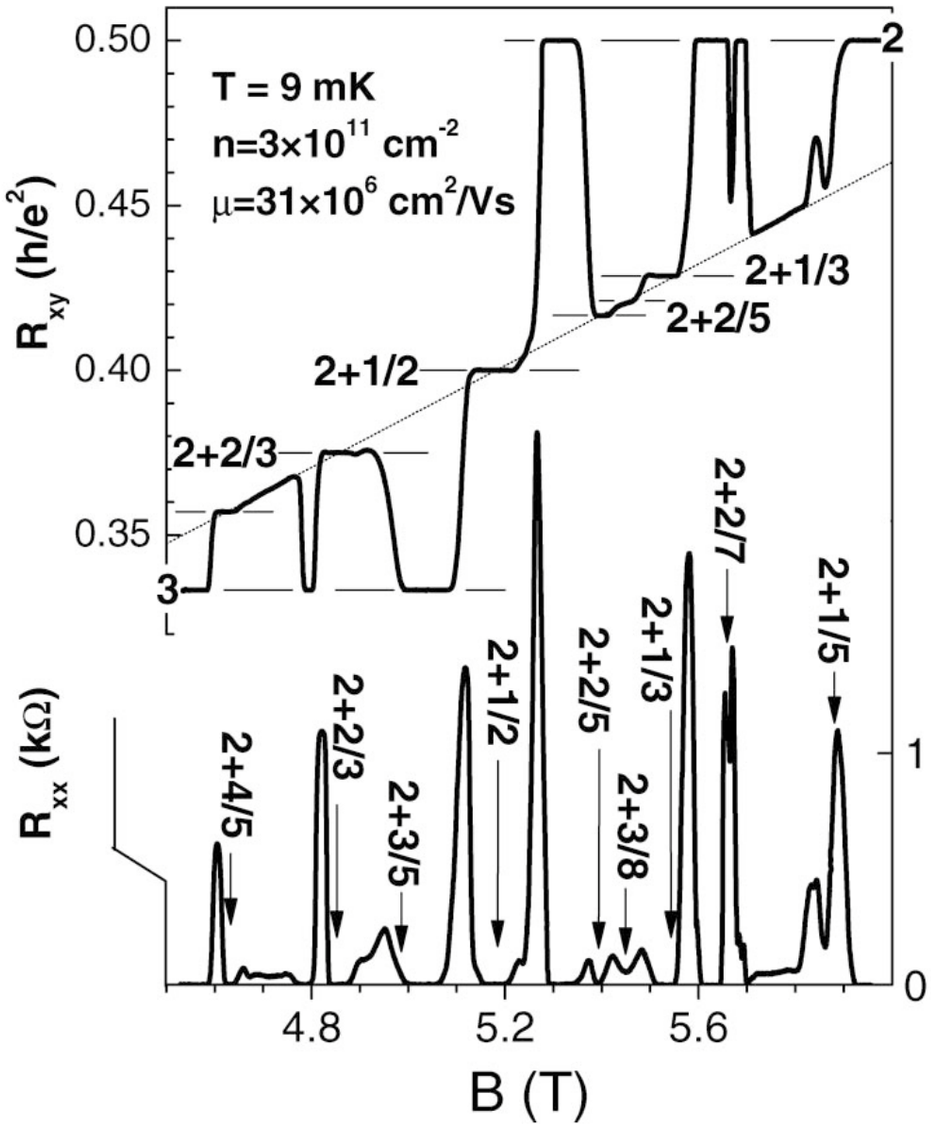
J. K. Jain and R. K. Kamilla (1998)

- Comparison of spectra obtained from exact diagonalization (dashes) and CF theory (dots).

FQHE in Second Landau level



H. L. Stormer, RMP (1999)



J. S. Xia et al., PRL (2004)

For $\nu = \frac{5}{2}$, the BCS-like gap would appear by the pairing of composite fermions

cf) Moore-Read Pfaffian wavefunction

G. Moore & N. Read, NPB (1991)
M. Greiter at al., NPB (1992)

$\nu = \frac{5}{2}$ FQHE in Second Landau level

Moore-Read Pfaffian (MR) wavefunction

G. Moore & N. Read, NPB (1991)

M. Greiter at al., NPB (1992)

$$\Psi_{\mathrm{Pf}} = \mathrm{Pf}\left(\frac{1}{Z_i - Z_j}\right)\Phi_1^2 \ \exp\left[-\frac{1}{4}\sum_k |Z_k|^2\right] \qquad \Phi_1^2 = \prod_{i<j}(Z_i - Z_j)^2$$

$$\mathrm{Pf}\,(M_{ij}) = A\,(M_{12}M_{34}\cdots M_{N-1,N})$$

cf) BCS wave function for fully polarized electrons (symmetric spinor is not shown)

$$\Psi_{\mathrm{BCS}} = A\left[\phi\left(\mathbf{r}_1 - \mathbf{r}_2\right)\phi\left(\mathbf{r}_3 - \mathbf{r}_4\right)\cdots\phi\left(\mathbf{r}_{N-1} - \mathbf{r}_N\right)\right] \qquad \phi\left(\mathbf{r}\right) = \sum_{\mathbf{k}} g_{\mathbf{k}} \exp\left[i\mathbf{k}\cdot\mathbf{r}\right]$$

A prototype state for non-Abelian statistics ⟶ fault-tolerant quantum computation

S. Das Sarma, M. Freedman, and C. Nayak, PRL (2005).

http://www.technologyreview.com/news/528256/digital-summit-microsofts-quantum-search-for-the-next-transistor/

MIT Technology Review

Digital Summit: Microsoft's Quantum Search for the "Next Transistor"

Microsoft is investing in quantum physics research that could lead to a whole new kind of computer.

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In an interview, he told *MIT Technology Review* that Microsoft had previously kept its quantum effort relatively quiet, but that positive results have convinced him to be more open. "One reason we've been a little cagey is that early on this was a fringe effort – now the physics community takes us seriously," he said. "We are very serious about our quantum physics research and we're expanding."

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A quantum computer should be able to complete calculations that are effectively impossible for any conventional machine today. None has ever been built. Although the Canadian company D-Wave Systems has sold several machines it says are quantum computers, experts say there is still no definitive proof that they exploit quantum principles and can beat conventional machines (see "The CIA and Jeff Bezos Bet on Quantum Computing").

. . . . . .

Microsoft's research focuses on a type of qubit known as a topological qubit that theory suggests would encode data in a much more robust way.

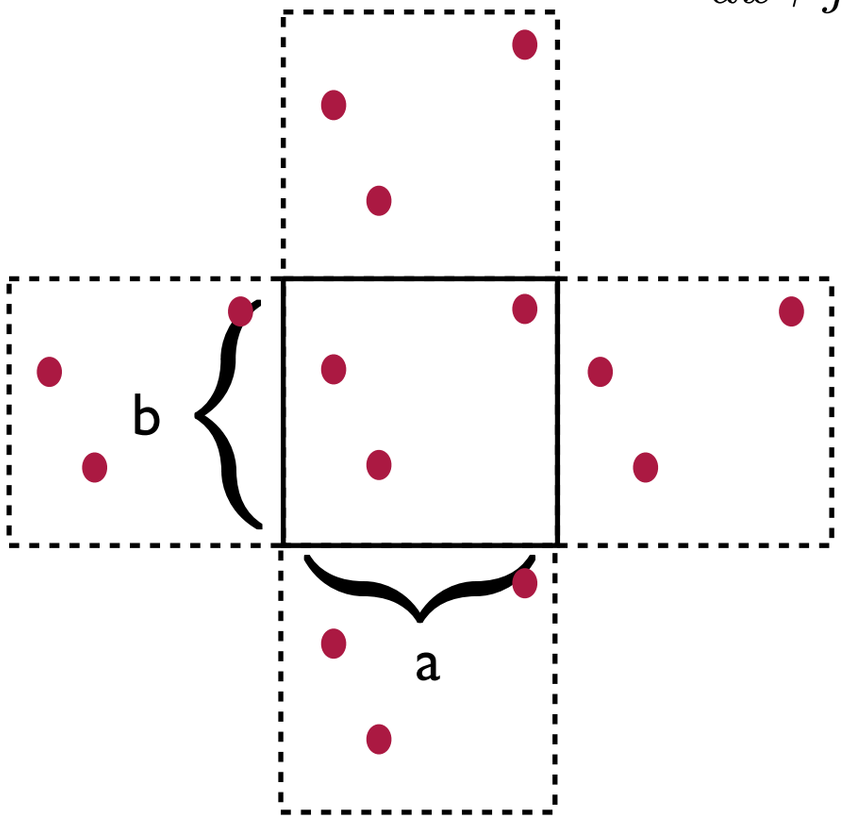
. . . . . .

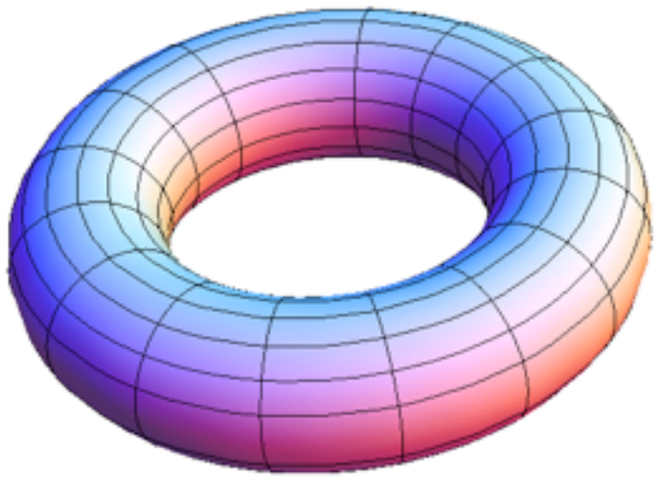
Exact diagonalization in Torus (1)

- The size of the Hamiltonian
  - For 1/2 single layer FQH system with N=14 & $N_\Phi = 28$, the size of H ~ 0.1million x 0.1million
  - For 1/2 bilayer FQH system with N=12 & $N_\Phi = 24$, the size of H ~ 63million x 63million
  - For 1/3 bilayer FQH system with N=10 & $N_\Phi = 30$, the size of H ~ 68million x 68million

- Torus → rectangular (square) geometry with periodic boundary conditions

$$\mathcal{T}_{a\hat{x}}\phi_j(x,y) = \mathcal{T}_{b\hat{y}}\phi_j(x,y) = \phi_j(x,y)$$





no curvature effect

Exact diagonalization in Torus (2)

$$H|\psi_i\rangle = E_i|\psi_i\rangle$$

1) Construct *H* matrix.
2) Diagonalize *H* matrix.

$$H = H_{\text{kinetic}} + H_{\text{Coulomb}} = \sum_j \frac{1}{2m_b}\left[\frac{\hbar}{i}\nabla_j + \frac{e}{c}\mathbf{A}(\mathbf{r}_j)\right]^2 + \frac{e^2}{\epsilon}\sum_{j<k}\frac{1}{|\mathbf{r}_j - \mathbf{r}_k|}$$

- Construction of *H*

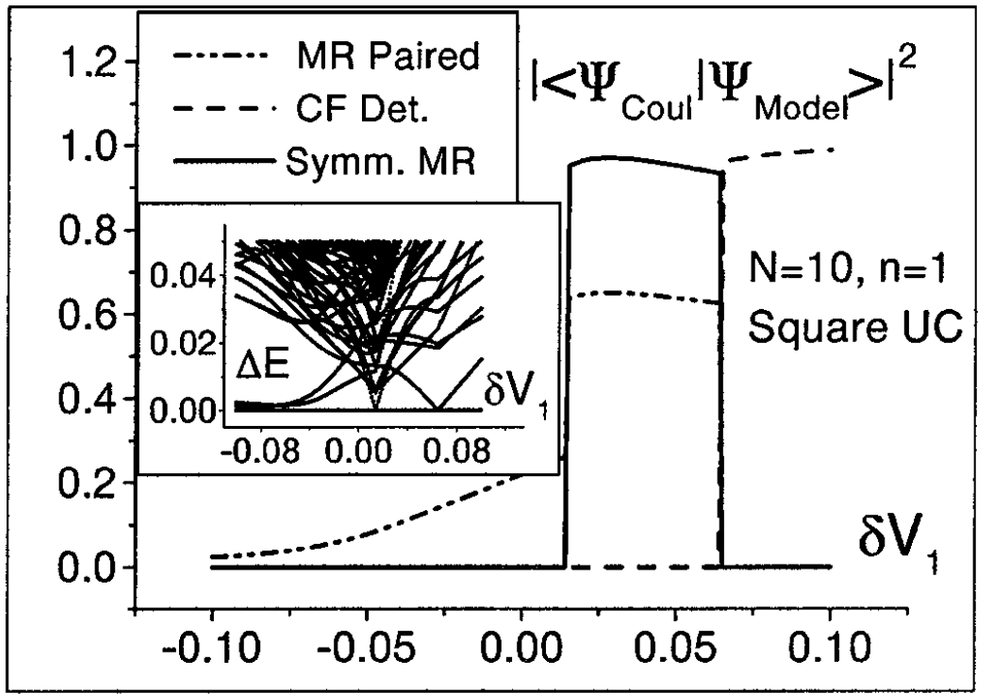
  - Find all possible many-body degenerate states in a Landau level

    of H_{kinetic} (w/o H_{Coulomb}) satisfying a certain momentum → Basis $|\phi_i\rangle$

  - The number of the basis → The size of the Hamiltonian matrix.
  - Evaluate the $H_{mn} = \langle\phi_m|H_{\text{Coulomb}}|\phi_n\rangle$

Numerical evidence $\nu = \frac{5}{2}\left(= 2 + \frac{1}{2}\right)$

N=10



E. H. Rezayi & F. D. M. Haldane, PRL (2000).

$$\left| \langle \text{MR Pfaffian} \left| \frac{5}{2} \right\rangle \right|^2$$

$$H = \sum_{m=0}^{\infty} V_m \frac{2}{N_\Phi} \sum_{\mathbf{q}} e^{-(1/2)q^2} L_m(q^2) \sum_{i<j} e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)}$$

$$N_\Phi = 2N$$

V_1 : pseudopotential parameter
describing the short-range interaction

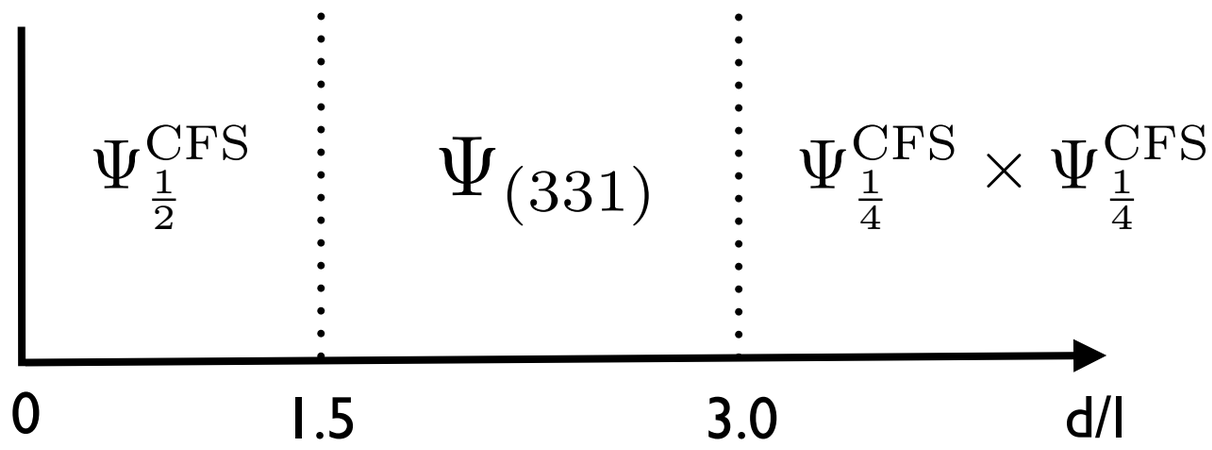
cf) For Coulomb potential, $V_1 = 0.415419$

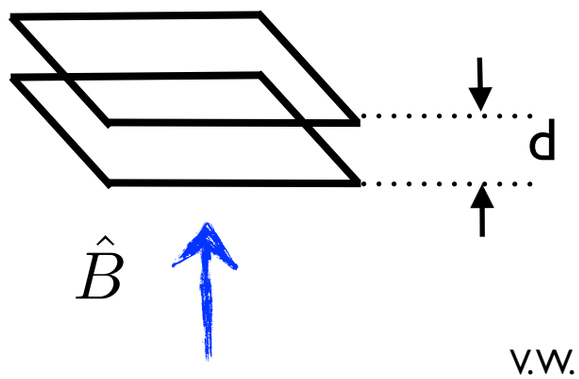
- The paired character of the 5/2 exact ground state is observed in a narrow window of δV_1.
- The overlap (squared) becomes 0.97 if the MR state is particle-hole symmetrized.

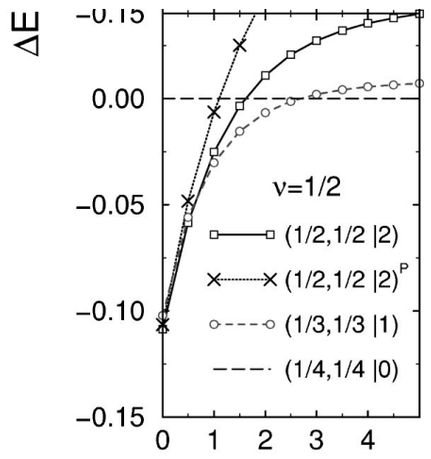
Bilayer mapping study

Jae-Seung Jeong & Kwon Park (in preparation)

Approximate analytic ground state of bilayer FQH system for $\nu = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}$







V.W. Scarola & J. K. Jain, PRB (2001)

$$\Psi_{(331)} = \prod_{i<j} \left[(z_i - z_j)^3 (\omega_i - \omega_j)^3 \right] \prod_{i,j} (z_i - \omega_j)$$

B. I. Halperin, Helv.Phys. Acta (1983)

$$A\left[\Psi_{(331)}\right] = \mathrm{Pf}\left(\frac{1}{Z_i - Z_j}\right) \Phi_1^2$$

M. Greiter, X. G. Wen, & F. Wilczek, PRB (1992)

A : antisymmetrization over spatial part

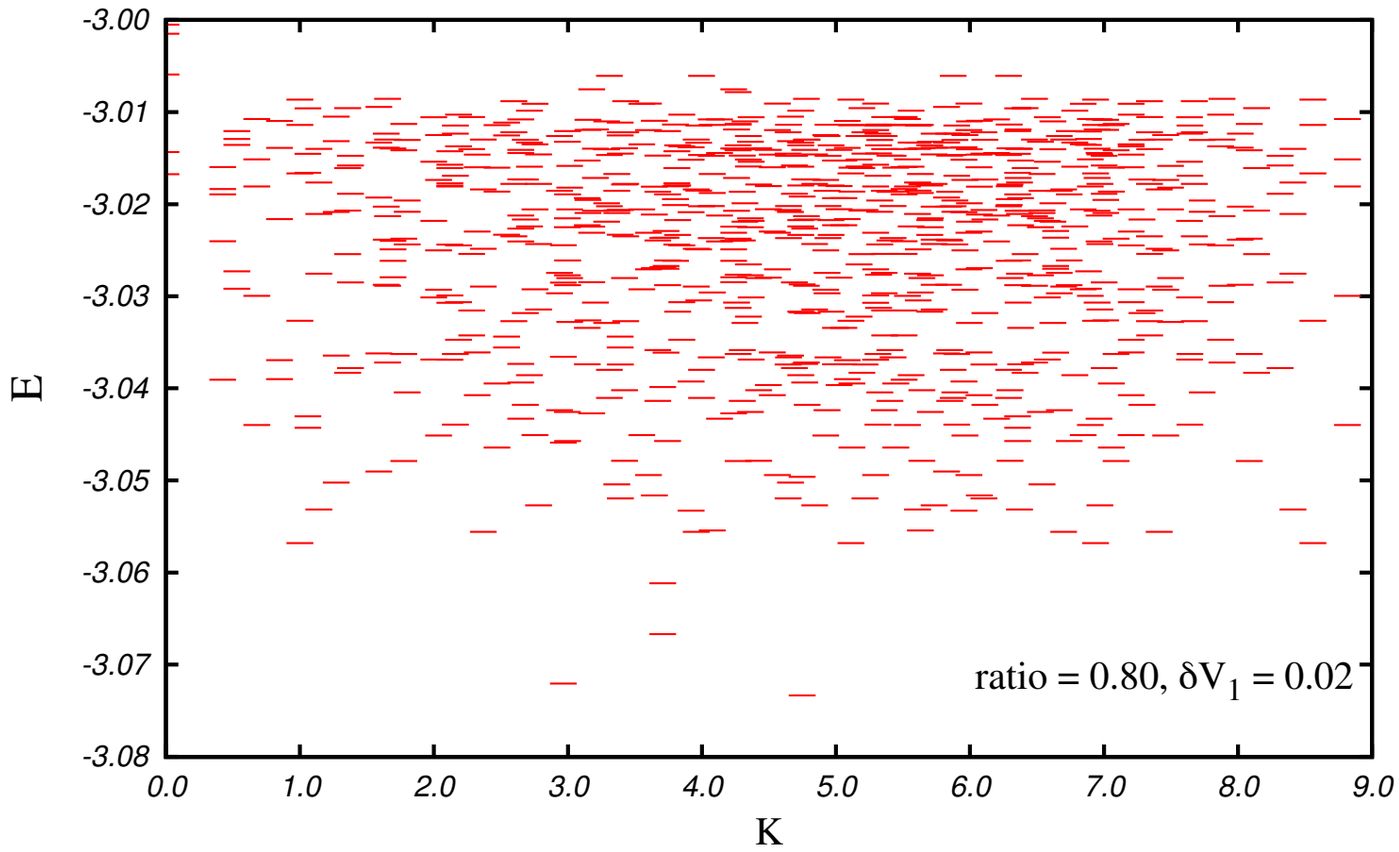
Then, what is the resulting state if we antisymmetrize the *exact bilayer FQH states* for entire interval of d/l ? (→ bilayer mapping)

Exact diagonalization - energy spectrum $\nu = \frac{5}{2}$

Jae-Seung Jeong & Kwon Park (in preparation)

$$N = 14 \quad N_\Phi = 28$$

- The size of the Hamiltonian ~ 0.1 million
- Lanczos method is used.



$$K = \sqrt{\left(\frac{2\pi P_x}{a}\right)^2 + \left(\frac{2\pi J}{b}\right)^2}$$

aspect ratio = $\frac{a}{b}$

Lanczos method

- Construct Krylov subspace S_m, spanned by a Krylov matrix, $K^m(f) = [f\ Hf\ \ldots\ H^{m-1}f]$

- Let Q_m be orthonormal basis obtained by QR factorization $K^m(f) = Q_mR$, then $T_m = Q_m^T H Q_m$ is a tridiagonal matrix. ($Q_m = [q_1\ q_2\ \ldots\ q_m]$)

$$T_m = \begin{pmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{m-2} & \alpha_{m-1} & \beta_{m-1} \\ & & & \beta_{m-1} & \alpha_m \end{pmatrix}$$

$$\alpha_j = \mathbf{q}_j^T H \mathbf{q}_j \qquad j = 1, \ldots, m$$
$$\beta_j = \mathbf{q}_{j+1}^T H \mathbf{q}_j \quad j = 1, \ldots, m-1$$

- Due to the tridiagonality of T_m,

$$H\mathbf{q}_i = \beta_{i-1}\mathbf{q}_{i-1} + \alpha_i\mathbf{q}_i + \beta_i\mathbf{q}_{i+1} \quad (2 \le i \le m-1)$$
$$\beta_i\mathbf{q}_{i+1} = H\mathbf{q}_i - \beta_{i-1}\mathbf{q}_{i-1} - \alpha_i\mathbf{q}_i \quad (1 \le i \le m-1)$$

$$Q_m^T H Q_m |\lambda_k\rangle = \lambda_k |\lambda_k\rangle$$
$$H Q_m |\lambda_k\rangle = \lambda_k Q_m |\lambda_k\rangle$$
$$H |\psi_k\rangle = \lambda_k |\psi_k\rangle$$

Parallel exact diagonalization

$$\frac{20000000000}{63000000 \times 63000000} \approx 5 \times 10^{-6}$$

$$\begin{pmatrix} \cdots & \cdots & \cdots & \cdots \\ \cdots & \text{Sparse} & M & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \cdots \\ a_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \cdots \\ b_n \end{pmatrix}$$

rank = 0

$$\begin{pmatrix} 1 & \cdots & \cdots & \cdots & \cdots \\ 8 & 3 & \cdots & \cdots & \cdots \\ 0 & 9 & 5 & \cdots & \cdots \\ 6 & 0 & 1 & 3 & \cdots \\ 9 & 0 & 0 & 0 & 7 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix} = \begin{pmatrix} b^1_{\text{tmp}} \\ b^2_{\text{tmp}} \\ b^3_{\text{tmp}} \\ b^4_{\text{tmp}} \\ b^5_{\text{tmp}} \end{pmatrix}$$

rank = 1

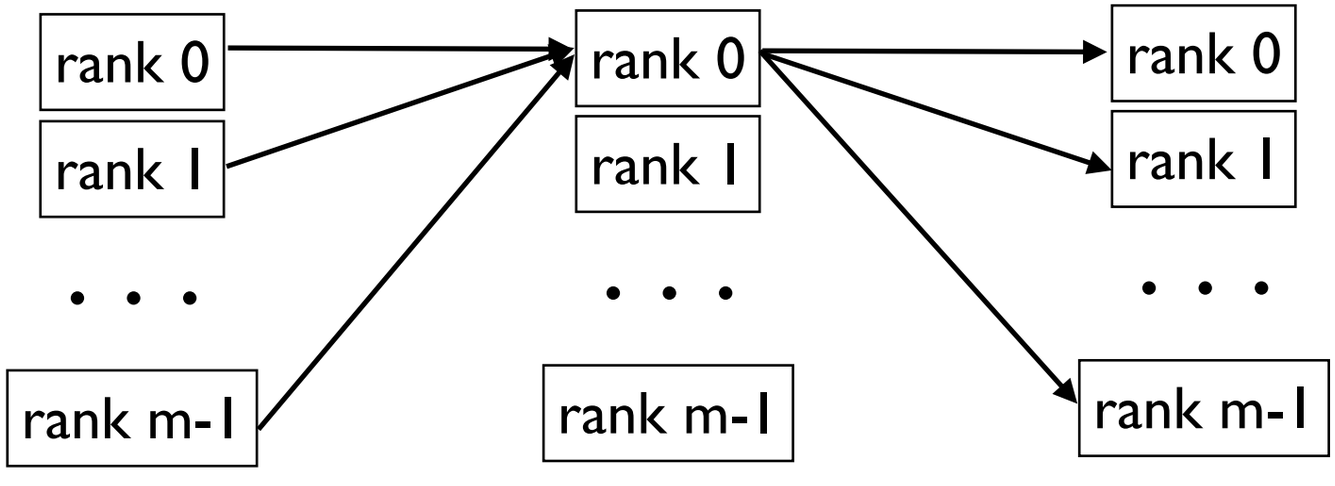
$$\begin{pmatrix} 1 & \cdots & \cdots & \cdots & \cdots \\ 8 & 3 & \cdots & \cdots & \cdots \\ 0 & 9 & 5 & \cdots & \cdots \\ 6 & 0 & 1 & 3 & \cdots \\ 9 & 0 & 0 & 0 & 7 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix} = \begin{pmatrix} b^1_{\text{tmp}} \\ b^2_{\text{tmp}} \\ b^3_{\text{tmp}} \\ b^4_{\text{tmp}} \\ b^5_{\text{tmp}} \end{pmatrix}$$

. . .

rank = m-1

$$\begin{pmatrix} 1 & \cdots & \cdots & \cdots & \cdots \\ 8 & 3 & \cdots & \cdots & \cdots \\ 0 & 9 & 5 & \cdots & \cdots \\ 6 & 0 & 1 & 3 & \cdots \\ 9 & 0 & 0 & 0 & 7 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix} = \begin{pmatrix} b^1_{\text{tmp}} \\ b^2_{\text{tmp}} \\ b^3_{\text{tmp}} \\ b^4_{\text{tmp}} \\ b^5_{\text{tmp}} \end{pmatrix}$$

MPI_Allreduce(b_tmp,b,n,MPI_DOUBLE,MPI_SUM,MPI_COMM_WORLD);



Modified Lanczos method

E. Dagotto, RMP (763)

1. $H\,|\psi_0\rangle = \epsilon_0\,|\psi_0\rangle + b|\tilde{\psi}_0\rangle$

$\epsilon_0\,[= \langle\psi_0|H|\psi_0\rangle]$

$\langle\psi_0|H|\psi_0\rangle = \epsilon_0 + b\langle\psi_0|\tilde{\psi}_0\rangle \rightarrow \langle\psi_0|\tilde{\psi}_0\rangle = 0.$

2. $b = \pm\left(\langle H^2\rangle_0 - \langle H\rangle_0^2\right)^{\frac{1}{2}}$

$b = \langle\tilde{\psi}_0|H|\psi_0\rangle = \langle\psi_0|H|\tilde{\psi}_0\rangle$

$\langle H^2\rangle_0 = \epsilon_0\,\langle H\rangle_0 + b\langle\psi_0|H|\tilde{\psi}_0\rangle,$

$\langle H^2\rangle_0 = \epsilon_0\,\langle H\rangle_0 + b^2,$

3. $|\psi_1\rangle = \dfrac{|\psi_0\rangle + \alpha_1|\tilde{\psi}_0\rangle}{(1+\alpha_1^2)^{\frac{1}{2}}}$

$\langle\tilde{\psi}_0|H|\tilde{\psi}_0\rangle = \dfrac{1}{b^2}\left[\langle H^3\rangle_0 - 2\epsilon_0\,\langle H^2\rangle_0 + \epsilon_0^2\,\langle H\rangle_0\right]$

$= \dfrac{1}{b^2}\left[\langle H^3\rangle_0 - 2\langle H\rangle_0\langle H^2\rangle_0 + \langle H\rangle_0^3\right]$

$\equiv c$

4. $\langle H\rangle_1 = \dfrac{1}{1+\alpha_1^2}\left[\langle H\rangle_0 + \alpha_1\langle\psi_0|H|\tilde{\psi}_0\rangle + \alpha_1\langle\tilde{\psi}_0|H|\psi_0\rangle + \alpha_1^2\langle\tilde{\psi}_0|H|\tilde{\psi}_0\rangle\right]$

$= \dfrac{1}{1+\alpha_1^2}\left[\langle H\rangle_0 + 2\alpha_1 b + \alpha_1^2 c\right].$

$\alpha_1 = f - \left(f^2+1\right)^{\frac{1}{2}}$

5. $\epsilon_1 = \epsilon_0 + \alpha_1 b$

$f = \dfrac{\langle H^3\rangle_0 - 3\langle H\rangle_0\langle H^2\rangle_0 + 2\langle H\rangle_0^3}{2b^3}$

Summary

- Exact diagonalization is a powerful numerical tool for studying many-body condensed matter physics.

- $n \geq 10^6$, parallel Lanczos method would be more efficient way to perform exact diagonalization

- Parallel exact diagonalization is a essential numerical method to reveal the character of 5/2 FQH state, which could be utilized for fault-tolerant quantum computation.