On the modeling and simulation of anyons systems

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SUMMARY OF THE TALK

Modeling anyons

Computing the ground state of a system of anyons

Quantum statistics: the textbook approach

Consider a system of N indistinguishable particles: $L^2((\mathbb{R}^d)^N) \simeq \otimes^N L^2(\mathbb{R}^d)$.

Particles exchange

Exchanging 2 particles doesn't change the configuration of the system: the wavefunction is modified only up to a phase factor $P_{j,k}$

$$|\psi(x_1, \cdots, x_j, \cdots, x_k, \cdots, x_N)\rangle = P_{j,k}|\psi(x_1, \cdots, x_k, \cdots, x_j, \cdots, x_N)\rangle,$$

and, thus,

$$|\psi(x_1, \cdots, x_j, \cdots, x_k, \cdots, x_N)\rangle = P_{j,k}^2|\psi(x_1, \cdots, x_j, \cdots, x_k, \cdots, x_N)\rangle.$$

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$$|\psi(x_1,\cdots,x_j,\cdots,x_k,\cdots,x_N)\rangle = P_{j,k}^2|\psi(x_1,\cdots,x_j,\cdots,x_k,\cdots,x_N)\rangle.$$

This gives $P_{j,k}^2 = 1$. Thus

- $P_{j,k} = 1$ for bosons (with the Bose-Einstein statistic),
- $P_{j,k} = -1$ for fermions (with the Dirac-Fermi statistic).

Hence

$$L^2((\mathbb{R}^d)^N) \simeq \bigotimes_{\text{sym}}^N L^2(\mathbb{R}^d) \quad \text{or} \quad \bigotimes_{\text{antisym}}^N L^2(\mathbb{R}^d).$$

A closer inspection: path integral formalism for 2 particles

Configuration space

Space of possible position for the particles. For 2 indistinguishables particles, we have

$$\mathcal{C}_2 = \{(x_1, x_2) \in \mathbb{R}^d; x_1 \neq x_2\} \backslash \{(x_1, x_2) = (x_2, x_1)\}.$$

Path integral formulation

Evolution of 2 particles[a][b]

$$|\psi_{\text{end}}\rangle = \sum_{[\gamma] \in \mathcal{P}_{\text{hom}}} e^{i\theta([\gamma])} \int_{\gamma \in [\gamma]} d\gamma \, e^{iS(\gamma)} |\psi_{\text{ini}}\rangle,$$

where $\mathcal{P}_{\text{hom}}$ is the set of homotopically equivalent classes of paths in $\mathcal{C}_2$. Two paths γ_1 and γ_2 are homotopic if there exists a continuous deformation F such that

$$F(\gamma_1) = \gamma_2.$$

[a] Schulman, Phys. Rev. **176**, 1558 (1968)
[b] Laidlaw & DeWitt, Phys. Rev. D **3**, 1375 (1971)

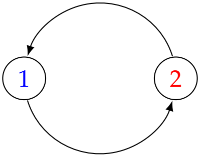

Figure: A loop in $\mathcal{C}_2$

Homotopic loops in $\mathcal{C}_2$

- For $d \geq 3$, $\mathcal{C}_2$ is simply connected so two classes of loops

  $$\mathcal{L}_{\text{hom}} \simeq \mathfrak{S}_2 = \{\sigma_1 = 1, \sigma_2\}$$

  thus,

  $$e^{i\theta([\sigma_1])} = 1 \quad \text{and} \quad e^{i\theta([\sigma_2])} = P_{1,2} = \pm 1,$$

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- For $d = 2$, $\mathcal{C}_2$ is multiply connected so there is an infinite number of classes

$$\mathcal{L}_{\text{hom}} \simeq \mathfrak{B}_2.$$

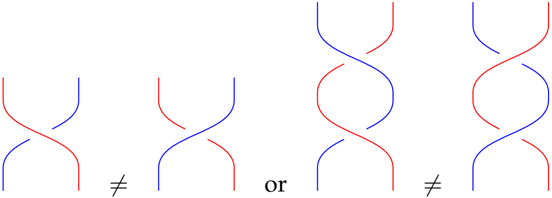

Figure: Homotopic classes of loops as braids

THE EMERGENCE OF ANYONS IN 2D

Anyons

Thus, for $d = 2$, we have

$$|\psi(x_1, \cdots, x_j, \cdots, x_k, \cdots, x_N)\rangle = e^{i\pi\beta}|\psi(x_1, \cdots, x_k, \cdots, x_j, \cdots, x_N)\rangle,$$

for **any** $\beta \in (0, 1)$. This gives a fractional quantum statistic: **any**ons.

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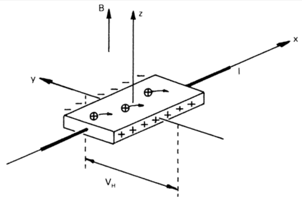
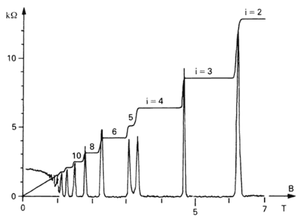
Fractional quantum Hall effect





"BOSONIC" ANYONS[1]

We define

"Bosonic" anyon

$$\psi(x_1, \cdots, x_N) := e^{-i\alpha \sum_{j<k} \theta_{j,k}} \psi_{\text{sym}}(x_1, \cdots, x_N),$$

where $\theta_{j,k} = \text{angle}\left(\frac{x_j - x_k}{|x_j - x_k|}\right)$.

One can then check that, by exchanging the particles n and m, we have

$$\theta_{n,m} = \theta_{m,n} \pm \pi,$$

and, thus,

$$\begin{aligned}
\psi(x_1, \cdots, x_n, \cdots, x_m, \cdots, x_N) &= e^{-i\alpha \sum_{j<k} \theta_{j,k}} \psi_{\text{sym}}(x_1, \cdots, x_n, \cdots, x_m, \cdots, x_N) \\
&= e^{-i\alpha \sum_{j<k} \theta_{j,k}} \psi_{\text{sym}}(x_1, \cdots, x_m, \cdots, x_n, \cdots, x_N) \\
&= e^{\mp i\alpha} \psi(x_1, \cdots, x_m, \cdots, x_n, \cdots, x_N).
\end{aligned}$$

This leads to a (bosonic) anyon wavefunction.

[1] S. Ouvry, *Anyons and Lowest Landau Level Anyons*, Séminaire Poincaré XI, 77–107 (2007).

Magnetic gauge picture

This amount to have a change of gauge on the bosonic wavefunction. Thus, if ψ evolves with respect to the free hamiltonian

$$H_N = \sum_{k=1}^{N} \frac{1}{2m} (p_k)^2$$

then the hamiltonian corresponding to ψ_{sym} is given by

Hamiltonian of "bosonic" anyons

$$H_{N,\text{sym}} = \sum_{k=1}^{N} \frac{1}{2m} (p_k - \alpha A(x_k))^2,$$

where

$$A(x_k) = \partial_{x_j} \sum_{\substack{j=1 \\ j\neq k}}^{N} \theta_{j,k} = \sum_{\substack{j=1 \\ j\neq k}}^{N} \frac{(x_k - x_j)^{\perp}}{|x_k - x_j|^2}.$$

MEAN-FIELD APPROXIMATION [2][3] WHEN $N \to +\infty$

We replace the magnetic potential $A(x_k)$ by a mean-field approximation

$$A[\varrho](x) := \int_{\mathbb{R}^2} \frac{(x-y)^\perp}{|x-y|^2}\varrho(y)dy = \nabla^\perp w * \varrho(x),$$

where

$$\varrho(x) := \int_{\mathbb{R}^{2(N-1)}} |\psi(x, x_2, \cdots, x_N)|^2 d\mathbf{x} \quad \text{and} \quad w(x) = \log|x|.$$

The dimensionless hamiltonian becomes

$$H_{N,\mathrm{sym}} = \sum_{k=1}^{N} (p_k - (N-1)\alpha A[\varrho](x_k))^2.$$

Taking $\psi = u^{\otimes N}$ (and $\varrho = |u|^2$) and assuming $(N-1)\alpha = \beta$, we derive

Mean-field energy of a pure state

$$\mathcal{E}(u) = N^{-1}\langle u^{\otimes N}, H_{N,\mathrm{sym}} u^{\otimes N}\rangle_{L^2} = \int_{\mathbb{R}^2} \left|(-i\nabla + \beta A[|u|^2])u\right|^2 dx.$$

[2] D. Lundholm & N. Rougerie, *The average field approximation for almost bosonic extended anyons*, J. Stat. Phys. 161, 1236-1267 (2015)

[3] M. Correggi, D. Lundholm & N. Rougerie, *Local density approximation for the almost-bosonic anyon gas*, Analysis & PDE 10, 1169-1200 (2017)

Modeling anyons

Computing the ground state of a system of anyons

Gradient method under constraint

Computing the ground state amounts to solve

$$\min_{u \in \mathbb{S}(L^2(\mathbb{R}^2)} \mathcal{E}(u),$$

where $\mathbb{S}(L^2(\mathbb{R}^2) = \{v \in L^2(\mathbb{R}^2);\ \|v\|_{L^2} = 1\}$.

Gradient of $\mathcal{E}$

$$D_{\bar{u}}\mathcal{E}(u) = -\Delta - 2\beta A[|u|^2] \cdot i\nabla + \beta^2 |A[|u|^2]|^2 - 2\beta A \left[A[|u|^2]|u|^2 - J[u]\right],$$

where

$$J[u] := -\Im\left(u\nabla\bar{u}\right) \quad \text{and} \quad A[v] = \nabla^{\perp} w * v.$$

We can recognize a kinetic term, a nonlinear transport term and a nonlinear potential. Also, A is a nonlocal functional.

The nonlinear conjugate gradient method

Classical nonlinear conjugate gradient (NCG)

$$
d_0 = -g_0,
$$

$$
\text{for } n = 1, 2, \ldots \begin{cases} d_n = -g_n + \beta_n d_{n-1}, \\ u_n = u_{n-1} + \tau_n d_n, \end{cases}
$$

where

$$
g_n = D_{\bar{u}}\mathcal{E}(u_n), \quad \tau_n = \underset{\tau>0}{\operatorname{argmin}}\, \mathcal{E}(u_{n-1} + \tau d_n),
$$

and

$$
\beta_n = \frac{\|g_n\|_{L^2}^2}{\|g_{n-1}\|_{L^2}^2} \ (\mathit{Fletcher-Reeves}) \quad \text{or} \quad \frac{\langle g_n - g_{n-1}, g_n\rangle_{L^2}}{\|g_{n-1}\|_{L^2}^2} \ (\mathit{Polak-Ribiere}).
$$

A projected and preconditionned nonlinear conjugate gradient method[4][5]

Projection on the constraint manifold

- Projection on the tangent space

$$g_n = \mathcal{T}_{\mathbb{S},u_n} D_{\bar{u}}\mathcal{E}(u_n) \quad \text{and} \quad d_n = \mathcal{T}_{\mathbb{S},u_n}\left(-g_n + \beta_n d_{n-1}\right)$$

where $\mathcal{T}_{\mathbb{S},u_n} v := v - \frac{\langle v, u_n\rangle_{L^2}}{\langle u_n, u_n\rangle_{L^2}} u_n$.

- Projection on space

$$\tau_n = \underset{\tau>0}{\operatorname{argmin}}\ \mathcal{E}(P_{\mathbb{S}}(u_{n-1} + \tau d_n)) \quad \text{and} \quad u_n = P_{\mathbb{S}}(u_{n-1} + \tau d_n),$$

where $P_{\mathbb{S}} v = \frac{v}{\|v\|_{L^2}}$.

[4] X. Antoine, A. Levitt & Q. Tang, *Efficient spectral computation of the stationary states of rotating Bose?Einstein condensates by preconditioned nonlinear conjugate gradient methods*, Journal of Computational Physics 343 (2017)

[5] I. Danaila & B. Protas, *Computation of Ground States of the Gross-Pitaevskii Functional via Riemannian Optimization*, SIAM J. Scientific Computing, 39(6), p. B1102-B1129-94 (2017)

A projected and preconditionned nonlinear conjugate gradient method

Preconditionning

We introduce

$$p_n = M g_n,$$

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Projected and preconditionned nonlinear conjugate gradient

$$d_0 = -p_0,$$

$$\text{for } n = 1, 2, \ldots \begin{cases} d_n = \mathcal{T}_{\mathbb{S},u_n}(-p_n + \beta_n d_{n-1}), \\ u_n = P_{\mathbb{S}}(u_{n-1} + \tau_n d_n), \end{cases}$$

where

$$g_n = \mathcal{T}_{\mathbb{S},u_n} D_{\bar{u}} \mathcal{E}(u_n), \quad p_n = (1-\Delta)^{-1} g_n, \quad \tau_n = \operatorname*{argmin}_{\tau>0} \mathcal{E}(P_{\mathbb{S}}(u_{n-1} + \tau d_n)),$$

and

$$\beta_n = \frac{\langle g_n - g_{n-1}, p_n \rangle_{L^2}}{\langle g_{n-1}, p_{n-1} \rangle_{L^2}}.$$

SPACE DISCRETIZATION

The pseudo-spectral discretization

- The problem is solved on a uniform cartesian grid

$$\mathcal{O}_{J,K} = \{\mathbf{x}_{j,k}, (j,k) \in \mathcal{P}_{J,K}\} \subset [-L_x, L_x] \times [-L_y, L_y]$$

  with $(J+1)(K+1)$ points,
- The boundary conditions are periodic, *i.e.* the unknown array $\boldsymbol{u} = (\boldsymbol{u}(\mathbf{x}_{j,k}))_{j,k}$ verifies

$$\boldsymbol{u}_{1,k} = \boldsymbol{u}_{J+1,k}, \quad \text{and} \quad \boldsymbol{u}_{j,1} = \boldsymbol{u}_{j,K+1}.$$

Pseudo-spectral approximation of the gradient

We need to approximate the operators from

Gradient of $\mathcal{E}$

$$D_{\bar{u}}\mathcal{E}(u) = -\Delta - 2\beta A[|u|^2] \cdot i\nabla + \beta^2 |A[|u|^2]|^2 - 2\beta A\left[A[|u|^2]|u|^2 - J[u]\right],$$

where

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- For the differential operators, we have the symbols

$$[\partial_x]\boldsymbol{u}_{j,k} = \mathsf{iFFT}\left(\xi_p\, \mathsf{FFT}(\boldsymbol{u})_{p,\ell}\right)_{j,k} \quad \text{and} \quad [\partial_y]\boldsymbol{u}_{j,k} = \mathsf{iFFT}\left(\eta_\ell\, \mathsf{FFT}(\boldsymbol{u})_{p,\ell}\right)_{j,k}.$$

- Hence, the main difficulty is to evaluate the operator A, *i.e.* the convolution with w.

THE SINGULAR INTEGRAL

By applying a FFT, we obtain

$$(\boldsymbol{w} * \boldsymbol{v})_{j,k} = \mathsf{iFFT}\left(\hat{\boldsymbol{w}}_{p,\ell}\mathsf{FFT}(\boldsymbol{v})_{p,\ell}\right)_{j,k}$$

Problem

Since $w(x) = \log|x|$ (Newton potential), we deduce

$$\hat{\boldsymbol{w}}_{p,\ell} = 2\pi(\xi_p^2 + \eta_\ell^2)^{-1}.$$

Kernel truncation method[6]

Since $\mathcal{O}$ is bounded, the idea is to replace w with a truncation

$$w_R(x) = w(x)\mathbf{1}_{|x|\leq R},$$

with $R = 3\max(L_x, L_y)$. This leads to

Fourier transform of truncated Kernel

$$\hat{\boldsymbol{w}}_{R,p,\ell} = \frac{1 - J_0(Rs_{p,\ell})}{s_{p,\ell}^2} - R\log(R)\frac{J_1(Rs_{p,\ell})}{s_{p,\ell}},$$

where J_0, J_1 are Bessel functions and

$$s_{p,\ell} = \sqrt{\xi_p^2 + \eta_\ell^2}.$$

This lifts the singularity since

$$\frac{1 - J_0(Rs)}{s^2} \underset{s\to 0}{\longrightarrow} \left(\frac{R}{2}\right)^2 \quad \text{and} \quad \frac{J_1(Rs)}{s} \underset{s\to 0}{\longrightarrow} \frac{R}{2}.$$

[6] F. Vico, L. Greengard & M. Ferrando, *Fast convolution with free-space Green's functions*, J. Comput. Phys. 323, 191–203 (2016)

SIMULATIONS

Computations of ground states for

$$\mathcal{E}(u) = \int_{\mathbb{R}^2} \left(\left| (-i\nabla + \beta A[|u|^2])u \right|^2 + V(x)|u|^2 \right) dx,$$

with $V(x) = \frac{1}{2}|x|^2$.

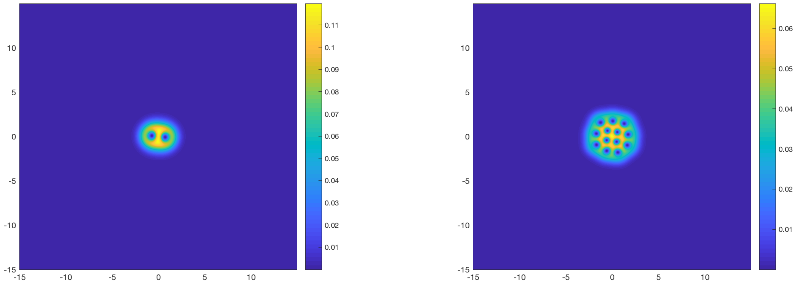

Figure: $\beta = 5$ on the left and $\beta = 20$ on the right.

SIMULATIONS

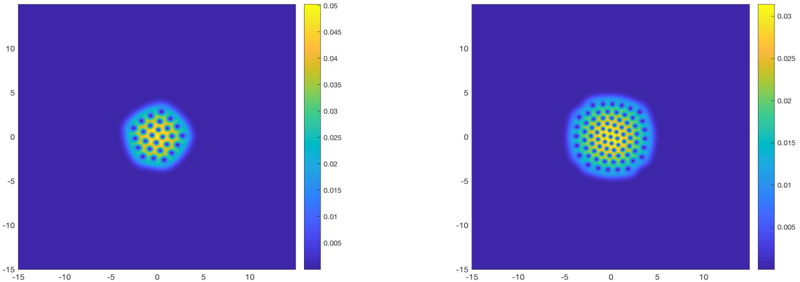

Figure: $\beta = 35$ on the left and $\beta = 90$ on the right.