On some methods for the numerical simulation of quantum systems

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SUMMARY OF THE TALK

Gradient methods to compute a groundstate
   Without constraints
   On a manifold

Application to an almost-bosonic anyon gas
   A mean-field energy for an almost-bosonic anyon gas
   Preconditionned Gradient method
   Pseudo-spectral discretization

Numerical results
   Ground states
   Comparaison with theory
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**Minimization of an Energy**

Let $\mathcal{E} : L^2(\mathbb{R}^d) \to \mathbb{R}$ be the energy of a quantum system in a mean-field regime.

**Goal: find a groundstate**

Numerically solve the minimization problem

$$\min_{u \in \mathcal{S}} \mathcal{E}(u),$$

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

Example: the Gross-Pitaevskii energy for Bose-Einstein condensate

$$\mathcal{E}(u) = \int_\Omega \frac{1}{2} |\nabla u|^2 + V|u|^2 + \frac{\beta}{4} |u|^4.$$
GRADIENT DESCENT METHOD

We wish to solve the minimization problem (without constraints)

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

under the assumption that $\mathcal{E}$ is differentiable.

The standard gradient descent

$$\begin{cases} u_0 \in L^2(\mathbb{R}^d), \\ u_{n+1} = u_n - \tau \nabla \mathcal{E}(u_n), \end{cases}$$

with $\tau > 0$.

- Easy to implement
- The step size $\tau$ needs to be adjusted
- Rather slow

Figure: Example: 24 iterations
**Gradient Descent Method**

The steepest gradient descent

\[
\begin{cases}
    u_0 \in L^2(\mathbb{R}^d), \\
    \tau_n = \min_{\tau \in \mathbb{R}} \mathcal{E}(u_n - \tau \nabla \mathcal{E}(u_n)) \\
    u_{n+1} = u_n - \tau_n \nabla \mathcal{E}(u_n).
\end{cases}
\]

- The step size is optimum
- Faster than the standard gradient
- The implementation of the scalar minimization is not straightforward (black-box)

Figure: Example: 10 iterations
**Gradient descent method**

The conjugate gradient descent

\[
\begin{align*}
  u_0 & \in L^2(\mathbb{R}^d), \\
  g_n &= -\nabla \mathcal{E}(u_n) \\
  \beta_n &= \langle g_n, g_n - g_{n-1} \rangle / \| g_n - 1 \|^2 \\
  d_n &= g_n + \beta_n d_{n-1} \\
  \tau_n &= \min_{\tau \in \mathbb{R}} \mathcal{E}(u_n + \tau d_n) \\
  u_{n+1} &= u_n + \tau_n d_n.
\end{align*}
\]

- The step size is optimum (but requires a scalar minimization)
- Faster than the steepest gradient
- Several possibilities for $\beta_n$ (here Polak-Ribière)
- $\mathcal{E}$ needs to be well-behaved (approximately quadratic near the minimum)

Figure: Example: 9 iterations
GRADIENT DESCENT METHOD ON A MANIFOLD

We wish to solve the minimization problem (with constraints)

$$\min_{u \in S} \mathcal{E}(u),$$

under the assumption that $S$ is a manifold. We consider the projection $\mathcal{P}_S(u) : L^2(\mathbb{R}^d) \to S$. Here, we have

$$S = \{ u \in L^2; \|u\|_2 = 1 \} \quad \text{and} \quad \mathcal{P}_S(u) = u/\|u\|_2.$$

The steepest gradient

$$\left\{ \begin{array}{l}
u_0 \in L^2(\mathbb{R}^d), \\
\tau_n = \min_{\tau \in \mathbb{R}} \mathcal{E}(\mathcal{P}_S(u_n - \tau \nabla \mathcal{E}(u_n))) \\
u_{n+1} = \mathcal{P}_S(u_n - \tau_n \mathcal{E}(u_n)) \end{array} \right.$$
The problem stems from the fact that, near the minimum,

\[ \langle -\nabla \mathcal{E}(u_n), u_n \rangle \simeq \| \nabla \mathcal{E}(u_n) \|_2 = O(1). \]

Thus, the error on the constraint is

\[
\| u_{n+1} \|_2^2 = \| u_n - \tau_n \nabla \mathcal{E}(u_n) \|_2^2 \\
= \| u_n \|_2^2 + 2\tau_n \langle -\nabla \mathcal{E}(u_n), u_n \rangle \\
+ \tau_n^2 \| \nabla \mathcal{E}(u_n) \|_2^2 \\
\sim 1 + 2\tau_n \| \nabla \mathcal{E}(u_n) \|_2.
\]

Figure: Near the minimum
GRADIENT DESCENT METHOD ON A MANIFOLD

We consider \( T_u S \) the tangent space of \( S \) at \( u \in S \) as well as a projection \( T_{T_u S} : L^2(\mathbb{R}^d) \rightarrow T_u S \). Here

\[
T_u S = \{ v \in L^2(\mathbb{R}^d); \langle u, v \rangle = 0 \} \quad \text{and} \quad T_{T_u S} v = v - \langle u, v \rangle u.
\]

The projected gradient

\[
\begin{cases}
u_0 \in L^2(\mathbb{R}^d), \\
g_n = -T_{T_{u_n} S} \nabla \mathcal{E}(u_n) \\
\tau_n = \min_{\tau \in \mathbb{R}} \mathcal{E}(P_S (u_n - \tau g_n)) \\
u_{n+1} = P_S (u_n - \tau_n g_n).
\end{cases}
\]

- \( P_S \) and \( P_{T_u S} \) depend on the manifold...
- Faster near the minimum

Figure: Example: 4 iterations
GRADIENT DESCENT METHOD ON A MANIFOLD

The projected conjugate gradient

\[ \begin{align*}
    u_0 &\in L^2(\mathbb{R}^d), \\
    g_n &=-\nabla E(u_n), \\
    h_{n-1} &= T_{u_n} g_{n-1}, \\
    \beta_n &= \langle g_n, g_n - h_{n-1} \rangle / \| h_{n-1} \|^2, \\
    d_n &= g_n + \beta_n T_{u_n} g_{n-1}, \\
    \tau_n &= \min_{\tau \in \mathbb{R}} E(\mathcal{P}_S(u_n + \tau d_n)), \\
    u_{n+1} &= \mathcal{P}_S(u_n + \tau_n d_n).
\end{align*} \]

- $\mathcal{P}_S$ and $\mathcal{P}_{T_{u}S}$ depend on the manifold...
- Faster than the projected gradient

Figure: Example: 5 iterations
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"BOSONIC" ANYONS\textsuperscript{1}

We define

\[ \psi(x_1, \cdots, x_N) := e^{-i\alpha \sum_{j<k} \theta(x_j, x_k)} \psi_{\text{sym}}(x_1, \cdots, x_N), \]

where \( \theta(x, y) = \text{angle} \left( \frac{x-y}{|x-y|} \right) \) and \( \alpha \in \mathbb{R} \).

By exchanging the particles \( n \) and \( m \), we have

\[ \theta(x_n, x_m) = \text{angle} \left( \frac{x_n - x_m}{|x_n - x_m|} \right) = \text{angle} \left( \frac{-(x_m - x_n)}{|x_m - x_n|} \right) = \theta(x_m, x_n) \pm \pi, \]

and, thus,

\[ \psi(x_1, \cdots, x_n, \cdots, x_m, \cdots, x_N) = e^{-i\alpha \sum_{j<k} \theta(x_j, x_k)} \psi_{\text{sym}}(x_1, \cdots, x_n, \cdots, x_m, \cdots, x_N) \]
\[ = e^{-i\alpha \sum_{j<k} \theta(x_j, x_k)} \psi_{\text{sym}}(x_1, \cdots, x_m, \cdots, x_n, \cdots, x_N) \]
\[ = e^{\mp i\alpha} \psi(x_1, \cdots, x_m, \cdots, x_n, \cdots, x_N). \]

This leads to a (bosonic) anyon wavefunction.

\textsuperscript{1}S. Ouvry, \textit{Anyons and Lowest Landau Level Anyons}, Séminaire Poincaré XI, 77–107 (2007).
**Magnetic Gauge Picture**

Thus, if $\psi$ evolves with respect to the free Hamiltonian

$$i\hbar \partial_t \psi(t, x) = H_N \psi(t, x) = \sum_{k=1}^{N} \frac{1}{2m} (p_k)^2 \psi(t, x_1, \ldots, x_N),$$

then, since

$$p_k \psi(t, x) = -i \partial_{x_k} (\psi_{\text{sym}}(t, x)) e^{-i \alpha \sum_{j<k} \theta(x_j, x_k)}$$

$$= \left( -\alpha \partial_{x_k} \sum_{j<k} \theta(x_j, x_k) \psi_{\text{sym}}(t, x) - i \partial_{x_k} \psi_{\text{sym}}(t, x) \right) e^{-i \alpha \sum_{j<k} \theta(x_j, x_k)}$$

the Hamiltonian corresponding to $\psi_{\text{sym}}$ 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

$$A(x_k) = \sum_{j=1}^{N} \left( \sum_{j \neq k} \partial_{x_j} \theta(x_j, x_k) \right) = \sum_{j=1}^{N} \frac{(x_k - x_j)^\perp}{|x_k - x_j|^2}.$$
MEAN-FIELD APPROXIMATION \(^{23}\) WHEN \(N \to +\infty\)

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

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

where

\[
\rho(x) := \int_{\mathbb{R}^2(N-1)} |\psi(x, x_2, \cdots, x_N)|^2 dx \quad \text{and} \quad w(x) = \log |x|.
\]

The dimensionless hamiltonian becomes

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

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

Mean-field energy of a pure state

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


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

**Mean-field energy**

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

with

\[
\text{curl}(A[\varrho](x)) = 2\pi \varrho(x).
\]

**Gradient of \( E \)**

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

where

\[
J[u] := -\Im (u \nabla \bar{u}).
\]
PRECONDITIONNING A CONJUGATE GRADIENT METHOD

**Gradient vs. Newton**

\[ \begin{align*}
\left\{ \begin{array}{l}
{u_0} \in L^2(\mathbb{R}^d), \\
{u_{n+1}} = {u_n} - \tau \nabla \mathcal{E}(u_n).
\end{array} \right. \\
\left\{ \begin{array}{l}
{u_0} \in L^2(\mathbb{R}^d), \\
{u_{n+1}} = {u_n} - \left( \nabla^2 \mathcal{E}(u_n) \right)^{-1} \nabla \mathcal{E}(u_n).
\end{array} \right.
\]

Newton uses the information from the second derivative to accelerate the convergence.

This can be interpreted as a gradient under a new scalar product

\[ \langle v, \nabla \mathcal{E}(u_n) \rangle_M = \langle \sqrt{M}v, \sqrt{M}\nabla \mathcal{E}(u_n) \rangle_{L^2} = \langle v, M\nabla \mathcal{E}(u_n) \rangle_{L^2}, \]

where \( M \) is symmetric definite positive. We can choose \( M \simeq \left( \nabla^2 \mathcal{E}(u_n) \right)^{-1} \) in order to avoid a computationally expensive inversion (e.g. \( M = (1 - \Delta)^{-1} \)).
The projected preconditioned conjugate gradient

\[ u_0 \in L^2(\mathbb{R}^d), \]
\[ g_n = -\mathcal{T}_{u_n} \nabla \mathcal{E}(u_n) \]
\[ h_{n-1} = \mathcal{T}_{u_n} g_{n-1} \]
\[ \beta_n = \langle g_n, g_n - h_{n-1} \rangle_M / \| h_{n-1} \|^2_M \]
\[ d_n = Mg_n + \beta_n \mathcal{T}_{u_n} d_{n-1} \]
\[ \tau_n = \min_{\tau \in \mathbb{R}} \mathcal{E}(\mathcal{P}_S(u_n + \tau d_n)) \]
\[ u_{n+1} = \mathcal{P}_S(u_n + \tau_n d_n). \]

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**SPACE DISCRETIZATION**

The pseudo-spectral discretization in 2D

- The problem is solved on a uniform cartesian grid

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

with \((J+1)(K+1)\) points,

- The boundary conditions are periodic, *i.e.* the unknown array \( u = (u(x_{j,k}))_{j,k} \) verifies

\[ u_{1,k} = u_{J+1,k}, \quad \text{and} \quad u_{j,1} = u_{j,K+1}. \]

For the differential operators, we have the symbols

\[ [\partial_x] u_{j,k} = \text{iFFT} \left( i \xi_p \text{FFT}(u)_{p,\ell} \right)_{j,k} \quad \text{and} \quad [\partial_y] u_{j,k} = \text{iFFT} \left( i \eta_\ell \text{FFT}(u)_{p,\ell} \right)_{j,k}. \]
PSEUDO-SPECTRAL APPROXIMATION OF THE GRADIENT

We need to approximate the operators from

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

where

\[ J[u] := -\mathcal{S}(u\nabla \bar{u}) \quad \text{and} \quad A[v] = \nabla^\perp w \ast v. \]

We have explicitely

\[ [\Delta] = [\partial_x]^2 + [\partial_y]^2 \quad \text{and} \quad [\nabla] = \begin{pmatrix} [\partial_x] \\ [\partial_y] \end{pmatrix}. \]

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

\[(w \ast v)_{j,k} = \text{iFFT} \left( \hat{w}_{p,\ell} \text{FFT}(v)_{p,\ell} \right)_{j,k} \cdot \]

Problem

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

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

A possible solution is to smooth the kernel

\[ \hat{w}_{p,\ell} = 2\pi (\xi_p^2 + \eta_{\ell}^2 + \varepsilon)^{-1}, \]

for \( \varepsilon > 0 \) small enough. But this can deteriorate the precision of the discretization (numerical locking phenomena\(^6\)).

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**Kernel Truncation Method**

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**

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

where $J_0, J_1$ are Bessel functions and

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

This lifts the singularity since

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

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GROUND STATES: HARMONIC TRAP
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 \( V(x) = |x|^2 \).

Figure: \( \beta = 5 \) on the left and \( \beta = 15 \) on the right.
GROUND STATES: HARMONIC TRAP

Figure: $\beta = 25$ on the left and $\beta = 140$ on the right.
**GROUND STATES: QUARTIC TRAP**

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 \( V(x) = |x|^4 \).

Figure: \( \beta = 55 \) on the left and \( \beta = 90 \) on the right.
**GROUND STATES: QUARTIC TRAP**

Figure: $\beta = 140$ on the left and $\beta = 195$ on the right.
**The Local Density Approximation**

For large $\beta$, it is expected that the energy of the ground state

$$ E(u) \approx E_{\beta}^{\text{TF}}(|u|^2) = \int_{\mathbb{R}^2} \left( e(\beta, |u|^2(x)) + V(x)|u|^2(x) \right) dx, $$

where $e(\beta, \rho)$ is the thermodynamic limit of the ground state energy of a homogeneous analogue with density $\rho$ and statistic parameter $\beta$.

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**The constant $e(1, 1)$**

By a scaling

$$ e(\beta, \rho) = \beta \rho^2 e(1, 1), $$

which yields a TF energy

$$ E_{\beta}^{\text{TF}}(\rho) = \int_{\mathbb{R}^2} \left( \beta \rho(x)^2 e(1, 1) + V(x)\rho(x) \right) dx, $$

and a TF ground state, with $\lambda_{\beta}^{\text{TF}}$ the chemical potential for $L^1$ normalization,

$$ \rho_{\beta}^{\text{TF}}(x) = (2\beta e(1, 1))^{-1} (\lambda_{\beta}^{\text{TF}} - V(x))_+. $$

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EVALUATING $e(1, 1)$

Suppose that $V(x) = |x|^s$, $s > 0$. Then, the length scale of the cloud is of the order $\beta^{1/(s+2)}$ and, by scaling,

$$\mathcal{E}_\beta^{TF}(\rho_{\beta}) = E_\beta^{TF} = \beta^{s/(s+2)} E_1^{TF},$$

where we compute

$$E_1^{TF} = \frac{1}{2} \frac{s}{s + 1} \left( \frac{s + 2}{s} \right)^{2 \frac{s+1}{s+2}} \left( \frac{2e(1, 1)}{\pi} \right)^{\frac{s}{s+2}}.$$

$e(1, 1)$ as a function of $E_\beta^{TF}$

We recover

$$e(1, 1) = \frac{\pi}{2} \left( 2 \frac{s + 1}{s} \right)^{\frac{s+2}{s}} \left( \frac{s}{s + 2} \right)^{2 \frac{s+1}{s}} \frac{(E_\beta^{TF})^{\frac{s+2}{2}}}{\beta}.$$
**Numerical evaluation of $e(1,1)$**

![Graphs](image)

Figure: $e(1,1)$ for harmonic ($s = 2$) on the left and quartic ($s = 4$) on the right.

**Numerical value of $e(1,1)$**

A frequently used first guess is in fact $e(1,1) \approx 2\pi$. Here, we obtain

$$e(1,1) \approx \frac{4\pi^{3/2}}{3} > 2\pi.$$
Density profile comparison

By using the numerical value of $e(1,1)$, we are able to deduce a theoretical density profile.

Figure: Theoretical profile of the density vs rotationally-averaged numerical profile for harmonic potential with $\beta = 90$ on the left and quartic potential with $\beta = 140$. 
**Vortex Density**

By separating the density and the phase, one obtains

$$\mathcal{E}(\sqrt{\rho}e^{i\varphi}) = \int_{\mathbb{R}^2} \left( |\nabla \sqrt{\rho}|^2 + (|\nabla \varphi + \beta A[\rho]|^2 + V)\rho \right) dx.$$  

A minimization of the second term suggests that

$$\nabla \varphi \approx -\beta A[\rho],$$

which gives, by taking the curl,

**Average Vortex Density**

$$\text{curl} \nabla \varphi \approx -2\pi \beta \rho.$$  

For the TF ground state, the expected number of vortices in a disk of radius $R$ is given by

$$N_v(R) = 4\pi^2 \beta \int_0^R \rho_{\beta}^{\text{TF}}(r) dr.$$
VORTEX DENSITY COMPARAISON

Figure: Theoretical vs numerical vortex density for harmonic potential with $\beta = 90$ on the left and quartic potential with $\beta = 140$. 
THE END

Thank you for your attention