The quantum N-body problem in Mathematics

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What is math useful for

Math is good for

- expressing a problem/model in an unambiguous way
- deriving exact properties of a model, which can then be used for calibration in empirical approximations
- proving the existence and properties of solutions, which helps to design adapted numerical methods
- developing validated numerical strategies
- explaining universal physical phenomena using abstract concepts (e.g. symmetry)

Math is really not efficient for

- showing fine properties of specific complex systems

In this talk: new abstract point of view, which explains the universal behavior of N-body systems in mean-field regime

Exchangeability and independence

- Famous result in probability theory says that for **many** events

Exchangeability (symmetry) $\Longrightarrow$ Independence

de Finetti '31, Hewitt-Savage '55

- $(X_n)_{n\geq 1}$ **infinite** set of random variables which are **exchangeable**

$$\mathbb{E}\left[f(X_{i_1},...,X_{i_k})\right] = \mathbb{E}\left[f(X_1,...,X_k)\right], \qquad \forall f, k \quad \forall i_1 \neq \cdots \neq i_k$$

then they are essentially **independent**: There exists a probability $\mathscr{P}$ over probabilities p's such that

$$\mathbb{E}\left[f(X_1,...,X_k)\right] = \int \bigg(\underbrace{\int f(x_1,...,x_k) dp(x_1)\cdots dp(x_k)}_{\text{i.i.d. random variables}} \bigg) \underbrace{d\mathscr{P}(p)}_{\text{mixture}}, \qquad \forall f, k$$

- exists quantitative estimates on error in the case of N random variables (Diaconis-Freedman '80)
- less known **quantum version** (Størmer '69, Hudson-Moody '75) important in quantum information theory, mean-field limits for quantum gases (Lewin-Nam-Rougerie '14–20)

Bosonic k-particle density matrices

N bosons in $\mathbb{R}^d$, wavefunction Ψ

$$\Gamma^{(k)}_\Psi(x_1,\dots,x_k;y_1,\dots,y_k)=\frac{N!}{(N-k)!}\int_{(\mathbb{R}^d)^{N-k}}\Psi(x_1,\dots,x_k,Z)\overline{\Psi(y_1,\dots,y_k,Z)}\,dZ$$

$\Gamma^{(k)}_\Psi\geq 0$, $\mathrm{tr}(\Gamma^{(k)}_\Psi)=N!/(N-k)!$ hence

$$\text{largest eigenvalue of } \Gamma^{(k)}_\Psi\leq\frac{N!}{(N-k)!}\underset{N\to\infty}{\sim}N^k$$

This is optimal for a Bose-Einstein condensate $\Psi(x_1,\dots,x_N)=u(x_1)\cdots u(x_N)$, then $\Gamma^{(k)}_\Psi=\frac{N!}{(N-k)!}|u^{\otimes k}\rangle\langle u^{\otimes k}|\sim N^k|u^{\otimes k}\rangle\langle u^{\otimes k}|$

Informal quantum de Finetti theorem for physicists

(Fragmented) Bose-Einstein condensation is the only way to create eigenvalues of order N^k in $\Gamma^{(k)}_\Psi$.

Quantum de Finetti

Assume $N^{-k}\Gamma_N^{(k)} \to \Upsilon^{(k)}$ in a sufficiently strong sense when $N \to \infty$, for all $k \geq 1$

Theorem (quantum de Finetti)

Let $(\Upsilon^{(k)})_{k\geq 1}$ *be an* **infinite** *sequence of* **bosonic** *density matrices so that* $\mathrm{tr}_k\, \Upsilon^{(k)} = \Upsilon^{(k-1)}$ *and* $\mathrm{tr}(\Upsilon^{(1)}) = 1$*. Then* $\exists\ \mathscr{P}$ *such that*

$$\Upsilon^{(k)} = \int_{\int_{\mathbb{R}^d} |u|^2=1} |u^{\otimes k}\rangle\langle u^{\otimes k}|\, d\mathscr{P}(u), \qquad \forall k \geq 1$$

(Størmer '69, Hudson-Moody '75)

Not all the particles need to be condensed!

Theorem (better quantum de Finetti)

Assume $N^{-k}\Gamma_N^{(k)} \to \Upsilon^{(k)}$ *in any sense that you can imagine, for all* $k \geq 1$*. Then* $\exists \mathscr{P}$ *such that*

$$\Upsilon^{(k)} = \int_{\int_{\mathbb{R}^d} |u|^2\leq 1} |u^{\otimes k}\rangle\langle u^{\otimes k}|\, d\mathscr{P}(u), \qquad \forall k \geq 1$$

(Lewin-Nam-Rougerie '14)

Quantum de Finetti theorem in finite dimension

Replace one-body space $L^2(\mathbb{R}^d)$ by a subspace $\mathfrak{H}$ of finite-dimension d
Call $S\mathfrak{H}$ the unit sphere of $\mathfrak{H}$

- **Coherent state representation** (Schur's lemma)

$$\mathbb{1}_{\bigotimes_s^N \mathfrak{H}} = \binom{N+d-1}{d-1} \int_{S\mathfrak{H}} |u^{\otimes N}\rangle\langle u^{\otimes N}| \, du$$

Over-complete basis $(u^{\otimes N})_{u \in S\mathfrak{H}}$ with $\left\langle u^{\otimes N}, v^{\otimes N}\right\rangle = \langle u, v\rangle^N \to 0$ as $N \to \infty$

Theorem (Quantitative de Finetti in dimension d)

For the Husimi measure $d\mu_\Psi(u) = \binom{N+d-1}{d-1} |\langle u^{\otimes N}, \Psi\rangle|^2 \, du$, *we have*

$$\left\| \frac{\Gamma_\Psi^{(k)}}{N^k} - \int_{S\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| \, d\mu_\Psi(u) \right\| \leq \frac{4kd}{N}.$$

(Christandl-Konig-Mitchitson-Renner '04, Lewin-Nam-Rougerie '15)

N-body problem in mean-field limit

$$H_N = \sum_{j=1}^{N} \underbrace{\frac{|-i\nabla_{x_j} + A(x_j)|^2}{2} + V(x_j)}_{:=h_{x_j}} + \frac{1}{N} \sum_{1\le k<\ell\le N} w(x_k - x_\ell)$$

Theorem (BEC in mean-field limit)

Assume that the system is confined (either by V or A). Let Ψ_N be a bosonic ground state for H_N. Then

$$\lim_{N\to\infty} \frac{\langle \Psi_N, H_N \Psi_N\rangle}{N} = \min_{\int_{\mathbb{R}^d} |u|^2=1} \left\{ \langle u, hu\rangle + \frac{1}{2} \iint_{\mathbb{R}^d\times\mathbb{R}^d} w(x-u)|u(x)|^2|u(y)|^2\, dx\, dy \right\}$$

and (maybe after extraction of a subsequence) there exists a probability measure $\mathscr{P}$ over the set $\mathcal{M}$ of Gross-Pitaevskii minimizers u such that

$$N^{-k}\Gamma^{(k)}_{\Psi_N} \to \int_{\mathcal{M}} |u^{\otimes k}\rangle\langle u^{\otimes k}|\, d\mathscr{P}(u), \qquad \forall k\ge 1$$

No particular condition on w, which can be repulsive, attractive or both

Comments

- Similar result when the system is not confined, but much more difficult (some particles may be lost at infinity)
- When u is unique and non-degenerate, one can identify the next order for every fixed eigenvalue of H_N, given by Bogoliubov theory
  (Seiringer '11, Grech-Seiringer '13, Lewin-Nam-Serfaty-Solovej '15, ...)
- This is a high density / small interaction regime
- A real trapped Bose gas does not have w/N. But in dilute regime and after scaling, one gets w_N/N where $w_N(x) = N^3 w(Nx)$
  $\rightsquigarrow$ Gross-Pitaevskii with $4\pi a \delta_0$ instead of w, with a =scattering length (3D)
  (Lieb-Seiringer-Yngvason '00s)

“Bosonic” atoms

Many ways to see why Pauli’s principle is so important. One is to remove it and see what happens!

Atom at scale x/N

$$\sum_{j=1}^{N} -\frac{\Delta_{x_j}}{2} - \frac{Z}{|x_j|} + \sum_{1\leq j<k<N} \frac{1}{|x_j - x_k|} \sim N^2 \left(\sum_{j=1}^{N} -\frac{\Delta_{x_j}}{2} - \frac{Z}{N|x_j|} + \frac{1}{N} \sum_{1\leq j<k<N} \frac{1}{|x_j - x_k|} \right)$$

In limit $N \to \infty$ with $N/Z = \kappa$ fixed, Hartree model

$$\frac{1}{2}\int_{\mathbb{R}^3} |\nabla u(x)|^2\,dx - \kappa^{-1}\int_{\mathbb{R}^3} \frac{|u(x)|^2}{|x|}\,dx + \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|u(x)|^2|u(y)|^2}{|x-y|}\,dx\,dy$$

- convergence of ground state energy and PDM
- bosonic atoms are stable for $N \lesssim 1.21\,Z$!

(Benguria-Lieb ’83, Solovej ’90, Bach ’91, Bach-Lewis-Lieb-Siedentop ’93, Lewin-Nam-Rougerie ’14)

Fermions

Theorem (Yang's inequalities)

For fermions, largest eigenvalue of $\Gamma_\Psi^{(k)} \leq C_k N^{[\frac{k}{2}]}$

(Yang '63)

Furthermore, $\Gamma_\Psi^{(k)}$ stays bounded when tested against Slater determinants:

$$\left\langle u_1 \wedge \cdots \wedge u_k, \Gamma_\Psi^{(k)} v_1 \wedge \cdots \wedge v_k \right\rangle = \left\langle a^\dagger(v_1) \cdots a^\dagger(v_k) a(u_k) \cdots a(u_1) \right\rangle_\Psi$$

hence both $N^{-k}\Gamma_\Psi^{(k)}$ and $N^{-[\frac{k}{2}]}\Gamma_\Psi^{(k)}$ always tend to 0

- **Open mathematical problem:** condensation of Cooper pairs for eigenvalues of order $N^{[\frac{k}{2}]}$ (Yang '63, Coleman-Yukalov)
- **Classical** de Finetti theorem useful in fermionic **semi-classical** limits (Fournais-Lewin-Solovej '18)

Wigner functions

N fermions in a domain $\Omega \subset \mathbb{R}^d$ satisfy the Li-Yau bound

$$\left\langle \Psi, \sum_{j=1}^N -\Delta_j \Psi \right\rangle \geq \sum_{j=1}^N \lambda_j(-\Delta_{|\Omega}) \geq 2c_{\rm TF} N^{1+\frac{2}{d}} |\Omega|^{-\frac{2}{d}}$$

Definition (Wigner function)

$$W_\Psi^{(k)}(x_1, p_1, ..., x_k, p_k) = \int_{(\mathbb{R}^d)^k} \Gamma_\Psi^{(k)}\Big(x_1 + \frac{y_1}{2}, ... ; x_1 - \frac{y_1}{2}, ...\Big)\, e^{-i\sum_{\ell=1}^k \frac{p_\ell \cdot y_\ell}{\varepsilon}} dy_1 \cdots dy_k$$

Then $\displaystyle\int_{\mathbb{R}^{2dk}} W_\Psi^{(k)} = \varepsilon^{dk} \frac{N!}{(N-k)!} \to 1$ for $\varepsilon = N^{-\frac{1}{d}}$

Theorem (Phase-space fermionic de Finetti theorem)

Let $\varepsilon = N^{-\frac{1}{d}}$. Let Ψ_N be fermionic states such that $\varepsilon^2 \left\langle \Psi_N, \sum_{j=1}^N -\Delta_j \Psi_N \right\rangle \leq CN$ and assume that $W_{\Psi_N}^{(k)} \to W^{(k)}$ (weakly) for every k. Then $\exists \mathscr{P}$ such that

$$W^{(k)} = \int_{\substack{0 \leq m \leq 1 \\ (2\pi)^{-d} \iint m \leq 1}} m^{\otimes k}\, d\mathscr{P}(m), \qquad \forall k \geq 1$$

Mean-field / semi-classical limit

$$H_N = \sum_{j=1}^N \frac12 \left|\frac{-i\nabla_{x_j}}{N^{\frac1d}} + A(x_j)\right|^2 + V(x_j) + \frac1N \sum_{1\le k<\ell\le N} w(x_k - x_\ell)$$

Theorem (Thomas-Fermi in mean-field limit)

Assume that $V \to +\infty$ at infinity. Let Ψ_N be a fermionic ground state for H_N. Then

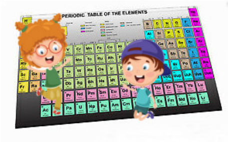
$$\lim_{N\to\infty} \frac{\langle \Psi_N, H_N \Psi_N\rangle}{N} = \min_{\int_{\mathbb{R}^d}\rho=1} \bigg\{ c_{TF}\int_{\mathbb{R}^d} \rho(x)^{1+\frac2d}\,dx + \int_{\mathbb{R}^d} V(x)\rho(x)\,dx + \frac12 \iint_{\mathbb{R}^d\times\mathbb{R}^d} w(x-y)\rho(x)\rho(y)\,dx\,dy \bigg\}$$

and (maybe after extraction of a subsequence) there exists a probability measure $\mathscr{P}$ over the set $\mathcal{M}$ of Thomas-Fermi minimizers ρ such that

$$N^{-k}\Gamma^{(k)}_{\Psi_N} \to \int_{\mathcal{M}} (m_\rho)^{\otimes k}\, d\mathscr{P}(\rho), \qquad \forall k \ge 1$$

with $m_\rho(x,p) := \mathbb{1}(|p + A(x)|^2 + V(x) + \rho * w \le \mu_\rho)$

Playing hopscotch on the periodic table



Atom at scale $x/N^{1/3}$

$$\sum_{j=1}^{N} -\frac{\Delta_{x_j}}{2} - \frac{Z}{|x_j|} + \sum_{1\leq j<k<N} \frac{1}{|x_j - x_k|} \sim N^{\frac{4}{3}} \left(\sum_{j=1}^{N} -\frac{\Delta_{x_j}}{2N^{\frac{2}{3}}} - \frac{Z}{N|x_j|} + \frac{1}{N} \sum_{1\leq j<k<N} \frac{1}{|x_j - x_k|} \right)$$

When $N \to \infty$ with $N/Z = \kappa$ fixed, get Thomas-Fermi model

$$c_{\rm TF} \int_{\mathbb{R}^3} \rho(x)^{\frac{5}{3}}\, dx - \kappa^{-1} \int_{\mathbb{R}^3} \frac{\rho(x)}{|x|}\, dx + \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|}\, dx\, dy$$

- convergence of ground state energy and Wigner functions
- atoms are stable for $N \lesssim Z$

(Lieb-Simon '77, Lieb-Sigal-Simon-Thirring '84, Fournais-Lewin-Solovej '18)

- Higher order corrections given by Scott and Dirac-Schwinger

(Siedentop-Weikard '87, Hughes '90, Fefferman-Seco '90)

Two famous open problems for periodic table

Ionization conjecture

A nucleus of charge Z can never bind more than $Z + C$ electrons (where C is a universal constant).

- $Z + o(Z)$ is known with a bad $o(Z)$
- very "fermionic" question, which needs a better math. understanding of Pauli...
- Many other open problems related to Thomas-Fermi (Solovej)

Affinity-ionization conjecture

For fixed Z, the ground state energy $N \mapsto E(Z, N)$ of an atom is convex in N.

- electron ionization energy $\geq$ electron affinity
- important for using grand-canonical states / fractional Kohn-Sham
  (Perdew-Parr-Levy-Balduz '82, Lewin-Lieb-Seiringer '19)