Effective Quantum Dynamics

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Area: Mathematical Physics
Framework: Non-relativistic Quantum Mechanics

Topics from physics:

- Non-equilibrium dynamics
- Non-equilibrium statistical physics

Topics from mathematics:

- analysis (mostly functional analysis, a bit of harmonic analysis)
- PDEs

central object: wave function $\psi^t \in L^2(\mathbb{R}^{3N} \to \mathbb{C})$ for all $t \in \mathbb{R}$
$\hookrightarrow$ basis for describing atoms, molecules (chemistry!), computers, ...

fundamental equation: **Schrödinger equation**

$$i\partial_t \psi^t = H\psi^t$$

H self-adjoint operator $\Rightarrow \psi^t = e^{-iHt}\psi^0$ for all $\psi^0 \in L^2$ (Stone's theorem)

$$i\partial_t \psi^t = H\psi^t$$

form of H:

$$H = \sum_{j=1}^{N}(-\Delta_{x_j}) + \lambda_N \sum_{1\le i<j\le N} v(x_i - x_j),$$

$\Delta =$ Laplacian, $v : \mathbb{R}^3 \to \mathbb{R}$ interaction potential, $v(x) = v(-x)$, $\lambda_N \in \mathbb{R}$

for large N: impossible to solve analytically or numerically ($L^2(\mathbb{R}^3)^{\otimes N}$!)

Goal: approximations for ψ^t
(large scale or average behavior of ψ^t)

two fundamental kinds of particles:

- bosons: $\psi^B(x_1, \ldots, x_N) = \psi^B(x_{\sigma(1)}, \ldots, x_{\sigma(N)})$
- fermions: $\psi^F(x_1, \ldots, x_N) = (-1)^\sigma \psi^F(x_{\sigma(1)}, \ldots, x_{\sigma(N)})$

($\sigma =$ permutation of $1, \ldots, N$, $(-1)^\sigma =$ sign of the permutation)

Bosons: most simple case is $\lambda_N = 1/N$

- uncorrelated initial state

$$\psi^0(x_1, \dots, x_N) = \prod_{i=1}^{N} \varphi^0(x_i), \quad \text{where } \varphi^0 \in L^2(\mathbb{R}^3)$$

- goal: show that

$$\psi^t(x_1, \dots, x_N) \approx \prod_{i=1}^{N} \varphi^t(x_i),$$

for all t, where φ^t is solution to the Hartree equation

$$i\partial_t \varphi^t = -\Delta\varphi^t + \left(v * |\varphi^t|^2\right)\varphi^t$$

More involved limits: $v(x) \to N^{3\beta} v(N^\beta x)$ (NLS or Gross-Pitaevskii)

$\hookrightarrow$ results by Hepp ('74), Spohn ('80), Erdös, Yau ('01), ..., Pickl ('11)

Fermions: $\psi(x_1, \dots, x_N) = (-1)^\sigma \psi(x_{\sigma(1)}, \dots, x_{\sigma(N)})$

most simple state: antisymmetric product state

$$\left(\bigwedge_{j=1}^{N} \varphi_j\right)(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} (-1)^\sigma \prod_{j=1}^{N} \varphi_{\sigma(j)}(x_j)$$

for orthonormal $\varphi_1, \dots, \varphi_N \in L^2(\mathbb{R}^3)$
due to orthonormality: for $v(x) = |x|^{-1}$ choose $\lambda_N = N^{-2/3}$ only

- initial state
$$\psi^0 = \bigwedge_{j=1}^{N} \varphi_j^0$$
- goal: show that
$$\psi^t \approx \bigwedge_{j=1}^{N} \varphi_j^t$$

  for all t, where φ_j^t's are solutions to the Hartree-Fock equations

$$i\partial_t \varphi_j^t = -\Delta \varphi_j^t + \lambda_N \sum_{k=1}^{N} \left(v * |\varphi_k^t|^2\right) \varphi_j^t - \lambda_N \sum_{k=1}^{N} \left(v * \overline{\varphi_k^t} \varphi_j^t\right) \varphi_k^t$$

$\hookrightarrow$ results by Narnhofer, Sewell ('81), Spohn ('81), Elgart, Erdös, Schlein, Yau ('04), Benedikter, Porta, Schlein ('14), SP, Pickl ('14–'16)

Theorem (Bach, Breteaux, SP, Pickl, Tzaneteas [J. Math. Pures Appl. (2016)])

Let $v(x) = |x|^{-1}$, $\lambda_N = N^{-2/3}$. *Assume* $\psi^0 = \bigwedge_{j=1}^N \varphi_j^0$ *with orthonormal* $\varphi_1^0, \ldots, \varphi_N^0$, *such that*

$$\sum_{j=1}^N \left|\left|\nabla \varphi_j^0\right|\right|^2 \leq CN.$$

Then, for all bounded operators $A : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$, *there is* $C > 0$ *such that* $(A_1 := A \otimes \mathbb{1} \ldots \otimes \mathbb{1})$

$$\left| \left\langle \psi^t, A_1 \psi^t \right\rangle - \left\langle \bigwedge_{j=1}^N \varphi_j^t, A_1 \bigwedge_{j=1}^N \varphi_j^t \right\rangle \right| \leq ||A|| \, e^{Ct} N^{-1/6}.$$

Theorem (SP ('16) [arXiv:1609.04754])

Assume additionally

$$\sum_{j=1}^N \left|\left|\nabla^4 \varphi_j^0\right|\right|^2 \leq CN.$$

Then

$$\left| \left\langle \psi^t, A_1 \psi^t \right\rangle - \left\langle \bigwedge_{j=1}^N \varphi_j^t, A_1 \bigwedge_{j=1}^N \varphi_j^t \right\rangle \right| \leq ||A|| \, e^{C(t)} N^{-1/2}.$$

Some open problems:

- For $v(x) = |x|^{-1}$: extend the time scales in the previous results $\hookrightarrow$ semiclassical analysis
- For bosons and $v(x) \to N^{3\beta} v(N^\beta x)$: more detailed approximation

$$\psi_t = \sum_{k=0}^{N} \varphi_t^{\otimes(N-k)} \otimes_s \chi_t^{(k)},$$

where $\chi_t^{(k)}$ comes from the Bogoliubov approximation

- Hartree-Fock equations for $v(x) = -|x|^{-1}$ (gravitation):

$$i\partial_t \varphi_j^t = \sqrt{-\Delta + m^2}\varphi_j^t + \lambda_N \sum_{k=1}^{N} \left(v * |\varphi_k^t|^2\right)\varphi_j^t - \lambda_N \sum_{k=1}^{N} \left(v * \overline{\varphi_k^t}\varphi_j^t\right)\varphi_k^t$$

Properties and time scales of finite time blow-up for large $N > N_{crit}$?

- Similar questions for spin systems, e.g., Heisenberg model

$$H = -\sum_{<x,y>\subset\Lambda} S_x \cdot S_y,$$

$\Lambda \subset \mathbb{Z}^d$, $< x, y >$ nearest neighbors, spin operators $[S^i, S^j] = i\varepsilon_{ijk} S^k$
$\hookrightarrow$ dynamics of low energy states $\Rightarrow$ interaction-free quasi particles
$\hookrightarrow$ spectral analysis

Thank you for your attention!