Effective Dynamics of Bose-Fermi Mixtures

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Texas A & M

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What are Bosons?

Bosons are quantum particles whose statistics are *symmetric*:

$$L_s^2(\mathbb{R}^{dN}) = \left\{ \Psi_N \in L^2(\mathbb{R}^{dN}) \,:\, \forall \sigma \in S_N,\, \Psi(x_{\sigma(1)}, \ldots, x_{\sigma(N)}) = \Psi(x_1, \ldots, x_N) \right\}$$

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Question: How do we effectively describe $\Psi_N(t)$ for $N \gg 1$?

Bose-Einstein Condensates

It was noticed by Bose and Einstein in 1924 that symmetric wave functions could *condense* and be represented by a single wave function,

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This was experimentally confirmed much later by cooling a gas of bosons to their lowest energy state [Cornell, Wieman 1995], [Ketterle 1995].

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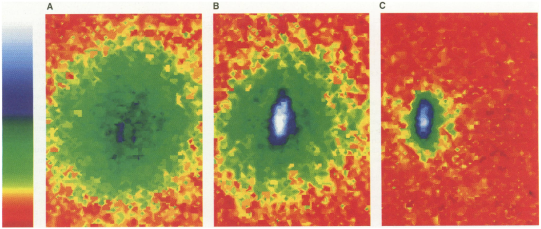

Fig. 2. False-color images display the velocity distribution of the cloud (**A**) just before the appearance of the condensate, (**B**) just after the appearance of the condensate, and (**C**) after further evaporation has left a sample of nearly pure condensate. The circular pattern of the noncondensate fraction (mostly yellow and green) is an indication that the velocity distribution is isotropic, consistent with thermal equilibrium. The condensate fraction (mostly blue and white) is elliptical, indicative that it is a highly nonthermal distribution. The elliptical pattern is in fact an image of a single, macroscopically occupied quantum wave function. The field of view of each image is 200 μm by 270 μm. The observed horizontal width of the condensate is broadened by the experimental resolution.

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Schrödinger → Hartree

Definition (Marginal)

Given $\Psi_N \in L^2(\mathbb{R}^{dN})$ define the first marginal

$$\begin{aligned}\gamma_N(t;x_1,x_1') &= N\int_{\mathbb{R}^{2d(N-1)}} \Psi_N(t,x_1,x_2,\dots,x_N)\overline{\Psi_N}(t,x_1',x_2,\dots,x_N)dx_2\dots dx_N \\ &= N\mathrm{Tr}_{2,\dots,N}|\Psi_N\rangle\langle\Psi_N|\end{aligned}$$

Question: Given the Hamiltonian

$$H_N := \frac{-\hbar^2}{2m}\sum_{i=1}^{N}\Delta_{x_i} + \frac{1}{N}\sum_{i,j=1}^{N} V(x_i - x_j),$$

and the initial data $\Psi_N(0) = \psi_0^{\otimes N}$, how does γ_N evolve under Schrödinger's equation?

Schrödinger → Hartree

Physicists answer: Let $\psi(t)$ solve

$$\begin{cases} i\hbar\partial\psi = -\frac{\hbar^2}{2m}\Delta\psi + (V * |\psi|^2)\psi \\ \psi(0) = \psi_0 \end{cases} . \tag{1}$$

Then by asymptotic expansions

$$\gamma_N(t) \approx |\psi(t)\rangle\langle\psi(t)| \qquad \text{as } N \to \infty. \tag{2}$$

Schrödinger → Hartree

Hartree derivation:

- [Spohn '80] for bounded interactions
- [Erdös, Yau '01] for Coulomb interactions
- [Rodnianski, Schlein '09], [Chen, Oon Lee, Schlein '11] with rates using Second Quantization
- [Dietze, Lee '22] uniform-in-time convergence

Gross-Pitaevskii/NLS:

- [Erdös, Schlein, Yau '06], [Adami, Golse, Teta '07] first results for deriving NLS
- [Kirkpatrick, Schlein, Staffilani '11] NLS on $\mathbb{T}^2$
- [Chen, Hainzl, Pavlović, Seiringer '15] Gross-Pitaevskii hierarchy unconditional uniqueness

What are Fermions?

Fermions are quantum particles whose statistics are *antisymmetric*:

$$L_a^2(\mathbb{R}^{dM}) =$$

$$\left\{ \Psi_M \in L^2(\mathbb{R}^{dM}) : \forall \sigma \in S_M, \Psi(x_{\sigma(1)}, \ldots, x_{\sigma(M)}) = (-1)^{\mathsf{sgn}(\sigma)} \Psi(x_1, \ldots, x_M) \right\}$$

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They also evolve according to Schrödinger's equation

$$i\hbar \partial_t \Psi_M = H_M \Psi_M$$

where H_M is the Hamiltonian encoding the physics of the system.

Fermi Gas: I

Fermionic gases obey the *Pauli Exclusion Principle* and cannot condense.

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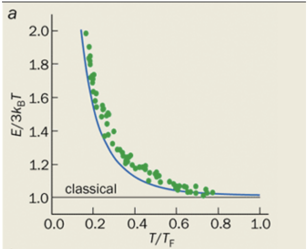
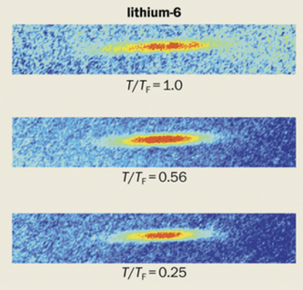
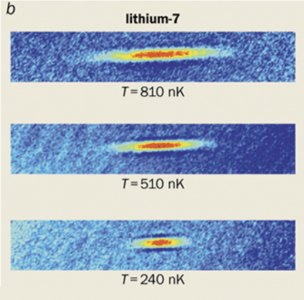


Fermi Pressure



$^6Li =$ Fermion



$^7Li =$ Boson

Fermi Gas: II

Given $\{\phi_i\}_{i=1}^M$ orthonormal set in $L^2(\mathbb{R}^d)$ we can construct *Slater determinants*

$$\Psi_M(x_1,\ldots,x_M) := \frac{1}{\sqrt{M!}} \det_{i,j}(\phi_i(x_j)) \in L_a^2(\mathbb{R}^{dM})$$

which are good approximations of the ground state of a weakly interacting fermionic gas.

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Their first marginal can be checked to be

$$\gamma_M = \sum_{i=1}^M |\phi_i\rangle\langle\phi_i|$$

Schrödinger → Hartree-Fock

For large M, physcists expect solutions of the Hartree-Fock equation

$$\begin{cases} i\hbar\partial_t \omega(t) = \left[\frac{-\hbar^2}{2m}\Delta + V * \rho(t) - X(t), \omega(t)\right] \\ \rho(t,x) = M^{-1}\omega(t;x,x) \\ \omega(0) = \omega_0 \in \mathscr{L}^2(L^2(\mathbb{R}^d)) \text{ with } \mathrm{Tr}\omega_0 = M \end{cases}$$

to approximate the Schrödinger evolution of $\gamma_M(t)$ under the Hamiltonian

$$H_M := \frac{-\hbar^2}{2m}\sum_{i=1}^{M}\Delta_{x_i} + \frac{1}{M}\sum_{i,j=1}^{M} V(x_i - x_j),$$

Schrödinger → Hartree-Fock

For $\hbar = 1$ regime:

- [Bardos, Golse, Gottlieb, Mauser '03] regular interactions
- [Frölich, Knowles '11] Coulomb interactions

For $\hbar = M^{-1/d}$ regime:

- [Elgart, Erdös, Schlein, Yau '04] for analytic potentials
- [Benedikter, Porta, Schlein '14] with rates using Second Quantization
- [Benedikter, Porta, Schlein '14] relativistic
- [Benedikter Jakšić, Porta, Saffirio, Schlein '16] for mixed states
- Porta Radamacher, Saffirio, Schlein '17] for Coulomb
- [Fresta, Porta, Schlein '23] for high density

Hartree-Fock $\to$ Vlasov

By considering a "macroscopic/semiclassical regime" where $\hbar = M^{-1/d}$ solutions of Hartree-Fock behave like solutions of the Vlasov equation:

$$\begin{cases} (\partial_t + p \cdot \nabla_x + F_f(t) \cdot \nabla_p) f(t,x,p) = 0 \\ F_f(t,x) = -\int \nabla V(x-y) f(t,y,p) dy dp \end{cases}$$

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- ▷ [Narnhofer, Sewell '81] [Spohn '81] first results (Schrödinger to Vlasov)
- ▷ [Lions, Paul '93], [Markowich, Mauser '93], [Gasser, Illner, Markowich '98] Hartree-Fock to Vlasov
- ▷ [Athanassoulis, Paul, Pezzotti, Pulverenti '11] improved convergence
- ▷ [Benedikter, Porta, Saffiro, Schlein '16] quantitative convergence for discontinuous initial data

Bose-Fermi Mixtures: Physics

Investigating degenerate mixtures of bosons and fermions is an extremely active area of research for understanding novel quantum bound states (e.g. superconductors, superfluids, and supersolids).

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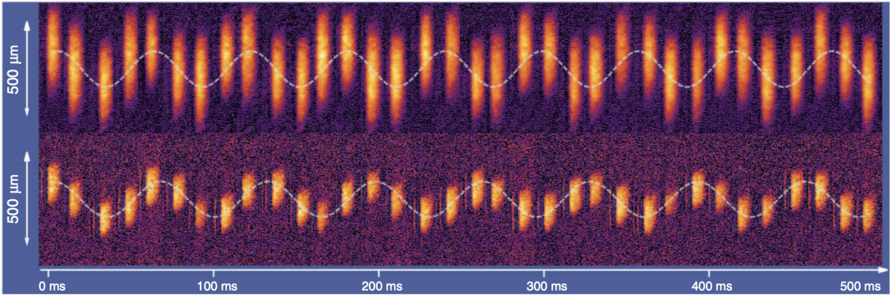

Bose-Fermi Mixtures: Mathematics

Define the Hamiltonian and phase space for N bosons and M fermions:

$$\mathscr{H} := L_s^2(\mathbb{R}^{dN}) \otimes L_a^2(\mathbb{R}^{dM})$$

$$H := \frac{\hbar^2}{2m_F}\sum_{i=1}^{M}(-\Delta_{x_i}) \otimes \mathbb{1} + \frac{\hbar^2}{2m_B}\sum_{j=1}^{N} \mathbb{1} \otimes (-\Delta_{y_j}) + \lambda \sum_{i,j=1}^{N,M} V(x_i - y_j)$$

Bose-Fermi Mixtures: Mathematics

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Our question: How do we obtain an effective description of Schrödinger's equation for large N, M?

Theorem 1: Deriving an Effective Description

Let γ_B, γ_F be the bosonic and fermionic marginals, and consider (ω, ψ) solutions to the Hartree-Hartree equation

$$\begin{cases} i\hbar\partial_t \omega = [-(\hbar^2/2m_F)\Delta + \lambda N (V * \rho_B), \omega] \\ i\hbar\partial_t \psi = -(\hbar^2/2m_B)\Delta\psi + \lambda M (V * \rho_F)\psi \end{cases} . \tag{1}$$

Theorem (Informal)

Under low temperature and propagation of semi-classical structure assumptions, we have

$$\frac{1}{M}\|\gamma_F(t) - \omega(t)\|_{Tr} \leq \frac{C}{\sqrt{M}} \exp\left[C\lambda\sqrt{\frac{NM}{\hbar}}\left(1 + \sqrt{\frac{\hbar M}{N}}\right)\exp|t|\right],$$

$$\frac{1}{N}\|\gamma_B(t) - N|\psi(t)\rangle\langle\psi(t)|\|_{Tr} \leq \frac{C}{\sqrt{N}} \exp\left[C\lambda\sqrt{\frac{NM}{\hbar}}\left(1 + \sqrt{\frac{\hbar M}{N}}\right)\exp|t|\right].$$

Theorem 1: Proof ideas

We use the language and tools of Second Quantization over a bosonic and fermionic Fock space to study the fluctuation dynamics:

$$\mathscr{F} := \bigoplus_{N=1}^{\infty} L_s^2(\mathbb{R}^{dN}) \otimes \bigoplus_{M=1}^{\infty} L_a^2(\mathbb{R}^{dM})$$

The main difficulties and novelties were:

- The identification of a scaling window,
- Controlling products of the bosonic and fermionic number operators when analyzing the fluctuation dynamics.

Theorem 2: Scaling and Vlasov-Hartree

From Theorem 1, we identified a scaling regime

$$\lambda = \frac{1}{N}\ , \qquad \hbar = \frac{1}{M^{\frac{1}{d}}}\ , \qquad m_B = \hbar\ , \qquad m_F = 1 \quad \text{and} \quad N = M^{1+\frac{1}{d}}\ . \tag{2}$$

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Now consider the Vlasov-Hartree

$$\begin{cases} (\partial_t + p\cdot\nabla_x + F_B(t,x)\cdot\nabla_p)f = 0 \\ i\partial_t\psi = -\frac{1}{2}\Delta\psi + (V*\rho_F)\psi \\ (f,\psi)(0) = (f_0,\psi_0) \in L^1_+(\mathbb{R}^{2d})\times L^2(\mathbb{R}^d) \end{cases} \quad (3)$$

Theorem 2: Convergence

Given a marginal $\omega \in \mathscr{L}^1(L^2(\mathbb{R}^d))$, define the *Wigner transform* by

$$W^\hbar[\omega](x,p) := \frac{1}{(2\pi)^{\frac{d}{2}}} \int_{\mathbb{R}^d} \omega\left(x+\frac{y}{2}, x-\frac{y}{2}\right) e^{-i\frac{y\cdot p}{\hbar}} dy \tag{4}$$

Theorem (Informal)

Let $(\omega_0^\hbar, \psi_0^\hbar)$ be an admissible family of initial data for the Hartree-Hartree equation with

$$W^\hbar[\omega_0^\hbar] \to f_0, \quad \textit{and} \quad \psi_0^\hbar \to \psi_0 \quad \textit{as } \hbar \to 0.$$

Let $(\omega^\hbar(t), \psi^\hbar(t))$ be the solutions of the Hartree-Hartree equation and $(f(t), \psi(t))$ be solutions of the Vlasov-Hartree equation with respect to the scaling (2). *Then we obtain (with estimates)*

$$W^\hbar[\omega^\hbar](t) \to f(t), \quad \textit{and} \quad \psi^\hbar(t) \to \psi(t) \quad \textit{as } \hbar \to 0.$$

Future Directions

- What about the ground state problem? What about other scaling regimes?
- Can anything interesting be said about the Vlasov-NLS system?

$$\begin{cases} (\partial_t + p\cdot\nabla_x + F_B(t,x)\cdot\nabla_p + F_f(t,x)\cdot\nabla_p)f = 0 \\ i\partial_t\psi = -\frac{1}{2}\Delta\psi + (V * \rho_F)\psi + |\psi|^2\psi \end{cases}$$

Thanks!

Thank you!

References for Figures

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