Effective dynamics for interacting magnetic fermions

Analytic and algebraic methods in physics

Domenico Monaco [arXiv:2406.15041, arXiv:2503.16001]
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Curse of dimensionality

YES,

$$\mathrm{i}\,\hbar\,\frac{\mathrm{d}\Psi}{\mathrm{d}t}(t) = H\,\Psi(t)$$

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BUT

$$\Psi(t) = \Psi(t;\vec{x}_1,\ldots,\vec{x}_N)\,,$$

$$\vec{x}_i \in \mathbb{R}^d, \qquad N \sim 10^{23}$$

Effective equations

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In this talk

Derive **Hartree–Fock equations** as effective equations for the many-body Schrödinger dynamics of fermions in a **magnetic field**

- From the **Dirac–Frenkel variational principle**
- Through a more refined semiclassical + many-body analysis (**Fock-space methods**)
- Discuss their “effectiveness” (scaling of the error w.r.t. time and number of fermions)

1-body picture: Landau in a box

Landau Hamiltonian

$$H_1 = \frac{1}{2m}\left(-\mathrm{i}\hbar\vec{\nabla} - \frac{q}{c}\vec{A}(\vec{x})\right)^2 \quad \text{in} \quad L^2(\Lambda)$$

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- $\vec{A}(x_1, x_2) = (0, B\,x_1)$ magnetic potential in the Landau gauge, $qB > 0$
  $\rightsquigarrow$ uniform magnetic field $(0, 0, B)$

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- **magnetic flux quantization condition** (MPBC):

$$\Phi_B = BL_1L_2 = M\,\Phi_0, \quad M \in \mathbb{N}, \quad \Phi_0 = hc/q$$

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allows to impose **magnetic periodic boundary conditions**

$$\varphi(-L_1/2, x_2) = \mathrm{e}^{-\mathrm{i}\,2\pi M\,x_2/L_2}\,\varphi(L_1/2, x_2)$$
$$\varphi(x_1, -L_2/2) = \varphi(x_1, L_2/2)$$

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Theorem

With MPBC, H_1 is self-adjoint on the **magnetic Sobolev space**

$$H^2_{\vec{A}}(\Lambda) = \left\{\psi \in L^2(\Lambda) : H_1\psi \in L^2(\Lambda)\right\} .$$

The spectrum of H_1 consists of **Landau levels**

$$E_n = \frac{\hbar^2}{2m} b\,(2n+1)\,, \quad n \in \mathbb{N}\,, \quad b := \frac{qB}{\hbar c}$$

and each Landau level has finite degeneracy M:

$$\ker\left(H_1 - E_n\,\mathbf{1}\right) = \mathrm{Span}\left\{\varphi_{n,m} : m \in \mathbb{Z}/M\mathbb{Z}\right\} .$$

N-body picture: Fermions

- N-particle Hilbert space:

$$L^2(\Lambda)^{\otimes N} = L^2(\Lambda) \otimes \overset{(N \text{ times})}{\cdots} \otimes L^2(\Lambda)$$

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totally antisymmetric wave functions

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- $\mathcal{H}_N$ is generated by **Slater determinants**: given $\{\psi_1, \ldots, \psi_N\} \subset L^2(\Lambda)$ o.n. **orbitals**

$$\Psi(\vec{x}_1, \ldots, \vec{x}_N) = (\psi_1 \wedge \cdots \wedge \psi_N)(\vec{x}_1, \ldots, \vec{x}_N) := \frac{1}{\sqrt{N!}} \det \left[\psi_i(\vec{x}_j)\right]_{1 \leq i, j \leq N} \in \mathcal{H}_N$$

N-body picture: Interacting fermions in a magnetic field

N-body Landau Hamiltonian

$$H_N = \sum_{1 \le i \le N} H_1^{(i)} + \sum_{1 \le i < j \le N} V(\vec{x}_i; \vec{x}_j) \quad \text{in} \quad \mathcal{H}_N$$

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- $V(\vec{x};\vec{y}) = V(\vec{y};\vec{x})$ bounded function on $\Lambda \times \Lambda$: 2-body interactions among fermions

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⚠ Interactions introduce **correlations**: even if $\Psi(0)$ is a Slater determinant, $\Psi(t) = e^{-iH_N t/\hbar}\Psi(0)$ will **not** be a Slater determinant

Dirac–Frenkel variational principle

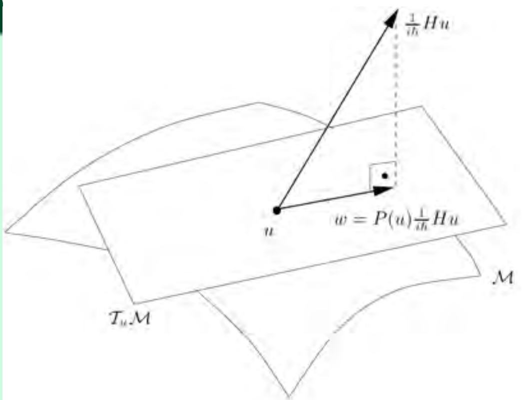
Effective equations

Project linear dynamics onto the nonlinear manifold of Slater determinants

$$\mathcal{M} := \{ u = a\,\varphi_1 \wedge \cdots \wedge \varphi_N : \\ a \in U(1)\,,\ \langle \varphi_i, \varphi_j \rangle = \delta_{i,j} \}$$

and study the effective (nonlinear) dynamics of the orbitals

$$\rightsquigarrow \quad \dot{u}(t) = \operatorname*{argmin}_{w \in \mathcal{T}_{u(t)}\mathcal{M}} \left\| w - \frac{1}{\mathrm{i}\hbar} H_N\, u(t) \right\|$$



Hartree–Fock effective equations

Theorem (see e.g. Lubich's book)

The solution $u(t) = a(t)\,\varphi_1(t) \wedge \cdots \wedge \varphi_N(t) \in \mathcal{M}$ to the Dirac–Frenkel principle has

- $a(t) = \mathrm{e}^{-\mathrm{i}\,\mathcal{E}_0^{(N)}\,t/\hbar}\,a(0)$, *with* $\mathcal{E}_0^{(N)} := \langle u(0), H_N\, u(0)\rangle = \langle \Psi(0), H_N\, \Psi(0)\rangle$
- $\{\varphi_1(t), \ldots, \varphi_N(t)\}$ *solutions of the* **Hartree–Fock equations**

$$\mathrm{i}\,\hbar\,\dot\varphi_\ell(t) = H_1\,\varphi_\ell(t) + K_\ell(t)\,\varphi_\ell(t) - \sum_{\ell' \neq \ell} X_{\ell,\ell'}(t)\,\varphi_{\ell'}(t)\,, \quad \ell \in \{1, \ldots, N\}\,, \quad \text{(HFE)}$$

where the **Hartree–Fock potential** K_ℓ *and the* **exchange potentials** $X_{\ell,n}$ *are*

$$K_\ell(t, \vec{x}) := \sum_{\ell' \neq \ell} \int_\Lambda \mathrm{d}\vec{y}\, V(\vec{x}; \vec{y})\, |\varphi_{\ell'}(t, \vec{y})|^2\,, \ell \in \{1, \ldots, N\}\,,$$

$$X_{\ell,\ell'}(t, \vec{x}) := \int_\Lambda \mathrm{d}\vec{y}\, V(\vec{x}; \vec{y})\, \overline{\varphi_{\ell'}(t, \vec{y})}\,\varphi_\ell(t, \vec{y})\,, \quad \ell, \ell' \in \{1, \ldots, N\}\,.$$

Hartree–Fock effective equations

Theorem (Cazenave, Esteban)

The system (HFE) *is (at least locally) well-posed: There exist a time interval* $0 \leq t \leq \bar{t}$ *for which a solution* $\varphi_\ell \in C^1([0,\bar{t}], L^2(\Lambda)) \cap C([0,\bar{t}], H^2_{\vec{A}}(\Lambda))$ *of the Hartree–Fock equations exists. Orthonormality of the* $\varphi_\ell(t)$*'s is preserved throughout the entire time interval.*

Effectiveness of the HFE

Theorem (Ferrero, M. arXiv:2406.15041)

Let $u(0) = \varphi_1(0) \wedge \cdots \wedge \varphi_N(0) \in \mathcal{M}$ *and* $u(t)$ *be the corresponding solution to the Dirac–Frenkel principle. Let also* $\Psi(t) := \mathrm{e}^{-\mathrm{i}H_N t/\hbar} u(0)$*. Then*

$$\|\Psi(t) - u(t)\|_{\mathcal{H}_N} \leq \frac{1}{\hbar} \sqrt{N(N-1)}\, \|V\|_{L^\infty(\Lambda\times\Lambda)}\, t\,.$$

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- Proof relies on decomposition

$$\mathcal{H}_N = \mathcal{H}_N^{(0)} \oplus \mathcal{H}_N^{(1)} \oplus \cdots \oplus \mathcal{H}_N^{(N)}$$

where $\mathcal{H}_N^{(s)}$ is spanned by Slater determinants in which s of the orbitals in $u(t)$ have been swapped with functions orthogonal to all of them

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- Error comes only from $\mathcal{H}_N^{(2)}$: 2-body correlations break Slater determinant structure
- Estimate is **linear** in time, in number of particles, and in strength of the interaction

Semiclassical mean-field scaling

- Hartree–Fock theory is believed to be relevant for fermions in the **semiclassical + mean-field scaling**:

$$\hbar \longrightarrow \hbar_{\text{eff}} := \hbar\, N^{-1/2}\,, \quad V(\vec{x};\vec{y}) \longrightarrow V_{\text{eff}}(\vec{x};\vec{y}) := N^{-1}\, V(\vec{x};\vec{y})$$

  in which both kinetic and interaction energy are $\mathcal{O}(N^2)$ and semiclassical times are of $\mathcal{O}(N^{-1/2})$

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- Our estimate becomes in this scaling

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  hence meaningful for times $t \ll N^{-1/2}$ much smaller than semiclassical scale
- Estimate is **not** expected to survive the **thermodynamic limit** ($N \to \infty, \Lambda \to \mathbb{R}^2$)

Hartree–Fock theory in the infinite-volume limit

- To treat the case $\Lambda \to \mathbb{R}^2$, it is best to switch to **reduced 1-body density matrices**:

$$\Psi(t) \rightsquigarrow \gamma^{(1)}(t)\,, \quad u(t) \rightsquigarrow \omega(t)$$

with

$$\gamma^{(1)}(t;\vec{x},\vec{y}) := N \int \mathrm{d}\vec{x}_2 \cdots \mathrm{d}\vec{x}_N \, \Psi(t;\vec{x},\vec{x}_2,\dots,\vec{x}_N)\,\overline{\Psi(t;\vec{y},\vec{x}_2,\dots,\vec{x}_N)}$$

$$\omega(t;\vec{x},\vec{y}) := \sum_{1\le\ell\le N} \varphi_\ell(t;\vec{x})\,\overline{\varphi_\ell(t;\vec{y})}$$

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- $\gamma^{(1)}(t)$, $\omega(t)$ are rank-N projections on $L^2(\mathbb{R}^2)$, satisfying respectively the **von Neumann equation**

$$\mathrm{i}\hbar_{\mathrm{eff}} \frac{\mathrm{d}\gamma^{(1)}}{\mathrm{d}t}(t) = \left[H_N\,, \gamma^{(1)}(t)\right]$$

and the **Hartree–Fock equation for density matrices**

$$\mathrm{i}\hbar_{\mathrm{eff}} \frac{\mathrm{d}\omega}{\mathrm{d}t}(t) = \left[H_{\mathrm{HF}}(\omega)\,, \omega(t)\right] \tag{HFEdm}$$

where[1] $H_{\mathrm{HF}}(\omega) = H_1 + V * \rho_\omega(t) - X_\omega(t)$ with

$$\rho_\omega(t;\vec{x}) := N^{-1}\,\omega(t;\vec{x},\vec{x})\,, \qquad X_\omega(t;\vec{x},\vec{y}) := N^{-1}\,\omega(t;\vec{x},\vec{y})\,V(\vec{x}-\vec{y})\,.$$

[1] Now $V(\vec{x};\vec{y}) \equiv V(\vec{x}-\vec{y})$.

Effectiveness of the infinite-volume Hartree–Fock equations

Theorem (Benedikter, Boccato, M., Nguyen arXiv:2503.16001)

Let $V(\vec{x})$ be an even function such that

$$\int (1 + |\vec{p}|^2) \left| \hat{V}(\vec{p}) \right| \, \mathrm{d}\vec{p} < \infty \, .$$

Then

$$\left\| \gamma^{(1)}(t) - \omega(t) \right\|_{\mathrm{tr}} \leq C \, N^{1/4} \, \mathrm{e}^{c_1 \, \mathrm{e}^{c_2 \, t}} \, .$$

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- Proof is based on **commutator estimates** to propagate the **semiclassical structure** of the HF projections:

$$\sup_{\vec{p}\in\mathbb{R}^2} \frac{1}{1+|\vec{p}|} \left\| \left[\omega(t)\,,\mathrm{e}^{\mathrm{i}\vec{p}\cdot\vec{x}} \right] \right\|_{\mathrm{tr}} \leq C(t)\,\hbar_{\mathrm{eff}}\, N\,, \qquad \left\| \left[\omega(t)\,, P_{\vec{A}} \right] \right\|_{\mathrm{tr}} \leq C(t)\,\hbar_{\mathrm{eff}}\, N$$

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- Passing to the **Fock space**, one can justify (HFEdm) and conclude the error bound by a double Gronwall estimate
- Estimate has much better scaling in N: $N^{1/4}$ vs $N^{1/2}$ $\rightsquigarrow$ meaningful for larger times $t \sim \log(\log N^{1/4})$ comparable to semiclassical

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Thank you for listening!
Any questions?