The Dirac-Frenkel Principle Revisited, and Optimality of the Bogoliubov-de-Gennes Equations

Niels Benedikter
Joint work with Jérémy Sok and Jan Philip Solovej

QMath
University of Copenhagen

Overview

1. The Classical Dirac-Frenkel Principle
2. The Dirac-Frenkel Principle for Reduced Densities
3. Application: The Bogoliubov-de-Gennes Equations

Overview

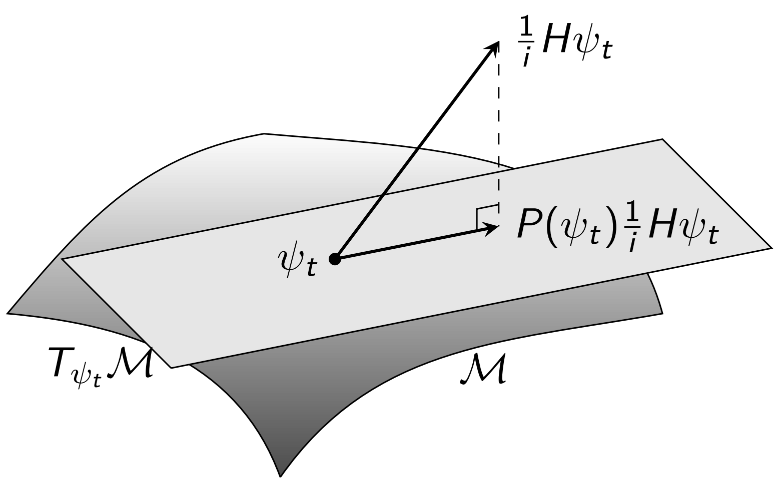
1. The Classical Dirac-Frenkel Principle
2. The Dirac-Frenkel Principle for Reduced Densities
3. Application: The Bogoliubov-de-Gennes Equations

Projecting the Schrödinger Equation to a Submanifold

Schrödinger equation: $\partial_t \psi_t = \frac{1}{i} H \psi_t$ in a Hilbert space $\mathcal{H}$.

Project evolution on a submanifold $\mathcal{M} \subset \mathcal{H}$:

Consider $\psi_t \in \mathcal{M}$ and "infinitisemal time step":



$P(\psi_t)$ = orthogonal projection onto the tangent space $T_{\psi_t}\mathcal{M}$

The Dirac-Frenkel Principle

The Dirac-Frenkel Principle: The optimal approximation to

$$\partial_t \psi_t = \frac{1}{i} H \psi_t$$

in $\mathcal{M}$ is given by

$$\partial_t \psi_t = P(\psi_t) \frac{1}{i} H \psi_t,$$

with $P(\psi_t)$ the orthog. projection of $\mathcal{H}$ to the tangent space $T_{\psi_t}\mathcal{M}$.

This is optimal w. r. t. the scalar product of $\mathcal{H}$.

Usually $\mathcal{H}$ is a space of wave-functions, e. g., $\psi_t \in \mathcal{H} = L^2_a(\mathbb{R}^{dN})$.

But in many-body theory the wave function is not a good starting point for effective equations!

Reduced Densities are Appropriate for Many-Body Systems

- One-particle reduced density matrix:

$$\gamma_t^{(1)} = N \operatorname{tr}_{2,\ldots N} |\psi_t\rangle\langle\psi_t| \quad \in \mathfrak{S}_1(L^2(\mathbb{R}^d))$$

- Recall typical results (e. g., B-Porta-Schlein 2014):

Theorem: Let ψ_t solve the SE (in m. f. & semiclassical scaling). Let $\gamma_t \in \mathfrak{S}_1(L^2(\mathbb{R}^d))$ solve the Hartree-Fock equation.

Then for all $t \in \mathbb{R}$

$$\|\gamma_t^{(1)} - \gamma_t\|_{\mathfrak{S}_2} \leq C(t) \text{ independent of } N.$$

Yau, Rodnianski, Fröhlich, Erdős, Knowles, Spohn, Pickl, Bardos, Petrat, Gottlieb,

Is HF the optimal effective evolution for reduced density matrices?

Overview

1 The Classical Dirac-Frenkel Principle

2 The Dirac-Frenkel Principle for Reduced Densities

3 Application: The Bogoliubov-de-Gennes Equations

Our Simplest Example: Fermions without Pairing

Goal: Formulate a Dirac-Frenkel principle for reduced densities—
to ensure optimality of the effective equations in e. g., $\mathfrak{S}_2 \equiv \mathfrak{S}_2(\mathbb{R}^d)$.

- Reduced density of many-body system:

$$\gamma_t^{(1)} \in \mathcal{H} := \{\gamma \in \mathfrak{S}_2 : \gamma^* = \gamma\}$$

- Submanifold of reduced densities of pure quasifree states (no pairing):

$$\mathcal{M} = \{\gamma \in \mathcal{H} : \gamma^2 = \gamma\} \quad \subset \quad \mathcal{H}$$

- Every $\gamma \in \mathcal{M}$ corresponds to a (unique up to a phase) $\psi_\gamma \in L^2_a(\mathbb{R}^{dN})$:

$$\gamma = \sum_{j=1}^{N} |f_j\rangle\langle f_j| \qquad \leftrightarrow \qquad \psi_\gamma = \frac{1}{\sqrt{N!}} f_1 \wedge \cdots \wedge f_N$$

The Dirac-Frenkel Principle for Reduced Densities

An "infinitesimal time step" optimally looks like this:

1. Consider a quasifree initial state given by $\gamma_0 \in \mathcal{M}$
2. Take the many-body evolution $\psi_t = e^{-iHt}\psi_{\gamma_0}$ and calculate

$$\partial_t \gamma_t^{(1)} = N\,\mathrm{tr}_{2,\ldots N}\,[\frac{1}{i}H, |\psi_t\rangle\langle\psi_t|] \quad \in \mathcal{H}$$

3. Evaluate the derivative at $t = 0$: $\partial_t \gamma_0^{(1)} = N\,\mathrm{tr}_{2,\ldots N}\,[\frac{1}{i}H, |\psi_{\gamma_0}\rangle\langle\psi_{\gamma_0}|]$
4. Project $\partial_t \gamma_0^{(1)}$ to the tangent space by $P(\gamma_0) : \mathcal{H} \to T_{\gamma_0}\mathcal{M}$

A Dirac-Frenkel Principle for Reduced Densities:

$$\partial_t \gamma_t = P(\gamma_t) N\,\mathrm{tr}_{2,\ldots N}\,[\frac{1}{i}H, |\psi_{\gamma_t}\rangle\langle\psi_{\gamma_t}|]$$

How is this compatible with "quasifree reduction"?

We have three different equations:

1. Many body: $\partial_t \gamma_t^{(1)} = N\,\mathrm{tr}_{2,\ldots N}\,[\frac{1}{i}H, |\psi_t\rangle\langle\psi_t|]$, $\psi_t = e^{-iHt}\psi_{\gamma_0}$
2. Dirac-Frenkel: $\partial_t \gamma_t = P(\gamma_t) N\,\mathrm{tr}_{2,\ldots N}\,[\frac{1}{i}H, |\psi_{\gamma_t}\rangle\langle\psi_{\gamma_t}|]$
3. Quasifree reduction: $\partial_t \gamma_t = N\,\mathrm{tr}_{2,\ldots N}\,[\frac{1}{i}H, |\psi_{\gamma_t}\rangle\langle\psi_{\gamma_t}|]$

Comments:

1. …is not a well-posed Cauchy problem: knowledge of $\partial_t \gamma_t^{(1)}$ does not determine evolution of ψ_t.
2. …is geometrically optimal & evolves in $\mathcal{M}$.
3. …is known to produce the Hartree-Fock equations;
   …does it stay in $\mathcal{M}$? Is it optimal?

We prove that Dirac-Frenkel implies Quasifree Reduction.

Tentative Proof

$$\partial_t \gamma_t = \cancel{P(\gamma_t)} N \,\mathrm{tr}_{2,\dots N} \left[\frac{1}{i} H, |\psi_{\gamma_t}\rangle\langle\psi_{\gamma_t}|\right] \qquad (1)$$

Does it stay in $\mathcal{M}$ at all? There is a (simple?) PDE-argument:

$$(1) \;\Rightarrow\; \partial_t \gamma_t = [\frac{1}{i} h_{\mathrm{HF}}(\gamma_t), \gamma_t], \quad h_{\mathrm{HF}}(\gamma_t) = -\Delta + V * \rho_{\gamma_t} - X(\gamma_t),$$

$$\Rightarrow\; \partial_t(\gamma_t^2) = [\frac{1}{i} h_{\mathrm{HF}}(\gamma_t), \gamma_t^2].$$

If $\gamma_0^2 = \gamma_0$, by uniqueness also $\gamma_t^2 = \gamma_t$, i. e., $\gamma_t \in \mathcal{M}$.

This is optimal only because it now agrees with Dirac-Frenkel!
Unlike $\partial_t \gamma_t = 2N \,\mathrm{tr}_{2,\dots N} \left[\frac{1}{i} H, |\psi_{\gamma_t}\rangle\langle\psi_{\gamma_t}|\right]$, or $\partial_t \gamma_t = 0$.

Anyway: We are going to give a more general argument, independent of PDE theory, regularity questions and form of H.

Dirac-Frenkel $\Rightarrow$ Quasifree Reduction

Lemma: The tangent space in a point $\gamma \in \mathcal{M}$ is given by

$$T_\gamma \mathcal{M} = \{A \in \mathcal{H} : \gamma A \gamma = 0 = (1-\gamma)A(1-\gamma)\}.$$

The orthogonal projection from $\mathcal{H}$ onto $T_\gamma \mathcal{M}$ is given by

$$P(\gamma) : A \mapsto \gamma A(1-\gamma) + (1-\gamma)A\gamma.$$

Proof. Let γ_t a curve in $\mathcal{M}$, then $\partial_t(\gamma_t^2) = \partial_t \gamma_t$. $\Rightarrow \gamma_0' \gamma_0 + \gamma_0 \gamma_0' = \gamma_0'$.
Multiply from left and right by γ_0 or $(1-\gamma_0)$:

$$\Rightarrow \quad \gamma_0 \gamma_0' \gamma_0 = 0 = (1-\gamma_0)\gamma_0'(1-\gamma_0).$$

Conversely, given such A, we take the curve $\gamma_t = e^{t[A,\gamma_0]} \gamma_0 e^{-t[A,\gamma_0]}$.
Obviously $\gamma_0' = A$. □

Dirac-Frenkel $\Rightarrow$ Quasifree Reduction

Quasifree reduction written with test functions $g_1, g_2 \in L^2(\mathbb{R}^d)$:

$$\langle g_1, \partial_t \gamma_t g_2 \rangle_{L^2(\mathbb{R}^d)} = \langle \psi_{\gamma_t}, [a^*(g_2)a(g_1), \frac{1}{i} H] \psi_{\gamma_t} \rangle_{\mathcal{F}_a}$$

in comparison to Dirac-Frenkel:

$$\langle g_1, \partial_t \gamma_t g_2 \rangle_{L^2(\mathbb{R}^d)} = \langle \psi_{\gamma_t}, \Big([a^*((1-\gamma_t)g_2)a(\gamma_t g_1), \frac{1}{i} H] + [a^*(\gamma_t g_2)a((1-\gamma_t)g_1), \frac{1}{i} H] \Big) \psi_{\gamma_t} \rangle_{\mathcal{F}_a}.$$

So to derive quasifree reduction from Dirac-Frenkel it is sufficient to show

$$\langle \psi_{\gamma_t}, [a^*(\gamma_t g_2)a(\gamma_t g_1), \frac{1}{i} H] \psi_{\gamma_t} \rangle_{\mathcal{F}_a} = 0$$
$$\langle \psi_{\gamma_t}, [a^*((1-\gamma_t)g_2)a((1-\gamma_t)g_1), \frac{1}{i} H] \psi_{\gamma_t} \rangle_{\mathcal{F}_a} = 0.$$

We treat the 1st case explicitly:

Dirac-Frenkel $\Rightarrow$ Quasifree Reduction

Pick the unitary implementation R_{γ_t} of the Bogoliubov transform

$$a^*(f) \mapsto a^*((1-\gamma_t)f) + a(\overline{\gamma_t f}).$$

This is a particle-hole transform: the transformed vacuum is $R^*_{\gamma_t}\Omega = \psi_{\gamma_t}$.

$$\begin{aligned}
&\langle \psi_{\gamma_t}, [a^*(\gamma_t g_2)a(\gamma_t g_1), \frac{1}{i} H] \psi_{\gamma_t} \rangle \\
&= \langle \Omega, R_{\gamma_t}[a^*(\gamma_t g_2)a(\gamma_t g_1), \frac{1}{i} H] R^*_{\gamma_t}\Omega \rangle \\
&= \langle \Omega, [a(\gamma_t g_2)a^*(\gamma_t g_1), \frac{1}{i} R_{\gamma_t} H R^*_{\gamma_t}]\Omega \rangle \\
&= \langle \Omega, [\underbrace{\langle g_2, \gamma_t g_1 \rangle_{L^2(\mathbb{R}^d)}}_{\in \mathbb{C}} - a^*(\gamma_t g_1)a(\gamma_t g_2), \frac{1}{i} R_{\gamma_t} H R^*_{\gamma_t}]\Omega \rangle \\
&= \langle \Omega, \Big(- a^*(\gamma_t g_1)a(\gamma_t g_2) \frac{1}{i} R_{\gamma_t} H R^*_{\gamma_t} + \frac{1}{i} R_{\gamma_t} H R^*_{\gamma_t} a^*(\gamma_t g_1)a(\gamma_t g_2) \Big)\Omega \rangle \\
&= 0 \qquad \square
\end{aligned}$$

Overview

1 The Classical Dirac-Frenkel Principle

2 The Dirac-Frenkel Principle for Reduced Densities

3 Application: The Bogoliubov-de-Gennes Equations

Fermionic Systems with Pairing

- Systems with pairing are described in Fock space: $\psi \in \mathcal{F}_a$.
- Generalized creation/annihilation operators:

$$A(F) = a(f_1) + a^*(\overline{f_2}), \quad \text{for } F = (f_1, f_2) \in L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d).$$

- Generalized reduced density $\Gamma : L^2 \oplus L^2 \to L^2 \oplus L^2$ defined by

$$\langle F_1, \Gamma F_2 \rangle_{L^2 \oplus L^2} = \langle \psi, A^*(F_2) A(F_1) \psi \rangle_{\mathcal{F}_a}$$

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ -\overline{\alpha} & 1 - \overline{\gamma} \end{pmatrix}, \qquad \begin{aligned} \gamma(x,y) &= \langle \psi, a_y^* a_x \psi \rangle \\ \alpha(x,y) &= \langle \psi, a_x a_y \psi \rangle \end{aligned} \tag{2}$$

- For $\Gamma^2 = \Gamma$, there is a corresponding unique quasifree $\psi \in \mathcal{F}_a$.
- Problem: $\operatorname{tr} \Gamma^* \Gamma = \operatorname{tr} 1 = \infty$. So $\Gamma \notin \mathfrak{S}_2 \equiv \mathfrak{S}_2(L^2 \oplus L^2)$.

Quasifree States Beyond Slater Determinants

- Split off the generalized reduced density of the vacuum

$$\Gamma = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} \gamma & \alpha \\ -\overline{\alpha} & -\overline{\gamma} \end{pmatrix} =: \Gamma_{\text{vac}} + \vec{\Gamma}$$

Introduce the affine space with Hilbert-Schmidt geometry

$$\mathcal{A} = \Gamma_{\text{vac}} + \vec{\mathcal{A}}, \quad \vec{\mathcal{A}} = \{\vec{\Gamma} \in \mathfrak{S}_2 : \vec{\Gamma}^* = \vec{\Gamma}\}.$$

- Generalized reduced density of many-body evolution with block structure (2) lives in the affine subspace

$$\mathcal{A}_- = \{\Gamma \in \mathcal{A} : \Gamma + \mathcal{J}\Gamma\mathcal{J} = 1\}, \quad \mathcal{J} = \begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix} : L^2 \oplus L^2 \to L^2 \oplus L^2.$$

- Generalized reduced densities of quasifree states form submanifold

$$\mathcal{M} = \{\Gamma \in \mathcal{A}_- : \Gamma^2 = \Gamma\} \quad \subset \quad \mathcal{A}_- \quad \subset \quad \mathcal{A}.$$

Result: Dirac-Frenkel $\Rightarrow$ Quasifree Reduction

Having identified the spaces, we generalize the no-pairing case:

Lemma: The projection $P(\Gamma) : T_\Gamma\mathcal{A} \to T_\Gamma\mathcal{M}$ satisfies

$$P(\Gamma) \restriction_{T_\Gamma\mathcal{A}_-} A = \Gamma A(1-\Gamma) + (1-\Gamma)A\Gamma.$$

Using some more refined theory of Bogoliubov transformations:

Theorem: The Dirac-Frenkel principle implies quasifree reduction

$$\langle F_1, \partial_t \Gamma_t F_2 \rangle_{L^2 \oplus L^2} = \langle \psi_{\Gamma_t}, \Big[A^*(F_2)A(F_1), \frac{1}{i}H\Big]\psi_{\Gamma_t}\rangle_{\mathcal{F}_a}.$$

Remark: Bosonic Bogoliubov states (condensate & quasifree part) can be treated by means of the mapping $\Gamma \mapsto -\Gamma\mathcal{S}$, where $\mathcal{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, and using symplectic analogues of the above constructions.