Mathematical analysis of the MCTDHF.
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\(N\)-body time dependent Schrödinger equation, and density. Binary interaction, \(N\) large but fixed and \(\hbar\) fixed.

\[
i\partial_t \psi(X_N, t) = -\frac{1}{2} \Delta \psi(X_N, t) + \sum_{1 \leq j < k \leq n} V(|x_j - x_k|) \psi(X_N, t).
\]

\(X_N = (x_1, x_2, \ldots, x_N) \in \mathbb{R}^{3N}\), \(i\partial_t \psi = H \psi\),

\[
\int_{\mathbb{R}^{3N}} |\psi(X_N, t)|^2 dX = 1.
\]

\(E(\psi) = (H \psi, \psi) = \int_{\mathbb{R}^{3N}} (H \psi(X_N, t), \psi(X_N, t)) dX_N = \int_{\mathbb{R}^{3N}} (H \psi(X_N, 0), \psi(X_N, 0)) dX_N\);

**Fermions**

\((\sigma \psi)(x_{\sigma(1)}, x_{\sigma(2)}, \ldots, x_{\sigma(N)}) = (-1)^{\sigma} \psi(x_1, x_2, \ldots, x_N)\)

\(D = \psi(X_N, t) \otimes \psi(Y_N, t), D_N \sigma = \sigma D_N\), Trace \(D = 1\), \(i\partial_t D(X_N, t) = [H, D]\).
Slaters determinants and MCHF Ansatz.

Hartree Fock:

\[ 1 \leq k \leq K = N, \phi_k(x), (\phi_{k_1}, \phi_{k_2}) = \delta_{k_1, k_2} \]

\[ \tilde{\Psi}_N(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \cdots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & \cdots & \phi_2(x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(x_1) & \phi_N(x_2) & \cdots & \phi_N(x_N) \end{vmatrix}. \]
The MCTDHF Ansatz

\[ K \gg N, 1 \leq k \leq K, L^2(\mathbb{R}^3) \text{ or } L^2(\Omega), r = C^{(K)}_N, \]
\[ \Phi = (\phi_1, \ldots, \phi_K) \in L^2(\Omega)^K, (\phi_{k_1}, \phi_{k_2}) = \delta_{k_1, k_2} \]
\[ \sigma \in \Sigma_{N,K}, \sigma : \{1, 2, \ldots, N\} \mapsto \{1, 2, \ldots, N\}, \sigma(1) < \sigma(2) < \ldots < \sigma(N) \]
\[ \{C = (c_\sigma) : \sum_\sigma |c_\sigma|^2 = 1\} \]
\[ \mathcal{F}_{N,K}(\Omega) = \{(C, \Phi)\} \subset S_{\ell^2(r)} \otimes L^2(\Omega)^K \]
\[ \pi : \mathcal{F}_{N,K} \mapsto L^2(\mathcal{\Omega}^N) \]
\[ \Psi = \pi(C, \Phi) = \sum_{\sigma \in \Sigma_{N,K}} c_\sigma \Phi_\sigma(x_1, \ldots, x_N). \]
\[ \Phi_\sigma(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \det(\phi_\sigma(j)(x_i)) \int_{\Omega_N} \Phi_\sigma(X_N)\Phi_\tau(X_N)dX_N = \delta_{\sigma, \tau}. \]
Basic Marginals

For an operator \( D = D(X_N, Y_N) \) in \( L^2(\Omega^N) \) commuting with transposition define the partial trace:

\[
[D]:n = \binom{N}{n} \int_{\Omega^{N-n}} D(X_n, Z_n^N; Y_n, Z_n^N) dZ_n^N.
\]

The mapping \((C, \Phi) \mapsto [\Psi \otimes \overline{\Psi}]:n\) is continuous from \( \mathcal{F}_{N,K}(\Omega) \) (with its natural topolgy) into the space of trace class operators in \( L^2(\Omega^n) \). In particular one has:

\[
[\Psi \otimes \Psi]:2(x_1, y_1, x_2, y_2) = \sum_{ipjq} \gamma_{ipjq} \phi_i(x_1) \phi_p(x_2) \overline{\phi}_j(y_1) \overline{\phi}_q(y_2)
\]

\[
[\Psi \otimes \Psi]:1(x_1, y_1) = \sum_{ij} \gamma_{ij} \phi_i(x_1) \overline{\phi}_j(y_1)
\]

\[
\gamma_{ipjq} = 0 \text{ if } i = p \text{ or } j = q \text{ else }
\]

\[
\gamma_{ipjq} = \sum_{\sigma, \tau \{i,p\} \in \sigma \{j,q\} \in \tau \setminus \{i,p\} = \tau \setminus \{j,q\}} (-1)_i^\sigma (-1)_j^\tau c_\sigma \overline{c}_\tau
\]

\[
\gamma_{ij} = \sum_{i \in \sigma, j \in \tau; \{\sigma \setminus i\} = \tau \setminus j} (-1)_i^\sigma (-1)_j^\tau c_\sigma \overline{c}_\tau
\]
Γ = \{γ_{ij}\}, \Gamma = \{γ_{ipjq}\} γ_{ij} = \sum_p γ_{ipjp}; \text{trace}(\Gamma) = N, \text{trace}(\Gamma) = \frac{N(N - 1)}{2}.

0 \leq γ_1 \leq γ_2 \ldots \leq γ_K \leq 1, \text{ eigenvalues of } \Gamma.

**Full rank hypothesis** $0 < γ_1 \iff \text{Rank}([Ψ \otimes Ψ]_1) = K$.

$\mathcal{F}^{FR}_{N,K}(Ω) = \{(C, Φ)\} \text{ Rank } ([Ψ \otimes Ψ]_1) = K \text{ is open.}$

**Under the full rank hypothesis given**

$(C_1, Φ_1), (C_2, Φ_2), \pi((C_1, Φ_1)) = \pi((C_2, Φ_2))$ there is a unique unitary transform $U$ such that $(C_2, Φ_2) = U(C_1, Φ_1)$.

$\mathcal{F}^{FR}_{N,K}(Ω)/U \simeq π(\mathcal{F}^{FR}_{N,K}(Ω))$. A fiber bundle.

$U = (U, U)$

$U : (\phi_1^1, \phi_2^1, \ldots, \phi_K^1) \mapsto (\phi_1^2, \phi_2^2, \ldots, \phi_K^2)$,

$U_{σ,τ}^* = \det (U_σ(i), τ(j))$. 

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Correlation, Non Freeness

\[ \text{Cor}(\Psi) = -Tr([\Psi \otimes \Psi]:_1 \log([\Psi \otimes \Psi]:_1 + Tr(1 - [\Psi \otimes \Psi]:_1) \log(1 - [\Psi \otimes \Psi]:_1) \right) + \text{Tr}(1 - [\Psi \otimes \Psi]:_1) \log(1 - [\Psi \otimes \Psi]:_1) \right] \]

\[ \text{Cor}(\Psi) = -\sum_{i=1}^{K} \left( \gamma_i \log(\gamma_i) + (1 - \gamma_i) \log(1 - \gamma_i) \right) \]

The correlation vanishes if and only if \( \Psi \) is a single Slater determinant. It reaches its maximum for:

\[ \Psi = \sum_{I_p} \frac{1}{\sqrt{k+1}} \Phi_p, \quad I_p = \{Np + 1, \ldots, N(p + 1)\}, \quad p = 0, \ldots, k \]

All the orbitals carry the same contribution to the wave function.
The working equations

\[ \psi(X_N, t) = \sum_{\sigma} c_{\sigma}(t) \phi_{\sigma}(X_N, t), \]

\[ i \frac{d}{dt} c_{\sigma}(t) = \langle \left( \sum_{1 \leq i < j \leq N} V(x_i - x_j) \psi \right) \phi_{\sigma} \rangle, \]

\[ i \frac{\partial \phi(t, x)}{\partial t} = -\frac{1}{2} \Delta \phi(t, x) + \]

\[ \Gamma(t)^{-1} (I - P_{\phi}) \left( 2 \int_{\Omega^2} V(x, z) [\psi \otimes \psi]_2 (x, z, y, z) \phi(y) dy dz \right), \]

\[ 2 \int_{\Omega^2} V(x, z) [\psi \otimes \psi]_2 (x, z, y, z) \phi(y) dy dz = (I - P_{\phi}) ([\nabla_{\phi} \psi]^* V \psi). \]
Testing the multi-configuration time-dependent Hartree–Fock method

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\[ H(x, y; t) = -\frac{1}{2}(\partial_x^2 + \partial_y^2) + \frac{\Omega^2}{2}(x^2 + y^2) + \frac{1}{\sqrt{(x - y)^2 + a^2}} + (x + y)\mathcal{E}_0 \sin(\omega t). \]

**Figure 1.** Electron density \( \rho(x, y; 0) \) for the ground-state wavefunction and an increasing number of configurations \( \eta \). (\( \eta = \infty \) refers to the numerically exact solution.) The result for 15 coincides with the exact result within the resolution of the plot.

**Figure 2.** Probability of being in the ground state \( |\langle \Psi_0(x, y; 0) | \Psi_0(x, y; t) \rangle|^2 \) for an increasing number of configurations \( \eta \) (\( \eta = \infty \) refers to the numerically exact solution) in the presence of an electric field of strength \( \mathcal{E}_0 = 1 \) and frequency \( \omega = 8 \Omega \). The result for \( \eta = 15 \) coincides with the exact result within the resolution of the plot.
Main issues

- Is the problem well posed?
- Does it defines a local flow on $\mathcal{F}_{N,K}^{F,R}(\Omega)$?
- Does it conserves energy $\mathcal{E}(\Psi) = \frac{1}{2}(H\Psi, \Psi)$?

$$\mathcal{E}(\Psi) = \frac{1}{2} \int_{\Omega}^{N} |\nabla_{X_N} \Psi(X_N)|^2 dX_N + \frac{N(N - 1)}{2} \int_{\Omega}^{N} V(x_1 - x_2)|\Psi(X_N)|^2 dX_N
= \text{trace}(-\frac{1}{2}\Delta[\Psi \otimes \Psi]:1) + \int_{\Omega^2} V(x_1 - x_2)[\Psi \otimes \Psi]:2(x_1, x_2, x_1, x_2)dx_1dx_2
= \frac{1}{2} \int_{\Omega} (\Gamma(t)\nabla \Phi, \nabla \Phi)dx + \sum_{i:pjq} \gamma_{ipjq} \int_{\Omega^2} V(x - y)\phi_i(x)\phi_p(y)\phi_j(x)\phi_q(y)dx dy .$$

- The invertibility of the density matrix $\Gamma(t)$ being an important issue, is it possible to give sufficient conditions implying the global in time invertibility of this matrix?
- How good is the approximation.

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• For bounded potential the structure of the working equation implies with a Cauchy Lipschitz theorem well posedness in $S_{\ell^2(r)} \otimes L^2(\Omega)^K$. Furthermore with the operator $(I - P_\Phi)$ the orthogonality of the $\phi_k$ is preserved and finally by continuity the local invertibility of $\Gamma(t)$ is also preserved.

• Analysis with the Coulomb potential requires conservation of energy. For this issues and the next ones use gauge transformation!
Gauge transformation and variational principle

Introduce the unitary matrix:

\[ U(0) = Id, \quad i \frac{dU}{dt} = -U(t)M(t), \quad \text{with} \quad (M(t))_{ij} = -\frac{1}{2} (\Delta \phi_i(t), \phi_j(t)) \]

Under the transformation which preserves the fiber

\[ (C, \Phi) \mapsto (C', \Phi') = (U(t)C, U(t)\Phi) \]

a flow solution of the “working equation” is changed into the solution of

\[ i \frac{d}{dt} c'_\sigma(t) = \langle H \Psi' \mid \Phi'_\sigma \rangle, \quad i \Gamma(t) \frac{\partial}{\partial t} \Phi'(t, x) = (I - P_{\Phi'}) \left[ [\nabla'_{\Phi} \Psi']^* H \Psi' \right] \]

\[ \Psi' = \pi(C'\Phi') = \phi(C, \Phi) = \Psi \]

whose solution satisfy the variational principle:

\[ \left\langle \left[ i \frac{\partial}{\partial t} - H \right] \Psi' \mid \delta \Psi' \right\rangle = 0, \quad \text{for all} \quad \delta \Psi' \in T'_\Psi F_{N,K}^{FR}(\Omega). \]
Consequence of the variational principle

- Conservation of energy.
- Sufficient conditions for global invertibility of the matrix $\Gamma(t)$.
- A posteriori error estimates.
Conservation of energy

\[ \langle \left[ i \frac{\partial}{\partial t} - H \right] \psi | \delta \psi \rangle = 0 \Rightarrow \langle \left[ i \frac{\partial}{\partial t} - H \right] \psi | \frac{\partial \psi}{\partial t} \rangle = 0 \]

\[ \Rightarrow \Re \langle H \psi, \frac{\partial \psi}{\partial t} \rangle = 0 \Rightarrow \frac{dE(\psi)}{dt} = 0. \]

Therefore for potentials \( V \) with Coulomb like singularities:

\[ V(x) = \frac{c \geq 0}{|x|} + V_{\text{reg}}(|x|) \]

local in time solutions (as long as \( \int_0^t (\gamma_1(s))^{-1} ds < \infty \)).
Conservation of full rank

\[ \mathcal{E}(K) = \inf_{(C, \Phi) \in \mathcal{F}_{N,K}} \mathcal{E}(\pi(C, \Phi)), \quad K' \geq K \Rightarrow \mathcal{E}(K') \leq \mathcal{E}(K). \]

**Theorem** A stability condition:

\[
V(x) = \frac{c \geq 0}{|x|} + V_{\text{reg}}(|x|), \quad (C_0, \Phi_0) \in \mathcal{F}_{N,K}^{FR}, \quad \Phi_0 \in H^1(\Omega)^K,
\]

\[ \mathcal{E}(\pi(C_0, \Phi_0)) < \mathcal{E}(K - 1) \]

implies global in time existence of a smooth solution.

**Proof** By contradiction:

\[
\lim_{n \to \infty} \gamma_m(t_n) = 0, \quad 0 < \beta \leq \gamma_i(t_n) \text{ for } i \geq m + 1
\]

\[
w - \lim_{n \to \infty} (C(t_n), \Phi(t_n)) = (C^*, \Phi^*) \in \mathcal{F}_{N,K-1}
\]

\[ \mathcal{E}(K - 1) > \mathcal{E}(\pi(C_0, \Phi_0)) = \mathcal{E}(\pi(C_{t_n}, \Phi_{t_n})) \geq \mathcal{E}(\pi(C^*, \Phi^*)) \geq \mathcal{E}(K - 1) \]
Introduce $U = (\mathcal{U}, U)$ with $U$ which diagonalizes $\Gamma$ then:

$$\psi^n = \sum_{\sigma \cap \{1,2,\ldots,m\} \neq \emptyset} c^m\sigma \Phi^m\sigma + \sum_{\sigma \cap \{1,2,\ldots,m\} = \emptyset} c'_\sigma \Phi^m\sigma.$$ 

$$C \geq \frac{1}{2} \sum_{1 \leq i \leq K} \gamma_i(t_n) \int_{\Omega} |\nabla \phi_i(t_n)|^2 dx \geq \beta \sum_{m+1 \leq i \leq K} \int_{\Omega} |\nabla \phi_i(t_n)|^2 dx$$

$$\psi^n = \sum_{\sigma \cap \{1,2,\ldots,m\} \neq \emptyset} c^m\sigma \Phi^m\sigma + \sum_{\sigma \cap \{1,2,\ldots,m\} = \emptyset} c'_\sigma \Phi^m\sigma.$$ 

$$\| \sum_{\sigma \cap \{1,2,\ldots,m\} \neq \emptyset} c^m\sigma \Phi^m\sigma \|_{L^2(\Omega^N)} = \sum_{\sigma \cap \{1,2,\ldots,m\} \neq \emptyset} |c'_\sigma|^2$$

$$\leq \sum_{1 \leq i \leq m} \sum_{i \in \sigma} |c'_\sigma|^2 = \sum_{1 \leq i \leq m} \gamma_i^n \to 0.$$ 

This implies strong convergence of the $\psi(t_n)$ and weak semi continuity for the energy.
How good is the approximation?

\[
\left[ i \frac{\partial}{\partial t} - H \right] \Psi = \mathcal{P}_{T \Psi} \mathcal{F}^{FR}_{N,K} \left( \left[ i \frac{\partial}{\partial t} - H \right] \Psi \right) \\
+ (I - \mathcal{P}_{T \Psi} \mathcal{F}^{FR}_{N,K}) \left( \left[ i \frac{\partial}{\partial t} - H \right] \Psi \right) \\
= (I - \mathcal{P}_{T \Psi} \mathcal{F}^{FR}_{N,K}) H \Psi.
\]

\[
\| \Psi(t)_{E} - \Psi(t) \|_{L^2(\Omega^N)} \leq \| \Psi^0_{E}(t) - \Psi^0 \|_{L^2(\Omega^N)} + \| \int_{0}^{t} (I - \mathcal{P}_{T \Psi} \mathcal{F}^{FR}_{N,K}) H \Psi(s) ds \|_{L^2(\Omega^N)}.
\]

A posteriori error estimate.
A priori Error estimate?

\[ \delta \Psi = \sum_{\sigma} \delta_{\sigma} \Phi_{\sigma} + \sum_{\sigma} c_{\sigma} \sum_{1 \leq i \leq K} \frac{\partial \Phi_{\sigma}}{\partial \phi_i} \delta \phi_i \]

With \( \delta \phi_i = 0 \) and freedom of choice of the \( \phi_i \)

\[ \| \int_0^t (I - \mathcal{P}_{T\Psi} \mathcal{F}_{N,K}^{FR}) H \Psi(s) \, ds \|_{L^2(\Omega_N)} \leq \int_0^t \min_{(C', \Phi')} \| (H \Psi)(s) - \pi(C', \Phi') \|_{L^2(\Omega_N)}(s) \, ds \]

Much better than Galerkin!! With standard choice of the \( \phi'_1, \phi'_2 \ldots \phi'_K \) (Fourier, spectral ) it is at least like \( K^{-s} \) with \( s \) depending on the regularity of \( \Psi \).
THANKS FOR THE INVITATION

AND FOR YOUR PATIENCE.