Towards the inclusion of dissipative effects in Quantum Time Dependent Mean-field Theories
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Dissipative mechanisms in finite quantum systems
Towards the inclusion of dissipative effects in Quantum Time Dependent Mean-field Theories

Dissipative mechanisms in finite quantum systems

An old story...
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An old story...

N. Bohr, Science, 1937
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An old story...

neutron on nucleus

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Dissipative mechanisms in finite quantum systems

An old story...

Dissipation
Dynamical picture
Microscopic description
Finite systems

N. Bohr, Science, 1937
Nuclei at finite temperature
Nuclei at finite temperature

Measurement of maximum deposited excitation energy

\[ \frac{E^*}{A} \propto T^2 \]

(heavy ion collisions, Fermi energy domain)
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Nuclei at finite temperature

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\[ \frac{E^*}{A} \propto T^2 \]

(heavy ion collisions, Fermi energy domain)

\[ \frac{T}{S_n} \approx 0.5 - 1 \]
\[ \frac{T}{\varepsilon_F} \approx 0.1 - 0.2 \]
Temperature in clusters and molecules
Temperature in clusters and molecules

\[ C_{60} \]
Temperature in clusters and molecules

$C_{60}$
Temperature in clusters and molecules

Laser polarization

$C_{60}$
Temperature in clusters and molecules

Laser polarization

Laser Polarization

Exp: Campbell 2010
Temperature in clusters and molecules

Laser polarization

Exp: Campbell 2010
Temperature in clusters and molecules

$L_k$, $\theta$, and $E_k$.

Exp: Campbell 2010
Temperature in clusters and molecules

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Temperature in clusters and molecules

Laser polarization

$C_{60}$

~20% Ioniz. Pot.

Exp: Campbell 2010
Temperature in clusters and molecules

Thermalization

Dissipation: collective (laser) $\rightarrow$ thermal

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Deposited energy [J.cm$^{-2}$] vs. Temperature [eV]

Exp: Campbell 2010
Temperature in clusters and molecules

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Thermalization

Dissipation: collective (laser) → thermal

Exp: Campbell 2010
Quantum mean-field: a « mother » theory
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- Time Dependent (TD) mean field theory (1-body: electrons/nucleons)
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\[ i\hbar \frac{\partial \psi_i}{\partial t} = h[\psi] \psi_i \]

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Nuclei

Clusters and molecules
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Nuclei

Clusters and molecules

Skyrme Hartree-Fock TDHF
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Density Functional Theo. TDDFT
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\[ h[\varrho] = -\frac{\hbar^2}{2m} \Delta + t_0 \varrho + t_3 \varrho^{1+\sigma} + \ldots \]

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- Strongly decreasing de Broglie wavelength in high energy dynamics

Semi classics possible at high energy
Beyond mean field : Boltzmann (+)
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\[ \partial_t f = \{ h(r, p, t), f(r, p, t) \} \quad \text{Vlasov} \]
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\[ I_{\text{coll}}[f_1] \sim \int dp_2 dp_3 dp_4 \delta(\sum p_i)\delta(\sum \varepsilon_i) \frac{d\sigma}{d\Omega} [f_1 f_2 (1 - f_3)(1 - f_4) - ...] \]
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In medium cross section/
Screened Coulomb

Pauli blocking
Fusion in nuclear collisions
Fusion in nuclear collisions

\(^{12}\text{C} + ^{12}\text{C} \quad b = 0 \quad E = 85 \text{ MeV/A}\)
Fusion in nuclear collisions

Quadrupole moment in momentum space

$^{12}\text{C} + ^{12}\text{C} \ b = 0 \ E = 85 \text{ MeV/A}$
Fusion in nuclear collisions

Quadrupole moment in momentum space

\[ Q_{20}^k = \sum_i \int d^3k \varphi_M^*(k) (2k_z^2 - k_x^2 - k_y^2) \varphi_M^i(k) \]

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\[ Q_{20}^k = \sum_i \int d^3k \varphi_M^*(k)(2k_z^2 - k_x^2 - k_y^2)\varphi_M \]

Relaxation in momentum space

\[ {}^{40}\text{Ca} + {}^{40}\text{Ca} \]

\[ b = 0, E = 60 \text{ MeV/A} \]
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\[ \tau \]
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Infinite matter
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Infinite matter

Fusion dynamics

Time scales
The importance of quantum mechanics
The importance of quantum mechanics

- Pauli principle
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  Difficulties with VUU/BUU
The importance of quantum mechanics

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Occupation numbers
The importance of quantum mechanics

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Molecular Dynamics (FMD, AMD)
The importance of quantum mechanics

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  Difficulties with VUU/BUU
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Molecular Dynamics (FMD, AMD)

- Genuine effects
  in fragment production
The importance of quantum mechanics

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  - Molecular Dynamics (FMD, AMD)

- Genuine effects
  - in fragment production

Xe + Sn  E = 50 MeV/A central colls.
The importance of quantum mechanics

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central colls.

![Graph showing multiplicity distribution for different particles (\( p, d, t, ^3\text{He}, \alpha, \text{Z} \geq 3, \text{Z} \geq 5 \)). Indra data is represented by solid circles, and AMD data by open circles. The graph illustrates the multiplicity distribution for various charged particles in nuclear collisions.]
Beyond semiclassics (Boltzmann+)?
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Standard classical kinetic equation is insufficient!
Beyond semiclassics (Boltzmann+)?

Standard \textit{classical kinetic equation} is \textit{insufficient}!
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Sodium clusters may be OK... but certainly not a properly bonded $C_{60}$?
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Caution with excitation energy $E^*$
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Caution with excitation energy $E^*$

- very small $E^*$: fully correlated quantum dynamics
- very large $E^*$: drift towards (semi) classics
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Involved object... Need of simplifications for realistic finite systems
A quantum relaxation time ansatz
A quantum relaxation time ansatz

\[ \hat{I}_{coll}[\hat{\rho}] \approx \frac{\hat{\rho}^{\text{"thermal"}}_{\leftrightarrow E^*(t)} - \hat{\rho}(t)}{\tau_{\text{relax}}(E^*(t))} \]
A quantum relaxation time ansatz

« Simplest » kinetic theory

\[ \hat{I}_{\text{coll}}[\hat{\rho}] \simeq \frac{\hat{\rho}^{\text{thermal}} \leftrightarrow E^*(t) - \hat{\rho}(t)}{\tau_{\text{relax}}(E^*(t))} \]
A quantum relaxation
time ansatz

« Simplest » kinetic theory

... but quantum: dissipative TDLDA

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starting point: \( \hat{\rho}(t) = \sum_\alpha |\phi_\alpha(t)\rangle W_\alpha(t) \langle \phi_\alpha(t)| \)

1. mean-field propagation:
   \[ |\phi_\alpha^{(mf)}\rangle = U(t + \Delta t, t)|\phi_\alpha(t)\rangle \]
   \( W_\alpha(t) = W_\alpha^{(mf)} = \text{const.} \)

2. \( \hat{\rho}_{mf} = \hat{\rho}_{mf}(t + \Delta t) = \sum_\alpha |\phi_\alpha^{(mf)}\rangle W_\alpha^{(mf)} \langle \phi_\alpha^{(mf)}| \)
   \( \varrho_{mf}(r, t + \Delta t), j_{mf}(r, t + \Delta t), E_{mf} \)

3. density-constrained mean field (DCMF)
   1. \( \hat{\rho}_{eq} = \hat{\rho}_{eq}[\varrho_{mf}(r), j_{mf}(r), E_{mf}] \)
      \( = \sum_\alpha |\phi'_\alpha\rangle W'_\alpha \langle \phi'_\alpha| \)
      relaxation time:
      \( h\tau_{\text{relax}}^{-1} = 0.40 \sigma_{ee} r_s^{-2} E_{\text{intr}}^*/N \)
   2. intrinsic excitation energy \( E_{\text{intr}}^* \)

4. \( \hat{\rho}(t + \Delta t) = \hat{\rho}_{mf} - \frac{\Delta t}{\tau_{\text{relax}}} [\hat{\rho}_{mf} - \hat{\rho}_{eq}] \)
   diagonalize to natural orbitals:
   \( \hat{\rho}(t + \Delta t) = \sum_\alpha |\phi_\alpha(t + \Delta t)\rangle \tilde{W}_\alpha \langle \phi_\alpha(t + \Delta t)| \)

5. final fine-tuning of \( W_\alpha \) to reproduce \( E_{mf} \)
   \( \hat{\rho}(t + \Delta t) = \sum_\alpha |\phi_\alpha(t + \Delta t)\rangle W_\alpha(t + \Delta t) \langle \phi_\alpha(t + \Delta t)| \)

6.
A quantum relaxation time ansatz

\[ \hat{I}_{\text{coll}}[\hat{\rho}] \approx \frac{\hat{\rho}^{\text{thermal}} \leftrightarrow E^*(t) - \hat{\rho}(t)}{\tau_{\text{relax}}(E^*(t))} \]

starting point: \( \hat{\rho}(t) = \sum_{\alpha} |\phi_{\alpha}(t)\rangle W_{\alpha}(t)\langle \phi_{\alpha}(t)\rangle \)

1. mean-field propagation:
   \( |\phi_{\alpha}^{(mf)}\rangle = \hat{U}(t + \Delta t, t)|\phi_{\alpha}(t)\rangle \)

   \( W_{\alpha}(t) = W_{\alpha}^{(mf)} = \text{const.} \)

   \( \hat{\rho}_{mf}(t + \Delta t) = \sum_{\alpha} |\phi_{\alpha}^{(mf)}\rangle W_{\alpha}^{(mf)}(t + \Delta t)\langle \phi_{\alpha}^{(mf)}| \)

2. density-constrained mean field (DCMF)
   \[ \hat{\rho}_{eq} = \hat{\rho}_{eq}[g_{mf}(r), j_{mf}(r), E_{mf}] \]
   \[ = \sum_{\alpha} |\phi_{\alpha}'\rangle W_{\alpha}'\langle \phi_{\alpha}'| \]

   1. intrinsic excitation energy \( E_{\text{intr}}^* \)

   2. relaxation time:
      \( h\tau_{\text{relax}}^{-1} = 0.40 \sigma ee r_s^{-2} E_{\text{intr}}^*/N \)

   \( \hat{\rho}(t + \Delta t) = \frac{\hat{\rho}_{mf}(t + \Delta t) - \hat{\rho}_{eq}(t + \Delta t)}{\tau_{\text{relax}}(E^*(t))} \)

   diagonalize to natural orbitals:

   \( \hat{\rho}(t + \Delta t) = \sum_{\alpha} |\phi_{\alpha}(t + \Delta t)\rangle \tilde{W}_{\alpha}(t + \Delta t)\langle \phi_{\alpha}(t + \Delta t)| \)

   \( \hat{\rho}(t + \Delta t) = \sum_{\alpha} |\phi_{\alpha}(t + \Delta t)\rangle W_{\alpha}(t + \Delta t)\langle \phi_{\alpha}(t + \Delta t)| \)

   final fine-tuning of \( W_{\alpha} \) to reproduce \( E_{mf} \)
A quantum relaxation time ansatz

« Simplest » kinetic theory
... but quantum: dissipative TDLDA

\[ \hat{I}_{\text{coll}}[\hat{\rho}] \simeq \frac{\hat{\rho}^{\text{thermal}} \leftrightarrow E^*(t) - \hat{\rho}(t)}{\tau_{\text{relax}}(E^*(t))} \]
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\[
\hat{I}_{\text{coll}}[\hat{\rho}] \approx \frac{\hat{\rho}\text{"thermal"} \leftrightarrow E^*(t) - \hat{\rho}(t)}{\tau_{\text{relax}}(E^*(t))}
\]
A quantum relaxation time ansatz

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$$\hat{I}_{\text{coll}}[\hat{\rho}] \simeq \frac{\hat{\rho}^{\text{thermal}} \leftrightarrow E^*(t) - \hat{\rho}(t)}{\tau_{\text{relax}}(E^*(t))}$$

Response to dipole boost
A quantum relaxation time ansatz

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Response to dipole boost
A quantum relaxation time ansatz

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\[ \hat{I}_{\text{coll}}[\hat{\rho}] \approx \frac{\hat{\rho}^\text{"thermal"} \leftrightarrow E^*(t) - \hat{\rho}(t)}{\tau_{\text{relax}}(E^*(t))} \]

Response to dipole boost

Ionization

\[ \text{Sizable effects (ionization, response, PAD...)} \]
\[ \text{Large temperature } \sim 1.5 \text{ eV} \]
\[ \text{First quantum theory; better than semi classics?} \]

PAD

\[ I = 6.10^{11} \text{W.cm}^{-2} \ \omega = 2.7 \text{ eV FWHM=25 fs} \]

Na\textsubscript{41} +  Quantum

s. class. kin. eq.

Diss-Quant.

Na\textsubscript{40}

0 1 2 3 4 5 6 7

Frequency [eV]

0 1 2 3 4 5 6 7

Strength [a.u.]

0 1 2 3 4 5 6 7

Yield [a.u.]

0 45 90 135 180

Angle [°]

0 2000 4000 6000 8000 100

N\textsubscript{esc}

0.01 0.02 0.03 0.04 0.05 0.06 0.07

N\textsubscript{esc}

0 1 2 3 4 5

Time [fs]
A quantum relaxation time ansatz

«Simplest» kinetic theory
... but quantum: dissipative TDLDA

\[
\hat{I}_{coll}[\hat{\rho}] \simeq \frac{\hat{\rho}^{\text{thermal}} \leftrightarrow E^*(t) - \hat{\rho}(t)}{\tau_{\text{relax}}(E^*(t))}
\]

PAD

\[I = 6.10^{11} \text{W.cm}^{-2}, \omega = 2.7 \text{ eV}, \text{FWHM=25 fs}\]

\[
\begin{array}{c}
\text{Na}_{41}^+ \quad \text{Quantum} \\
\text{s. class.} \\
\text{s. class. kin. eq.} \\
\text{Diss-Quant.}
\end{array}
\]

Sizable effects (ionization, response, PAD...)
Large temperature \( \sim 1.5 \text{ eV} \)
First quantum theory; better than semi classics?

\[
\text{Response to dipole boost}
\]

\[
\begin{array}{c}
\text{Na}_{40} \\
\text{Dissip. Quantum} \\
\text{Quantum}
\end{array}
\]

\[
\begin{array}{c}
\text{Ionization} \\
\text{relax} \\
\text{no relax}
\end{array}
\]

\[
\begin{array}{c}
\text{Ions} \\
\text{0} \\
\text{100} \\
\text{200} \\
\text{300} \\
\text{400} \\
\text{500}
\end{array}
\]

\[
\begin{array}{c}
\text{Time [fs]} \\
\text{0} \\
\text{1} \\
\text{2} \\
\text{3} \\
\text{4} \\
\text{5} \\
\text{6} \\
\text{7}
\end{array}
\]

\[
\begin{array}{c}
\text{Frequency [eV]} \\
\text{0} \\
\text{1} \\
\text{2} \\
\text{3} \\
\text{4} \\
\text{5} \\
\text{6} \\
\text{7}
\end{array}
\]

\[
\begin{array}{c}
\text{Strength [a.u.]} \\
\text{0} \\
\text{1} \\
\text{2} \\
\text{3} \\
\text{4} \\
\text{5} \\
\text{6} \\
\text{7}
\end{array}
\]

\[
\begin{array}{c}
\text{0} \\
\text{0.5} \\
\text{1} \\
\text{1.5} \\
\text{2} \\
\text{2.5}
\end{array}
\]

\[
\begin{array}{c}
\text{Yield [a.u.]} \\
\text{0} \\
\text{0.5} \\
\text{1} \\
\text{1.5} \\
\text{2} \\
\text{2.5}
\end{array}
\]

\[
\begin{array}{c}
\text{Angle [°]} \\
\text{0} \\
\text{45} \\
\text{90} \\
\text{135} \\
\text{180}
\end{array}
\]

\
\[
\text{\text{PAD}}
\]

\
\[
\text{\text{I=6.10^{11} W.cm^{-2}, \omega=2.7 eV, FWHM=25 fs}}
\]

\
\[
\text{\text{\text{Na}_{41}^+ Quantum}}
\]

\
\[
\text{\text{\text{s. class.}}} \\
\text{\text{s. class. kin. eq.}} \\
\text{\text{Diss-Quant.}}
\]

\
\[
\text{\text{Sizable effects (ionization, response, PAD...)}}
\]

\
\[
\text{\text{Large temperature \sim 1.5 eV}}
\]

\
\[
\text{\text{First quantum theory; better than semi classics?}}
\]
A complementing view: Stochastic TDHF
A complementing view: Stochastic TDHF

- Basic idea: Ensemble of TDHF states \( \hat{\rho} \rightarrow \{ \hat{\rho}_\alpha, \alpha = 1, \ldots \} \)
A complementing view: Stochastic TDHF

- Basic idea: **Ensemble** of TDHF states \( \hat{\rho} \longrightarrow \{ \hat{\rho}_\alpha, \alpha = 1, \ldots \} \)

- Second order perturb. theory on top of TDHF evolution *(Fermi Golden rule)*

\[
\hat{\rho}_\alpha \longrightarrow \hat{\mathcal{D}}_\alpha = \sum_\beta W_{\alpha \beta} \hat{\rho}_\beta
\]
A complementing view: Stochastic TDHF

- Basic idea: Ensemble of TDHF states \( \hat{\rho} \rightarrow \{ \hat{\rho}_\alpha, \alpha = 1, \ldots \} \)

  - Second order perturb. theory on top of TDHF evolution (Fermi Golden rule)

  - **Coherence loss**: occasional statistical reduction on TDHF states

\[
\hat{\rho}_\alpha \rightarrow \hat{D}_\alpha = \sum_\beta W_{\alpha\beta} \hat{\rho}_\beta
\]
A complementing view: Stochastic TDHF

- **Basic idea**: Ensemble of TDHF states
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  - **Coherence loss**: occasional statistical reduction on TDHF states

\[ \hat{\rho}_\alpha \longrightarrow \hat{D}_\alpha = \sum_{\beta} W_{\alpha \beta} \hat{\rho}_\beta \]

\[
\left\{ \begin{array}{c}
\hat{\rho}_\alpha \xrightarrow{\tau_{\text{STDHF}}} \{ \hat{\rho}_\beta, W_{\alpha \beta} \} \\
\hat{\rho}_{\alpha_0} \xrightarrow{\tau_{\text{STDHF}}} \{ \hat{\rho}_\gamma, W_{M_{\alpha_0 \gamma}} \} \\
\ldots \end{array} \right\}_{\alpha=1,\ldots}
\]
A complementing view: Stochastic TDHF

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  \[ \hat{\rho} \longrightarrow \{\hat{\rho}_\alpha, \alpha = 1, \ldots\} \]

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- Coherence loss: occasional statistical reduction on TDHF states

\[ \hat{\rho}_\alpha \longrightarrow \hat{D}_\alpha = \sum W_{\alpha\beta} \hat{\rho}_\beta \]

\[
\left\{ \begin{array}{l}
\hat{\rho}_\alpha \xrightarrow{\tau_{STDHF}} \{\hat{\rho}_\beta, W_{\alpha\beta}\} \\
\hat{\rho}_{\alpha_0} \xrightarrow{\tau_{STDHF}} \{\hat{\rho}_\gamma, W_{M_{\alpha_0}\gamma}\}
\end{array} \right\}_\alpha \]

0 \quad \tau_{STDHF} \quad 2\tau_{STDHF}
A complementing view: Stochastic TDHF

- Basic idea: Ensemble of TDHF states
  \[ \hat{\rho} \longrightarrow \{ \hat{\rho}_\alpha, \alpha = 1, \ldots \} \]

- Second order perturb. theory on top of TDHF evolution (Fermi Golden rule)

- Coherence loss: occasional statistical reduction on TDHF states

\[ \hat{\rho}_\alpha \longrightarrow \hat{D}_\alpha = \sum_{\beta} W_{\alpha \beta} \hat{\rho}_\beta \]

TDHF Propagation

\[ \hat{\rho}_\alpha \quad \tau_{\text{STDHF}} \quad \{ \hat{\rho}_\beta, W_{\alpha \beta} \} \]

\[ \hat{\rho}_{\alpha_0} \quad \tau_{\text{STDHF}} \quad \{ \hat{\rho}_\gamma, W_{\alpha_0 \gamma} \} \quad \text{etc.} \]
A complementing view: Stochastic TDHF

- Basic idea: Ensemble of TDHF states
  \[ \hat{\rho} \rightarrow \{ \hat{\rho}_\alpha, \alpha = 1, \ldots \} \]

- Second order perturb. theory on top of TDHF evolution (Fermi Golden rule)

- Coherence loss: occasional statistical reduction on TDHF states

- Stochastic reduction

\[ \hat{\rho}_\alpha \rightarrow \hat{D}_\alpha = \sum W_{\alpha\beta} \hat{\rho}_\beta \]

TDHF Propagation

\[ \{ \hat{\rho}_\beta, W_{\alpha\beta} \} \]

\[ \{ \hat{\rho}_\gamma, W_{M\alpha\gamma} \} \]

\[ \hat{\rho}_\alpha \rightarrow \hat{\rho}_\beta \]

\[ \boxed{\tau_{\text{STDHF}} \rightarrow \hat{R} \rightarrow 2\tau_{\text{STDHF}}} \]
A complementing view: Stochastic TDHF

- Basic idea: Ensemble of TDHF states
  \[ \hat{\rho} \rightarrow \{\hat{\rho}_\alpha, \alpha = 1, \ldots\} \]

- Second order perturb. theory on top of TDHF evolution (Fermi Golden rule)

- Coherence loss: occasional statistical reduction on TDHF states

\[ \hat{\rho}_\alpha \rightarrow \hat{D}_\alpha = \sum W_{\alpha\beta} \hat{\rho}_\beta \]

\[ \tau_{\text{STDHF}} \]

Stochastic reduction

Sampling
A complementing view: Stochastic TDHF

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  \[ \hat{\rho} \longrightarrow \{ \hat{\rho}_\alpha, \alpha = 1, \ldots \} \]

- Second order perturb. theory on top of TDHF evolution (Fermi Golden rule)

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- Interests
A complementing view: Stochastic TDHF

- Basic idea: Ensemble of TDHF states

\[ \hat{\rho} \rightarrow \{ \hat{\rho}_\alpha, \alpha = 1, \ldots \} \]

- Second order perturb. theory on top of TDHF evolution (Fermi Golden rule)

- Coherence loss: occasional statistical reduction on TDHF states

\[ \hat{\rho}_\alpha \rightarrow \hat{D}_\alpha = \sum W_{\alpha \beta} \hat{\rho}_\beta \]

- Interests

- Reducible to a Quantum Stochastic kinetic equation

\[ i\partial_t \hat{\rho} = [\hat{h}[\hat{\rho}], \hat{\rho}] + \hat{I}_{\text{coll}}[\hat{\rho}] + \delta\hat{I}_{\text{coll}} \]
A complementing view: Stochastic TDHF

- Basic idea: Ensemble of TDHF states
  \( \hat{\rho} \rightarrow \{ \hat{\rho}_\alpha, \alpha = 1, \ldots \} \)

  - Second order perturb. theory on top of TDHF evolution (Fermi Golden rule)
  - Coherence loss: occasional statistical reduction on TDHF states

\[
\hat{\rho}_\alpha \rightarrow \hat{\mathcal{D}}_\alpha = \sum_{\beta} W_{\alpha \beta} \hat{\rho}_\beta
\]

- Interests
  - Reducible to a Quantum Stochastic kinetic equation
    \[
    i\partial_t \hat{\rho} = [\hat{h}[\hat{\rho}], \hat{\rho}] + \hat{I}_{\text{coll}}[\hat{\rho}] + \delta \hat{I}_{\text{coll}}
    \]
  - Simple practical scheme ...
STDHF in wavefunction form
STDHF in wavefunction form

- STDHF directly in terms of wavefunctions (Slater) \( \hat{\rho}_\alpha \rightarrow |\Phi_\alpha\rangle \)
STDHF in wavefunction form

- STDHF directly in terms of wavefunctions (Slater)  \( \hat{\rho}_\alpha \rightarrow |\Phi_\alpha\rangle \)
- Ensemble strategy of stochastic jumps:  \( |\Phi_\alpha\rangle \rightarrow \{|\Phi_\beta\rangle, W_{\alpha\beta}\} \)
**STDHF in wavefunction form**

- STDHF directly in terms of wavefunctions (Slater) \( \hat{\rho}_\alpha \rightarrow |\Phi_\alpha\rangle \)
- Ensemble strategy of stochastic jumps: \( |\Phi_\alpha\rangle \rightarrow \{|\Phi_\beta\rangle, W_{\alpha\beta}\} \)
- Assume 2p 2h excitations on \( |\Phi_\alpha\rangle : |\Phi_\beta\rangle \simeq \hat{a}_p^\dagger \hat{a}_{p'}^\dagger \hat{a}_{h'} \hat{a}_h |\Phi_\alpha\rangle \)
STDHF in wavefunction form

- STDHF directly in terms of wavefunctions (Slater) \[ \hat{\rho}_\alpha \rightarrow |\Phi_\alpha \rangle \]
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- Assume 2p 2h excitations on \[ |\Phi_\alpha \rangle : |\Phi_\beta \rangle \simeq \hat{a}_p^{\dagger}\hat{a}^{\dagger}_{p'}\hat{a}_h\hat{a}_{h'}|\Phi_\alpha \rangle \]
- Perturbative correlations on \( \tau_{STDHF} \) for residual interaction \( \hat{V}_{res} \)

\[ W_{\alpha\beta} \simeq \tau_{STDHF} |\langle \Phi_\beta | \hat{V}_{res} |\Phi_\alpha \rangle|^2 \delta(E_\beta - E_\alpha) \]
STDHF in wavefunction form

- STDHF directly in terms of wavefunctions (Slater) \( \hat{\rho}_\alpha \rightarrow |\Phi_\alpha\rangle \)
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- Perturbative correlations on \( \tau_{STDHF} \) for residual interaction \( \hat{V}_{res} \)
  \( W_{\alpha\beta} \sim \tau_{STDHF} |\langle \Phi_\beta | \hat{V}_{res} | \Phi_\alpha \rangle|^2 \delta(E_\beta - E_\alpha) \)
- 1D typical «organic» system
  \( h(x) = -\frac{\hbar^2}{2m} \Delta + V_{ext}(x) + \kappa g(x)^\sigma \quad V_{res} \sim V_0 \delta(x - x') \)
STDHF in wavefunction form

- STDHF directly in terms of wavefunctions (Slater) \[ \hat{\rho}_\alpha \rightarrow |\Phi_\alpha\rangle \]
- Ensemble strategy of stochastic jumps: \[ |\Phi_\alpha\rangle \rightarrow \{ |\Phi_\beta\rangle, W_{\alpha\beta} \} \]
- Assume 2p 2h excitations on \[ |\Phi_\alpha\rangle : |\Phi_\beta\rangle \simeq \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} \hat{a}_{h'} \hat{a}_{h}|\Phi_\alpha\rangle \]
- Perturbative correlations on \( \tau_{STDHF} \) for residual interaction \( \hat{V}_{res} \)
  \[ W_{\alpha\beta} \simeq \tau_{STDHF} |\langle \Phi_\beta | \hat{V}_{res} | \Phi_\alpha \rangle|^2 \delta(E_\beta - E_\alpha) \]
- 1D typical «organic» system
  \[ h(x) = -\frac{\hbar^2}{2m} \Delta + V_{ext}(x) + \kappa \varrho(x)^\sigma \quad \text{for residual interaction} \]
  \[ V_{res} \sim V_0 \delta(x - x') \]
- Random, initial multi particle hole (1ph, 2ph, 3ph...) excitation \[ \rightarrow E^* \]
STDHF in wavefunction form

- STDHF directly in terms of wavefunctions (Slater) \( \hat{\rho}_\alpha \rightarrow |\Phi_\alpha\rangle \)
- Ensemble strategy of stochastic jumps: \( |\Phi_\alpha\rangle \rightarrow \{ |\Phi_\beta\rangle, W_{\alpha\beta} \} \)
- Assume 2p 2h excitations on \( |\Phi_\alpha\rangle : |\Phi_\beta\rangle \simeq \hat{a}_{p}\hat{a}_{p}^{\dagger}\hat{a}_{p'}\hat{a}_{h'}\hat{a}_{h}|\Phi_\alpha\rangle \)
- Perturbative correlations on \( \tau_{STDHF} \) for residual interaction \( \hat{V}_{res} \)
  \[ W_{\alpha\beta} \simeq \tau_{STDHF} |\langle \Phi_\beta |\hat{V}_{res} |\Phi_\alpha\rangle|^2 \delta(E_\beta - E_\alpha) \]
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  \[ h(x) = -\frac{\hbar^2}{2m} \Delta + V_{ext}(x) + \kappa \varrho(x)^\sigma \]
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- Random, initial **multi** particle hole (1ph, 2ph, 3ph...) excitation \( \rightarrow E^* \)
- Compute dynamics of the ensemble of «Slater» states
STDHF in wavefunction form

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  \[ W_{\alpha\beta} \simeq \tau_{STDHF} |\langle \Phi_\beta | \hat{V}_{res} | \Phi_\alpha \rangle|^2 \delta(E_\beta - E_\alpha) \]
- 1D typical «organic» system
  \[ h(x) = -\frac{\hbar^2}{2m} \Delta + V_{ext}(x) + \kappa \varrho(x) \sigma \quad \text{\( V_{res} \sim V_0 \delta(x - x') \)} \]
- Random, initial multi particle hole (1ph, 2ph, 3ph...) excitation \( \rightarrow E^* \)
- Compute dynamics of the ensemble of «Slater» states
- Note the «forgiving» excitations (laser,...) in terms of phase space
Test case
• Compute dynamics of the ensemble of «Slater» states

\[ \{ |\Phi_\alpha(t)\rangle, \alpha = 1, \ldots, N \} \]

\[ |\Phi_\alpha\rangle = \prod_{i=1,N} |\varphi_{\alpha,i}\rangle \]
Compute dynamics of the ensemble of «Slater» states

\[ \{ |\Phi_\alpha(t)\rangle, \alpha = 1, \ldots, N \} \]

\[ |\Phi_\alpha\rangle = \prod_{i=1,N} \varphi_{\alpha,i} \]

Extract correlated 1-body density matrix from the ensemble
Test case

- Compute dynamics of the ensemble of «Slater» states
  \[ \{ |\Phi_\alpha(t)\rangle, \alpha = 1, \ldots, N \} \]
  \[ |\Phi_\alpha\rangle = \prod_{i=1,N} |\varphi_{\alpha,i}\rangle \]
- Extract correlated 1-body density matrix
  from the ensemble
  \[ \hat{\rho} = \frac{1}{N} \sum_{\alpha} \hat{\rho}_\alpha = \frac{1}{N} \sum_{\alpha} \sum_{i=1}^{N} |\varphi_{\alpha,i}\rangle \langle \varphi_{\alpha,i}| \]
Test case

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- Extract occupation numbers \( n_i \) from \( \hat{\rho} \) by diagonalization
**Test case**

- Compute dynamics of the ensemble of «Slater» states
  \[
  \{|\Phi_\alpha(t)\rangle, \alpha = 1, \ldots, N\}\]
  \[
  |\Phi_\alpha\rangle = \prod_{i=1,N} |\varphi_{\alpha,i}\rangle
  \]

- Extract correlated 1-body density matrix from the ensemble
  \[
  \hat{\rho} = \frac{1}{N} \sum_\alpha \hat{\rho}_\alpha = \frac{1}{N} \sum_\alpha \sum_{i=1}^N |\varphi_{\alpha,i}\rangle \langle \varphi_{\alpha,i}|
  \]

- Extract occupation numbers \(n_i\) from \(\hat{\rho}\) by diagonalization

1 ph excitation - 100 events - \(E^* = 2.3\) Ry

![Graph showing occupation numbers versus energy for different times](image)
Test case

- Compute dynamics of the ensemble of «Slater» states
  \[ \{ |\Phi_\alpha(t)\rangle, \alpha = 1, \ldots, N \} \]
  \[ |\Phi_\alpha\rangle = \prod_{i=1, N} |\varphi_{\alpha,i}\rangle \]

- Extract correlated 1-body density matrix from the ensemble
  \[ \hat{\rho} = \frac{1}{N} \sum_{\alpha} \hat{\rho}_{\alpha} = \frac{1}{N} \sum_{\alpha} \sum_{i=1}^{N} |\varphi_{\alpha,i}\rangle \langle \varphi_{\alpha,i}| \]

- Extract occupation numbers \( n_i \) from \( \hat{\rho} \) by diagonalization
Towards the inclusion of dissipative effects in Quantum Time Dependent Mean-field Theories

Dissipative mechanisms in finite quantum systems

An old story...
Towards the inclusion of dissipative effects in Quantum Time Dependent Mean-field Theories

Dissipative mechanisms in finite quantum systems

An old story...

With a bright future ...?
Towards the inclusion of dissipative effects in Quantum Time Dependent Mean-field Theories

Dissipative mechanisms in finite quantum systems

Several important results
- Key role of quantum effects
- Semi classical kinetic equations sometimes applicable
- Relaxation time ansatz done\ in the oven
- Stochastic extension of TDLDA done\ in the oven
- Tractable dissipative mean field in the near future
Towards the inclusion of dissipative effects in Quantum Time Dependent Mean-field Theories

Dissipative mechanisms in finite quantum systems

Many directions to be investigated
- Further analysis of relaxation time ansatz (quantum rate, systematics, photoelectron spectra,...)
- (Re)derivation of a kinetic-like theory
- Tests of kinetic-like approaches
- ...

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neutron on nucleus
Towards the inclusion of dissipative effects in Quantum Time Dependent Mean-field Theories

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Several important results
- Key role of quantum effects
- Semi classical kinetic equations sometimes applicable
- Relaxation time ansatz done/ in the oven
- Stochastic extension of TDLDA done/ in the oven
- Tractable dissipative mean field in the near future
Thank you for your attention.
Thank you too...

People

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« Palm tree »
Jacobins church, Toulouse