Chapter 8: Time-dependent Hartree-Fock (TDHF) and Time-dependent Density Functional Theory (TDDFT)

1. TDHF

References for formalism

- J. W. Negele, Rev. Mod. Phys. 54 (1982) 913
- P. Ring and P. Schuck, "The Nuclear Many-Body Problem", chapter 12

Main assumption:

Many-body WF = a single time-dependent Slater determinant

\[ \Phi(x_1, \ldots, x_N; t) = \frac{1}{\sqrt{N!}} \det \phi(x_i, t) \]

\[ \Rightarrow \text{s.p. UF's} \]

As a result, the system acquires a time-dependent density

\[ \rho(\vec{r}) \rightarrow \rho(\vec{r}, t) \]

The TDHF equations can be derived in different ways. By analogy to the quantities \( \rho_{HF} \) in static HF, one defines new quantities

\[ \rho_{HF}^{TDHF} = \langle \phi(t) | \hat{c}_\beta^+ \hat{c}_\alpha | \phi(t) \rangle \]
which results in the following comparison:

<table>
<thead>
<tr>
<th>Static HF</th>
<th>TDHF</th>
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<tbody>
<tr>
<td>Var. principle</td>
<td>Var. principle</td>
</tr>
<tr>
<td>$[\mathbf{H}, \Psi(t)] = 0$</td>
<td>$[\mathbf{H}, \Psi(t)] = i \hbar \frac{\partial}{\partial t}$</td>
</tr>
<tr>
<td>$\mathbf{H}(\mathbf{r}) \Psi_{\alpha}(\mathbf{r}) = E_{\alpha} \Psi_{\alpha}(\mathbf{r})$</td>
<td>$\mathbf{H}(\mathbf{r}, t) \Psi_{\alpha}(\mathbf{r}, t) = i \hbar \frac{2}{\hbar} \Psi_{\alpha}(\mathbf{r}, t)$</td>
</tr>
<tr>
<td>HF-eqns</td>
<td>TDHF-eqns</td>
</tr>
</tbody>
</table>

2 important practical applications

a) quantum system in time-dep. external field $V(t)$

- atom in strong time-dep. laser field
- nucleus in time-dep. field

e. g.

b) collision of two nuclei / atoms

- create static HF solutions for 2 nuclei / atoms: $\Psi_{\alpha}^{(1)}, \Psi_{\alpha}^{(2)}$
- "boost" static WF's: $\Psi_{\alpha}^{(1)} \rightarrow e^{i \mathbf{K}_{\alpha} \cdot \mathbf{R}_{1}} \Psi_{\alpha}^{(1)}$, $\Psi_{\alpha}^{(2)} \rightarrow e^{i \mathbf{K}_{\alpha} \cdot \mathbf{R}_{2}} \Psi_{\alpha}^{(2)}$
Nuclear TDHF as example

Phys-365 Website, "Additional lecture materials" section:

Chapter 8:
- TDHF calculations of nuclear reactions
- TDHF move: heavy-ion fusion
- TDHF move: deep-inelastic reaction

Suggested term paper topics (atomic TDHF):

1. Multi-electron atom in strong time-dep. laser field

2. Atomic collision (He + He)

2. TDDFT

Ref.:
Straightforward generalization of static Kohn-Sham formalism (see ch. 7, p. 46):

\[ H = H_{KS} \quad \rightarrow \quad H(t) = H_{KS}(t) + V_{\text{ext}}(\vec{r}_t) \]

with

\[ H_{KS}(t) = -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ion}}(\vec{r}_t) + V_{H}\left[ \rho(\vec{r}_t) \right] + V_{XC}\left[ \rho(\vec{r}_t) \right] \]

electron-electron interaction Hartree pot. exchange-correlation

time-dep. density functional theory (TDDFT) equs:

\[ H(t) \psi(t) = \frac{i}{\hbar} \frac{\partial}{\partial t} \psi(t) \]

Note: motion of ions is treated classically using quantum potentials (Ehrenfest's theorem).

⇒ Suggested term papers (TDDFT)

check recent papers by UU cond. matt. theorists (Professors Vargor and Pantelides)