On the Existence and Uniqueness of the Current-Density to Vector-Potential Mapping in Time-Dependent Current-Density Functional Theory

a Global Fixed-Point Proof

Paul L. de Boeij

Scientific Computing & Modeling, Amsterdam

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Outline

Definition of the N-Electron System

Starting point is the time-dependent Schrödinger equation,

$$i\frac{\partial}{\partial t}\Psi(t) = \hat{H}(t)\Psi(t), \ \ with \ \Psi(t_0) = \Psi_0.$$

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with kinetic, two-particle interaction, and external potential operators,

$$\hat{T} = \frac{1}{2}\sum_{i=1}^{N}|\hat{\mathbf{p}}_i|^2,\ \ with\ \hat{\mathbf{p}}_i = -\frac{i}{2}(\nabla_i - \nabla_i^\dagger),$$

$$\hat{W} = \frac{1}{2}\sum_{i,j\neq i} w(|\mathbf{r}_i - \mathbf{r}_j|),$$

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\hat{W} &= \frac{1}{2}\sum_{i,j\neq i} w(|\mathbf{r}_i - \mathbf{r}_j|), \\
\hat{V}(t) &= \sum_{i=1}^{N}\left\{\frac{1}{2}|\hat{\mathbf{p}}_i + \mathbf{A}(\mathbf{r}_i, t)|^2 + v(\mathbf{r}_i, t)\right\} - \hat{T}.
\end{aligned}$$

Hydrodynamical Description

We define the particle density, and the density operator

$$n(\mathbf{r},t) = \langle \Psi(t) \mid \hat{n}(\mathbf{r}) \mid \Psi(t) \rangle, \; \textit{with} \; \hat{n}(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i).$$

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$$\begin{aligned} \widehat{\frac{\partial n}{\partial t}}(\mathbf{r},t) &= -i[\hat{n}(\mathbf{r}), \hat{H}(t)], \\ &= -\frac{i}{2}\sum_{i=1}^{N}[\delta(\mathbf{r}-\mathbf{r}_i), |\hat{\mathbf{v}}_i(t)|^2], \;\; \textit{with} \;\; \hat{\mathbf{v}}_i(t) = \hat{\mathbf{p}}_i + \mathbf{A}(\mathbf{r}_i,t) \end{aligned}$$

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$$\textit{using}: \begin{cases} [a, b^2] = \{[a,b], b\} \\ [\delta(\mathbf{r}-\mathbf{r}_i), \hat{\mathbf{v}}_i(t)] = -i\nabla\delta(\mathbf{r}-\mathbf{r}_i) \end{cases}$$

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The time-derivative is obtained using the Heisenberg equation of motion,

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in which the current operator is

$$\hat{\mathbf{j}}(\mathbf{r},t) = \frac{1}{2} \sum_{i=1}^{N} \{\delta(\mathbf{r} - \mathbf{r}_i), \hat{\mathbf{v}}_i(t)\}$$

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defining the current density, and the continuity equation,

$$\mathbf{j}(\mathbf{r},t) = \langle \Psi(t) \mid \hat{\mathbf{j}}(\mathbf{r},t) \mid \Psi(t) \rangle \Rightarrow \frac{\partial n}{\partial t}(\mathbf{r},t) + \nabla \cdot \mathbf{j}(\mathbf{r},t) = 0$$

EOM Current Density

The equation of motion for the current operator reads,

$$\widehat{\frac{\partial \mathbf{j}_\mu}{\partial t}}(\mathbf{r},t) = \frac{\partial}{\partial t}\hat{\mathbf{j}}_\mu(\mathbf{r},t) - i[\hat{\mathbf{j}}_\mu(\mathbf{r},t), \hat{H}(t)]$$

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$$\textit{using}: \begin{cases} \hat{\mathbf{j}}(\mathbf{r},t) = \frac{1}{2}\sum_i \{\delta(\mathbf{r}-\mathbf{r}_i), \hat{\mathbf{v}}_i(t)\} \\ [\{a,b\},c] = \{[a,c],b\} + \{a,[b,c]\} \end{cases}$$

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The equation of motion for the current operator reads,

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with momentum stress tensor, and acceleration

$$\begin{aligned}\hat{\mathcal{T}}_{\nu\mu}(\mathbf{r},t) &= \frac{1}{4}\sum_i \{\{\delta(\mathbf{r}-\mathbf{r}_i), \hat{\mathbf{v}}_{i\nu}(t)\}, \hat{\mathbf{v}}_{i\mu}(t)\} \\ \widehat{\frac{\partial \mathbf{v}_{i\mu}}{\partial t}}(t) &= \frac{\partial}{\partial t}\hat{\mathbf{v}}_{i\mu}(t) - i[\hat{\mathbf{v}}_{i\mu}(t),\hat{H}(t)]\end{aligned}$$

EOM Current Density

Acceleration contributions: $v(\mathbf{r}, t)$, $w(\mathbf{r} - \mathbf{r}')$,

$$[\hat{\mathbf{v}}_{i\mu}(t), \sum_k v(\mathbf{r}_k, t)] \;=\; -i\nabla_{i\mu} v(\mathbf{r}_i, t)$$

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[\hat{\mathbf{v}}_{i\mu}(t), \sum_k v(\mathbf{r}_k, t)] &= -i\nabla_{i\mu} v(\mathbf{r}_i, t), \\
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\end{aligned}
$$

Contribution $\frac{1}{2}|\mathbf{p} + \mathbf{A}(\mathbf{r}, t)|^2$,

$$
[\hat{\mathbf{v}}_{i\mu}(t), \frac{1}{2}\sum_{k,\nu} \hat{\mathbf{v}}_{k\nu}(t)\hat{\mathbf{v}}_{k\nu}(t)] = \frac{1}{2}\sum_{\nu}\{[\hat{\mathbf{v}}_{i\mu}(t), \hat{\mathbf{v}}_{i\nu}(t)], \hat{\mathbf{v}}_{i\nu}(t)\}
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Acceleration contributions: $v(\mathbf{r}, t)$, $w(\mathbf{r} - \mathbf{r}')$,

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$$\begin{aligned} [\hat{\mathbf{v}}_{i\mu}(t), \frac{1}{2}\sum_{k,\nu} \hat{\mathbf{v}}_{k\nu}(t)\hat{\mathbf{v}}_{k\nu}(t)] &= \frac{1}{2}\sum_{\nu}\{[\hat{\mathbf{v}}_{i\mu}(t), \hat{\mathbf{v}}_{i\nu}(t)], \hat{\mathbf{v}}_{i\nu}(t)\}, \\ [\hat{\mathbf{v}}_{i\mu}(t), \hat{\mathbf{v}}_{i\nu}(t)] &= -i(\nabla_{\mu}\mathbf{A}_{\nu}(\mathbf{r}_i, t) - \nabla_{\nu}\mathbf{A}_{\mu}(\mathbf{r}_i, t)) \end{aligned}$$

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[\hat{\mathbf{v}}_{i\mu}(t), \hat{\mathbf{v}}_{i\nu}(t)] &= -i(\nabla_{\mu}\mathbf{A}_{\nu}(\mathbf{r}_i, t) - \nabla_{\nu}\mathbf{A}_{\mu}(\mathbf{r}_i, t)) \\
&= -i\sum_{\lambda} \epsilon_{\lambda\mu\nu}(\nabla \times \mathbf{A})_{\lambda}(\mathbf{r}_i, t)
\end{aligned}$$

EOM Current Density

Collecting all terms, and reorganizing,

$$
\begin{aligned}
\widehat{\frac{\partial \mathbf{j}_\mu}{\partial t}}(\mathbf{r},t) = & -\sum_\nu \nabla_\nu \hat{\mathcal{T}}_{\nu\mu}(\mathbf{r},t) \\
& -\sum_{i,j\neq i} \delta(\mathbf{r}-\mathbf{r}_i)\nabla_{i\mu} w(|\mathbf{r}_i-\mathbf{r}_j|) \\
& -\sum_i \delta(\mathbf{r}-\mathbf{r}_i)\cdot\left(-\frac{\partial}{\partial t}\mathbf{A}(\mathbf{r},t)+\nabla v(\mathbf{r},t)\right) \\
& -\frac{1}{2}\sum_i \{\delta(\mathbf{r}-\mathbf{r}_i),\hat{\mathbf{v}}_{i\nu}(t)\}\cdot\sum_{\lambda\nu}\epsilon_{\lambda\mu\nu}(\nabla\times\mathbf{A})_\lambda(\mathbf{r},t)
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&\quad - \sum_i \delta(\mathbf{r}-\mathbf{r}_i)\cdot\left(-\frac{\partial}{\partial t}\mathbf{A}(\mathbf{r},t) + \nabla v(\mathbf{r},t)\right) \\
&\quad - \frac{1}{2}\sum_i \{\delta(\mathbf{r}-\mathbf{r}_i), \hat{\mathbf{v}}_{i\nu}(t)\}\cdot\sum_{\lambda\nu}\epsilon_{\lambda\mu\nu}(\nabla\times\mathbf{A})_\lambda(\mathbf{r},t)
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Final result, local force balance relation,

$$\frac{\partial \mathbf{j}}{\partial t}(\mathbf{r},t) = -\nabla\cdot\mathcal{T}(\mathbf{r},t) + \mathbf{f}_W(\mathbf{r},t) \underbrace{-n(\mathbf{r},t)\mathbf{E}(\mathbf{r},t) - \mathbf{j}(\mathbf{r},t)\times\mathbf{B}(\mathbf{r},t)}_{\mathbf{f}_L(\mathbf{r},t)}$$

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& -\frac{1}{2}\sum_i \{\delta(\mathbf{r}-\mathbf{r}_i),\hat{\mathbf{v}}_{i\nu}(t)\}\cdot\sum_{\lambda\nu}\epsilon_{\lambda\mu\nu}(\nabla\times\mathbf{A})_\lambda(\mathbf{r},t)
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$$

Gauge Invariance

Gauge Shift Λ

$$
\begin{aligned}
v(\mathbf{r},t) &\rightarrow v(\mathbf{r},t) + \frac{\partial}{\partial t}\Lambda(\mathbf{r},t) \\
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\Psi(t) &\rightarrow e^{-i\sum_j \Lambda(\mathbf{r}_j,t)}\Psi(t)
\end{aligned}
$$

$$\Downarrow$$

Gauge Invariant Operators

$$\hat{o}[v,\mathbf{A}] = e^{i\sum\Lambda}\hat{o}[v + \frac{\partial\Lambda}{\partial t}, \mathbf{A} + \nabla\Lambda]e^{-i\sum\Lambda}$$

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Examples

$$\begin{aligned} \mathbf{E} &= \nabla v - \frac{\partial}{\partial t}\mathbf{A} \\ \mathbf{B} &= \nabla \times \mathbf{A} \end{aligned}$$

$$\Downarrow$$

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Examples

$$\sum_i v(\mathbf{r}_i,t) - i\frac{\partial}{\partial t}$$

$$\hat{\mathbf{v}}_i(t) = \hat{\mathbf{p}}_i + \mathbf{A}(\mathbf{r}_i,t)$$

$$\Rightarrow \hat{H}[v,\mathbf{A}] - i\frac{\partial}{\partial t}$$

$\Downarrow$

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\hat{o}[v,\mathbf{A}] &= e^{i\sum\Lambda}\hat{o}[v + \frac{\partial\Lambda}{\partial t}, \mathbf{A} + \nabla\Lambda]e^{-i\sum\Lambda} \\
\widehat{\frac{\partial o}{\partial t}} &= -i[\hat{o}, \hat{H}[v,\mathbf{A}] - i\frac{\partial}{\partial t}]
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$$

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$$\sum_i v(\mathbf{r}_i,t) - i\frac{\partial}{\partial t}$$

$$\hat{\mathbf{v}}_i(t) = \hat{\mathbf{p}}_i + \mathbf{A}(\mathbf{r}_i,t)$$

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$$\begin{aligned} \hat{o}[v,\mathbf{A}] &= e^{i\sum\Lambda}\hat{o}[v + \frac{\partial\Lambda}{\partial t}, \mathbf{A} + \nabla\Lambda]e^{-i\sum\Lambda} \\ \widehat{\frac{\partial o}{\partial t}} &= -i[\hat{o}, \hat{H}[v,\mathbf{A}] - i\frac{\partial}{\partial t}] \end{aligned}$$

Key Operators

$\hat{\mathcal{T}}, \hat{\mathbf{f}}_W \rightarrow \hat{\mathbf{f}}$

$\hat{n}, \hat{\mathbf{j}}, \mathbf{E}, \mathbf{B}$

Resumé

Hydrodynamicla description

- Density $\hat{n}(\mathbf{r}) \to n(\mathbf{r}, t)$ and current density $\hat{\mathbf{j}}(\mathbf{r}, t) \to \mathbf{j}(\mathbf{r}, t)$
- EOM's: $\begin{cases} \frac{\partial}{\partial t} n &= -\nabla \cdot \mathbf{j} \\ \frac{\partial}{\partial t} \mathbf{j} &= \mathbf{f} - n\mathbf{E} - \mathbf{j} \times \mathbf{B} \end{cases}$
- Internal force density $\mathbf{f} = -\nabla \cdot \mathcal{T} + \mathbf{f}_W$
- All properties depend on $(v, \mathbf{A})$, with gauge invariance!
- Establish direct relation between $(v, \mathbf{A})_\Lambda$ and $(n, \mathbf{j})_P$

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- Internal force density $\mathbf{f} = -\nabla \cdot \mathcal{T} + \mathbf{f}_W$
- All properties depend on $(v, \mathbf{A})$, with gauge invariance!
- Establish direct relation between $(v, \mathbf{A})_\Lambda$ and $(n, \mathbf{j})_P$

What is the information content ?

One-to-One Mapping

Quantum Dynamics

$$i\frac{\partial}{\partial t}\Psi = \hat{H}[v, \mathbf{A}]\Psi$$

$$\Psi(t_0) = \Psi_0$$

One-to-One Mapping

Quantum Dynamics

$$i\frac{\partial}{\partial t}\Psi = \hat{H}[v, \mathbf{A}]\Psi$$

$$\Psi(t_0) = \Psi_0$$

$$\Downarrow$$

Map & Functional

$$(v, \mathbf{A})_\Lambda \rightarrow (n, \mathbf{j})_P \; ; \; \mathbf{f}[v, \mathbf{A}]$$

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$\Rightarrow$

Hydrodynamics

$$\begin{aligned}\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{j} &= 0 \\ \frac{\partial \mathbf{j}}{\partial t} + n\mathbf{E} + \mathbf{j} \times \mathbf{B} &= \mathbf{f}[v, \mathbf{A}]\end{aligned}$$

$$n(t_0) = n_0,\ \mathbf{j}(t_0) = \mathbf{j}_0$$

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$$(v, \mathbf{A})_\Lambda \overset{\mathbf{f}[v,\mathbf{A}]}{\longrightarrow} (n, \mathbf{j})_P$$

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Potentials to Densities

Hydrodynamics

$$\begin{aligned} 0 &= \frac{\partial n}{\partial t} + \nabla \cdot \mathbf{j} \\ \mathbf{f} &= \frac{\partial \mathbf{j}}{\partial t} + \mathbf{E} n + \mathbf{B} \times \mathbf{j} \end{aligned}$$

with $\begin{cases} n(\mathbf{r}, t_0) = n_0(\mathbf{r}) \\ \mathbf{j}(\mathbf{r}, t_0) = \mathbf{j}_0(\mathbf{r}) \end{cases}$.

Mathematical Structure

Define $\begin{cases} u_0 = \delta n, & u_{i\neq 0} = \delta j_i \\ x_0 = t, & x_{i \neq 0} = r_i \end{cases}$.

$$0 = \sum_{j=0}^{4} \left\{ \sum_{k=0}^{4} c_{k,ij} \frac{\partial u_j}{\partial x_k} + b_{ij} u_j \right\}$$

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Potentials to Densities

Hydrodynamics

$$
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$$

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with $\mathbf{u}(\mathbf{x} = (t_0, \mathbf{r})) = \mathbf{0}$.

Analysis Characteristics

$c_{0,ij} = \delta_{ij}$, $c_{k\neq 0,ij} = \delta_{i0}\delta_{kj} \Rightarrow \det\{c_k\} = \delta_{k0}$, so only $\partial \mathbf{u}/\partial t$ well defined.

Potentials to Densities

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$\Rightarrow$ Initial value problem integrates to $\mathbf{u}(\mathbf{x}) = 0$

$$(v, \mathbf{A})_\Lambda \overset{\mathbf{f}[v,\mathbf{A}]}{\rightarrow} (n, \mathbf{j})_P$$

Densities to Potentials

Local Force Balance

Given n, $\mathbf{j}$, with $\partial_t n + \nabla \cdot \mathbf{j} = 0$, and $\mathbf{f}[v, \mathbf{A}]$

$$\mathbf{f}[v, \mathbf{A}] = \frac{\partial}{\partial t}\mathbf{j} + n(\nabla v - \frac{\partial}{\partial t}\mathbf{A}) + \mathbf{j} \times (\nabla \times \mathbf{A})$$

4 unknowns $(v, \mathbf{A})$, 3 eqs. $\Rightarrow$ 1 extra gauge-fixing relation $\lambda(v, \mathbf{A}) = 0$

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Compare Primed-Unprimed Systems

Unprimed

$\Psi_0,\ w,\ (v, \mathbf{A}) \rightarrow \mathbf{f}[v, \mathbf{A}]$

$\Leftrightarrow$

Primed

$\Psi_0',\ w',\ (v', \mathbf{A}') \rightarrow \mathbf{f}'[v', \mathbf{A}']$

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Define $\nu = v - v'$, $\mathbf{a} = \mathbf{A} - \mathbf{A}'$ and $\Delta\mathbf{f}[\nu, \mathbf{a}] = \mathbf{f}[v, \mathbf{A}] - \mathbf{f}'[v', \mathbf{A}']$.

$$\Delta\mathbf{f}[\nu, \mathbf{a}] = n(\nabla \nu - \frac{\partial}{\partial t}\mathbf{a}) + \mathbf{j} \times (\nabla \times \mathbf{a})$$

Densities to Potentials: Vignale's proof

Choose $\nu = 0$, and $t_0 = 0$, and Taylor-expansions for **a**, n, and **j**,

$$\mathbf{a}(\mathbf{r},t) = \sum_{n=0}^{\infty} \frac{t^n}{n!}\mathbf{a}_n(\mathbf{r}) \Rightarrow \begin{cases} \dfrac{\partial^k}{\partial t^k}\mathbf{a}(\mathbf{r},t) = \sum_{n=0}^{\infty} \dfrac{t^n}{n!}\mathbf{a}_{n+k}(\mathbf{r}) \\ \mathbf{a}_k(\mathbf{r}) = \dfrac{\partial^k}{\partial t^k}\mathbf{a}(\mathbf{r},t)\,\big|_{t=0} \end{cases}$$

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Repeated use of Heisenberg equation of motion,

$$\left.\begin{aligned} \hat{\mathbf{f}}_0(\mathbf{r},t) &= -\nabla\cdot\hat{\mathcal{T}}(\mathbf{r},t) + \hat{\mathbf{f}}_W(\mathbf{r}) \\ \hat{\mathbf{f}}_{k+1}(\mathbf{r},t) &= -i[\hat{\mathbf{f}}_k(\mathbf{r},t), \hat{H}(t) - i\frac{\partial}{\partial t}] \end{aligned}\right\} \frac{\partial^k}{\partial t^k}\mathbf{f}(\mathbf{r},t) = \langle\Psi(t)\mid\hat{\mathbf{f}}_k(\mathbf{r},t)\mid\Psi(t)\rangle$$

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Hence

$$\mathbf{f}(\mathbf{r},t) = \sum_{n=0}^{\infty} \frac{t^n}{n!}\mathbf{f}_n(\mathbf{r}) \Rightarrow \mathbf{f}_k(\mathbf{r}) = \langle \Psi_0 \mid \hat{\mathbf{f}}_k(\mathbf{r},t_0) \mid \Psi_0\rangle = \mathbf{f}_k[\mathbf{a}_0 \cdots \mathbf{a}_k](\mathbf{r})$$

Densities to Potentials: Vignale's proof

Inserting Taylor series, and equating orders in t,

$$\Delta \mathbf{f}[\mathbf{a}](\mathbf{r},t) + n(\mathbf{r},t)\frac{\partial}{\partial t}\mathbf{a}(\mathbf{r},t) - \mathbf{j}(\mathbf{r},t) \times (\nabla \times \mathbf{a}(\mathbf{r},t)) = 0$$

yields a hierarchy for $a_{n+1}(\mathbf{r})$ in terms of $\mathbf{a}_0(\mathbf{r})\cdots\mathbf{a}_n(\mathbf{r})$.

$$\sum_{n=0}^{\infty}\frac{t^n}{n!}\left[\Delta \mathbf{f}_n[\mathbf{a}_0\cdots\mathbf{a}_n] + \sum_{k=0}^{n}\binom{n}{k}\left[n_{n-k}\mathbf{a}_{k+1} - \mathbf{j}_{n-k} \times (\nabla \times \mathbf{a}_k)\right]\right] = 0$$

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Initial value $n_0(\mathbf{r})$ and $\mathbf{j}_0(\mathbf{r})$ fix $\mathbf{a}_0(\mathbf{r}) = \mathbf{A}_0(\mathbf{r}) - \mathbf{A}'_0(\mathbf{r})$ with given Ψ_0, Ψ'_0

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$$\boxed{(v, \mathbf{A})_\Lambda \overset{\mathbf{f}[v,\mathbf{A}]}{\longleftarrow} (n, \mathbf{j})_P} \text{ and } \boxed{(v', \mathbf{A}')_\Lambda \overset{\mathbf{f}'[v',\mathbf{A}']}{\longleftarrow} (n, \mathbf{j})_P}$$

Resumé

Hydrodynamics establishes

- Invertible map: $(v, \mathbf{A})_\Lambda \overset{\Psi_0, \mathbf{f}[v,\mathbf{A}]}{\leftrightarrow} (n, \mathbf{j})_P$.
- Kohn-Sham construction: $(v', \mathbf{A}')_\Lambda \overset{\Psi_0', \mathbf{f}[v',\mathbf{A}']}{\leftrightarrow} (n, \mathbf{j})_P$.

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BUT

- No easy access to Ψ_0, $\mathbf{f}[v, \mathbf{A}]$.
- No easy propagation, requires high order $d^k/dt^k\, \mathbf{f}[v, \mathbf{A}]$.
- Only n, $\mathbf{j}$, v, $\mathbf{A}$ analytic in t.

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How to make it practicle ?

Many-Body Perturbation Theory

Unprimed

Ψ_0, w, $(v, \mathbf{A})$

Primed

Ψ'_0, w', $(v', \mathbf{A}')$

Many-Body Perturbation Theory

Unprimed

$\Psi_0,\ w,\ (v, \mathbf{A})$

$\overset{\lambda=1}{\longleftarrow}$

Intermediate

$\Psi_{\lambda,0},\ w_\lambda,\ (v_\lambda, \mathbf{A}_\lambda)$

$\overset{\lambda=0}{\longrightarrow}$

Primed

$\Psi'_0,\ w',\ (v', \mathbf{A}')$

Many-Body Perturbation Theory

Unprimed		Intermediate		Primed
$\Psi_0,\ w,\ (v,\mathbf{A})$	$\overset{\lambda=1}{\longleftarrow}$	$\Psi_{\lambda,0},\ w_\lambda,\ (v_\lambda,\mathbf{A}_\lambda)$	$\overset{\lambda=0}{\longrightarrow}$	$\Psi'_0,\ w',\ (v',\mathbf{A}')$

$$\hat{H}_\lambda(t) = \hat{H}'(t) + f_\eta(t)\hat{H}_1(\lambda,t),\ \ with\ \hat{H}_1(\lambda,t) = \hat{W}_\lambda - \hat{W}' + \hat{V}_\lambda(t) - \hat{V}'(t)$$

in which:

$$\hat{W}_\lambda = \lambda\hat{W} + (1-\lambda)\hat{W}'$$

$$\hat{V}_\lambda(t) = \sum_{i=1}^{N}\left\{\frac{1}{2}[-i\nabla_i + \mathbf{A}_\lambda(\mathbf{r}_i,t)]^2 + v_\lambda(\mathbf{r}_i,t)\right\} - \hat{T}$$

Many-Body Perturbation Theory

Unprimed		Intermediate		Primed
$\Psi_0,\ w,\ (v, \mathbf{A})$	$\overset{\lambda=1}{\longleftarrow}$	$\Psi_{\lambda,0},\ w_\lambda,\ (v_\lambda, \mathbf{A}_\lambda)$	$\overset{\lambda=0}{\longrightarrow}$	$\Psi'_0,\ w',\ (v', \mathbf{A}')$

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Adiabatic switch-on:

$$f_\eta(t \geq t_0) = 1, \text{ but } f_\eta(t)\hat{H}_1(\lambda, t) = e^{\eta t}\hat{H}_1(\lambda, t_0) \text{ for } t \to -\infty.$$

$$\Psi(-\infty) = \Psi_\lambda(-\infty) = \Psi'(-\infty) \doteq \Psi'_0$$

Expectation values in orders of $\hat{H}_1(\lambda, t)$

Perturbation expansion

$$\langle \Psi_\lambda(t) \mid \hat{o}(\mathbf{r}, t) \mid \Psi_\lambda(t) \rangle = \langle \Psi'(t) \mid \hat{o}(\mathbf{r}, t) \mid \Psi'(t) \rangle +$$
$$\lim_{\eta \to 0} \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_C dt_1 f_\eta(t_1) \ldots \int_C dt_n f_\eta(t_n) \times$$
$$\langle \Psi'_0 \mid T_C \Delta\hat{o}(\mathbf{r}, t) \Delta\hat{H}_1(\lambda, t_1) \ldots \Delta\hat{H}_1(\lambda, t_n) \mid \Psi'_0 \rangle.$$

Fluctuation operators in Heisenberg picture wrt $\hat{H}'(t)$,

$$\Delta\hat{o}(t) = \hat{o}_H(t) - \langle \hat{o}_H(t) \rangle', \text{ with } \hat{o}_H(t) = \hat{U}'(-\infty, t)\hat{o}(t)\hat{U}'(t, -\infty).$$

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$$\langle \Psi'_0 \mid T_C \Delta\hat{o}(\mathbf{r}, t) \Delta\hat{H}_1(\lambda, t_1) \dots \Delta\hat{H}_1(\lambda, t_n) \mid \Psi'_0 \rangle.$$

Fluctuation operators in Heisenberg picture wrt $\hat{H}'(t)$,

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Density expansion

$$\hat{n}_\lambda(\mathbf{r}) = \hat{n}'(\mathbf{r}) \Rightarrow n_\lambda(\mathbf{r}, t) = n'(\mathbf{r}, t) + \textstyle\sum_n \langle\langle \Delta\hat{n}'(\mathbf{r}, t) \Delta\hat{H}_1^n(\lambda) \rangle\rangle'$$

Expectation values in orders of $\hat{H}_1(\lambda, t)$

Diamagnetic contribution to current operator,

$$\hat{\mathbf{j}}_\lambda(\mathbf{r}, t) = \hat{\mathbf{j}}'(\mathbf{r}, t) + \hat{n}'(\mathbf{r})\mathbf{a}_\lambda(\mathbf{r}, t), \text{ with } \mathbf{a}_\lambda = \mathbf{A}_\lambda - \mathbf{A}'$$

Expectation values in orders of $\hat{H}_1(\lambda, t)$

Diamagnetic contribution to current operator,

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Current-density expansion

$$\mathbf{j}_\lambda(\mathbf{r}, t) = \mathbf{j}'(\mathbf{r}, t) + \hat{n}_\lambda(\mathbf{r}, t)\mathbf{a}_\lambda(\mathbf{r}, t) + \sum_n \langle\langle T_C \Delta\hat{\mathbf{j}}'(\mathbf{r}, t)\Delta\hat{H}_1^n(\lambda)\rangle\rangle'$$

$\hat{H}_1(\lambda, t)$ in orders of λ

Potential energy operator

$$\hat{V}_\lambda(t) - \hat{V}'(t) = \int d\mathbf{r} \left[\hat{\mathbf{j}}'(\mathbf{r}, t) \cdot \mathbf{a}_\lambda(\mathbf{r}, t) + \hat{n}'(\mathbf{r}) \left(\nu_\lambda(\mathbf{r}, t) + \frac{1}{2} |\mathbf{a}_\lambda(\mathbf{r}, t)|^2 \right) \right]$$

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Expansion of the vector potential in orders of λ, with $\mathbf{a}_\lambda = \mathbf{A}_\lambda - \mathbf{A}'$

$$\mathbf{a}_\lambda(\mathbf{r}, t) = \sum_{n=1}^{\infty} \lambda^n \mathbf{a}_n(\mathbf{r}, t)$$

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$$\mathbf{a}_\lambda(\mathbf{r}, t) = \sum_{n=1}^{\infty} \lambda^n \mathbf{a}_n(\mathbf{r}, t) \Rightarrow \frac{1}{2} |\mathbf{a}_\lambda|^2 = \frac{1}{2} \sum_{n=2}^{\infty} \lambda^n \sum_{p=1}^{n-1} \mathbf{a}_p \cdot \mathbf{a}_{n-p}.$$

$\hat{H}_1(\lambda, t)$ in orders of λ

Potential energy operator

$$\hat{V}_\lambda(t) - \hat{V}'(t) = \int d\mathbf{r} \left[\hat{\mathbf{j}}'(\mathbf{r}, t) \cdot \mathbf{a}_\lambda(\mathbf{r}, t) + \hat{n}'(\mathbf{r}) \left(\nu_\lambda(\mathbf{r}, t) + \frac{1}{2} |\mathbf{a}_\lambda(\mathbf{r}, t)|^2 \right) \right]$$

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The same for the apparent scalar potential, with $\nu_\lambda = v_\lambda - v'$

$$\nu_\lambda(\mathbf{r}, t) + \frac{1}{2} |\mathbf{a}_\lambda(\mathbf{r}, t)|^2 = \sum_{n=1}^{\infty} \lambda^n \nu_n(\mathbf{r}, t)$$

$\hat{H}_1(\lambda, t)$ in orders of λ

Potential energy operator

$$\hat{V}_\lambda(t) - \hat{V}'(t) = \int d\mathbf{r} \left[\hat{\mathbf{j}}'(\mathbf{r}, t) \cdot \mathbf{a}_\lambda(\mathbf{r}, t) + \hat{n}'(\mathbf{r}) \left(\nu_\lambda(\mathbf{r}, t) + \frac{1}{2} |\mathbf{a}_\lambda(\mathbf{r}, t)|^2 \right) \right]$$

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$$\nu_\lambda(\mathbf{r}, t) + \frac{1}{2} |\mathbf{a}_\lambda(\mathbf{r}, t)|^2 = \sum_{n=1}^{\infty} \lambda^n \nu_n(\mathbf{r}, t)$$

So we arrive at

$$\hat{V}_\lambda(t) - \hat{V}'(t) = \sum_{n=1}^{\infty} \lambda^n \left\{ \int d\mathbf{r} \left[\hat{\mathbf{j}}'(\mathbf{r}, t) \cdot \mathbf{a}_n(\mathbf{r}, t) + \hat{n}'(\mathbf{r}) \nu_n(\mathbf{r}, t) \right] \right\}$$

$\hat{H}_1(\lambda, t)$ in orders of λ

Define $\Delta w(r) = w(r) - w'(r)$, then

$$\hat{W}_\lambda - \hat{W}' = \frac{\lambda}{2} \sum_{i,j \neq i} \Delta w(|\mathbf{r}_i - \mathbf{r}_j|)$$

Separate Hartree term, using $n_\lambda \to n'$,

$$u_\lambda(\mathbf{r}, t) = \int d\mathbf{r}'\, w_\lambda(|\mathbf{r}-\mathbf{r}'|) n_\lambda(\mathbf{r}', t) \to u'(\mathbf{r}, t) + \lambda \underbrace{\int d\mathbf{r}'\, \Delta w(|\mathbf{r} - \mathbf{r}'|) n'(\mathbf{r}', t)}_{\Delta u(\mathbf{r}, t)}$$

$\to$ first order in λ

$$\hat{V}_{h,\lambda}(t) - \hat{V}'_h(t) = \int d\mathbf{r}\, \hat{n}'(\mathbf{r})(u_\lambda(\mathbf{r}, t) - u'(\mathbf{r}, t)) \to \lambda \int d\mathbf{r}\, \hat{n}'(\mathbf{r}) \Delta u(\mathbf{r}, t)$$

Include in apparent scalar potential

$$\nu_1(\mathbf{r}, t) \to \nu_1(\mathbf{r}, t) + \Delta u(\mathbf{r}, t)$$

Expectation values in orders of λ

$$\hat{H}_1(\lambda, t) = \lambda\Big(\overbrace{\hat{W} - \hat{W}' - \hat{V}_h(t) + \hat{V}_h'(t)}^{\hat{\omega}(t)}\Big) + \sum_{n=1}^{\infty} \lambda^n \int d\mathbf{r} \left[\hat{\mathbf{j}}'(\mathbf{r}, t) \cdot \mathbf{a}_n(\mathbf{r}, t) + \hat{n}'(\mathbf{r}, t)\nu_n(\mathbf{r}, t)\right]$$

$$\Rightarrow \hat{h}_n(t) = \delta_{n1}\hat{\omega}(t) + \int d\mathbf{r} \left[\hat{\mathbf{j}}'(\mathbf{r}, t) \cdot \mathbf{a}_n(\mathbf{r}, t) + \hat{n}'(\mathbf{r}, t)\nu_n(\mathbf{r}, t)\right]$$

Expectation values in orders of λ

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Re-order summation in perturbation expansion

$$\langle \hat{o}(\mathbf{r}, t)\rangle_\lambda - \langle \hat{o}(\mathbf{r}, t)\rangle' = \sum_{n=1}^{\infty} \lambda^n \Bigg\{ \sum_{p=1}^{n} \frac{(-i)^p}{p!} \lim_{\eta\to 0} \int_C dt_1 f_\eta(t_1) \dots \int_C dt_p f_\eta(t_p) \times \sum_{\{n_1 \cdots n_p\}} \langle \Psi'_0 \mid T_C \Delta\hat{o}(\mathbf{r}, t) \Delta\hat{h}_{n_1}(t_1) \dots \Delta\hat{h}_{n_p}(t_p) \mid \Psi'_0 \rangle \Bigg\}.$$

with $1 \le n_i \le n - p + 1$ and $\sum_i n_i = n \Rightarrow$ highest $n_1 = n$ only for $p = 1$

Optimized Potential Method (x-only...)

To all orders $n_\lambda(\mathbf{r},t) = n'(\mathbf{r},t)$ and $\mathbf{j}_\lambda(\mathbf{r},t) = \mathbf{j}'(\mathbf{r},t)$

$$\int d\mathbf{r}' \int_C dt' \begin{bmatrix} \chi_{nn}(\mathbf{r}t,\mathbf{r}'t') & \chi_{n\mathbf{j}}(\mathbf{r}t,\mathbf{r}'t') \\ \chi_{\mathbf{j}n}(\mathbf{r}t,\mathbf{r}'t') & \Delta\chi_{\mathbf{jj}}(\mathbf{r}t,\mathbf{r}'t') \end{bmatrix} \cdot \begin{bmatrix} \nu_n(\mathbf{r}'t') \\ \mathbf{a}_n(\mathbf{r}'t') \end{bmatrix} = \begin{bmatrix} q_n(\mathbf{r}t) \\ \mathbf{q}_n(\mathbf{r}t) \end{bmatrix}$$

with response functions

$$\Delta\chi_{\mathbf{jj}}(\mathbf{r}t,\mathbf{r}'t') = \chi_{\mathbf{jj}}(\mathbf{r}t,\mathbf{r}'t') + n'(\mathbf{r},t)\delta(\mathbf{r}-\mathbf{r}')\delta(t,t')$$

$$\chi_{ab}(\mathbf{r}t,\mathbf{r}'t') = -i\langle\Psi_0' \mid T_C \Delta\hat{a}'(\mathbf{r},t)\Delta\hat{b}'(\mathbf{r}',t') \mid \Psi_0'\rangle$$

and inhomogeneous part $(n=1)$

$$\begin{bmatrix} q_1(\mathbf{r}t) \\ \mathbf{q}_1(\mathbf{r}t) \end{bmatrix} = -i \lim_{\eta\to 0} \int_C dt_1 f_\eta(t_1) \langle\Psi_0' \mid T_C \begin{bmatrix} \Delta n'(\mathbf{r}t) \\ \Delta\mathbf{j}'(\mathbf{r}t) \end{bmatrix} \Delta\hat{\omega}(t_1) \mid \Psi_0'\rangle$$

Optimized Potential Method (...and beyond)

Higher order terms ($n > 1$)

$$\begin{bmatrix} q_n(\mathbf{r}t) \\ \mathbf{q}_n(\mathbf{r}t) \end{bmatrix} = \sum_{p=2}^{n} \frac{(-i)^p}{p!} \lim_{\eta\to 0} \int_C dt_1 f_\eta(t_1) \ldots \int_C dt_p f_\eta(t_p) \times \sum_{\{n_1 \cdots n_p\}} \langle \Psi_0' \mid T_C \begin{bmatrix} \Delta n'(\mathbf{r}t) \\ \Delta \mathbf{j}'(\mathbf{r}t) \end{bmatrix} \underbrace{\Delta \hat{h}_{n_1}(t_1) \ldots \Delta \hat{h}_{n_p}(t_p)}_{=\Delta \hat{h}^n[\nu_1 \ldots \nu_{n-p+1}, \mathbf{a}_1 \ldots \mathbf{a}_{n-p+1}]} \mid \Psi_0' \rangle .$$

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Self-consistency loop

$$(v', \mathbf{A}')_{i-1} \to \begin{pmatrix} (q_1, \mathbf{q}_1) \to (\nu_1, \mathbf{a}_1) \\ \downarrow \\ (q_m, \mathbf{q}_m) \to (\nu_m, \mathbf{a}_m) \end{pmatrix}_i \to (v', \mathbf{A}')_i$$

Update for potentials

$$(v', \mathbf{A}')_i = (v, \mathbf{A}) - \sum_{k=1}^{m} (\nu_k, \mathbf{a}_k)_i - (\Delta u - \frac{1}{2} \Big| \sum_{k=1}^{m} \mathbf{a}_k \Big|^2, \mathbf{0})_i$$

Resumé

MBPT establishes

- Access to Ψ_0, $\mathbf{f}[v, \mathbf{A}]$.
- Propagation in time, already for lowest order (x-only OEP).

BUT

- Inverting response-kernel techniquely problematic
- Not an existence/uniqueness proof!
- Not using hydrodynamics

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Best of both approaches ?

Densities to Potentials: Global Fixed Point

Unprimed (Fixed)

$\Psi_0,\ w,\ (v, \mathbf{A}) \rightarrow \mathbf{f}[v, \mathbf{A}]$

$\leftarrow$

Primed (Variable)

$\Psi_0',\ w',\ (v', \mathbf{A}') \rightarrow \mathbf{f}'[v', \mathbf{A}']$

Define $\nu = v - v'$, $\mathbf{a} = \mathbf{A} - \mathbf{A}'$, $\Delta\mathbf{f}[\nu, \mathbf{a}] = \mathbf{f}[v, \mathbf{A}] - \mathbf{f}'[v', \mathbf{A}']$.

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Quantum Dynamics (MBPT) to get $\Delta\mathbf{f}[\nu, \mathbf{a}]$,

$$\hat{H}(t) = \hat{H}'(t) + f_\eta(t)\hat{H}_1(t)$$

$$\hat{H}_1(t) = \hat{\omega}(t) + \int d\mathbf{r}\left[\hat{\mathbf{j}}'(\mathbf{r}, t)\cdot\mathbf{a}(\mathbf{r}, t) + \hat{n}'(\mathbf{r})\underbrace{\left(\nu(\mathbf{r}, t) + \Delta u(\mathbf{r}, t) + \frac{1}{2}|\mathbf{a}(\mathbf{r}, t)|^2\right)}_{\tilde{\nu}(\mathbf{r},t)}\right]$$

Densities to Potentials: Global Fixed Point

Unprimed (Fixed)		Primed (Variable)
$\Psi_0,\ w,\ (v, \mathbf{A}) \rightarrow \mathbf{f}[v, \mathbf{A}]$	$\leftarrow$	$\Psi'_0,\ w',\ (v', \mathbf{A}') \rightarrow \mathbf{f}'[v', \mathbf{A}']$

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Hydrodynamics to get $(\nu, \mathbf{a})$ for fixed $(n, \mathbf{j})$.

$$\Delta\mathbf{f}[\nu, \mathbf{a}] = n(\nabla\nu - \frac{\partial}{\partial t}\mathbf{a}) + \mathbf{j} \times (\nabla \times \mathbf{a})$$

Global Fixed Point

Define iteration process, with e.g. $(\nu_0, \mathbf{a}_0) = (-\Delta u, \mathbf{0})$,

$$(\nu_i, \mathbf{a}_i) \stackrel{QD}{\rightarrow} \Delta\mathbf{f}[\nu_i, \mathbf{a}_i] \stackrel{HD}{\rightarrow} (\nu_{i+1}, \mathbf{a}_{i+1}) \stackrel{QD}{\rightarrow} \Delta\mathbf{f}[\nu_{i+1}, \mathbf{a}_{i+1}] \stackrel{HD}{\rightarrow} \cdots \stackrel{HD}{\rightarrow} (\nu_\infty, \mathbf{a}_\infty)$$

If convergent, then fixed point.

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If convergent, then fixed point. Global fixed point if for any initial $(\nu_0, \mathbf{a}_0)$,

$$||(\nu_{i+1}, \mathbf{a}_{i+1}) - (\nu_i, \mathbf{a}_i)||_\alpha \leq C_\alpha ||(\nu_i, \mathbf{a}_i) - (\nu_{i-1}, \mathbf{a}_{i-1})||_\alpha \; \textit{with} \; C_\alpha < 1$$

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Fixed gauge $\nu + \mathbf{v} \cdot \mathbf{a} - \lambda = 0$ ($\mathbf{v}, \lambda$ constant), so $||\nu - \nu'||_\alpha \propto ||\mathbf{a} - \mathbf{a}'||_\alpha$

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$$||\mathbf{a}(\mathbf{r}, t)||_\alpha = \int d\mathbf{r} \int_{t_0}^{T} dt\, e^{-\alpha(t-t_0)} |\mathbf{a}(\mathbf{r}, t)|$$

Similar for $||\mathbf{f}(\mathbf{r}, t)||_\alpha$

Force-Density to Potentials: Mathematical Structure

$$\frac{1}{n}\Delta\mathbf{f}[\nu,\mathbf{a}] \quad = \quad \nabla\nu - \frac{\partial}{\partial t}\mathbf{a} + \mathbf{v} \times (\nabla \times \mathbf{a})$$

Force-Density to Potentials: Mathematical Structure

$$\begin{aligned}\frac{1}{n}\Delta\mathbf{f}[\nu,\mathbf{a}] &= \nabla\nu - \frac{\partial}{\partial t}\mathbf{a} + \mathbf{v}\times(\nabla\times\mathbf{a}),\\ &= \nabla\nu - \frac{\partial}{\partial t}\mathbf{a} + \nabla(\mathbf{v}\cdot\mathbf{a}) - (\nabla\mathbf{v})\cdot\mathbf{a} - (\mathbf{v}\cdot\nabla)\mathbf{a}\end{aligned}$$

Force-Density to Potentials: Mathematical Structure

$$
\begin{aligned}
\frac{1}{n}\Delta \mathbf{f}[\nu, \mathbf{a}] &= \nabla\nu - \frac{\partial}{\partial t}\mathbf{a} + \mathbf{v} \times (\nabla \times \mathbf{a}), \\
&= \nabla\nu - \frac{\partial}{\partial t}\mathbf{a} + \nabla(\mathbf{v} \cdot \mathbf{a}) - (\nabla \mathbf{v}) \cdot \mathbf{a} - (\mathbf{v} \cdot \nabla)\mathbf{a}, \\
&= -\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\right)\mathbf{a} + \nabla(\nu + \mathbf{v} \cdot \mathbf{a}) - (\nabla \mathbf{v}) \cdot \mathbf{a}.
\end{aligned}
$$

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\end{aligned}
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Gauge fixing relation,

$$
\nu(\mathbf{r},t) + \mathbf{v}(\mathbf{r},t)\cdot\mathbf{a}(\mathbf{r},t) - \lambda(\mathbf{r},t) = 0
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Co-moving frame

$$\mathbf{r} = \mathbf{r}(\mathbf{r}_0,t),\ \mathbf{r}_0 = \mathbf{r}(\mathbf{r}_0,t_0),$$

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$$\mathbf{r} = \mathbf{r}(\mathbf{r}_0,t),\ \mathbf{r}_0 = \mathbf{r}(\mathbf{r}_0,t_0),\ \textit{with}\ \frac{d}{dt}\mathbf{r}(\mathbf{r}_0,t) = \mathbf{v}(\mathbf{r}(\mathbf{r}_0,t),t)$$

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Co-moving frame

$$\mathbf{r} = \mathbf{r}(\mathbf{r}_0,t),\ \mathbf{r}_0 = \mathbf{r}(\mathbf{r}_0,t_0),\ \textit{with}\ \frac{d}{dt}\mathbf{r}(\mathbf{r}_0,t) = \mathbf{v}(\mathbf{r}(\mathbf{r}_0,t),t)$$

$$\frac{d}{dt}a(\mathbf{r}(\mathbf{r}_0,t),t) = \left[\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right)a(\mathbf{r},t)\right]_{\mathbf{r}=\mathbf{r}(\mathbf{r}_0,t)}$$

Force-Density to Potentials: Mathematical Structure

Define quantities in comoving frame,

$$\bar{\mathbf{a}}(t) = \mathbf{a}(\mathbf{r}(\mathbf{r}_0, t), t), \ \textit{etc.}$$

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$$\bar{\mathbf{f}}[\bar{\mathbf{a}}](t) = \frac{1}{n}\Delta\mathbf{f}[\lambda - \mathbf{v}\cdot\mathbf{a}, \mathbf{a}](\mathbf{r}(\mathbf{r}_0, t), t) - \nabla\lambda(\mathbf{r}(\mathbf{r}_0, t), t)$$

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$$\bar{\mathbf{f}}[\bar{\mathbf{a}}](t) = \frac{1}{n}\Delta \mathbf{f}[\lambda - \mathbf{v}\cdot\mathbf{a}, \mathbf{a}](\mathbf{r}(\mathbf{r}_0, t), t) - \nabla\lambda(\mathbf{r}(\mathbf{r}_0, t), t)$$

$$\bar{S}_{\mu\nu}(t) = (\nabla_\mu \mathbf{v}_\nu)(\mathbf{r}(\mathbf{r}_0, t), t)$$

Force-Density to Potentials: Mathematical Structure

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Structure of 'simple' set of ODE's,

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Gauge relation $\nu \to \nu + \partial_t\Lambda$ and $\mathbf{a} \to \mathbf{a} + \nabla\Lambda$

$$\nu + \mathbf{v}\cdot\mathbf{a} = \lambda \to \lambda + \left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right)\Lambda \Rightarrow \bar{\lambda} \to \bar{\lambda} + \frac{d}{dt}\bar{\Lambda}$$

HD Step, Given $\bar{\mathbf{f}}$, Update $\bar{\mathbf{a}}$

$$\bar{\mathbf{f}}(t) = \frac{d}{dt}\bar{\mathbf{a}}(t) - \bar{S}(t)\cdot\bar{\mathbf{a}}(t),\ \ \textit{with}\ \bar{\mathbf{a}}(t_0) = \mathbf{a}(\mathbf{r}_0, t_0)$$

$$\bar{\mathbf{a}}(t) = \bar{\mathbf{a}}(t_0) + \int_{t_0}^{t} dt'\ \bar{G}(t,t')\cdot\bar{\mathbf{f}}(t'),\ \ \textit{with}\ \ \bar{G}(t,t') = \exp\left(\int_{t'}^{t} d\tau\ \bar{S}(\tau)\right)$$

Consider norm

$$\int_{t_0}^{T} dt\, e^{-\alpha(t-t_0)}|\bar{\mathbf{a}}_i(t) - \bar{\mathbf{a}}_j(t)|$$

$$\leq \int_{t_0}^{T} dt \int_{t_0}^{t} dt'\, e^{-\alpha(t-t')}||\bar{G}(t,t')||\cdot e^{-\alpha(t'-t_0)}|\bar{\mathbf{f}}_i(t') - \bar{\mathbf{f}}_j(t')|$$

$$= \int_{t_0}^{T} dt' \Bigg(\underbrace{\int_{t'}^{T} dt\, e^{-\alpha(t-t')}||\bar{G}(t,t')||}_{\leq \frac{1}{\alpha - \bar{s}_{max}}\ \ \textit{for}\ \ \alpha > \bar{s}_{max}} \Bigg)\cdot e^{-\alpha(t'-t_0)}|\bar{\mathbf{f}}_i(t') - \bar{\mathbf{f}}_j(t')|$$

$$\Rightarrow ||\mathbf{a}_i - \mathbf{a}_j||_\alpha \leq \frac{1}{\alpha - s_{max}}||\frac{1}{n}||\cdot||\mathbf{f}_i - \mathbf{f}_j||_\alpha$$

QD Step, Given **a**, Update **f**

Diamagnetic contribution to $\hat{\mathbf{j}}$

$$\left.\begin{array}{r}\hat{n} = \hat{n}' \\ \hat{\mathbf{j}} = \hat{\mathbf{j}}' + \hat{n}'\mathbf{a}\end{array}\right\} \Rightarrow \left\{\begin{array}{l} n = n' + \sum_n \langle\langle T_C \Delta\hat{n}' \Delta\hat{H}_1^n \rangle\rangle' \\ \mathbf{j} = \mathbf{j}' + \sum_n \langle\langle T_C \Delta\hat{\mathbf{j}}' \Delta\hat{H}_1^n \rangle\rangle' + n\mathbf{a}\end{array}\right.$$

and similarly for $\hat{\mathcal{T}}$

$$\hat{\mathcal{T}}_{\mu\nu} = \hat{\mathcal{T}}'_{\mu\nu} + \hat{n}'\mathbf{a}_\mu\mathbf{a}_\nu + \hat{\mathbf{j}}'_\mu\mathbf{a}_\nu + \mathbf{a}_\mu\hat{\mathbf{j}}'_\nu$$

$$\Rightarrow \mathcal{T} = \mathcal{T}' + \sum_n \langle\langle T_C \Delta\hat{\mathcal{T}}' \Delta\hat{H}_1^n \rangle\rangle' + \mathbf{ja} + \mathbf{aj} - n\mathbf{aa}$$

Two particle interaction $\omega = w - w'$

$$\hat{\mathbf{f}}_W = \hat{\mathbf{f}}'_W \underbrace{- \sum_{i,j\neq i} \delta(\mathbf{r} - \mathbf{r}_i)\nabla\omega(\mathbf{r}_i - \mathbf{r}_j)}_{\hat{\mathbf{f}}_\omega}$$

$$\Rightarrow \mathbf{f}_W = \mathbf{f}'_W + \langle\hat{\mathbf{f}}_\omega\rangle' + \sum_n \langle\langle T_C \Delta(\hat{\mathbf{f}}'_W + \hat{\mathbf{f}}_\omega)\Delta\hat{H}_1^n \rangle\rangle'$$

QD Step, Given **a**, Update **f**

$$\mathbf{a} \to \nu = \lambda - \mathbf{v}\cdot\mathbf{a} \to \left\{ \begin{array}{c} \hat{H}'[v', \mathbf{A}'] \to \Psi'(t) \to \mathcal{T}', \mathbf{f}'_W \\ \hat{H}_1[\nu, \mathbf{a}] \to \mathcal{T}, \mathbf{f}_W \end{array} \right\} \to \mathbf{f}$$

Consider a change

$$\mathbf{a} \to \mathbf{a} + \delta\mathbf{a}, \nu \to \nu + \delta\nu = \nu - \mathbf{v}\cdot\delta\mathbf{a}$$

Then unchanged unprimed system,

$$\hat{H}[v, \mathbf{A}] = \hat{H}'[v' - \delta\nu, \mathbf{A}' - \delta\mathbf{a}] + \hat{H}_1[\nu + \delta\nu, \mathbf{a} + \delta\mathbf{a}] \to \mathcal{T}, \mathbf{f}_W$$

But modified primed system

$$\hat{H}'[v' - \delta\nu, \mathbf{A}' - \delta\mathbf{a}] = \hat{H}'[v', \mathbf{A}'] + \int d\mathbf{r}\,[(\hat{\mathbf{j}}' - \hat{n}'\mathbf{v})\cdot\delta\mathbf{a} + \frac{1}{2}\hat{n}'|\delta\mathbf{a}|^2]$$

Perturbation theory yields

$$\mathbf{f} \to \mathbf{f} + \delta\mathbf{f} = \mathbf{f} + \delta\{\nabla\cdot\mathcal{T}' - \mathbf{f}'_W\}$$

QD Step, Given **a**, Update **f**

Response formulation

$$\delta\mathbf{f}(\mathbf{r},t) = \int_{t_0}^{t} dt' \int d\mathbf{r}\, \chi_{\mathbf{f}\,(\mathbf{j}-n\mathbf{v})}(\mathbf{r},t;\mathbf{r}',t') \cdot \delta\mathbf{a}(\mathbf{r}',t')$$

with integrated intermediate response functions

$$\chi_{\mathbf{f}\,(\mathbf{j}-n\mathbf{v})}(\mathbf{r},t;\mathbf{r}',t') = -i \int_0^1 d\lambda \langle \Psi_0' \mid T_C \Delta_\lambda \hat{\mathbf{f}}(\mathbf{r},t) \Delta_\lambda (\hat{\mathbf{j}} - \mathbf{v}\hat{n})(\mathbf{r}' t') \mid \Psi_0' \rangle$$

Leading to α-norm

$$\Rightarrow ||\delta\mathbf{f}||_\alpha \leq \frac{\chi_{max}}{\alpha} ||\delta\mathbf{a}||_\alpha$$

Resumé

Global-Fixed-Point Approach establishes

- Access to Ψ_0, $\mathbf{f}[v, \mathbf{A}]$.
- Propagation in time, already for lowest order.
- Inverting response-kernel not needed
- Existence/uniqueness proof!
- Using hydrodynamics $\Rightarrow$ Directly constructing potentials

BUT

- More rigorous derivation needed, e.g.
  -replace α-norm with simple mixing scheme
  -remove $\frac{1}{n}$-factor in HD-map by constructing QM $\mathbf{a} \rightarrow \mathbf{f}/n$-map
- More-complicated perturbation matrix elements

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Discussion and Conclusions

- Perturbation route from primed-to-unprimed system assumed
- Scalar-potential-only & TDDFT
- Connection with TD-DefFT
- Connection with viscoelastic stress-tensor