$\mathcal{V}$-representability in the Time-Dependent Current Density Functional Theory

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Outline

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DFT: A theory of collective variables

Most experiments probe dynamics of some local observables

Typical example:

$n(\mathbf{r},t)$ and $\mathbf{j}(\mathbf{r},t)$ are controlled and probed by $\varphi(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$

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Time-dependent (current) density functional theory: $\{\varphi, \mathbf{A}\} \mapsto \{n, \mathbf{j}\}$

In TD(C)DFT the “intermediate” many-body problem is avoided because the local observables completely determine the state

TDDFT: $n \mapsto |\Psi\rangle = |\Psi[n]\rangle$ TDCDFT: $\mathbf{j} \mapsto |\Psi\rangle = |\Psi[\mathbf{j}]\rangle$

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TDDFT: $n \mapsto |\Psi\rangle = |\Psi[n]\rangle$ TDCDFT: $\mathbf{j} \mapsto |\Psi\rangle = |\Psi[\mathbf{j}]\rangle$

Conceptually TDDFT is a theory of collective variables, which operates only with observables.

The observable to wave function mapping in DFT

Any DFT relies on the existence of the unique observable-to-WF map $\mathcal{N} \mapsto |\Psi\rangle$, which can be viewed as a consequence of the map from the observable to the conjugated potential $\mathcal{N} \mapsto \mathcal{V}$

- The standard quantum mechanics solves the "direct problem":

$$\mathcal{V} \mapsto \mathcal{N} : \; i\partial_t|\Psi\rangle = \hat{H}[\mathcal{V}]|\Psi\rangle, \; \mathcal{N}[\mathcal{V}] = \langle\Psi|\hat{\mathcal{N}}|\Psi\rangle$$

- TD(C)DFT assumes that the "inverse problem" is also solvable:

$$\mathcal{N} \mapsto \mathcal{V}$$

Two key problems of TD(C)DFT (setting up the terminology)

- uniqueness of the "inverse map" $\equiv$ Runge-Gross theorem
- existence of the "inverse map" $\equiv$ $\mathcal{V}$-representability problem

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Question: How to formulate the inverse problem mathematically?

Formulation of the TDCDFT problem (temporal gauge)

$$\hat{H}[\mathbf{A}] = \sum_{j=1}^{N} \frac{(i\nabla_j + \mathbf{A}(\mathbf{r}_j, t))^2}{2m} + \frac{1}{2}\sum_{j\neq k} V(\mathbf{r}_j - \mathbf{r}_k)$$

Direct problem (given $\mathbf{A}$, $|\Psi_0\rangle$): Linear Schrödinger equation

$$i\partial_t|\Psi(t)\rangle = H[\mathbf{A}]|\Psi(t)\rangle, \quad |\Psi(0)\rangle = |\Psi_0\rangle$$

$$\hat{n}(\mathbf{r}) = \sum_{j=1}^{N}\delta(\mathbf{r}-\mathbf{r}_j), \quad \hat{\mathbf{j}}^p(\mathbf{r}) = \frac{-i}{2m}\sum_{j=1}^{N}\{\nabla_j, \delta(\mathbf{r}-\mathbf{r}_j)\}$$

$$\mathbf{j}(\mathbf{r},t) = \langle\Psi(t)|\hat{\mathbf{j}}^p(\mathbf{r})|\Psi(t)\rangle - \frac{n(\mathbf{r},t)}{m}\mathbf{A}(\mathbf{r},t), \quad n(\mathbf{r},t) = \langle\Psi(t)|\hat{n}(\mathbf{r})|\Psi(t)\rangle$$

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Inverse problem (given $\mathbf{j}$, $|\Psi_0\rangle$): Nonlinear many-body problem

$$i\partial_t|\Psi(t)\rangle = H[\mathbf{A}]|\Psi(t)\rangle, \quad |\Psi(0)\rangle = |\Psi_0\rangle$$

$$\mathbf{A}(\mathbf{r},t) = \frac{m}{n(\mathbf{r},t)}\left[\langle\Psi(t)|\hat{\mathbf{j}}^p(\mathbf{r})|\Psi(t)\rangle - \mathbf{j}(\mathbf{r},t)\right]$$

The solution, if exists, gives us the functionals $\Psi[\mathbf{j},\Psi_0]$ and $\mathbf{A}[\mathbf{j},\Psi_0]$

Simple example of the inverse problem: N=1

$$i\partial_t \Psi(\mathbf{r},t) = \frac{1}{2m}\left(i\nabla + \mathbf{A}(\mathbf{r},t)\right)^2 \Psi(\mathbf{r},t), \quad \Psi(\mathbf{r},0) = \Psi_0(\mathbf{r}) \equiv \sqrt{n_0(\mathbf{r})}e^{i\varphi_0(\mathbf{r})}$$

$$\mathbf{A}(\mathbf{r},t) = \frac{1}{|\Psi|^2}\left[\frac{-i}{2}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) - m\mathbf{j}(\mathbf{r},t)\right]$$

This nonlinear problem is exactly solvable!

Exact solution of the inverse TDCDFT problem for one particle

$$\Psi[\Psi_0, \mathbf{j}](\mathbf{r},t) = \sqrt{n(\mathbf{r},t)}e^{i\varphi(\mathbf{r},t)},$$

$$\mathbf{A}[\Psi_0, \mathbf{j}](\mathbf{r},t) = \nabla\varphi(\mathbf{r},t) - m\frac{\mathbf{j}(\mathbf{r},t)}{n(\mathbf{r},t)},$$

where the functions $n(\mathbf{r},t)$ and $\varphi(\mathbf{r},t)$ are defined as follows

$$n(\mathbf{r},t) = n_0(\mathbf{r}) - \int_0^t dt' \nabla\mathbf{j}(\mathbf{r},t),$$

$$\varphi(\mathbf{r},t) = \varphi_0(\mathbf{r}) + \int_0^t dt' \left[\frac{\nabla^2\sqrt{n(\mathbf{r},t')}}{2m\sqrt{n(\mathbf{r},t')}} - \frac{m\mathbf{j}^2(\mathbf{r},t')}{2n^2(\mathbf{r},t')}\right]$$

General N-body inverse problem of TDCDFT

Nonlinear many-body problem – finding $|\Psi\rangle$ for a given $\mathbf{j}(\mathbf{r},t)$

$$i\partial_t|\Psi(t)\rangle = H[\mathbf{A}]|\Psi(t)\rangle, \quad |\Psi(0)\rangle = |\Psi_0\rangle \tag{1}$$

$$\mathbf{A}(\mathbf{r},t) = \frac{m}{\langle\Psi(t)|\hat{n}(\mathbf{r})|\Psi(t)\rangle}\left[\langle\Psi(t)|\hat{\mathbf{j}}^p(\mathbf{r})|\Psi(t)\rangle - \mathbf{j}(\mathbf{r},t)\right] \tag{2}$$

"NLSE" approach to the TDCDFT problem – Plug $\mathbf{A}[\Psi]$ from Eq. (2) into Eq. (1). The results is a nonlinear Schrödinger equation (NLSE):

$$i\partial_t|\Psi(t)\rangle = \tilde{H}_{\mathbf{j}}[\Psi]|\Psi(t)\rangle, \quad |\Psi(0)\rangle = |\Psi_0\rangle$$

TDCDFT is valid if there exists a unique solution to this NLSE.

Current status of the TD(C)DFT problem

TD(C)DFT in continuum

- Assuming V-representability (the existence) we can prove the uniqueness for t-analytic potentials using RG-type arguments [E. Runge and E. K. U. Gross, PRL **52**, 997 (1984)]
- The V-representability problem remains unsolved (all existing proofs rely on some reasonable, but unjustified assumptions)

TD(C)DFT on a lattice

For lattice systems both the uniqueness and the existence has been proved rigorously without any additional assumption.

TDCDFT: IVT, PRB, **83**, 035127 (2011);
TDDFT: M. Farzanehpour and IVT, PRB, **86**, 125130 (2012)

Outline

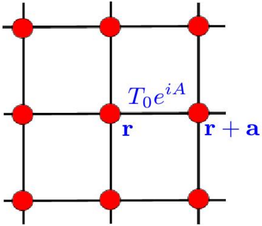
Many-body theory on a lattice (temporal gauge)

N particles on M-site lattice $(N_{\mathcal{H}} = M^N)$

Many-body wave function: $\psi(\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_N, t)$

Vector potential enters via hopping phases:

$$T(\mathbf{r}, \mathbf{r}+\mathbf{a}) \to T_0 e^{iA(\mathbf{r},\mathbf{r}+\mathbf{a};t)}$$



$A(\mathbf{r}, \mathbf{r}+\mathbf{a}; t) = \int_{\mathbf{r}}^{\mathbf{r}+\mathbf{a}} \mathbf{A}(\mathbf{x}, t) d\mathbf{x}$ – link vector potential (two-point object)

Schrödinger equation on a lattice (Cauchy problem for $N_{\mathcal{H}}$ ODE!)

$$\begin{aligned} i\partial_t \psi(\mathbf{r}_1 \dots \mathbf{r}_N; t) = & - \sum_{j=1}^{N} \sum_{\mathbf{a}} T_0 e^{iA(\mathbf{r}_j, \mathbf{r}_j+\mathbf{a}; t)} \psi(\dots \mathbf{r}_j + \mathbf{a} \dots; t) \\ & + \sum_{i>j} V_{\mathbf{r}_i - \mathbf{r}_j} \psi(\mathbf{r}_1 \dots \mathbf{r}_N; t) \\ \psi(\mathbf{r}_1 \dots \mathbf{r}_N; t_0) = & \ \psi_0(\mathbf{r}_1 \dots \mathbf{r}_N) \end{aligned}$$

Basic one-particle observables (identical particles)

On-site density: $n(\mathbf{r};t) = \sum_{\mathbf{r}_2\ldots\mathbf{r}_N} |\psi(\mathbf{r},\mathbf{r}_2\ldots\mathbf{r}_N;t)|^2$

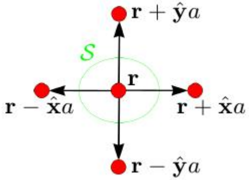
Local current is expressed in terms of the link density matrix:

$$\rho(\mathbf{r},\mathbf{r}+\mathbf{a}) = \sum_{\mathbf{r}_2\ldots\mathbf{r}_N} \psi^*(\mathbf{r},\mathbf{r}_2\ldots\mathbf{r}_N,t)\psi(\mathbf{r}+\mathbf{a},\mathbf{r}_2\ldots\mathbf{r}_N;t)$$

Current on a lattice link: $J(\mathbf{r},\mathbf{r}+\mathbf{a};t) = 2\mathrm{Im}\left\{T_0 e^{iA(\mathbf{r},\mathbf{r}+\mathbf{a};t)}\rho(\mathbf{r},\mathbf{r}+\mathbf{a};t)\right\}$

Continuity equation on a lattice:

$$\partial_t n(\mathbf{r};t) = -\sum_{\mathbf{a}} J(\mathbf{r},\mathbf{r}+\mathbf{a};t)$$



Kinetic energy on a link: $K(\mathbf{r},\mathbf{r}+\mathbf{a};t) = 2\mathrm{Re}\left\{T_0 e^{iA(\mathbf{r},\mathbf{r}+\mathbf{a};t)}\rho(\mathbf{r},\mathbf{r}+\mathbf{a};t)\right\}$

Outline

Many-body NLSE on a lattice (1)

I. Start from the definition of the current:

$$J(\mathbf{r},\mathbf{r}+\mathbf{a};t) = 2\text{Im}\left\{T_0 e^{iA(\mathbf{r},\mathbf{r}+\mathbf{a};t)}\rho(\mathbf{r},\mathbf{r}+\mathbf{a};t)\right\}$$

$$|J(\mathbf{r},\mathbf{r}+\mathbf{a};t|^2 + |K(\mathbf{r},\mathbf{r}+\mathbf{a};t)|^2 = 4T_0^2|\rho(\mathbf{r},\mathbf{r}+\mathbf{a};t)|^2$$

II. Express the vector potential as $A[J,\psi]$:

$$T_0 e^{iA(\mathbf{r},\mathbf{r}+\mathbf{a})} = \frac{s_0\sqrt{4T_0^2|\rho(\mathbf{r},\mathbf{r}+\mathbf{a};t)|^2 - |J(\mathbf{r},\mathbf{r}+\mathbf{a};t)|^2} + iJ(\mathbf{r},\mathbf{r}+\mathbf{a};t)}{2\rho(\mathbf{r},\mathbf{r}+\mathbf{a};t)}$$

$$s_0 \equiv s(\psi_0) = \text{sgn}\left\{K(\mathbf{r},\mathbf{r}+\mathbf{a};t_0)\right\}$$

Initial state enters via the sign of the initial link kinetic energy!

III. Final step in the derivation of the lattice NLSE:

Insert $T_0 e^{iA[\psi](\mathbf{r},\mathbf{r}+\mathbf{a};t)} = T_J[\psi](\mathbf{r},\mathbf{r}+\mathbf{a};t)$ into the lattice SE

Many-body NLSE on a lattice (2)

Nonlinear Schrödinger equation on a lattice

$$i\partial_t \psi(\mathbf{r}_1 \dots \mathbf{r}_N; t) = -\sum_{j=1}^{N} \sum_{\mathbf{a}} T_J[\psi](\mathbf{r}_j, \mathbf{r}_j + \mathbf{a}; t)\psi(\dots \mathbf{r}_j + \mathbf{a} \dots; t)$$

$$+ \sum_{i>j} V_{\mathbf{r}_i - \mathbf{r}_j} \psi(\mathbf{r}_1 \dots \mathbf{r}_N; t),$$

$$\psi(\mathbf{r}_1 \dots \mathbf{r}_N; t_0) = \psi_0(\mathbf{r}_1 \dots \mathbf{r}_N)$$

The problem of TDCDFT reduces a system of $N_{\mathcal{H}}$ nonlinear ODE

$$\dot{\boldsymbol{\psi}} = \mathbf{F}(\boldsymbol{\psi}, t), \quad \boldsymbol{\psi}(t_0) = \boldsymbol{\psi}_0$$

which by Picard's theorem has a unique solution if $\mathbf{F}(\psi, t)$ is continuous in time and Lipschitz continuous in ψ-variables.

Lipschitz condition: $\|\mathbf{F}(\boldsymbol{\psi}_1) - \mathbf{F}(\boldsymbol{\psi}_2)\| < L\|\boldsymbol{\psi}_1 - \boldsymbol{\psi}_2\|$

Many-body NLSE on a lattice (3)

$$T_J[\psi](\mathbf{r},\mathbf{r}+\mathbf{a};t) = \frac{s_0\sqrt{4T_0^2|\rho(\mathbf{r},\mathbf{r}+\mathbf{a};t)|^2 - |J(\mathbf{r},\mathbf{r}+\mathbf{a};t)|^2} + iJ(\mathbf{r},\mathbf{r}+\mathbf{a};t)}{2\rho(\mathbf{r},\mathbf{r}+\mathbf{a};t)}$$

On a lattice physical (A-representable) currents are bounded

$$|J(\mathbf{r},\mathbf{r}+\mathbf{a})| < 2T_0|\rho(\mathbf{r},\mathbf{r}+\mathbf{a})| \qquad (3)$$

The reason is that the maximal "hopping rate" is bounded by T_0.

$|J(\mathbf{r},\mathbf{r}+\mathbf{a})| = 2T_0|\rho(\mathbf{r},\mathbf{r}+\mathbf{a})|$ implies $|K(\mathbf{r},\mathbf{r}+\mathbf{a})| = 0$:
vanishing kinetic energy on a link

Inequality (3) determines a subset of "A-representability" in the Hilbert space $\mathcal{H}$

Theorem 1 (existence of the lattice TDCDFT)

$NLSE: \quad i\partial_t\psi(t) = \hat{T}_J[\psi]\psi(t) + \hat{W}\psi(t)$

Let $J(\mathbf{r}, \mathbf{r}+\mathbf{a}; t)$ be continuous functions of t, such that in the extended phase space $\mathcal{H} \times \mathbb{R}$ there exists a subset Ω defined by

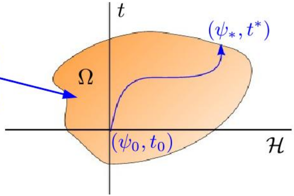
$$2T_0|\rho(\mathbf{r}, \mathbf{r}+\mathbf{a})| > |J(\mathbf{r}, \mathbf{r}+\mathbf{a}; t)|.$$

If the initial point $(\psi_0, t_0) \in \Omega$, then:

(i) There is a neighborhood of (ψ_0, t_0) where $\psi(t)$ is a unique functional of $J(t)$ and the map $J \mapsto A$ is bijective.

(ii) The statement (i) holds globally in time unless at some t^* the boundary of Ω is reached.

A-representability subset (non-zero kinetic energy)



The solution is not global only if it hits the boundary, i. e., at least for one link:
$t \to t^*, \; |K(\mathbf{r}, \mathbf{r}+\mathbf{a}; t)| \to 0$

Exact solution of the Lattice NLSE for $N = 1$

$$i\partial_t \psi(\mathbf{r};t) = -\sum_{\mathbf{a}} T_J[\psi](\mathbf{r},\mathbf{r}+\mathbf{a};t)\psi(\mathbf{r}+\mathbf{a};t), \quad \psi(\mathbf{r};t_0) = |\psi_0(\mathbf{r})|e^{i\chi_0(\mathbf{r})}$$

The exact solution for one particle: $\psi(\mathbf{r};t) = |\psi(\mathbf{r};t)|e^{i\chi(\mathbf{r};t)}$

$$|\psi(\mathbf{r};t)| = \sqrt{|\psi_0(\mathbf{r})|^2 - \int_{t_0}^{t} \sum_{\mathbf{a}} J(\mathbf{r},\mathbf{r}+\mathbf{a};t')dt'},$$

$$\chi(\mathbf{r};t) = \chi_0(\mathbf{r}) + \int_{t_0}^{t} \frac{\sum_{\mathbf{a}} K(\mathbf{r},\mathbf{r}+\mathbf{a};t')}{2|\psi(\mathbf{r};t')|^2} dt',$$

$$K(\mathbf{r},\mathbf{r}+\mathbf{a};t) = s_0\sqrt{4T_0^2|\psi(\mathbf{r};t)|^2|\psi(\mathbf{r}+\mathbf{a};t)|^2 - J^2(\mathbf{r},\mathbf{r}+\mathbf{a};t)}$$

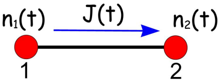
The maximal existence time t^* is determined by $K(\mathbf{r},\mathbf{r}+\mathbf{a};t^*) = 0$

The behavior of one-particle system is generic!

There is no conceptual difference between $N = 1$ and $N > 1$.

Simplest case: One particle on two sites

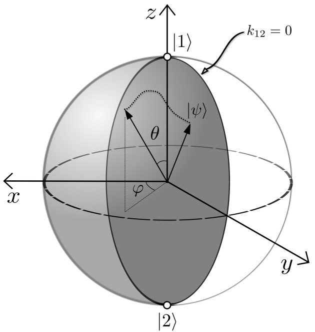
$$|\psi\rangle = \cos\theta e^{i\phi/2}|1\rangle + \sin\theta e^{-i\phi/2}|2\rangle$$



$$n_{1,2}(t) = n_{1,2}(t_0) \mp \int_{t_0}^{t} J(t')dt'$$

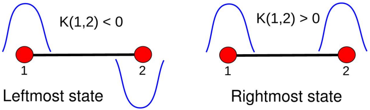
$$\dot{A}[J] = V[J] = s_0 \frac{\dot{J} - 2T_0^2(n_1 - n_2)}{\sqrt{4T_0^2 n_1 n_2 - J^2}}$$

$$s_0 = \text{sgn}\{K(t_0)\}$$



- On the left/right hemispheres:

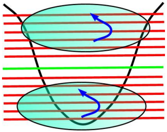
$$V^{L/R}[J] = \pm \frac{\dot{J} - 2T_0^2(n_1 - n_2)}{\sqrt{4T_0^2 n_1 n_2 - J^2}}$$



$K(1,2) = 0 \mapsto$ prime meridian

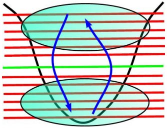
Overview of the lattice TDCFT

“Weakly” nonequilibrium state



- sgn$K(t)$ stays unchanged $\Rightarrow$ A-representable currents.

“Strongly” nonequilibrium state



- sgn$K(t)$ changes $\Rightarrow$ problems with A-representability

The A-representability problem originates from the fixed hopping rate.

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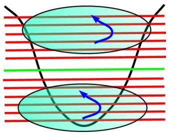

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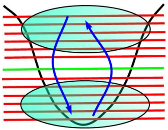

- sgn$K(t)$ changes $\Rightarrow$ problems with A-representability

The A-representability problem originates from the fixed hopping rate.

Solution: Generalized lattice TDCDFT

- Allow for variations of the hopping rate $|T(\mathbf{r}, \mathbf{r}')|$
- Expand the set of basic variables, $\{\mathcal{N}\} = \{J, K\}$

Outline

Basic variables, conjugated fields, and NLSE

- Basic collective variable – “complex link current”:

$$Q(\mathbf{r},\mathbf{r}+\mathbf{a};t) = T(\mathbf{r},\mathbf{r}+\mathbf{a};t)\rho(\mathbf{r},\mathbf{r}+\mathbf{a};t),$$

$$2Q(\mathbf{r},\mathbf{r}+\mathbf{a};t) = \underbrace{K(\mathbf{r},\mathbf{r}+\mathbf{a};t)}_{\text{kinetic energy}} + i\,\underbrace{J(\mathbf{r},\mathbf{r}+\mathbf{a};t)}_{\text{current}}$$

- Conjugated driving field – complex hopping parameters

$$T(\mathbf{r},\mathbf{r}+\mathbf{a};t) = |T(\mathbf{r},\mathbf{r}+\mathbf{a};t)|e^{iA(\mathbf{r},\mathbf{r}+\mathbf{a};t)}$$

- The inverse problem in the generalized TDCDFT:

  Finding $|\psi(t)\rangle$ and $\{T(t)\}$ from given $\{Q(t)\}$ and $|\psi_0\rangle$.

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Construction of the corresponding NLSE

$$T(\mathbf{r},\mathbf{r}+\mathbf{a};t) \to T[Q,\psi](\mathbf{r},\mathbf{r}+\mathbf{a};t) = \frac{Q(\mathbf{r},\mathbf{r}+\mathbf{a};t)}{\rho(\mathbf{r},\mathbf{r}+\mathbf{a};t)}$$

Theorem 2 (existence of the generalized TDCDFT)

$NLSE: \quad i\partial_t \psi(t) = \hat{T}_Q[\psi]\psi(t) + \hat{W}\psi(t); \quad T_Q[\psi] = \frac{Q(\mathbf{r},\mathbf{r}';t)}{\rho(\mathbf{r},\mathbf{r}';t)}$

Let complex link currents $Q(\mathbf{r}, \mathbf{r}+\mathbf{a}; t)$ be continuous functions of t, and the initial state ψ_0 is such that for all links $|\rho(\mathbf{r}, \mathbf{r}+\mathbf{a}; t_0)| \neq 0$. Then the following statements hold true.

(i) The wave function $\psi(t)$ is a unique functional of $Q(t)$ and ψ_0.

(ii) There is a bijective map $Q \leftrightarrow T$ between the set of complex currents and the set of complex hopping integrals.

(iii) The statements (i) and (ii) hold globally in time unless at some $t^* > t_0$ at least for one link $|\rho(\mathbf{r}, \mathbf{r}+\mathbf{a}; t^*)| = 0$, which corresponds to $|T(\mathbf{r}, \mathbf{r}+\mathbf{a}; t^*)| \to \infty$.

- $\mathcal{V}$-representability is violated only if there are broken lattice links!
- Any current is (locally in t) reproducible by adjusting hoping rates.

Overview of the generalized lattice TDCDFT

- Using $Q(\mathbf{r},\mathbf{r}') = \frac{1}{2}K(\mathbf{r},\mathbf{r}') + i\frac{1}{2}J(\mathbf{r},\mathbf{r}')$ as a basic variable we can access “strongly” nonequilibrium dynamics within “TDDFT“.
- The corresponding Kohn-Sham system reproduces exactly both the current/density and the local kinetic energy.

In the continuum limit: $K(\mathbf{r},\mathbf{r}';t) \mapsto \tau(\mathbf{r},t) = \langle \nabla\hat{\psi}^{\dagger}(\mathbf{r})\nabla\hat{\psi}(\mathbf{r})\rangle$

Therefore we recover a theory of collective variables, which has

- $\{\mathbf{j}(\mathbf{r},t), \tau(\mathbf{r},t)\}$ as a set basic observables
- $\{\mathbf{A}(\mathbf{r},t), m^{*}(\mathbf{r},t)\}$ as a set driving/selfconsistent fields

Closely related phenomenological constructions

- Skyrme Hartree-Fock theory in nuclear physics
- meta-GGA construction in the electronic structure theory

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Outline

Summary

- The existence of any TDDFT reduces to the existence and uniqueness problem for a certain many-body NLSE.
- NLSE for TDCDFT has the simplest structure. However, in the continuum a rigorous proof of existence is still lacking.
- In the lattice setting the existence has been proved for different theories: TDCDFT, generalized TDCDFT, and TDDFT.
- Generalized TDCDFT provides us with the most flexible theoretical setup with no $\mathcal{V}$-representability restrictions.
- The existence of the plain lattice TD(C)DFT is linked to the properties of the $\mathcal{V}$-representability subset in the Hilbert space. Characterization of geometry/topology of this subset is an interesting unsolved problem.
- Accurate continuum limit of the lattice TDDFT-type theories remains an open issue.
- As usual in DFT the approximations is the eternally open question. In connection with this links to the Skyrme HF theory and meta-GGA deserve special attention.

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