Linear Continuum Mechanics for Quantum Many-Body Systems

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Dynamics of Quantum Many-Body systems

1. Solution of a Full N-body time-dependent Schrödinger Equation
   (a hopeless task)

2. Approximate Quantum Kinetics Approaches:
   i. Keldysh-Kadanoff-Baym with approximate self-energy
   ii. Decoupled at some level BBGKY hierarchy

(almost hopeless in many cases + formally unjustified approximations)

3. Kohn-Sham formulation of TDDFT/TDCDFT
   (still quite complex for large N and complex geometries
   + real big problems with approximations)

In this talk I present an alternative approach:

Quantum Continuum Mechanics

Quantum Continuum Mechanics (QCM)

Like classical theories of continuum media it describes dynamics of many-body systems without explicit reference to individual particles

Direct calculation of collective variables of interest n(r,t) and j(r,t)

Why this is possible in general?

Conceptually QCM = TD(C)DFT

By the first step of the Runge-Gross mapping theorem

$$\Psi(t) = \Psi[\mathbf{j}(\mathbf{r},t)](t) \quad \rightarrow$$

A closed theory for calculation of the current density does exist!

Formal structure of the Quantum Continuum Mechanics

$$\hat{H} = \underbrace{\hat{T} + \hat{W} + \hat{V}_0}_{H_0} + \hat{V}_1(t) = \hat{H}_0 + \int d\mathbf{r}\hat{n}(\mathbf{r})V_1(\mathbf{r},t)$$

Exact Heisenberg equation of motion for the current

Quantum stress force

$$m\partial_t j_\mu(\mathbf{r},t) = -n(\mathbf{r},t)\partial_\mu\left[V_0(\mathbf{r}) + V_1(\mathbf{r},t)\right] + \partial_\nu P_{\mu\nu}(\mathbf{r},t)$$

Exact stress tensor: $P_{\mu\nu}(\mathbf{r},t) = P_{\mu\nu}[\mathbf{j}](\mathbf{r},t)$

In the following: New non-local approximation for the stress tensor, exact at high frequency (anti-adiabatic limit)

Connection to KS TDCDFT: $F_\mu^{xc} = \frac{1}{n}\partial_\nu\left(P_{\mu\nu}[\mathbf{j}] - P_{\mu\nu}^S[\mathbf{j}]\right)$

Linear Quantum Continuum Mechanics

Basic variable is the displacement field u(r,t)

$$\mathbf{j}(\mathbf{r},t) = n_0(\mathbf{r})\partial_t \mathbf{u}(\mathbf{r},t)$$

$$n(\mathbf{r},t) = n_0(\mathbf{r}) + \delta n(\mathbf{r},t); \qquad \delta n(\mathbf{r},t) = -\nabla n_0(\mathbf{r})\mathbf{u}(\mathbf{r},t)$$

Linearized Heisenberg equation of motion

$$m n_0(\mathbf{r})\partial_t^2 \mathbf{u}(\mathbf{r},t) = -n_0(\mathbf{r})\nabla V_1(\mathbf{r},t) + \mathbf{F}[\mathbf{u}](\mathbf{r},t)$$

$$F_\mu(\mathbf{r},t) = -\int dt' d\mathbf{r}' Q_{\mu\nu}(\mathbf{r},\mathbf{r}',t-t') u_\nu(\mathbf{r}',t')$$

Connection to KS formulation: **The knowledge of $Q_{\mu\nu}$(r,r',ω) is equivalent to to the knowledge of the exact exchange-correlation kernel in TDCDFT**

$$n_0(\mathbf{r})\, f_{\mu\nu}^{xc}(\mathbf{r},\mathbf{r}',\omega) n_0(\mathbf{r}') = Q_{\mu\nu}(\mathbf{r},\mathbf{r}',\omega) - Q_{\mu\nu}^{S}(\mathbf{r},\mathbf{r}',\omega)$$

High-frequency (anti-adiabatic) limit of QCM

$$m n_0(\mathbf{r})\partial_t^2 \mathbf{u}(\mathbf{r},t) = -n_0(\mathbf{r})\nabla V_1(\mathbf{r},t) + \mathbf{F}[\mathbf{u}](\mathbf{r},t)$$

In the high-frequency limit F[u] is expressed in terms of the energy functional

$$E[\mathbf{u}] = \left\langle \Psi_0[\mathbf{u}] \middle| \hat{H}_0 \middle| \Psi_0[\mathbf{u}] \right\rangle$$

Expectation value of the GS Hamiltonian with a "deformed" GS wave function

$$\left|\Psi_0[\mathbf{u}]\right\rangle = \Psi_0\left(\mathbf{r}_1 - \mathbf{u}(\mathbf{r}_1), \mathbf{r}_2 - \mathbf{u}(\mathbf{r}_2), \ldots, \mathbf{r}_N - \mathbf{u}(\mathbf{r}_N)\right)$$

$$F_\mu(\mathbf{r},t) = -\int d\mathbf{r}' \left. \frac{\delta^2 E[\mathbf{u}]}{\delta u_\mu(\mathbf{r})\,\delta u_\nu(\mathbf{r}')} \right|_{\mathbf{u}=0} u_\nu(\mathbf{r}',t)$$

Physics: The wave function in a co-moving stays stationary

Direct derivation of the high-frequency limit of QCM

$$j_\mu(\mathbf{r},\omega) = \int d\mathbf{r}'\,\chi_{\mu\nu}(\mathbf{r},\mathbf{r}',\omega)\,A_\nu(\mathbf{r}',\omega) \qquad (1)$$

$$-i\omega n_0(\mathbf{r})\,u_\mu(\mathbf{r},\omega)$$

$$\frac{1}{i\omega}\partial_\mu V_1(\mathbf{r},\omega)$$

$$\chi_{\mu\nu}(\mathbf{r},\mathbf{r}',\omega) \underset{\omega\to\infty}{\approx} \frac{n_0(\mathbf{r})}{m}\delta(\mathbf{r}-\mathbf{r}')\,\delta_{\mu\nu} + \frac{M_{\mu\nu}(\mathbf{r},\mathbf{r}')}{m^2\omega^2}$$

$$M_{\mu\nu}(\mathbf{r},\mathbf{r}') = -m^2\left\langle \Psi_0 \left| \left[\left[\hat{H}_0, \hat{j}_\mu(\mathbf{r})\right], \hat{j}_\nu(\mathbf{r}')\right] \right| \Psi_0 \right\rangle$$ -- **first spectral moment**

Inverting (1) to the leading order in $1/\omega^2$ we obtain the equation of motion

$$-mn_0(\mathbf{r})\,\omega^2 u_\mu(\mathbf{r},\omega) = -n_0(\mathbf{r})\,\partial_\mu V_1(\mathbf{r},\omega) - \int d\mathbf{r}'\,M_{\mu\nu}(\mathbf{r},\mathbf{r}')\,u_\mu(\mathbf{r}',\omega)$$

Identity for the first spectral moment of the current response function

$$M_{\mu\nu}(\mathbf{r},\mathbf{r}') = -m^2 \left\langle \Psi_0 \left| \left[\left[\hat{H}_0, \hat{j}_\mu(\mathbf{r}) \right], \hat{j}_\nu(\mathbf{r}') \right] \right| \Psi_0 \right\rangle = \left. \frac{\delta^2 E[\mathbf{u}]}{\delta u_\mu(\mathbf{r})\, \delta u_\nu(\mathbf{r}')} \right|_{\mathbf{u}=0}$$

Proof:

$$E[\mathbf{u}] = \left\langle \Psi_0[\mathbf{u}] \right| \hat{H}_0 \left| \Psi_0[\mathbf{u}] \right\rangle \qquad \text{(A)}$$

Current density operator is a generator of a position-dependent translation

$$\left| \Psi_0[\mathbf{u}] \right\rangle \rightarrow e^{-im\int d\mathbf{r}\hat{\mathbf{j}}(\mathbf{r})\mathbf{u}(\mathbf{r})} \left| \Psi_0 \right\rangle \qquad \text{(B)}$$

Inserting (B) into (A) and expanding to the second order in u(r) we find

$$E[\mathbf{u}] = E_0 + \frac{1}{2}\int d\mathbf{r} d\mathbf{r}'\, u_\mu(\mathbf{r}')\, M_{\mu\nu}(\mathbf{r}',\mathbf{r})\, u_\nu(\mathbf{r})$$

Lagrangian of QCM in the elastic approximation

$$L=\frac{1}{2}\int d\mathbf{r}\Big\{n_0\Big[m\left(\partial_t\mathbf{u}\right)^2-u_\mu u_\nu\partial_\mu\partial_\nu V_0\Big]-T_{\mu\nu}\Big[4u_{\mu\alpha}u_{\nu\alpha}-\partial_\mu u_\alpha\partial_\mu u_\alpha\Big]$$

$$-\frac{n_0}{2m}\Big[\partial_\mu u_{\nu\nu}\partial_\mu u_{\alpha\alpha}+2\partial_\mu u_{\nu\alpha}\partial_\mu u_{\nu\alpha}-2\partial_\mu u_{\nu\mu}\partial_\nu u_{\alpha\alpha}\Big]\Big\}$$

$$-\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'K_{\mu\nu}\left(\mathbf{r},\mathbf{r}'\right)\Big[u_\mu\left(\mathbf{r}\right)-u_\mu\left(\mathbf{r}'\right)\Big]\Big[u_\nu\left(\mathbf{r}\right)-u_\nu\left(\mathbf{r}'\right)\Big]$$

$$u_{\mu\nu}=\frac{1}{2}\left(\partial_\mu u_\nu+\partial_\nu u_\mu\right)$$ **strain tensor**

$$T_{\mu\nu}\left(\mathbf{r}\right)=\frac{1}{2m}\left(\partial_\mu\partial'_\nu+\partial_\nu\partial'_\mu\right)\rho_1\left(\mathbf{r},\mathbf{r}'\right)\Big|_{\mathbf{r}'=\mathbf{r}}-\frac{\delta_{\mu\nu}}{4m}\nabla^2 n_0$$ **Kinetic stress tensor**

$$K_{\mu\nu}\left(\mathbf{r},\mathbf{r}'\right)=\rho_2\left(\mathbf{r},\mathbf{r}'\right)\partial_\nu\partial_\mu w\left(\left|\mathbf{r}-\mathbf{r}'\right|\right)$$ **“dipole-dipole” interaction kernel**

An illustrative example: One-dimensional system

$$L = \frac{1}{2}\int dx \left\{ n_0(x)\left[m(\partial_t u)^2 - u^2 \partial_x^2 V_0 \right] - 3T(x)(\partial_x u)^2 - \frac{n_0(x)}{4m}\left(\partial_x^2 u\right)^2 \right\}$$

$$-\frac{1}{2}\int dx dx' K(x,x')\left[u(x) - u(x')\right]^2$$

Corresponding equation of motion for the displacement

$$m n_0 \partial_t^2 u = -u n_0 \partial_x^2 V_0 + 3\partial_x T \partial_x u - \frac{\partial_x^2 n_0 \partial_x^2 u}{4m} - \frac{1}{2}\int dx' K(x,x')\left[u(x) - u(x')\right]$$

Where

$$T(x) = \frac{1}{2m}\partial_x \partial'_x \rho_1(x,x')\Big|_{x'=x} - \frac{1}{4m}\partial_x^2 n_0(x)$$

$$K(x,x') = \rho_2(x,x')\, w''\left(\left|x - x'\right|\right)$$

QCM for one particle in a harmonic potential

$$m\partial_t^2 u = -u\partial_x^2 V_0 + \frac{3}{n_0}\partial_x\left(T\partial_x u\right) - \frac{1}{4mn_0}\partial_x^2\left(n_0\partial_x^2 u\right)$$

Harmonic oscillator

$$V_0(x) = \frac{1}{2}\omega_0 x^2 \quad \rightarrow \quad n_0(x) \sim e^{-m\omega_0 x^2}, \quad T(x) = \frac{1}{2}\omega_0 n_0(x)$$

$$x = \frac{\xi}{\sqrt{m\omega_0}}$$

$$\omega^2 u = u - \frac{3}{2}e^{\xi^2}\partial_\xi\left(e^{-\xi^2}\partial_\xi u\right) + \frac{1}{4}e^{\xi^2}\partial_\xi^2\left(e^{-\xi^2}\partial_\xi^2 u\right)$$

Using the identities for Hermite polynomials $H_l(x)$:

$$e^{x^2}\partial_x\left(e^{-x^2}\partial_x H_l\right) = -2lH_l, \quad e^{x^2}\partial_x^2\left(e^{-x^2}\partial_x^2 H_l\right) = 4l(l-1)H_l$$

we find the following exact solution of the QCM equation

$$\Omega_l^2 = \omega_0^2 l^2, \ \ l = 1, 2, \ldots; \quad u_l(x) = H_{l-1}\left(x\sqrt{m\omega_0}\right) \sim \frac{\langle 0|\hat{j}(x)|l\rangle}{n_0(x)}$$

General QCM eigenvalue problem

(orthogonality, completeness, and the QCM current response function)

$$m n_0 \Omega_l^2 u_\mu^l = \hat{M}_{\mu\nu} u_\mu^l$$

Stability of GS ensures that $M_{\mu\nu}(r,r')$ is symmetric and positively definite

$$\int d\mathbf{r} n_0(\mathbf{r}) u_\mu^l(\mathbf{r}) u_\mu^{l'}(\mathbf{r}) = \delta_{ll'}; \qquad \sum_l u_\mu^l(\mathbf{r}) u_\nu^l(\mathbf{r}') = \delta_{\mu\nu}\delta(\mathbf{r}-\mathbf{r}')/n_0(\mathbf{r})$$

Spectral decomposition of the M-operator

$$\hat{M}_{\mu\nu} = m \sum_l \Omega_l^2 n_0(\mathbf{r}) u_\mu^l(\mathbf{r}) n_0(\mathbf{r}') u_\nu^l(\mathbf{r}')$$

QCM current response function

$$\chi_{\mu\nu}^{\mathrm{QCM}}(\mathbf{r},\mathbf{r}',\omega) = \frac{1}{m}\sum_l \frac{\omega^2}{\omega^2 - \Omega_l^2} n_0(\mathbf{r}) u_\mu^l(\mathbf{r}) n_0(\mathbf{r}') u_\nu^l(\mathbf{r}')$$

The third moment sum rule

From the spectral decomposition and the QCM response function

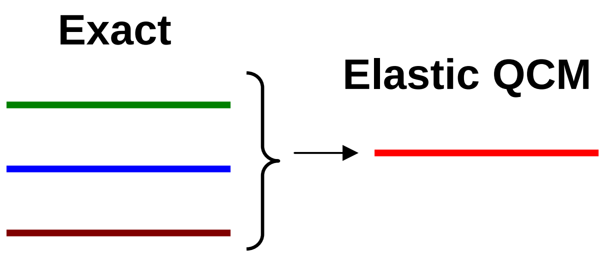
$$\hat{M}_{\mu\nu} = m\sum_l \Omega_l^2 n_0(\mathbf{r}) u_\mu^l(\mathbf{r}) n_0(\mathbf{r}') u_\nu^l(\mathbf{r}') = -\frac{2}{\pi} m^2 \int_0^\infty \omega \, \mathrm{Im}\, \chi_{\mu\nu}^{\mathrm{QCM}}(\mathbf{r},\mathbf{r}') \, d\omega$$

The 3d moment sum rule is automatically satisfied since by construction:

$$\hat{M}_{\mu\nu} = -\frac{2}{\pi} m^2 \int_0^\infty \omega \, \mathrm{Im}\, \chi_{\mu\nu}^{\mathrm{exact}}(\mathbf{r},\mathbf{r}') \, d\omega = m^2 \sum_l \Delta E_n \langle 0 | \hat{j}_\mu(\mathbf{r}) | n \rangle \langle n | \hat{j}_\nu(\mathbf{r}') | 0 \rangle$$

QCM eigenfrequency is a weighted sum of the exact excitation energies:

$$\Omega_l = \sum_n f_n^l \Delta E_n; \qquad f_n^l = \frac{m}{\Omega_l} \left| \int d\mathbf{r} \langle 0 | \hat{\mathbf{j}}(\mathbf{r}) | n \rangle \mathbf{u}^l(\mathbf{r}) \right|^2$$



A group of levels collapses into one but the spectral weight is preserved within each group!

Two interacting 1D particles in a harmonic potential

$$\hat{H}_0 = \frac{1}{2m}\left(\hat{\mathbf{p}}_1^2 + \hat{\mathbf{p}}_2^2\right) + \frac{1}{2} m\omega_0^2 \left(x_1^2 + x_2^2\right) + \frac{e^2}{\sqrt{\left(x_1 - x_2\right)^2 + a^2}}$$

$\lambda = e^2 m \big/ \sqrt{m\omega_0} = \ell_0 / a_B$ -- dimensionless coupling constant

Excitation spectrum

States

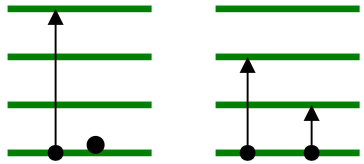
1. Exact: $(n, 2m) \equiv (n, m)$

Center of mass relative

Energies

$$\Delta E_{nm} = \begin{cases} \omega_0 \left(n + 2m\right), & \lambda = 0 \\ \omega_0 \left(n + \sqrt{3}m\right), & \lambda \gg 1 \end{cases}$$

Degeneracy at λ=0



n+2m=3

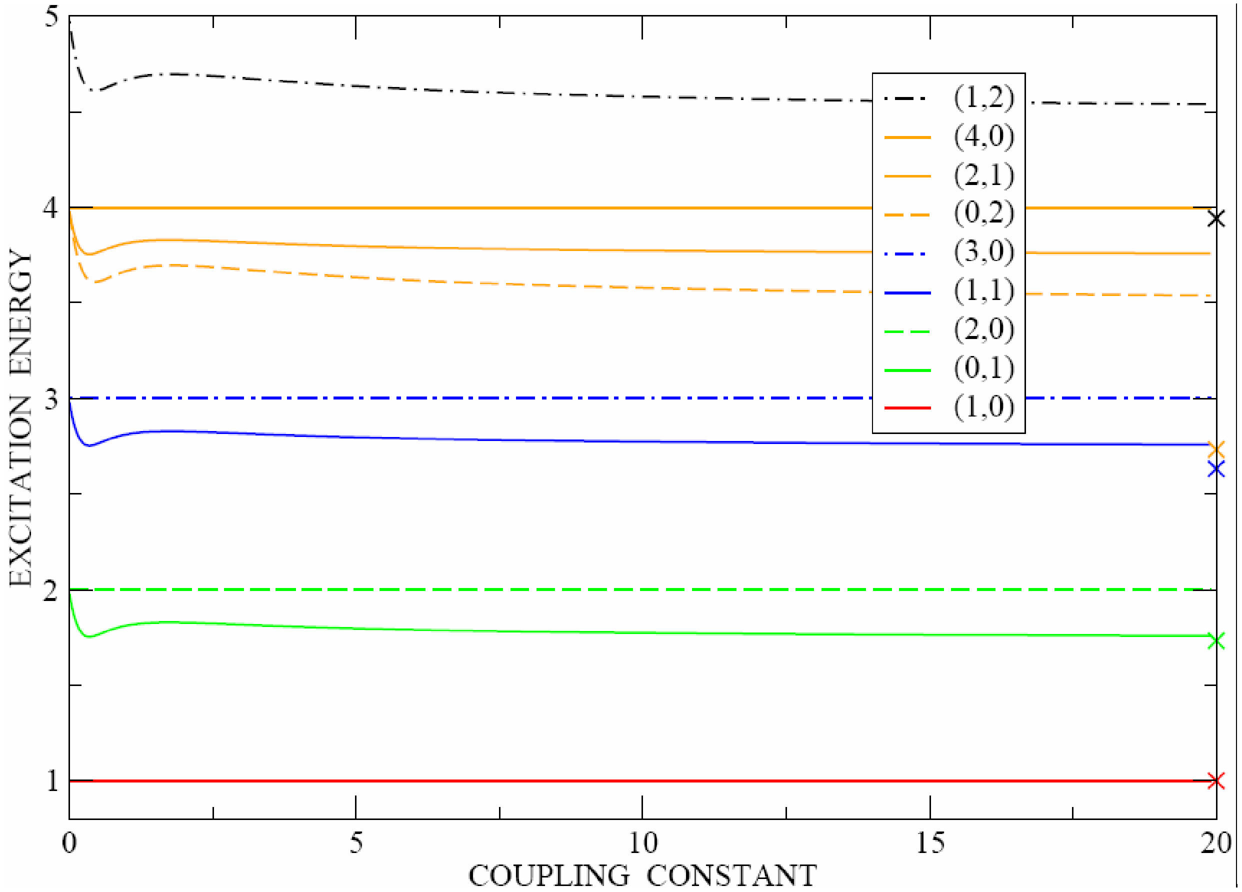
2. QCM: $\lambda = 0,$ the results are exact;

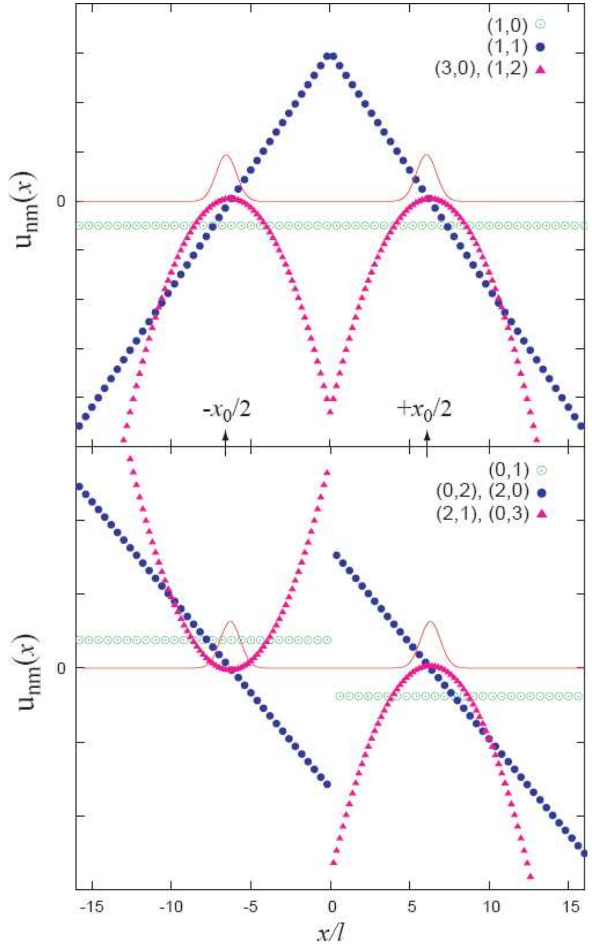
$$\lambda \gg 1, \qquad \Omega_k = \omega_0 \sqrt{2 + 3\sqrt{3}k + 6k\left(k-1\right)\left(2-\sqrt{3}\right) - \left(-1\right)^m \left(2-\sqrt{3}\right)^k}$$

$$k = n + m - 1$$

Excitation energies and displacement fields for 2 interacting particles

States with the same $n+m$ and the same parity of m have identical $\langle 0|\hat{j}(x)|nm\rangle \sim u_{nm}(x)$ → **At the QCM level they collapse into one mode**





Displacements at strong coupling

Concluding remarks + speculations

1. Our Quantum Continuum Mechanics is a direct extension of the collective approximation ("plasmon pole") for the homogeneous electron gas to inhomogeneous quantum systems. Therefore it should be useful for

- The theory of dispersive VdW forces, especially in complex geometries
- Possible nonlocal refinement of the plasmon pole approximation in GW
- Studying dynamics in the strongly correlated regime, which is dominated by a collective response

2. As a byproduct we got an explicit analytic representation of the exact xc kernel in the high-frequency (anti-adiabatic) limit

- This kernel should help us to study an importance of the space and time nonlocalities in the KS formulation of TD(C)DFT
- It is interesting to try to interpolate between the adiabatic and anti-adiabatic extremes to construct a reasonable frequency-dependent functional