From Basic Concepts to Real Materials

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Continuum Mechanics of Quantum Many-Body Systems

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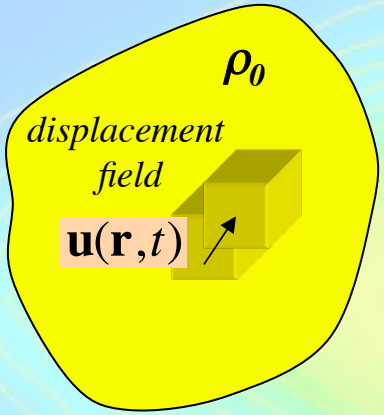
Continuum Mechanics: what is it?

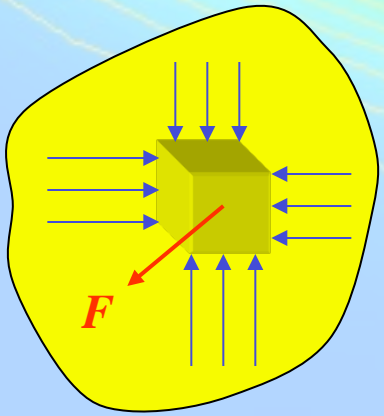
An attempt to describe a complex many-body system in terms of a few collective variables -- density and current -- without reference to the underlying atomic structure. Classical examples are "Hydrodynamics" and "Elasticity".



Elasticity

$$\rho_0 \frac{\partial^2 \mathbf{u}(\mathbf{r},t)}{\partial t^2} = \underbrace{\vec{\nabla} \cdot \underbrace{\vec{\vec{\sigma}}(\mathbf{r},t)}_{\text{Stress tensor}}}_{\text{Internal Force}} + \underbrace{\mathbf{F}(\mathbf{r},t)}_{\text{External Volume force}}$$

$$\sigma_{ij}(\vec{r},t) = \underbrace{B}_{\substack{\text{Bulk} \\ \text{modulus}}} \vec{\nabla} \cdot \vec{u} \delta_{ij} + \underbrace{S}_{\substack{\text{Shear} \\ \text{modulus}}} \left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} - \frac{2}{3} \vec{\nabla} \cdot \vec{u} \delta_{ij} \right)$$



$$\rho_0 \frac{\partial^2 \mathbf{u}(\mathbf{r},t)}{\partial t^2} = \underbrace{\left[B + \left(1 - \frac{2}{3} \right) S \right] \nabla (\nabla \cdot \mathbf{u}) + S \nabla^2 \mathbf{u}}_{\text{Internal forces}} + \underbrace{\mathbf{F}(\mathbf{r},t)}_{\text{Volume force}}$$

Can continuum mechanics be applied to quantum *many-body* systems?

In principle, yes!

Hamiltonian:

$$\hat{H}(t) = \underbrace{\hat{T}}_{\text{Kinetic Energy}} + \underbrace{\hat{W}}_{\text{Interaction Energy}} + \underbrace{\hat{V}_0}_{\text{External static potential}} + \int d\mathbf{r}\ \underbrace{V_1(\mathbf{r},t)}_{\text{External time-dependent potential (small)}}\ \hat{n}(\mathbf{r},t)$$

Heisenberg Equations of Motion:

Local conservation of particle number

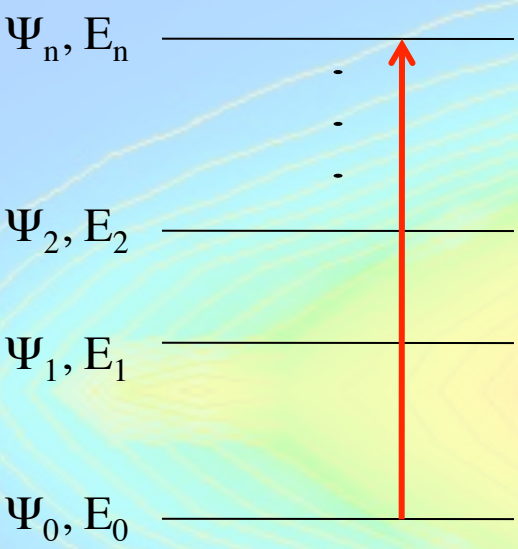
$$\underbrace{\frac{\partial n(\mathbf{r},t)}{\partial t}}_{\text{Derivative of particle density}} = -\nabla \cdot \underbrace{\mathbf{j}(\mathbf{r},t)}_{\text{Current density}}$$

Local conservation of momentum

$$\frac{\partial \mathbf{j}(\mathbf{r},t)}{\partial t} = -\nabla \cdot \underbrace{\vec{\mathbf{P}}(\mathbf{r},t)}_{\text{Stress tensor}} - \mathrm{n}(\mathbf{r},t)\ \nabla V(\mathbf{r},t)$$

The Runge-Gross theorem asserts that P(**r**,t) is a unique functional of the current density (and of the initial quantum state) -- thus closing the equations of motion.

Continuum mechanics in the linear response regime



"Linear response regime" means that we are in a non-stationary state that is "close" to the ground-state, e.g.

$$\left|\Psi_{n0}(t)\right\rangle = \left|\Psi_0\right\rangle e^{-iE_0 t} + \lambda\left|\Psi_n\right\rangle e^{-iE_n t}$$

$$\lambda << 1$$

The *displacement field* associated with this excitation is

$$u_{n0}(\mathbf{r},t) = \frac{\left\langle \Psi_n \left| \hat{\mathbf{j}}(\mathbf{r}) \right| \Psi_0 \right\rangle}{i\left(E_n - E_0\right) n_0(\mathbf{r})} e^{-i\left(E_n - E_0\right)t} + c.c.$$

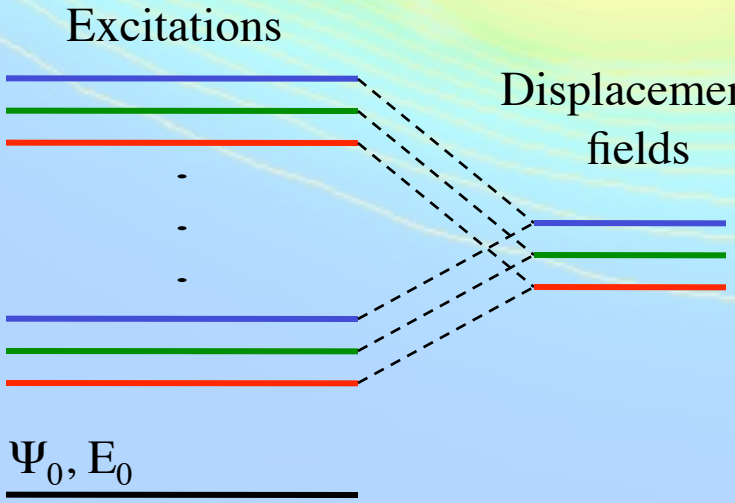
up to a proportionality constant.

Continuum mechanics in the linear response regime - continued

Excitation energies in linear continuum mechanics are obtained by Fourier analyzing the displacement field

$$u_{n0}(\mathbf{r},t) = \frac{\langle \Psi_n | \hat{\mathbf{j}}(\mathbf{r}) | \Psi_0 \rangle}{i(E_n - E_0) n_0(\mathbf{r})} e^{-i(E_n - E_0)t} + c.c.$$

However, the correspondence between excited states and displacement fields can be many-to-one. Different excitations can have the same displacement fields (up to a constant). This implies that the equation for the displacement field, while linear, cannot be rigorously cast as a conventional eigenvalue problem.



Continuum Mechanics in the Elastic Approximation

Objective: to obtain an approximate linear equation of motion for **j** (or **u**) that involves only ground-state properties, thus bypassing the solution of the time-dependent Kohn-Sham equation.

The Idea:

1) Go to the "comoving frame" -- an accelerated reference frame that moves with the electron liquid so that ***the density is constant and the current density is zero everywhere.***

2) In the comoving frame assume that the wave function remain time-independent - the time evolution of the system being entirely governed by the changing metric. We call this assumption the ***"elastic approximation".***

This approximation is expected to work best in strongly correlated systems, and is fully justified for **(1) High-frequency limit (2) One-electron systems.**

Notice that this is the **opposite** of an **adiabatic** approximation.

Elastic equation of motion: an elementary derivation

Start from the equation for the linear response of the current:

$$\mathbf{j}(\omega) = n_0 \mathbf{A}_1(\omega) + \mathbf{K}(\omega) \cdot \mathbf{A}_1(\omega)$$

and go to the high frequency limit:

$$\mathbf{K}(\omega) = \langle\langle \mathbf{j};\mathbf{j} \rangle\rangle_\omega \xrightarrow[\omega \to \infty]{} \frac{\mathbf{M}}{\omega^2}$$

$$\mathbf{M} = -\langle \Psi_0 | [[\hat{H},\mathbf{j}],\mathbf{j}] | \Psi_0 \rangle$$

First spectral moment : $-\frac{2}{\pi}\int_0^\infty d\omega\, \omega \,\mathrm{Im}K(\omega)$

Inverting Eq. (1) to first order we get

$$\mathbf{A}_1(\omega) = \frac{1}{n_0}\mathbf{j}(\omega) + \frac{1}{n_0}\frac{\mathbf{M}}{\omega^2}\frac{1}{n_0} \cdot \mathbf{j}(\mathbf{r}',\omega)$$

Finally, using

$$\mathbf{j}(\omega) = -i\omega n_0 \mathbf{u}(\omega)$$

$$\mathbf{A}_1(\omega) = -\frac{\nabla V_1(\omega)}{i\omega}$$

$$\Rightarrow \quad n_0(\mathbf{r})\ddot{\mathbf{u}}(\mathbf{r},t) = \int d\mathbf{r}' \mathbf{M}(\mathbf{r},\mathbf{r}') \cdot \mathbf{u}(\mathbf{r}',t) - n_0(\mathbf{r})\nabla V_1(\mathbf{r},t)$$

$$\mathbf{F}[\mathbf{u}] = \frac{\delta E_2[\mathbf{u}]}{\delta \mathbf{u}(\mathbf{r},t)}$$

The elastic equation of motion

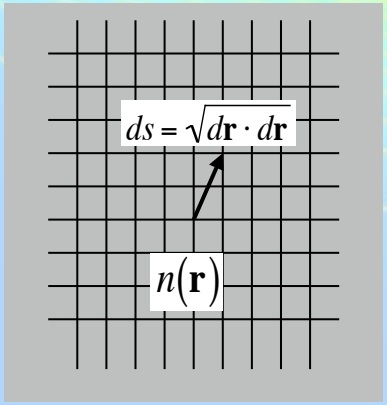
$$-\omega^2 n_0(\mathbf{r})\mathbf{u}(\mathbf{r},t) = F[\mathbf{u}] - n_0(\mathbf{r})\nabla V_1(\mathbf{r},t)$$

External force

$$\mathbf{F}[\mathbf{u}] = -\frac{\delta}{\delta \mathbf{u}(\mathbf{r},t)}\left\langle \Psi_0[\mathbf{u}]\middle|\hat{T} + \hat{W} + \hat{V}_0\middle|\Psi_0[\mathbf{u}]\right\rangle_2$$

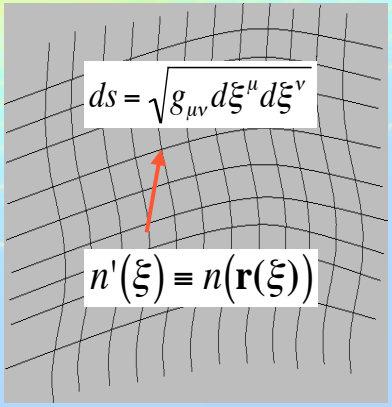
Second order in **u**

$$\left\langle \mathbf{r}_1,\ldots,\mathbf{r}_N\middle|\Psi_0[\mathbf{u}]\right\rangle = \Psi_0(\mathbf{r}_1 - \mathbf{u}(\mathbf{r}_1),\ldots,\mathbf{r}_N - \mathbf{u}(\mathbf{r}_N))g^{-1/4}(\mathbf{r}_1)\ldots g^{-1/4}(\mathbf{r}_N)$$



Euclidean space

$$\mathbf{r} \rightarrow \xi(\mathbf{r},t) = \mathbf{r} - \underbrace{\mathbf{u}(\mathbf{r},t)}_{\text{Displacement Field}}$$



Curved space

The elastic equation of motion: discussion

1. The linear functional **F**[**u**] is calculable from the exact one- and two body density matrices of the ground-state. The latter can be obtained from Quantum Monte Carlo calculations.

2. The eigenvalue problem is hermitian and yields a complete set of orthonormal eigenfunction. Orthonormality defined with respect to a modified scalar product with weight $n_0(r)$.

$$\int \mathbf{u}_\lambda(\mathbf{r}) \cdot \mathbf{u}_{\lambda'}(\mathbf{r}) n_0(\mathbf{r}) d\mathbf{r} = \delta_{\lambda\lambda'}$$

3. The positivity of the eigenvalues (=excitation energies) is guaranteed by the stability of the ground-state

4. All the excitations of one-particle systems are exactly reproduced.

The sum rule

Let $\mathbf{u}_\lambda(\mathbf{r})$ be a solution of the elastic eigenvalue problem with eigenvalue ω_λ^2. The following relation exists between ω_λ^2 and the exact excitation energies:

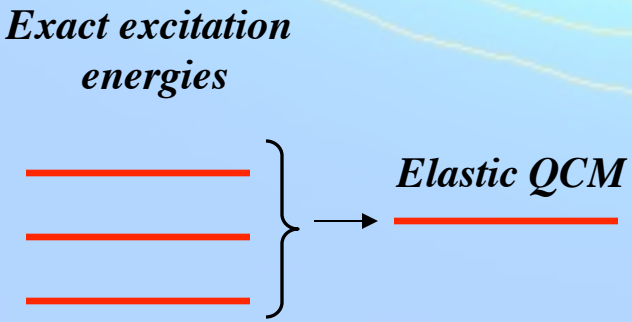
$$\omega_\lambda^2 = \sum_n f_n^\lambda \left(E_n - E_0\right)^2$$

Oscillator strength

$$f_n^\lambda = \frac{2\left|\int d\mathbf{r}\, \mathbf{u}_\lambda(\mathbf{r}) \cdot \mathbf{j}_{0n}(\mathbf{r})\right|^2}{E_n - E_0} \qquad \left(\mathbf{j}_{0n}(\mathbf{r}) = \left\langle \Psi_0 \left| \hat{\mathbf{j}}(\mathbf{r}) \right| \Psi_n \right\rangle\right)$$

f-sum rule

$$\sum_n f_n^\lambda = 1$$



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

Example 1: Homogeneous electron gas

LONGITUDINAL

$$\mathbf{u}_{L\mathbf{q}}(\mathbf{r}) = \hat{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}}$$

$$\omega_L^2(\mathbf{q}) = \omega_p^2 + 2t(n)q^2 + \frac{q^4}{4}$$

$$+\frac{\omega_p^2}{n}\int \frac{d\mathbf{q}'}{(2\pi)^3}(\hat{\mathbf{q}}\cdot\hat{\mathbf{q}}')^2\left[S(\mathbf{q}-\mathbf{q}') - S(\mathbf{q}')\right]$$

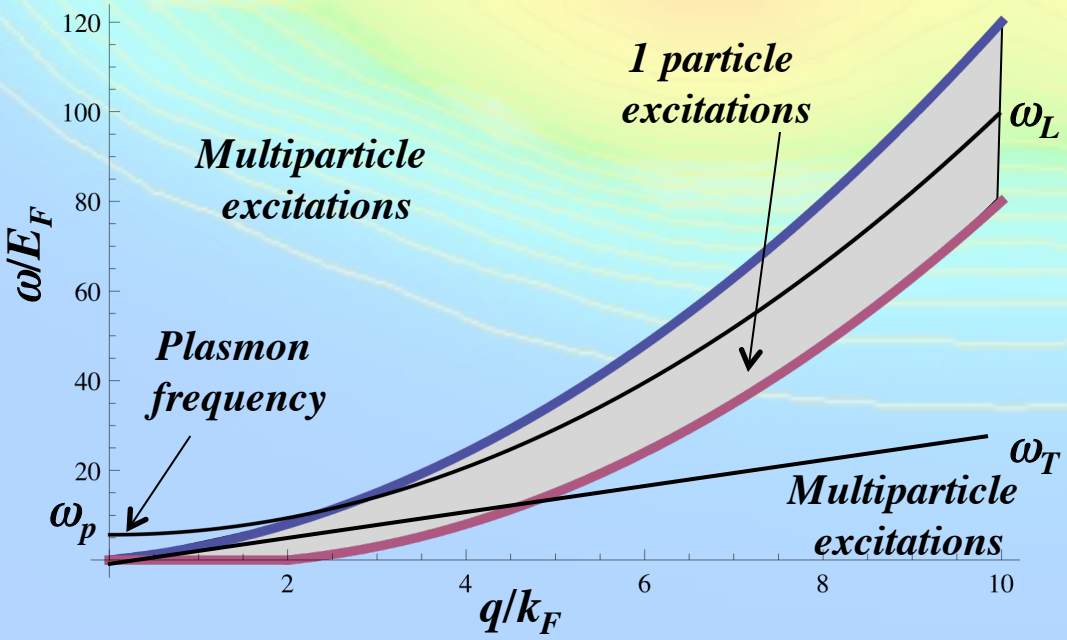
TRANSVERSAL

$$\mathbf{u}_{T\mathbf{q}}(\mathbf{r}) = \hat{\mathbf{t}}_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}}$$

static structure factor

$$\omega_T^2(\mathbf{q}) = \frac{2t(n)}{3}q^2$$

$$+\frac{\omega_p^2}{n}\int \frac{d\mathbf{q}'}{(2\pi)^3}|\hat{\mathbf{q}}\times\hat{\mathbf{q}}'|^2\left[S(\mathbf{q}-\mathbf{q}') - S(\mathbf{q}')\right]$$



Similar, but not identical to Bijl-Feynman theory:

$$|\Psi_{\mathbf{q}}\rangle \propto \hat{n}_{\mathbf{q}}|\Psi_0\rangle$$

$$\omega_L(\mathbf{q}) = \frac{q^2}{2S(q)}$$

Example 2
Elastic equation of motion for 1-dimensional systems

$$m\ddot{u} = -uV_0'' + \frac{(3T_0u')'}{n_0} - \frac{(n_0u'')''}{4n_0} + \int dx'K(x,x')\left[u(x) - u(x')\right]$$

a fourth-order integro-differential equation

$$T_0(x) = \frac{1}{2}\partial_x\partial_{x'}\underbrace{\rho(x,x')\big|_{x=x'}}_{\text{One-particle density matrix}} - \frac{n_0''(x)}{4}$$

From Quantum Monte Carlo

$$K(x,x') = \underbrace{\rho_2(x,x')}_{\text{Two-particle density matrix}}\ \underbrace{w''(x-x')}_{\text{Second derivative of interaction}}$$

A. Linear Harmonic Oscillator

$$\frac{1}{4}\frac{d^4\mathrm{u}}{dx^4} - x\frac{d^3\mathrm{u}}{dx^3} + (x^2-2)\frac{d^2\mathrm{u}}{dx^2} + 3x\frac{d\mathrm{u}}{dx} + \left(1-\frac{\omega^2}{\omega_0^2}\right)\mathrm{u} = 0$$

This equation can be solved analytically by expanding u(x) in a power series of x and requiring that the series terminates after a finite number of terms (thus ensuring zero current at infinity).

Eigenvalues: $\omega_n = \pm n\omega_0$

Eigenfunctions: $\mathrm{u}_n(x) = H_{n-1}(x)$

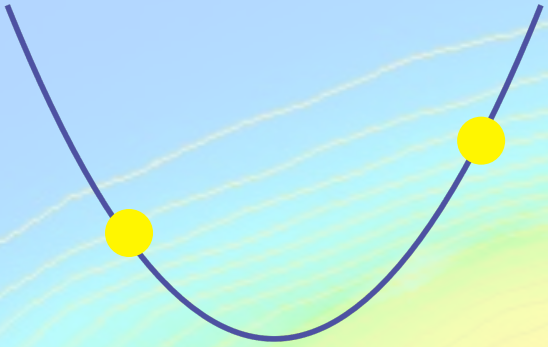
B. Hydrogen atom (l=0)

$$\frac{1}{4}\frac{d^4\mathrm{u}_r}{dr^4} - \left(1-\frac{1}{r}\right)\frac{d^3\mathrm{u}_r}{dr^3} + \left(1-\frac{2}{r}-\frac{1}{r^2}\right)\frac{d^2\mathrm{u}_r}{dr^2} + \frac{3}{r^2}\frac{d\mathrm{u}_r}{dr} + \left(\frac{2}{r^3}+\frac{\omega^2}{Z^4}\right)\mathrm{u}_r = 0$$

Eigenvalues: $\omega_n = \frac{Z^2}{2}\left(1-\frac{1}{n^2}\right)$

Eigenfunctions: $\mathrm{u}_{nr}(r) = L_{n-2}^2\left(\frac{2r}{n}\right)$

C. Two interacting particles in a 1D harmonic potential – Spin singlet



Parabolic trap

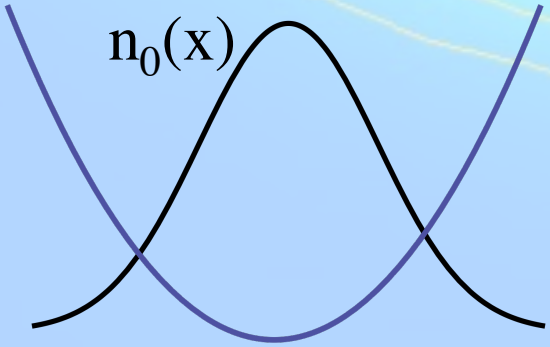
$$H = \overbrace{\frac{P^2}{4} + \frac{\omega_0^2}{2} X^2}^{\text{Center of Mass}} + \overbrace{p^2 + \frac{\omega_0^2}{8} x^2 + \underbrace{\frac{1}{\sqrt{x^2 + a^2}}}_{\text{Soft Coulomb repulsion}}}^{\text{Relative Motion}}$$

$$\Psi_{nm}(X,x) = \phi_n(X)\psi_m(x)$$

n,m non-negative integers

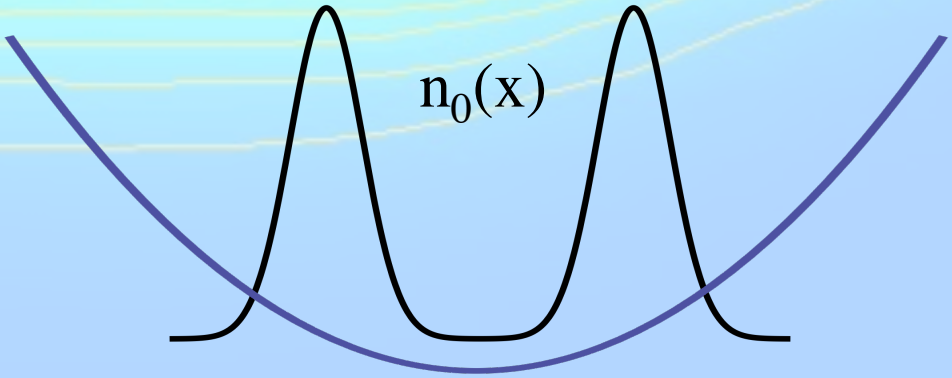
WEAK CORRELATION ω_0>>1

$$E_{nm} = \omega_0(n + 2m)$$

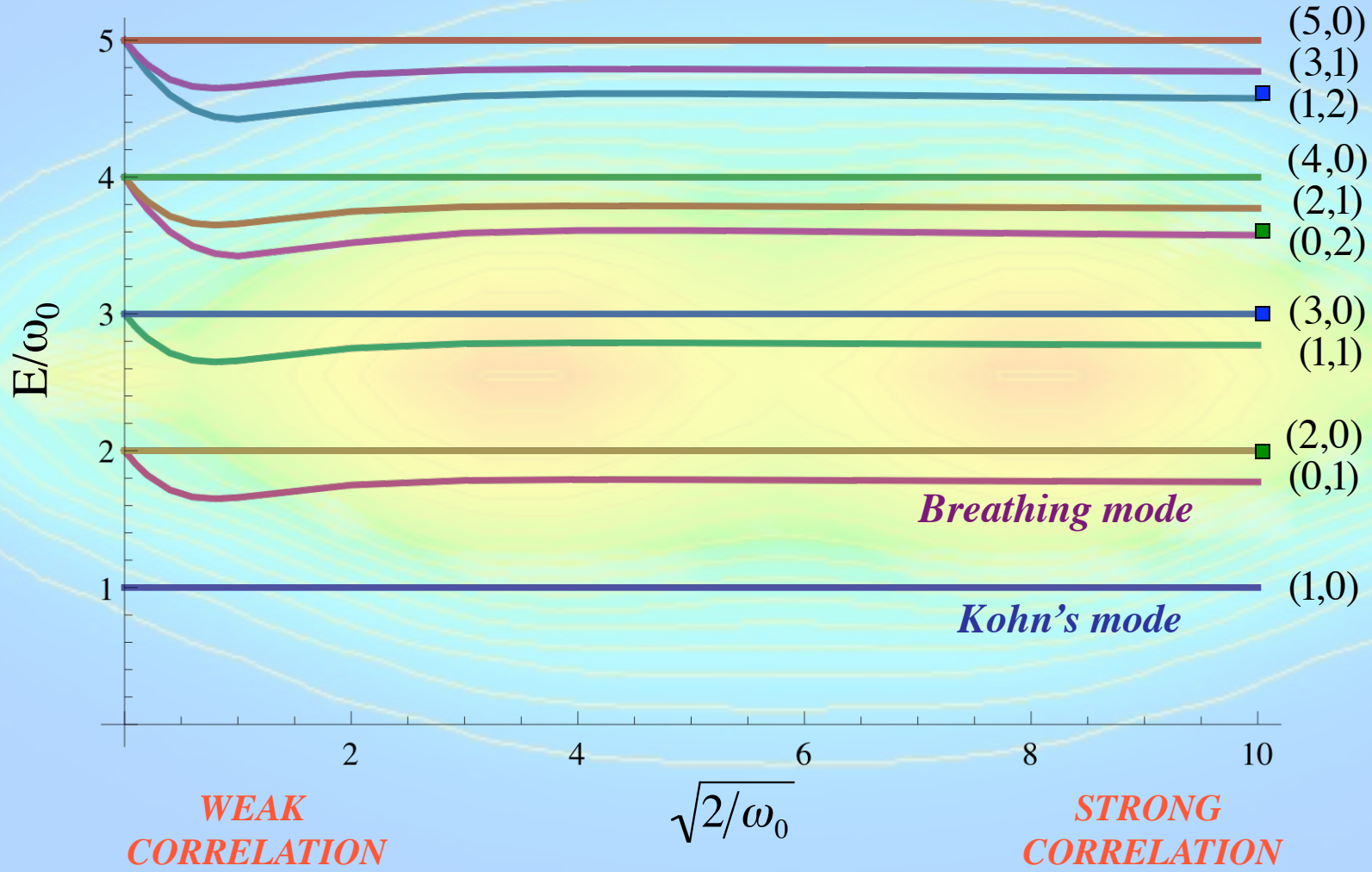


STRONG CORRELATION ω_0<<1

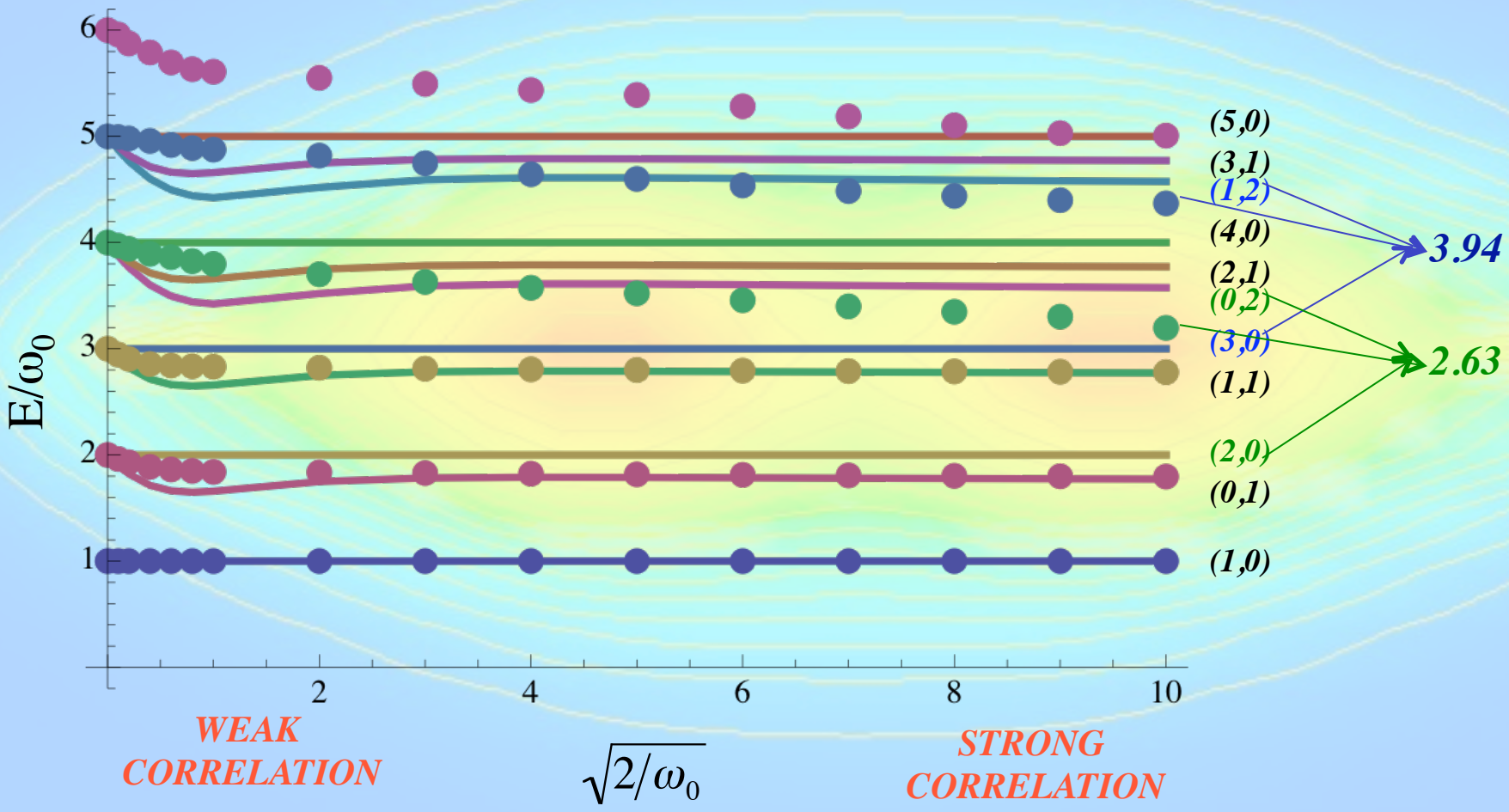
$$E_{nm} = \omega_0\left(n + m\sqrt{3}\right)$$



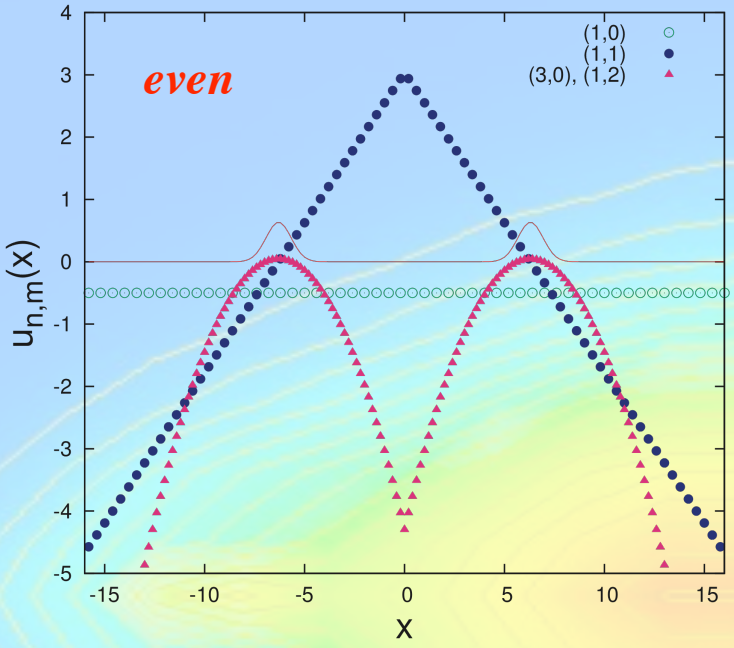
Evolution of exact excitation energies

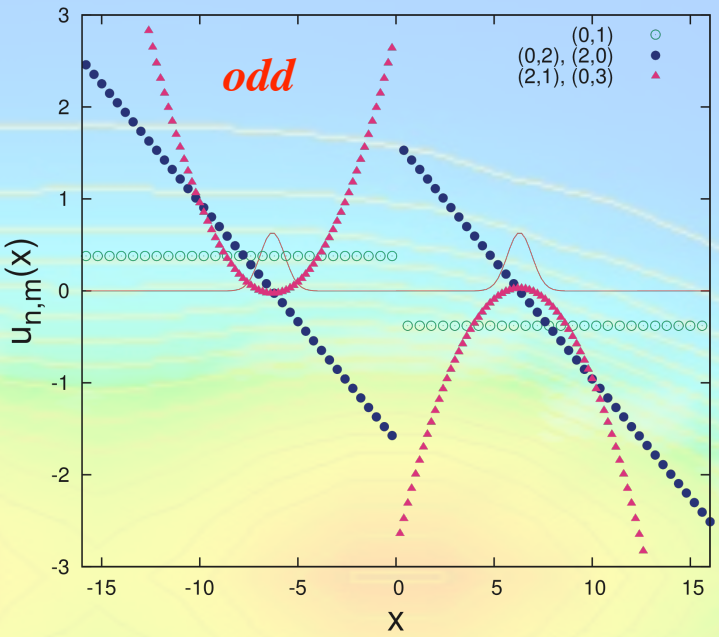


Exact excitation energies (lines) vs QCM energies (dots)



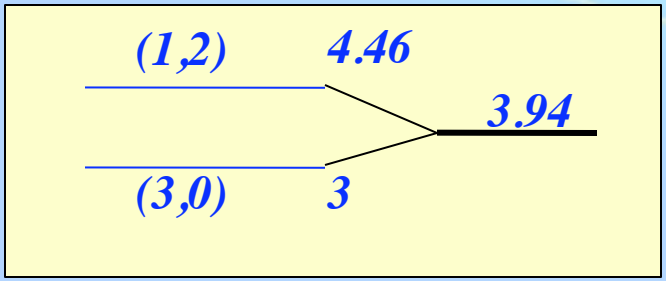
Strong Correlation Limit

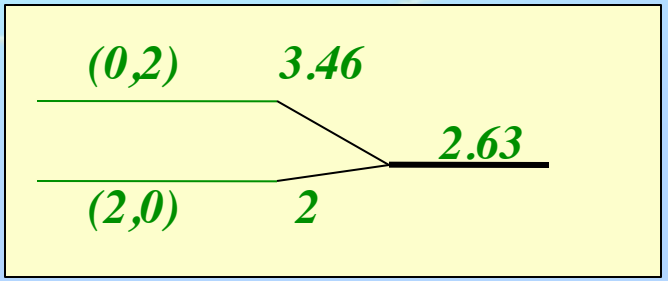




States with the same n+m and the same parity of m have identical displacement fields. At the QCM level they collapse into a single mode with energy $(k = n + m - 1)$

$$\omega_{nm} = \omega_0 \sqrt{2 + 3\sqrt{3}k + 6k(k-1)\left(2-\sqrt{3}\right) - (-1)^m \left(2-\sqrt{3}\right)^k}$$





Conclusions and speculations I

1. Our Quantum Continuum Mechanics is a direct extension of the collective approximation ("Bijl-Feynman") for the homogeneous electron gas to inhomogeneous quantum systems. We expect it to be useful for

- The theory of dispersive Van derWaals forces, especially in complex geometries

- Possible nonlocal refinement of the plasmon pole approximation in GW calculations

- Studying dynamics in the strongly correlated regime, which is dominated by a collective response (e.g., collective modes in the quantum Hall regime)

Conclusions and speculations II

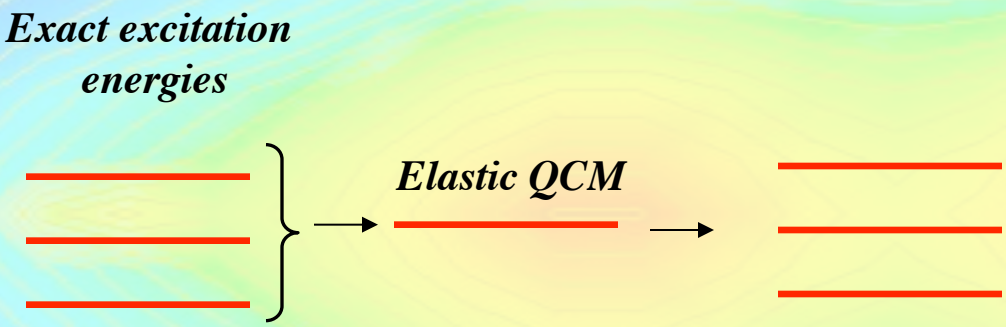
2. As a byproduct we got an explicit analytic representation of the exact xc kernel in the high-frequency (anti-adiabatic) limit

-This kernel should help us to study an importance of the space and time nonlocalities in the KS formulation of time-dependent CDFT.

-It is interesting to try to interpolate between the adiabatic and anti-adiabatic extremes to construct a reasonable frequency-dependent functional

The ultimate challenge: Including retardation

In the elastic theory, a group of levels may collapse into one. How can we recover the correct splitting of energy levels?



Answer: by making the force functional F[**u**] frequency-dependent: F[**u**,ω] – i.e., by including retardation.