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Quantum Continuum Mechanics for Many-Body Systems

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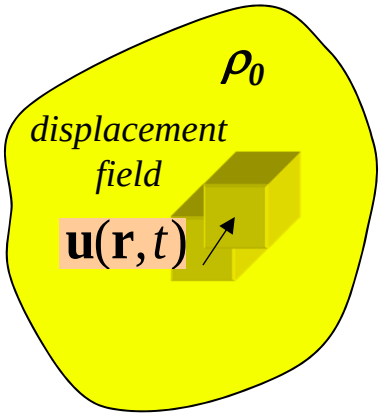
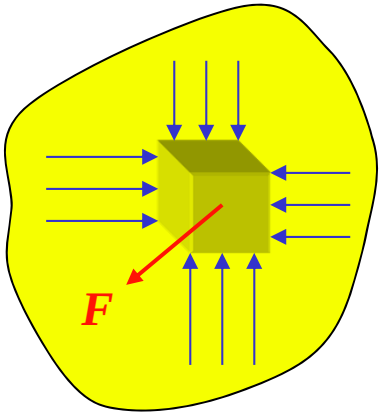
Continuum Mechanics: what is it?

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. A classical example is "Elasticity Theory".



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

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



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

Density and current in a quantum many-body system

In a quantum many-body system, the particle density n and the particle current density $\mathbf{j}$ are the relevant collective variables: they are *much simpler* than the quantum-mechanical wave function Ψ.

Particle density: $$n(\mathbf{r},t) = N \int d\mathbf{r}_2 ... d\mathbf{r}_N \left| \Psi(\mathbf{r},\mathbf{r}_2 ..., \mathbf{r}_N, t) \right|^2$$

Current density: $$\mathbf{j}(\mathbf{r},t) = N \,\mathrm{Im} \int d\mathbf{r}_2 ... d\mathbf{r}_N \Psi^*(\mathbf{r},\mathbf{r}_2 ..., \mathbf{r}_N, t) \nabla_{\mathbf{r}} \Psi(\mathbf{r},\mathbf{r}_2 ..., \mathbf{r}_N, t)$$

Velocity: $$\mathbf{v}(\mathbf{r},t) = \frac{\mathbf{j}(\mathbf{r},t)}{n(\mathbf{r},t)}$$

Displacement: $$\mathbf{u}(\mathbf{r},t) = \int dt\, \mathbf{v}(\mathbf{r},t)$$

Continuum mechanics of a single quantum particle

$$\Psi(\mathbf{r},t) = \left|\Psi(\mathbf{r},t)\right| e^{i\varphi(\mathbf{r},t)}$$

Density

$$n(\mathbf{r},t) = \left|\Psi(\mathbf{r},t)\right|^2$$

Current density

$$\mathbf{j}(\mathbf{r},t) = n(\mathbf{r},t)\nabla\varphi(\mathbf{r},t)$$

Velocity

$$\mathbf{v}(\mathbf{r},t) = \nabla\varphi(\mathbf{r},t)$$

Displacement

$$\mathbf{u}(\mathbf{r},t) = \int dt\, \nabla\varphi(\mathbf{r},t)$$

The Schrödinger equation, in this case, is completely equivalent to hydrodynamic equations

$$\begin{cases} \left(\dfrac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right)\mathbf{v} = -\nabla\cdot\underbrace{\vec{\vec{\mathbf{P}}}(\mathbf{r},t)}_{\substack{\text{Stress}\\ \text{tensor}}} - \nabla\underbrace{V(\mathbf{r},t)}_{\substack{\text{External}\\ \text{potential}}} \\ P_{ij} = \left(\partial_i\sqrt{n}\right)\left(\partial_j\sqrt{n}\right) - \dfrac{1}{4}\nabla^2 n\delta_{ij} \end{cases}$$

Can continuum mechanics be applied to quantum mechanical systems?

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

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

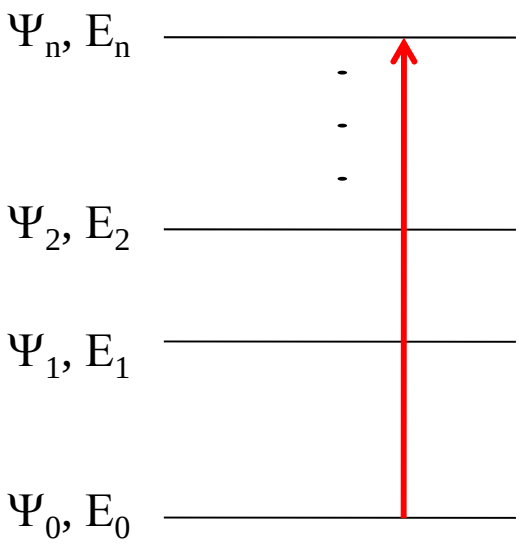
Local conservation of momentum

$$\frac{\partial \mathbf{j}(\mathbf{r},t)}{\partial t} = -\nabla \cdot \underbrace{\vec{\vec{\mathbf{P}}}(\mathbf{r},t)}_{\text{Stress tensor}} - \mathrm{n}(\mathbf{r},t)\ \nabla\left[V_0(\mathbf{r}) + V_1(\mathbf{r},t)\right]$$

P is a unique functional of the current density (by Runge-Gross theorem)

At variance with classical continuum mechanics quantum continuum mechanics aspires to be valid at *all* length scales.

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.

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

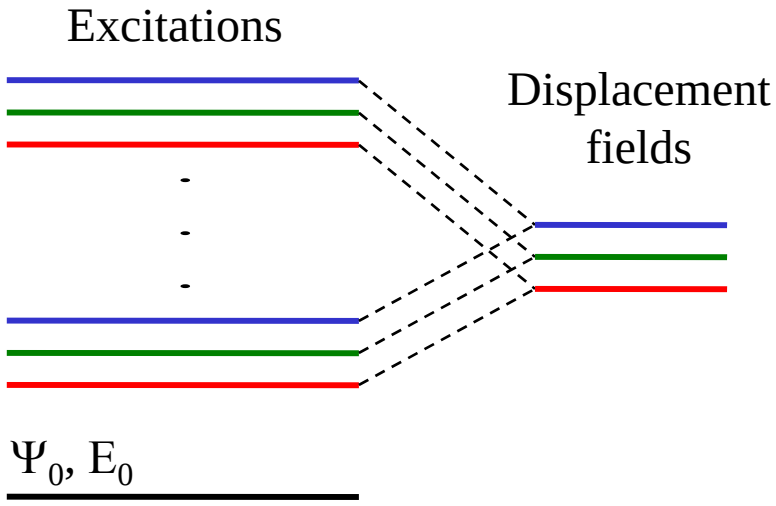
$$\lambda << 1$$

The *displacement field* associated with this excitation is the expectation value of the current in Ψ_{n0} divided by the ground-state density n_0 and integrated over time

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

Continuum mechanics in the linear response regime - continued

Excitation energies in linear continuum mechanics are obtained by solving a linear equation of motion for the Fourier transform of the displacement field $\boldsymbol{u}(\boldsymbol{r},\omega)$. The existence of a non-vanishing, normalizable solutions at frequency ω means that $\hbar\omega$ is an excitation energy.



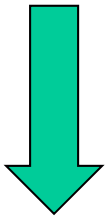
WARNING

Displacements associated with different excitations need not be linearly independent. Different excited states can have the same displacement.

Exception

In 1-particle systems (and only in 1-particle systems) there is a 1-1 correspondence between excitations and displacement fields

$$\int d\boldsymbol{r} n_0(\boldsymbol{r}) \frac{\boldsymbol{j}_{0n}(\boldsymbol{r})}{n_0(\boldsymbol{r})} \cdot \frac{\boldsymbol{j}_{k0}(\boldsymbol{r})}{n_0(\boldsymbol{r})} = 0 \qquad (n \neq k)$$

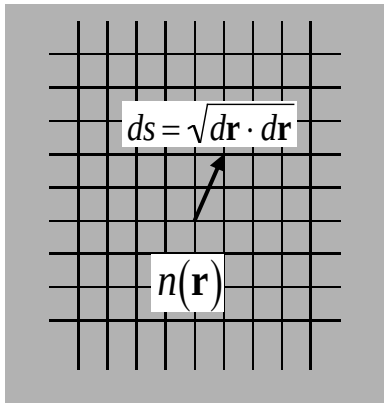


In a 1-particle system (and only in a 1-particle system) different excitations have orthogonal displacement fields

Continuum Mechanics – Lagrangian formulation

I. V. Tokatly, PRB 71, 165104 & 165105 (2005); PRB 75, 125105 (2007)

Make a change of coordinates 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.***



Cartesian coordinates

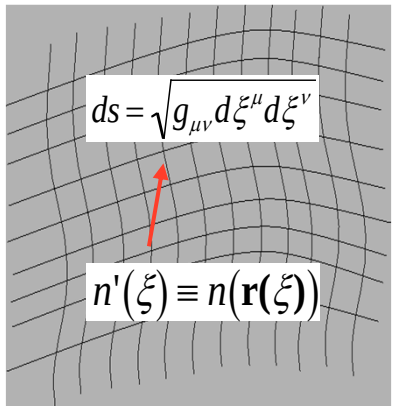
$$\mathbf{r}(\xi,t) = \xi + \underbrace{\mathbf{u}(\xi,t)}_{\text{Displacement Field}}$$

Metric tensor

$$g_{\mu\nu} = \delta_{\mu\nu} + \partial_\mu u_\nu + \partial_\nu u_\mu$$

Stress tensor

$$\hat{P}_{\mu\nu} = \frac{2}{\sqrt{g}} \frac{\delta \hat{H}[\mathbf{u}]}{\delta g_{\mu\nu}}$$



Curvilinear coordinates

Wave function in Lagrangian frame

Hamiltonian in Lagrangian frame

$$m \frac{\partial^2 u_\mu(\xi,t)}{\partial t^2} + \mathbf{u} \cdot \nabla \frac{\partial V_0}{\partial \xi_\mu} = -\frac{1}{n_0(\xi)} \underbrace{\left\langle \tilde{\psi}(t) \middle| \frac{\delta \tilde{H}[\mathbf{u}]}{\delta u_\mu} \middle| \tilde{\psi}(t) \right\rangle}_{\text{Generalized force}} \Bigg|_1 - \frac{\partial V_1}{\partial \xi_\mu}$$

Continuum Mechanics: the Elastic Approximation

Assume that the wave function in the Lagrangian frame is time-independent - the time evolution of the system being entirely governed by the changing metrics. We call this assumption the ***"elastic approximation". This gives...***

The elastic equation of motion:

$$m\ddot{\mathbf{u}} = F[\mathbf{u}] - \nabla V_1$$

$$\mathbf{F}[\mathbf{u}] = -\frac{1}{n_0}\frac{\delta\left\langle \Psi_0[\mathbf{u}]\middle|\hat{T}+\hat{W}+\hat{V}_0\middle|\Psi_0[\mathbf{u}]\right\rangle_2}{\delta\mathbf{u}} \equiv -\frac{1}{n_0}\frac{\delta E_2[\mathbf{u}]}{\delta\mathbf{u}}$$

$\Psi_0[\mathbf{u}]$ is the deformed ground state wave function:

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

The elastic approximation is expected to work best for highly collective excitations, and it is **exact** for **(1) High-frequency limit (2) One-electron systems.** Notice that this is the **opposite** of an **adiabatic** approximation.

An elementary derivation of the elastic equation of motion

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

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

Go the high frequency limit:

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

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

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

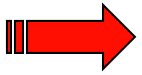
Inverting Eq. (1) to first order we get

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

Finally, using

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

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



$$-n_0(\mathbf{r})\omega^2 \tilde{\mathbf{u}}(\mathbf{r}) = \int d\mathbf{r}' \mathbf{M}(\mathbf{r},\mathbf{r}') \cdot \tilde{\mathbf{u}}(\mathbf{r}') - n_0(\mathbf{r}) \nabla \tilde{V}_1(\mathbf{r})$$

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

Full expression for the *instantaneous* force

The elastic equation of motion:

$$m\ddot{\mathbf{u}} = F[\mathbf{u}] - \nabla V_1$$

$$\mathbf{F}[\mathbf{u}] = -\frac{1}{n_0}\frac{\delta\left\langle \Psi_0[\mathbf{u}]\middle|\hat{T}+\hat{W}+\hat{V}_0\middle|\Psi_0[\mathbf{u}]\right\rangle_2}{\delta\mathbf{u}}$$

$$-\frac{\delta T_2[\mathbf{u}]}{\delta u_\mu} = \partial_\alpha[2T_{\nu\mu,0}u_{\nu\alpha} + T_{\nu\alpha,0}\partial_\mu u_\nu] - \frac{1}{4m}\partial_\nu\partial_\mu(n_0\partial_\nu\nabla\cdot\mathbf{u})$$
$$+\frac{1}{4m}\partial_\nu\{2(\nabla^2 n_0)u_{\nu\mu} + (\partial_\nu n_0)\partial_\mu\nabla\cdot\mathbf{u}$$
$$+(\partial_\mu n_0)\partial_\nu\nabla\cdot\mathbf{u} - 2\partial_\mu[(\partial_\alpha n_0)u_{\nu\alpha}]\}.$$

$$-\mathbf{u}\cdot\nabla\partial_\mu V_0$$

$$-\frac{\delta W_2[\mathbf{u}]}{\delta u_\mu(\mathbf{r})} = \int d\mathbf{r}' K_{\mu\nu}(\mathbf{r},\mathbf{r}')[u_\nu(\mathbf{r}) - u_\nu(\mathbf{r}')].$$

This expression has been simplified by Gould et al., JCP 136, 204115 (2012).

$$K_{\mu\nu}(\mathbf{r},\mathbf{r}') = \rho_2(\mathbf{r},\mathbf{r}')\partial_\mu\partial'_\nu\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}.$$

Pair correlation function

The one-particle case

The linear QCM equation of motion takes the form

$$-\omega^2 \mathbf{u}(r,t) = -\nabla\left[\frac{1}{2\sqrt{n_0}}\left(\frac{\nabla^2}{2} - \frac{\nabla^2\sqrt{n_0}}{2\sqrt{n_0}}\right)\frac{\nabla\cdot\left(n_0\mathbf{u}\right)}{\sqrt{n_0}}\right]$$

which coincides with what one gets from the Schrödinger equation

$$i\frac{\partial\psi(r,t)}{\partial t} = \left[-\frac{\nabla^2}{2m} + V_0(r) + V_1(r,t)\right]\psi(r,t)$$

with

$$\psi(r,t) = \sqrt{n(r,t)}\; e^{i\varphi(r,t)} \qquad \vec{\nabla}\varphi(r,t) \equiv \dot{\vec{u}}(r,t)$$

The elastic equation of motion: discussion

1. The linear force functional **F**[**u**] is calculable from the exact one- and two body density matrices of the ground-state. These 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 $\omega_\lambda{}^2$. The following relation exists between $\omega_\lambda{}^2$ and the exact excitation energies:

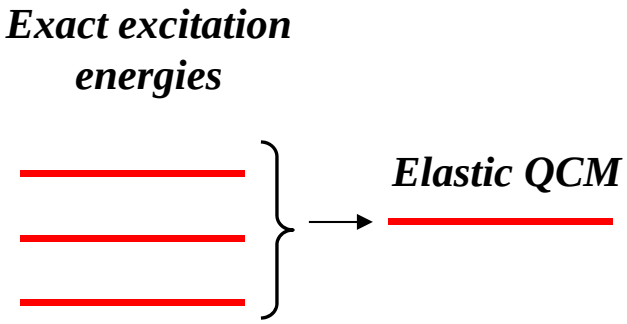
$$\omega_\lambda^2 = \sum_n f_n^\lambda \left(E_n - E_0\right)^2$$

Oscillator strengths

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

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!

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

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

The homogeneous electron gas

LONGITUDINAL

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

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

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

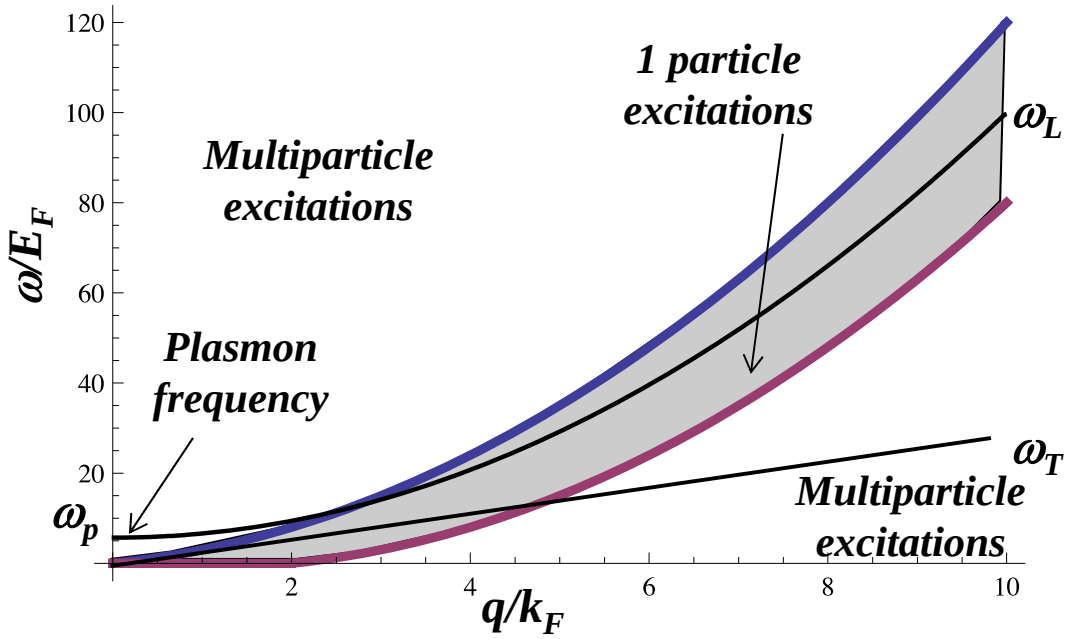
TRANSVERSAL

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

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

static structure factor

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



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

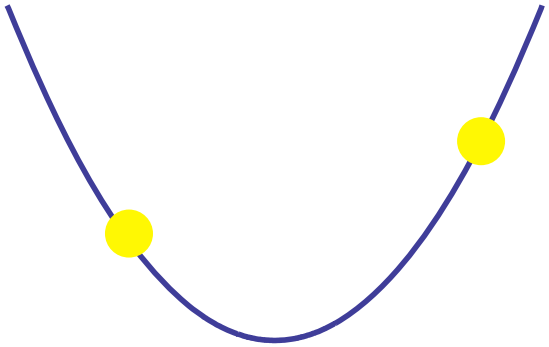
B. Hydrogen atom (l=0)

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

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

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

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



Parabolic trap

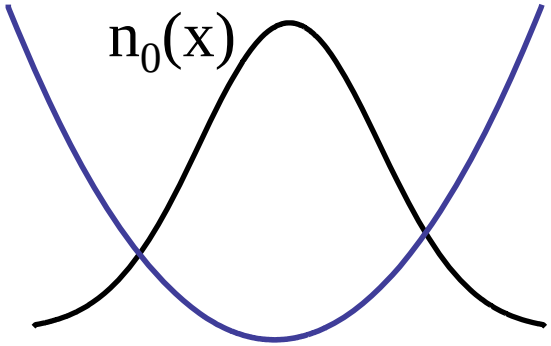
$$H = \overbrace{\frac{P^2}{4} + \frac{\omega_0^2}{2} X^2}^{\text{Center of Mass}} + \overbrace{p^2 + \frac{\omega_0^2}{4} x^2 + \underbrace{\frac{1}{\sqrt{x^2 + a^2}}}_{\text{Soft Coulomb repulsion}}}^{\text{Relative Motion}}$$

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

n,m non-negative integers

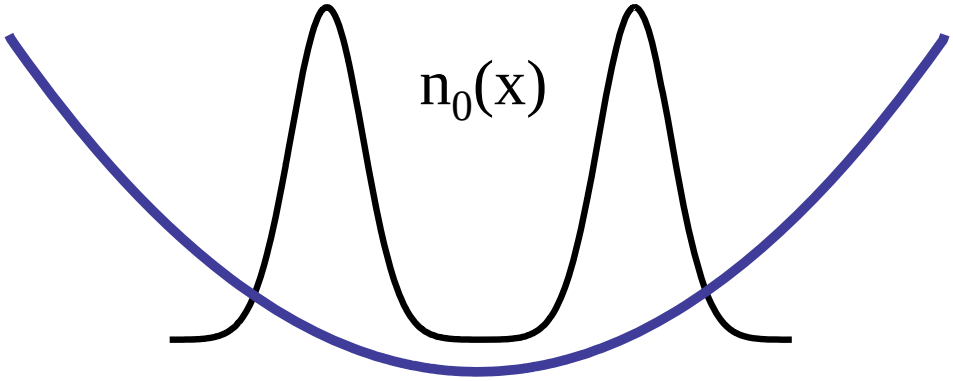
WEAK CORRELATION ω_0>>1

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

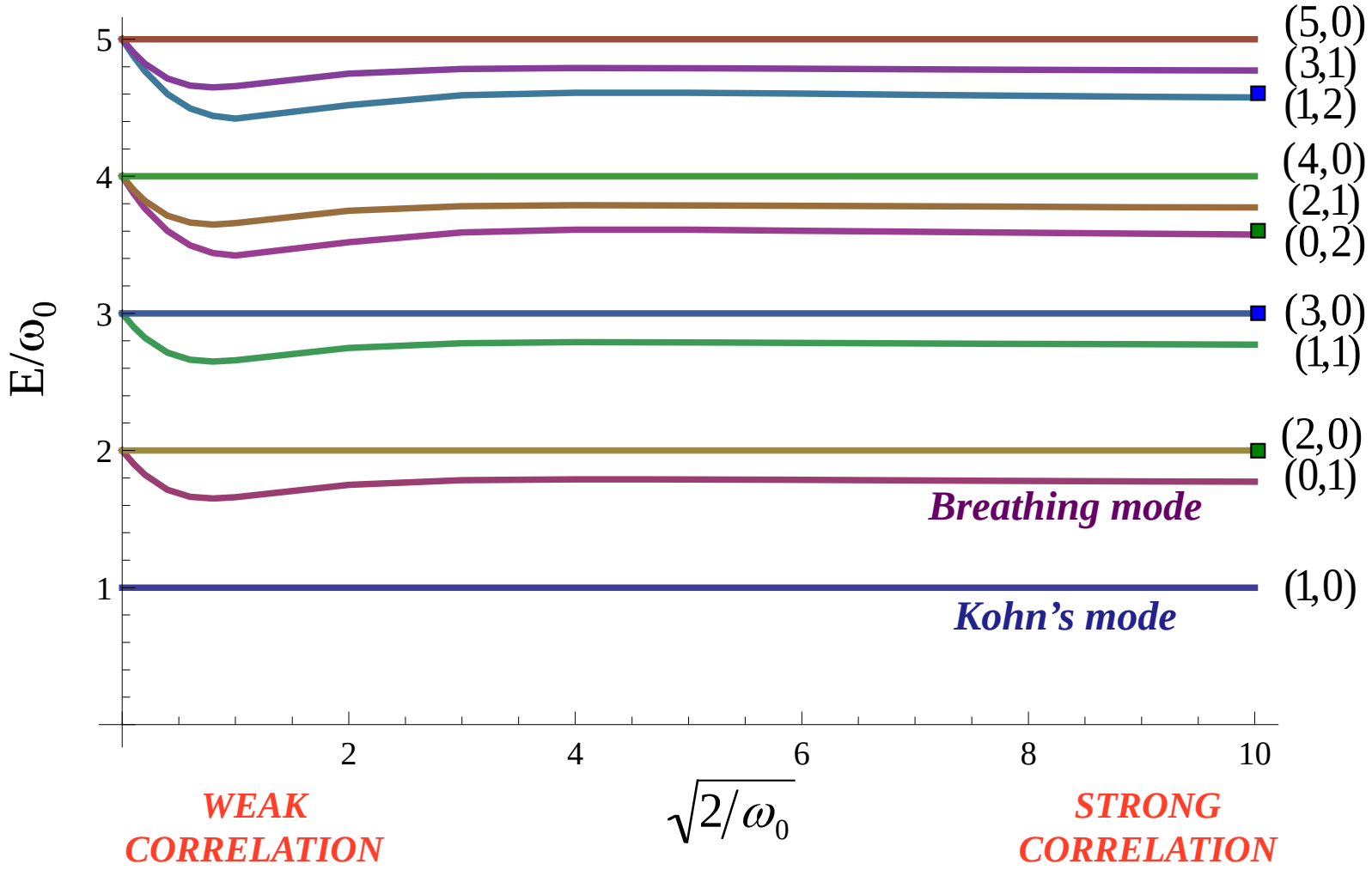


STRONG CORRELATION ω_0<<1

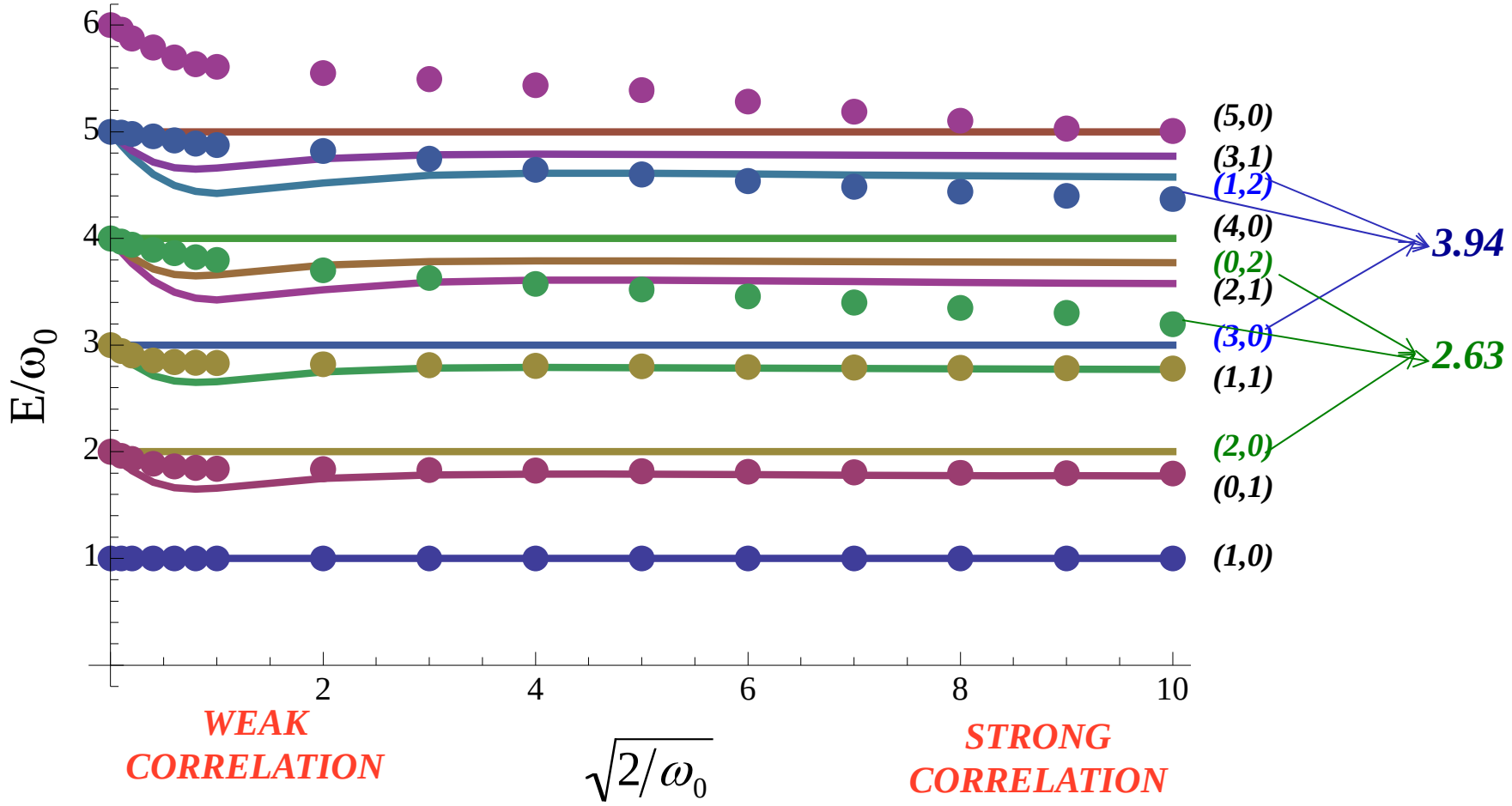
$$E_{nm} = \omega_0\left(n + m\sqrt{3}\right)$$



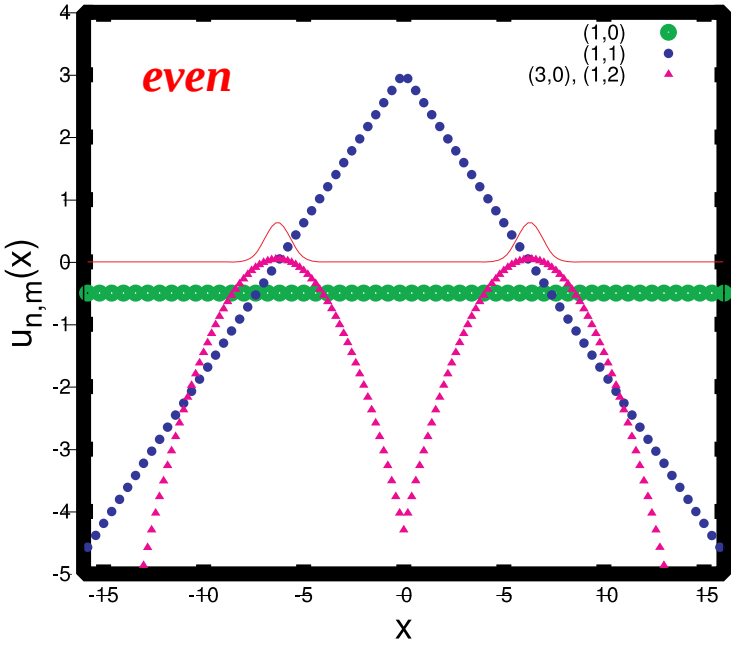
Evolution of exact excitation energies

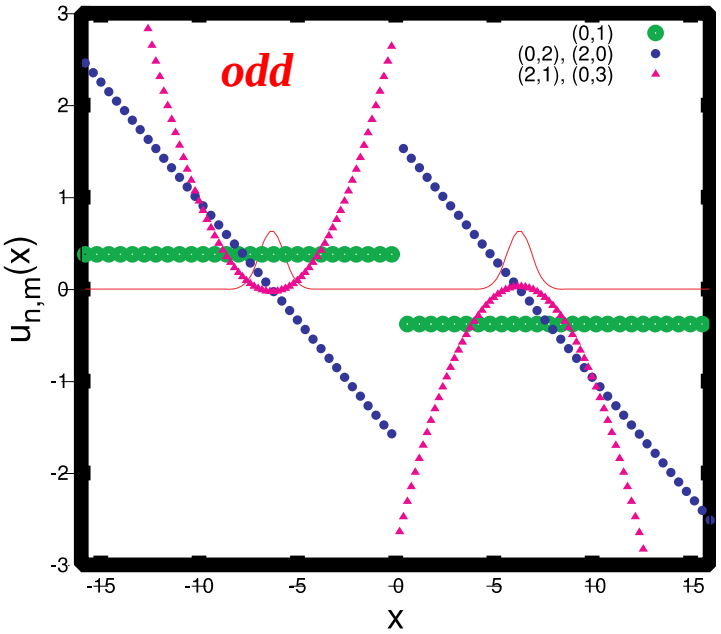


Exact excitation energies (lines) vs QCM energies (dots)



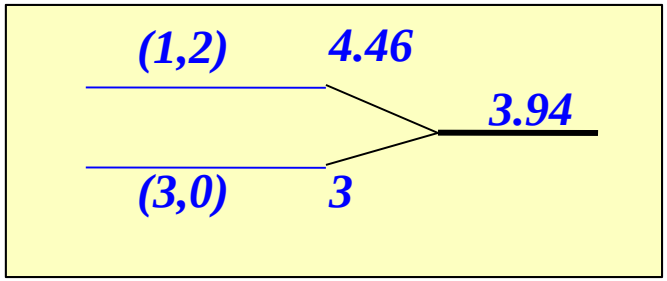
Strong Correlation Limit

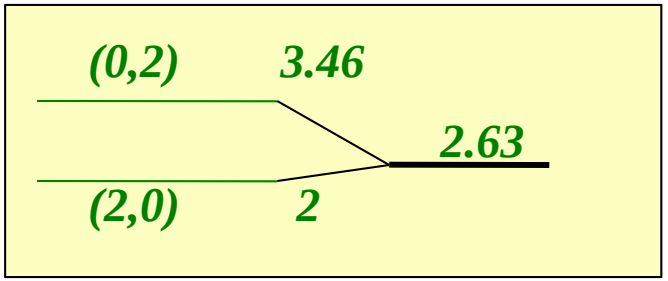


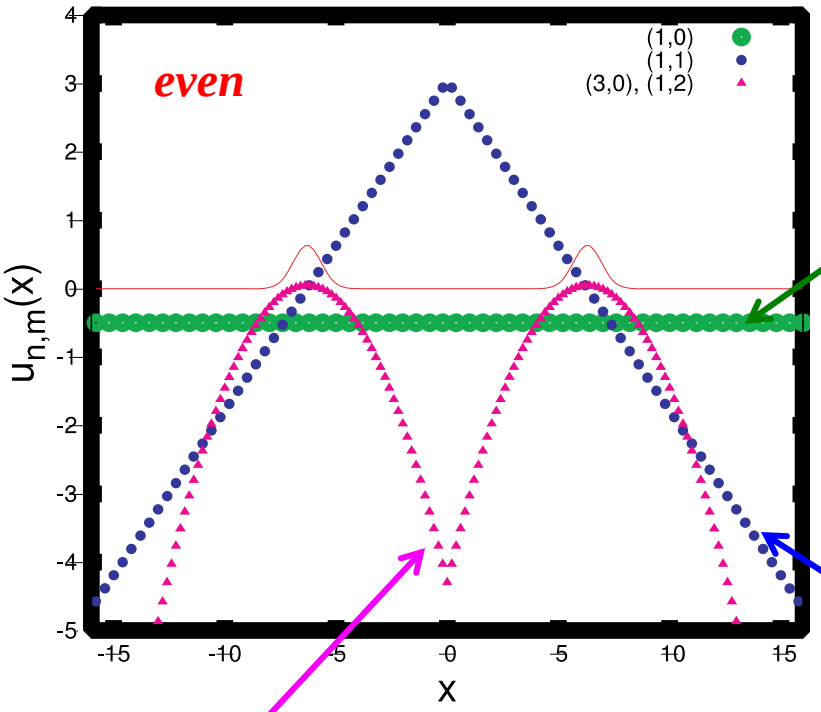


States with the same n+m and the same parity of m have identical displacement fields. At the QCM level they collapse into a single mode with energy $(k = n + m - 1)$

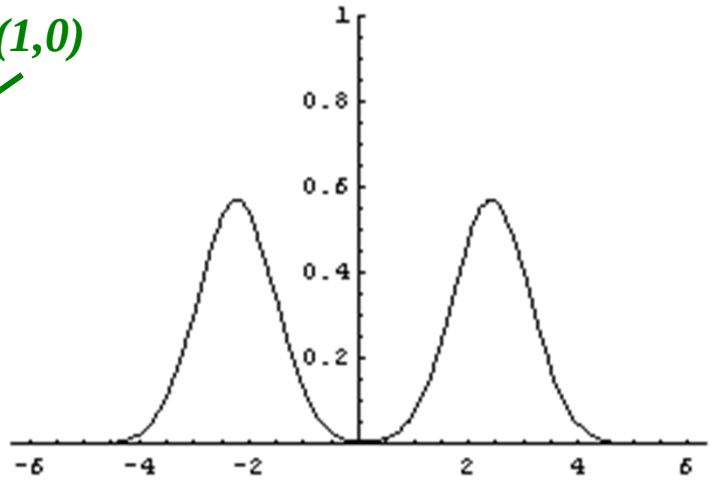
$$\omega_{k\pm} = \omega_0 \sqrt{2 + 3\sqrt{3}k + 6k(k-1)\left(2-\sqrt{3}\right) \square (-1)^k \left(2-\sqrt{3}\right)^k}$$







(1,0)



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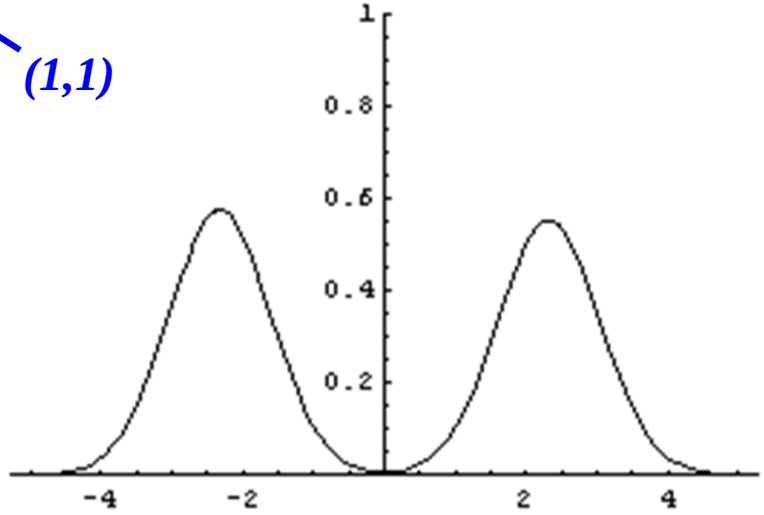

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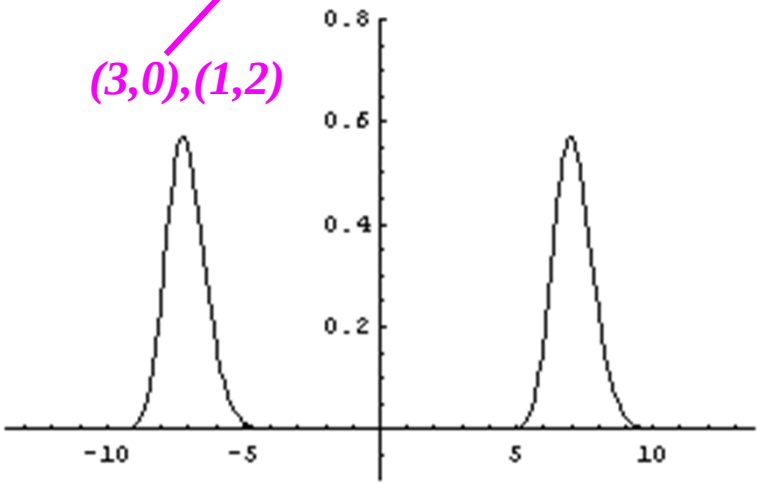

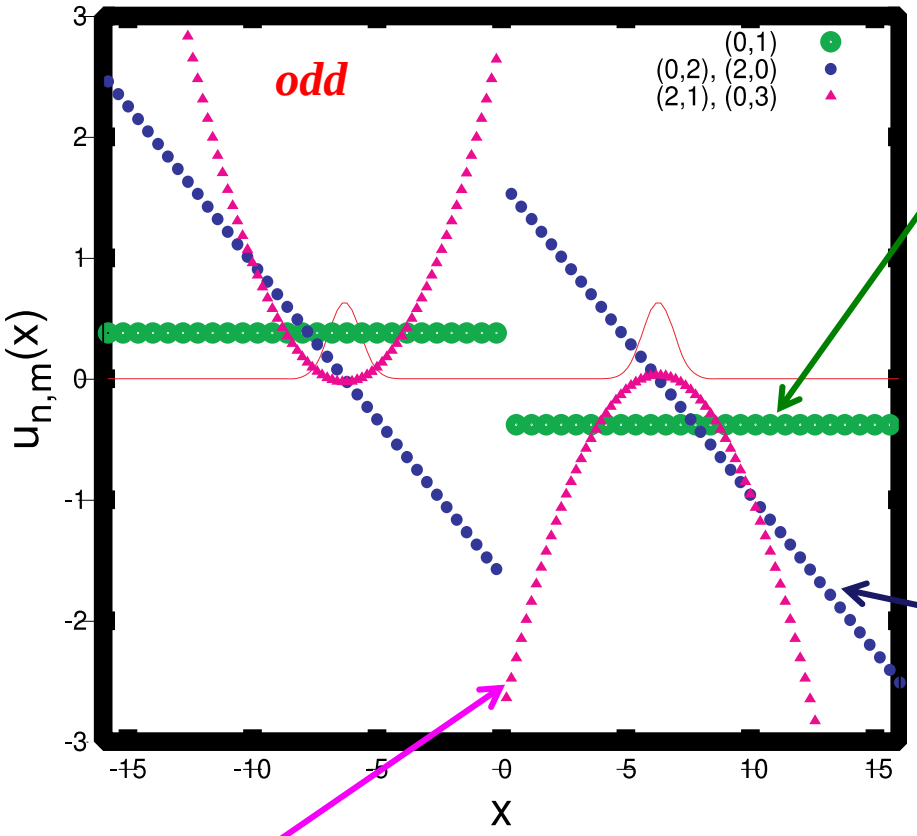

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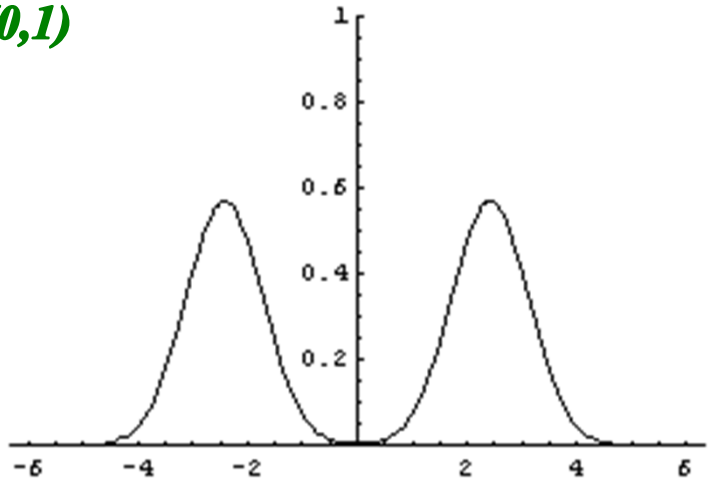
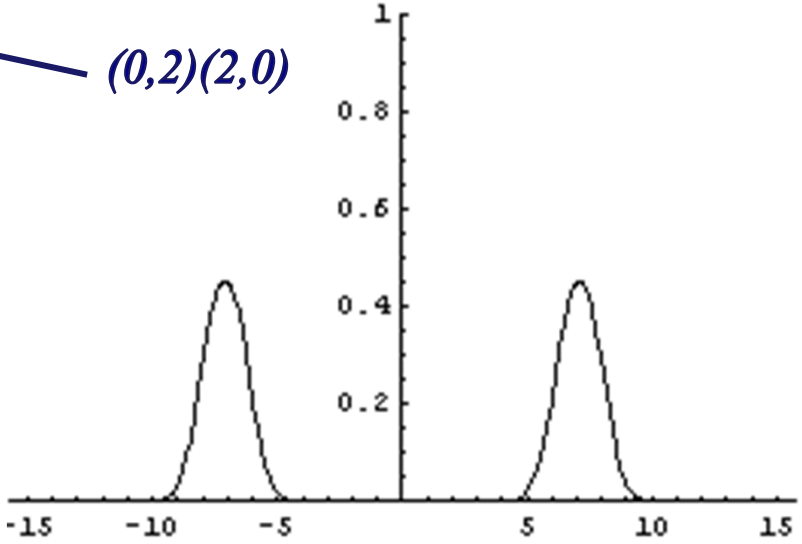
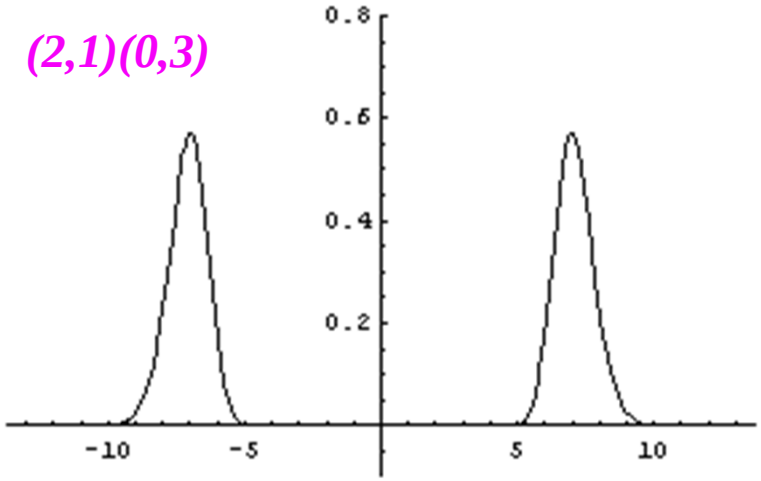


(0,2)(2,0)



(2,1)(0,3)



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 following applications:

- Theory of dispersive Van derWaals forces, especially in complex geometries (Gould-Dobson)

- Nonlocal refinement of the plasmon pole approximation in GW calculations

- Dynamics in the strongly correlated regime (e.g., collective modes in the quantum Hall regime)

Conclusions and speculations II

- As a byproduct we got an explicit analytic representation of the exact xc functional in the high-frequency (anti-adiabatic) limit [Nazarov *et al.*, PRB **81**, 245101 (2010)]. This functional should help us to study an importance of the space and time nonlocalities in the Kohn-Sham formulation of time-dependent current DFT.

- We are trying to interpolate between the adiabatic and anti-adiabatic extremes by including relaxation of the wave function in the co-moving frame. This can be done by assigning a finite width to the eigenmodes of the QCM.

- Prospected generalizations: (1) Combining electronic and ionic displacements in a single formulation (2) Including local temperature variations.