

Workshop on Dynamics and Correlation in Exotic Nuclei
Kyoto, Japan, September 2011

Quantum Continuum Mechanics for Many-Body Systems

J. Tao^{1,2}, X. Gao^{1,3}, G. Vignale², I. V. Tokatly⁴,
S. Pittalis²

1. *Los Alamos National Lab*
2. *University of Missouri-Columbia*
3. *Zhejiang Normal University, China*
4. *Universidad del País Vasco*



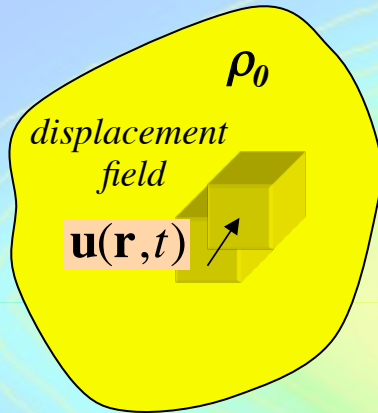
Los Alamos
NATIONAL LABORATORY



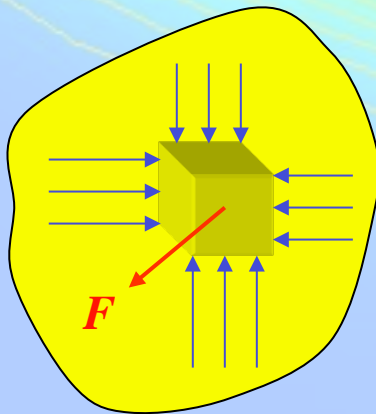
ikerbasque
Basque Foundation for Science

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”.



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



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

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

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

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

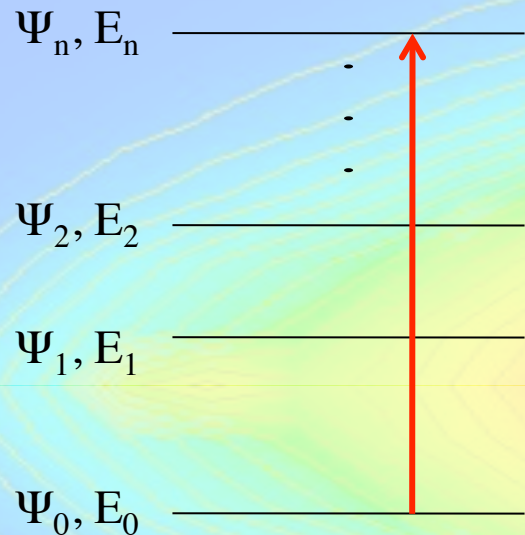
A unique functional of the current density (by Runge-Gross theorem)

Local conservation of momentum

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

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.

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

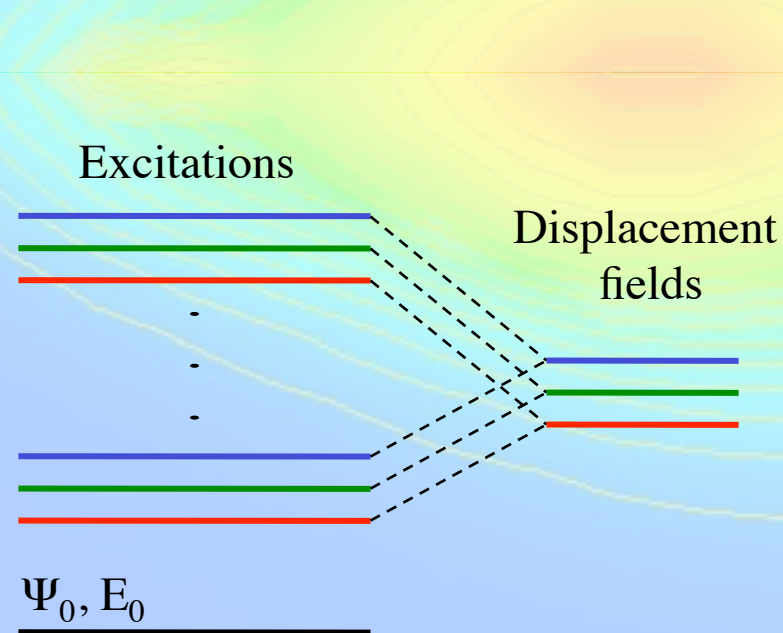
$$\lambda \ll 1$$

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

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

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 $\mathbf{u}(\mathbf{r}, \omega)$. The existence of a non-vanishing, normalizable solutions at frequency ω means that $\hbar\omega$ is an excitation energy.



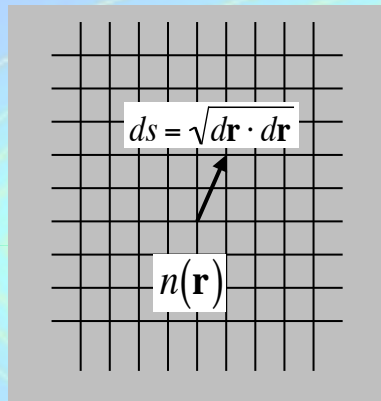
WARNING

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

Continuum Mechanics – Lagrangian formulation

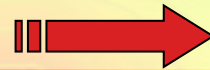
I. V. Tokatly, PRB 71, 165104 & 165105 (2005); PRB 75, 125105 (2007)

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.*

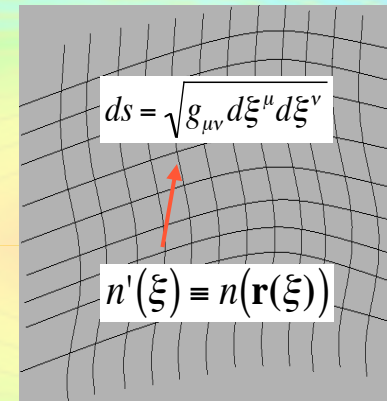


Cartesian coordinates

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



$$\frac{\partial \mathbf{u}(\xi, t)}{\partial t} = \frac{\mathbf{j}(\xi, t)}{n(\xi, t)},$$



Curvilinear coordinates

Wave function in
Lagrangian frame

Hamiltonian in
Lagrangian frame

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

Generalized force

Continuum Mechanics: the Elastic Approximation



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

The elastic equation of motion:

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

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

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

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

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 an **anti-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 to the high frequency limit:

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

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

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

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

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

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



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

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

The one-particle case

Polar representation of the wave function

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

Inserting into the Schrödinger equation

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

Linearizing about the ground-state and Fourier-transforming we get

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

Since the right hand side does not depend on frequency, we conclude that it is given exactly by the high-frequency limit of the linear response theory.

The homogeneous electron gas

LONGITUDINAL

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

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

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

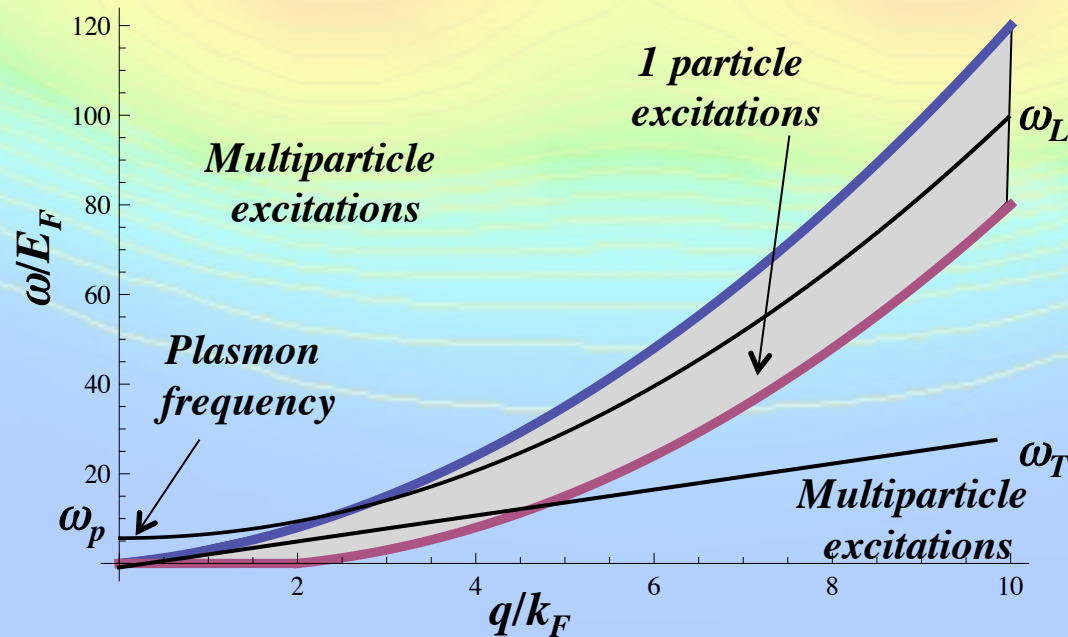
TRANSVERSAL

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

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

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

static structure factor



The elastic equation of motion: discussion

1. The linear functional $\mathbf{F}[\mathbf{u}]$ 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 $n_0(\mathbf{r})$.

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

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:

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

Oscillator strengths

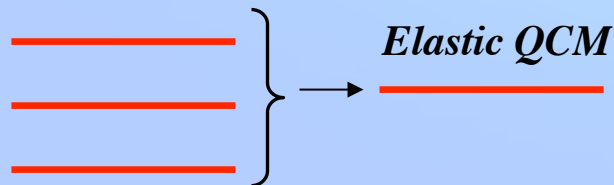
$$f_n^\lambda = \frac{2 \left| \int d\mathbf{r} \mathbf{u}_\lambda(\mathbf{r}) \cdot \mathbf{j}_{0n}(\mathbf{r}) \right|^2}{E_n - E_0} \quad \left(\mathbf{j}_{0n}(\mathbf{r}) = \langle \Psi_0 | \hat{\mathbf{j}}(\mathbf{r}) | \Psi_n \rangle \right)$$

f-sum rule

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

*rigorously satisfied
in 1D systems*

*Exact excitation
energies*



*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

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

a fourth-order integro-differential equation

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

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

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

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).

$$\text{Eigenvalues: } \omega_n = \pm n\omega_0$$

$$\text{Eigenfunctions: } u_n(x) = H_{n-1}(x)$$

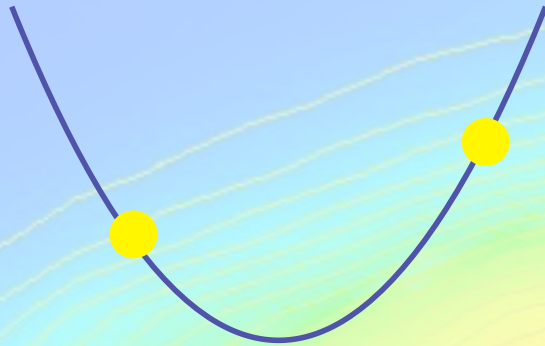
B. Hydrogen atom ($l=0$)

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

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

$$\text{Eigenfunctions: } u_{nr}(r) = L_{n-2}^2\left(\frac{2r}{n}\right)$$

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



Parabolic trap

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

Soft Coulomb repulsion

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

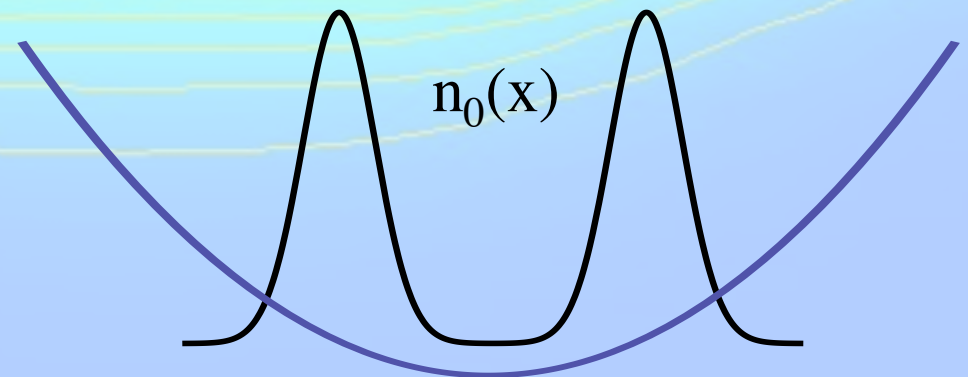
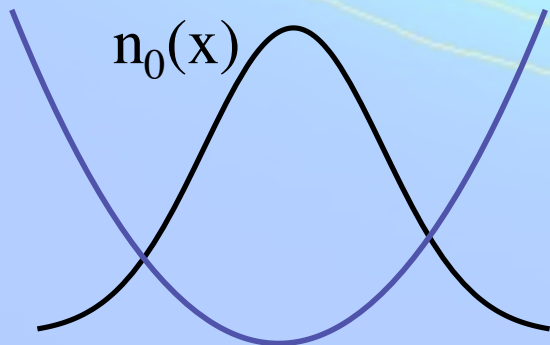
n, m non-negative integers

WEAK CORRELATION $\omega_0 \gg 1$

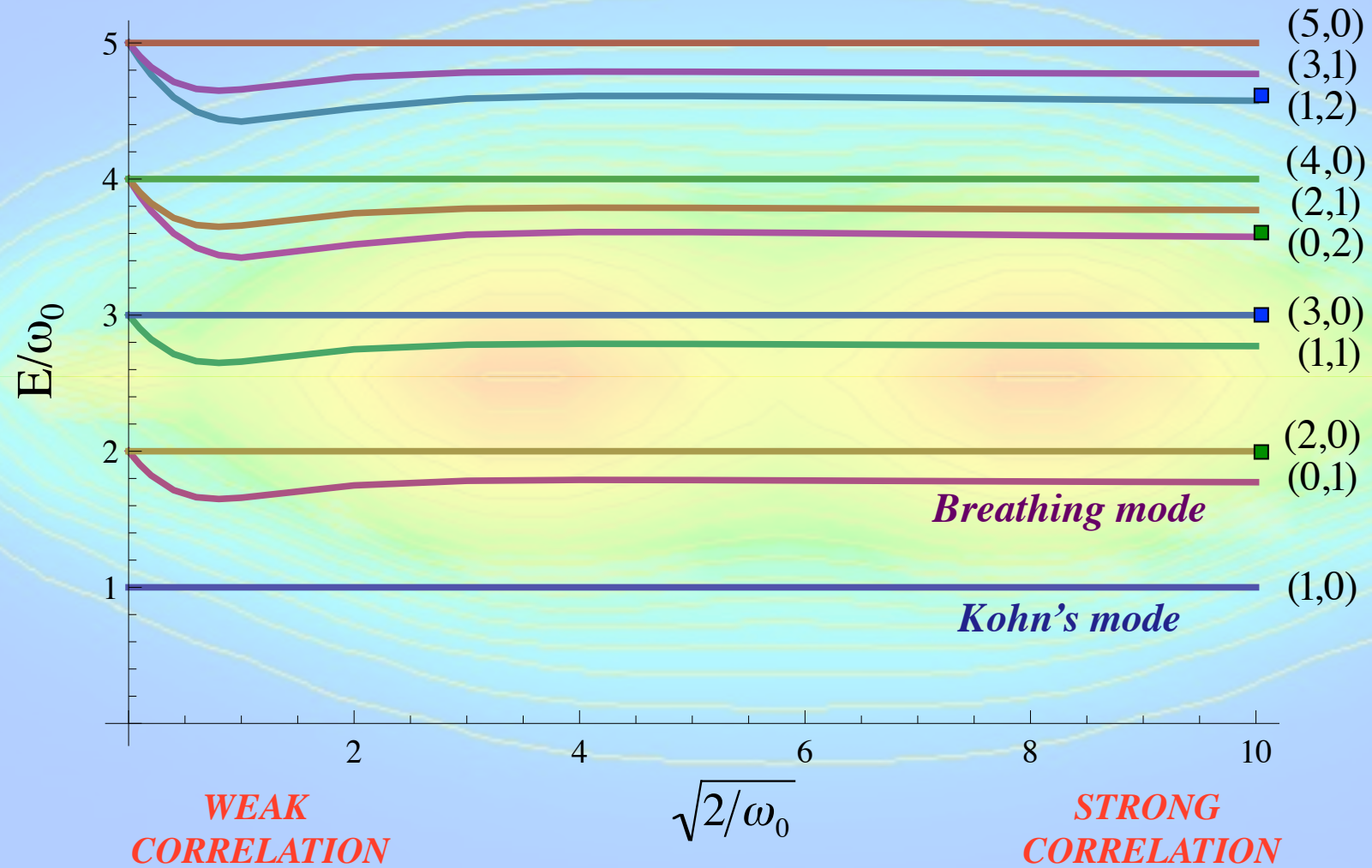
STRONG CORRELATION $\omega_0 \ll 1$

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

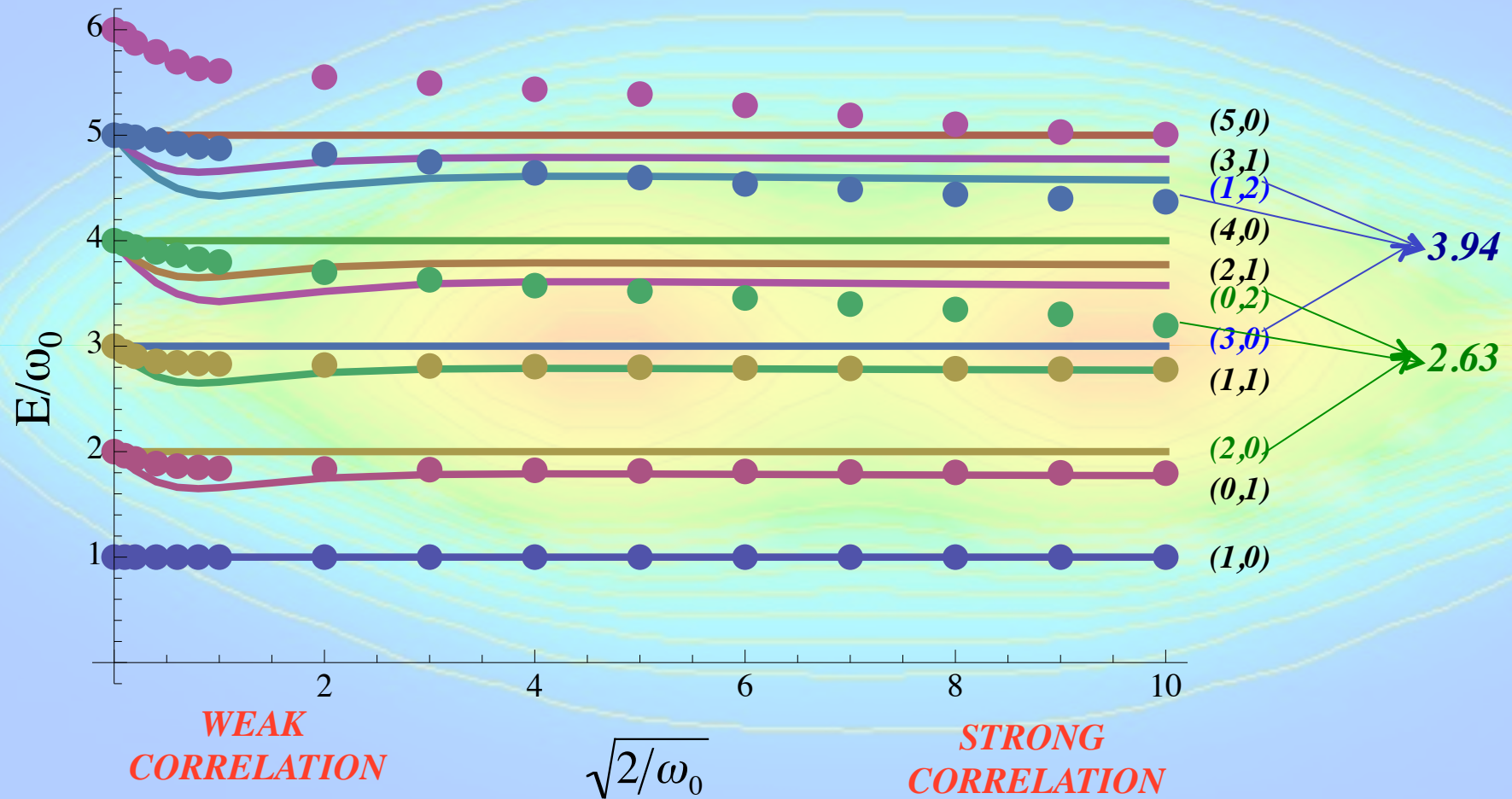
$$E_{nm} = \omega_0 (n + m\sqrt{3})$$



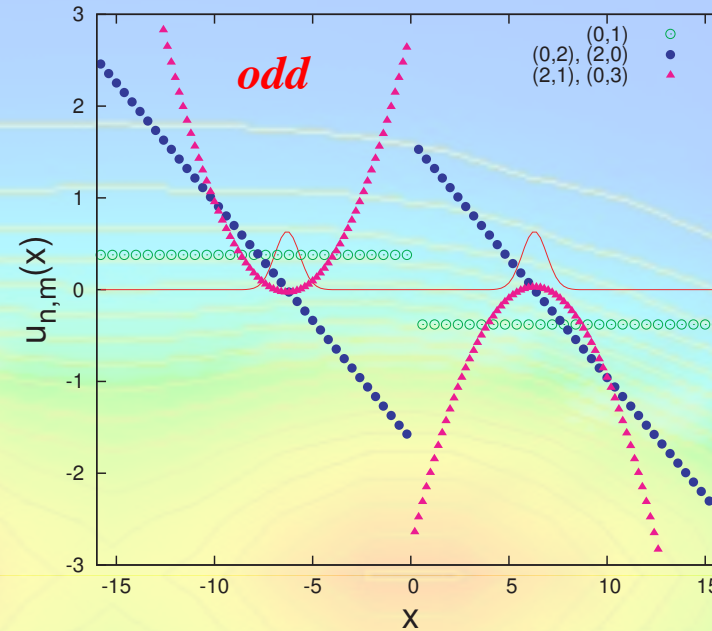
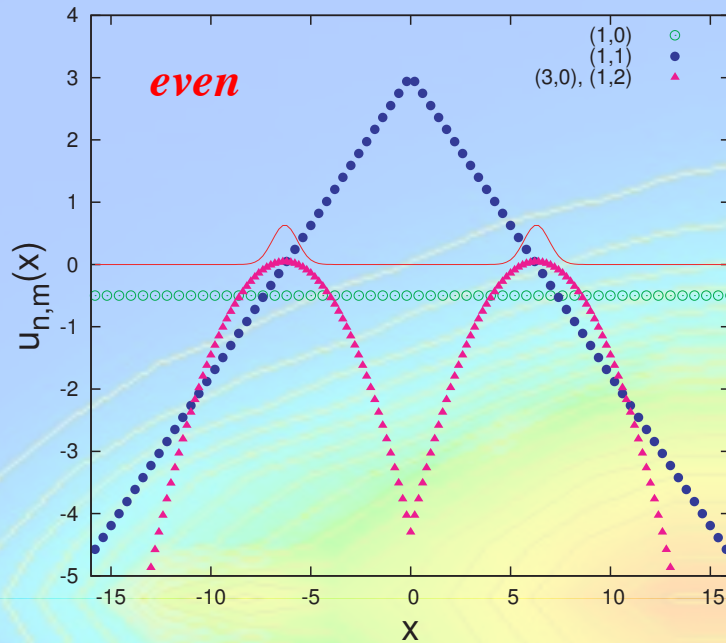
Evolution of exact excitation energies



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



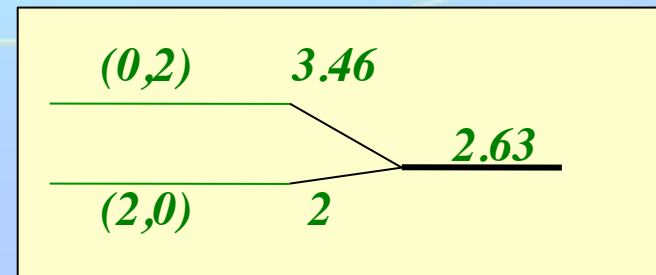
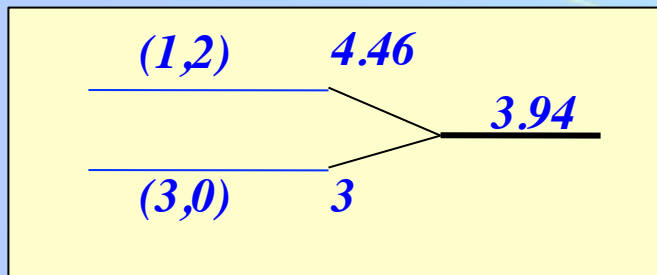
Strong Correlation Limit

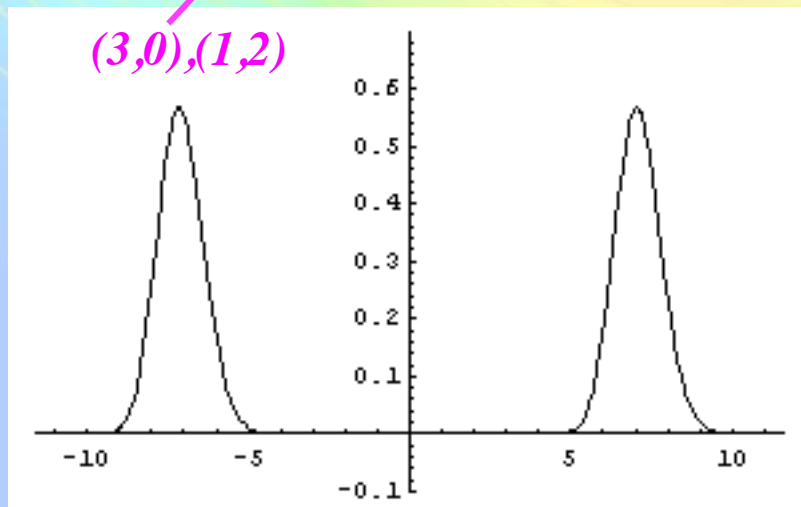
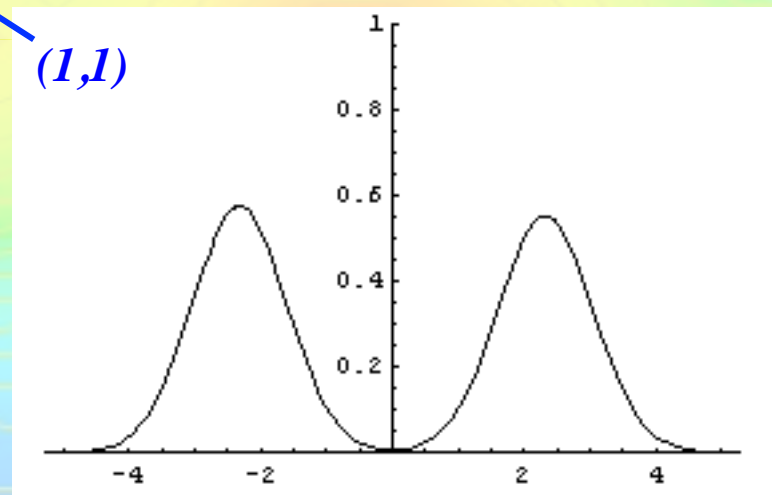
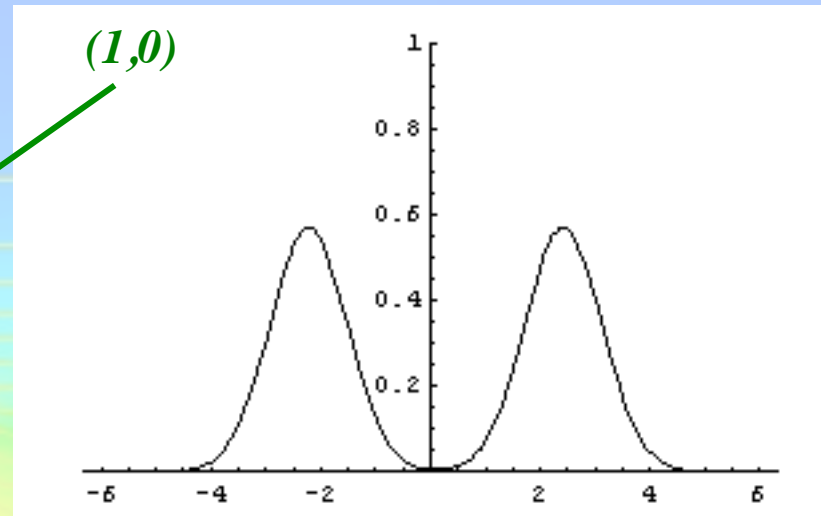
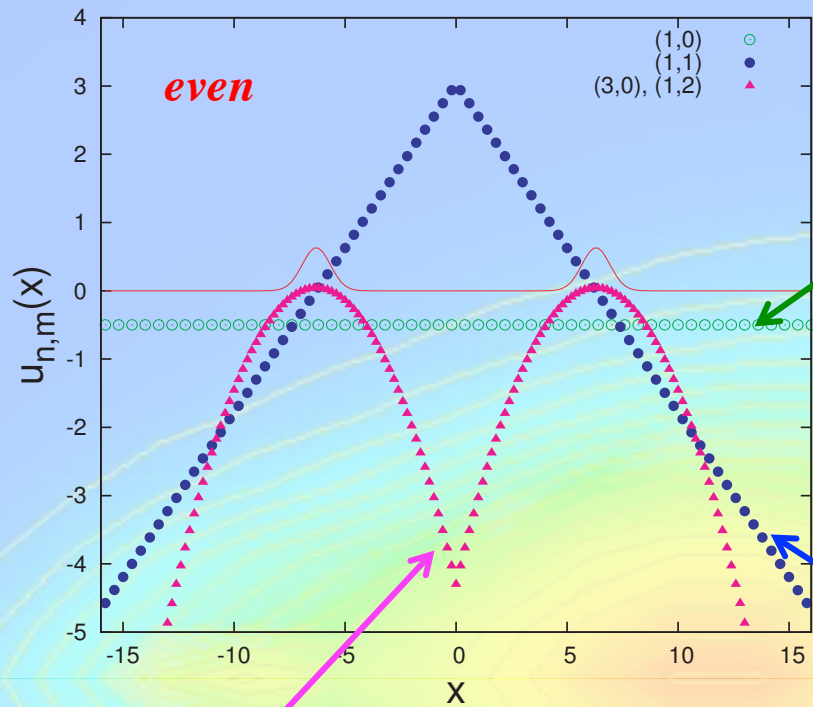


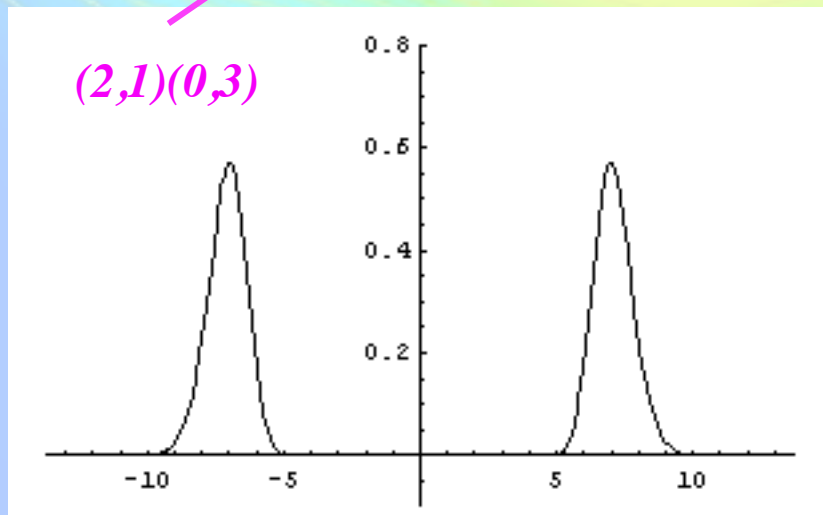
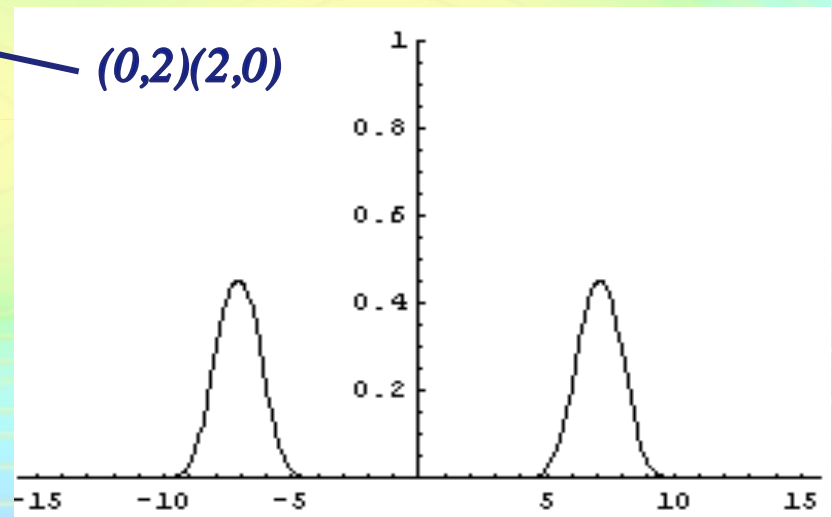
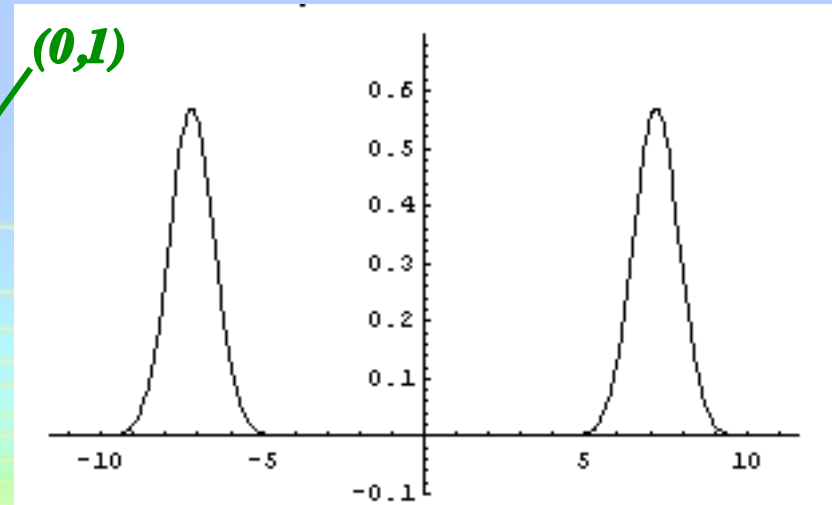
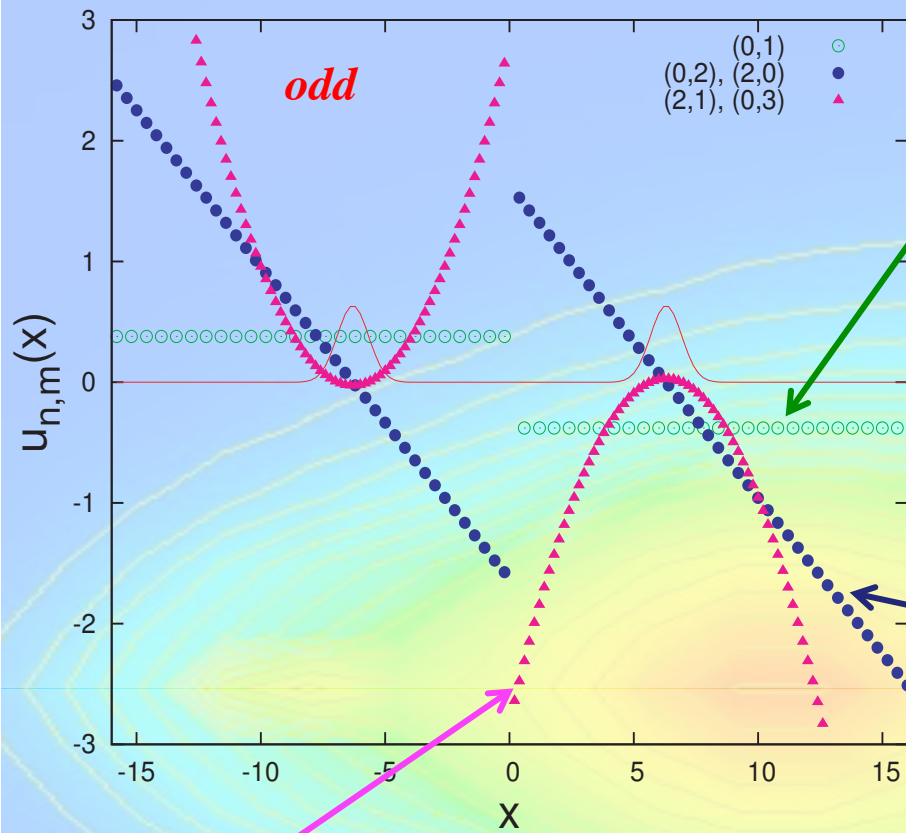
States with the same $n+m$ and the same parity of m have identical displacement fields. At the QCM level they collapse into a single mode with energy

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

$(k = n + m - 1)$







Quantum Continuum Mechanics and DFT

1. Replace the physical system by a non-interacting system subjected to the static Kohn-Sham potential $V_{KS0}(\mathbf{r})$.
2. Add to the external force the internally generated time-dependent Hartree+exchange-correlation forces

$$m\ddot{\mathbf{u}} = \mathbf{F}_s[\mathbf{u}] + \mathbf{F}_{Hxc}[\mathbf{u}] - \nabla V_1$$

3. Elastic approximation is applied only to the non-interacting kinetic response. Exchange-correlation forces can be retarded.

$$\mathbf{F}_s[\mathbf{u}] = -\frac{1}{n_0} \frac{\delta \langle \Psi_{0,s}[\mathbf{u}] | \hat{T} + \hat{V}_{KS,0} | \Psi_{0,s}[\mathbf{u}] \rangle_2}{\delta \mathbf{u}} \equiv -\frac{1}{n_0} \frac{\delta E_{s,2}[\mathbf{u}]}{\delta \mathbf{u}}$$

exchange-correlation
stress tensor

$$\mathbf{F}_{xc,i}(\mathbf{r}, \omega) = \underbrace{-\nabla_i V_{xc,0}(\mathbf{r}, \omega)}_{\text{Adiabatic LDA}} - \frac{1}{\underbrace{n_0(\mathbf{r})}_{\text{equilibrium density}}} \sum_j \frac{\overbrace{\partial \sigma_{xc,ij}(\mathbf{r}, \omega)}}{\partial r_j}$$

Kohn-Sham response in the elastic approximation: the Gould-Dobson approach

$$-\omega^2 n_0(\mathbf{r}) u_\mu(\mathbf{r}) = F_{s,\mu}(\mathbf{r}) = -\sum_\nu \hat{K}_{\mu\nu} u_\nu(\mathbf{r}) - \sum_\nu [\partial_\mu \partial_\nu V_{KS,0}(\mathbf{r})] u_\nu(\mathbf{r})$$



$\chi_{KS}(\mathbf{r}, \mathbf{r}', \omega)$
(Kohn-Sham response function)

Strong feature: Minimum excitation energy in elastic approximation $>$ Kohn-Sham HOMO-LUMO gap

From χ_{KS} , one calculates the RPA correlation energy as a functional of density. This is a sophisticated functional, which captures van der Waals forces between widely separated parts of the system.

Gould-Dobson approach – Energy of two parallel metallic slabs

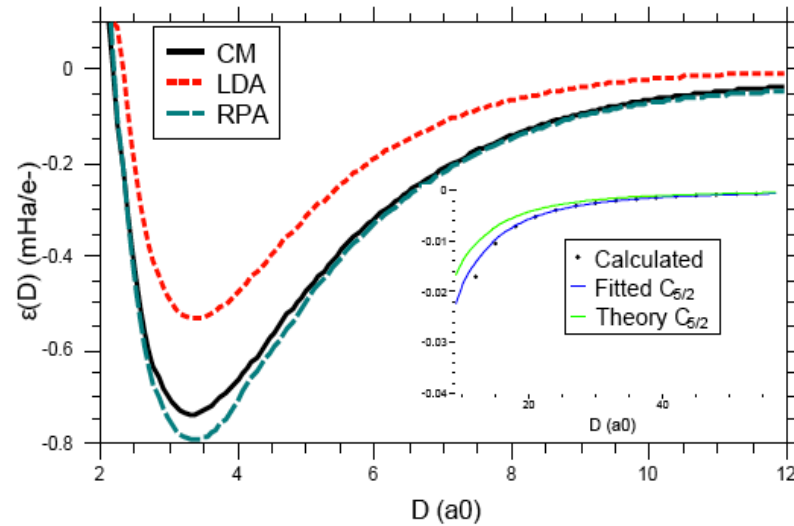


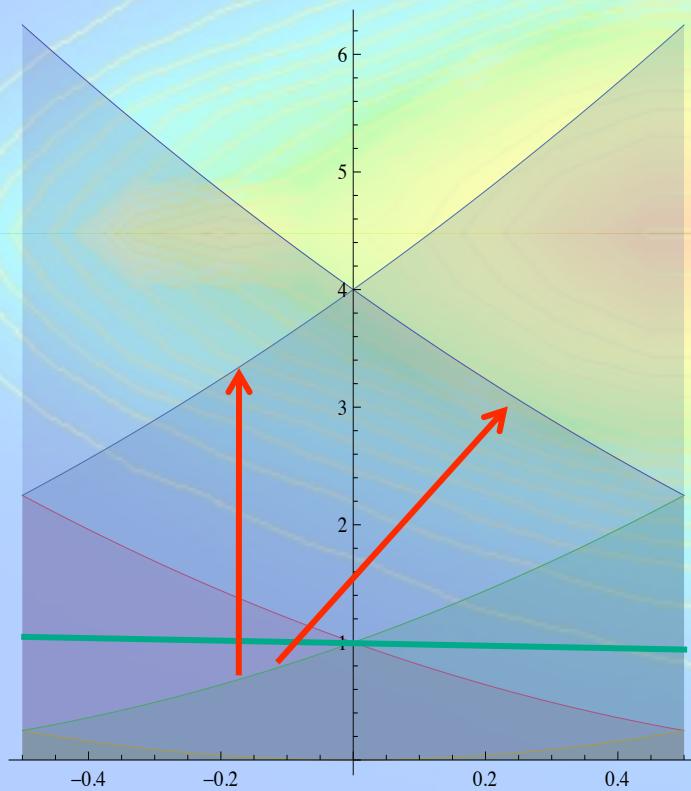
FIG. 1. $\bar{\epsilon}(D)$ graph for $r_s = 1.25$, $s = 3$. RPA data from [24]. Inset data shows the vdW dominated region.

	CM	LDA	dRPA	CM	LDA	dRPA
	$r_s = 1.25, s = 3$			$r_s = 2.07, s = 5$		
D_0	3.33	3.38	3.32‡	1.57	1.56	1.62±0.1§
ϵ_b	0.74	0.53	0.79‡	1.78	1.72	1.85±0.1§
C_{zz}	0.51	0.45	0.55‡	1.31	1.38	1.32±0.1§

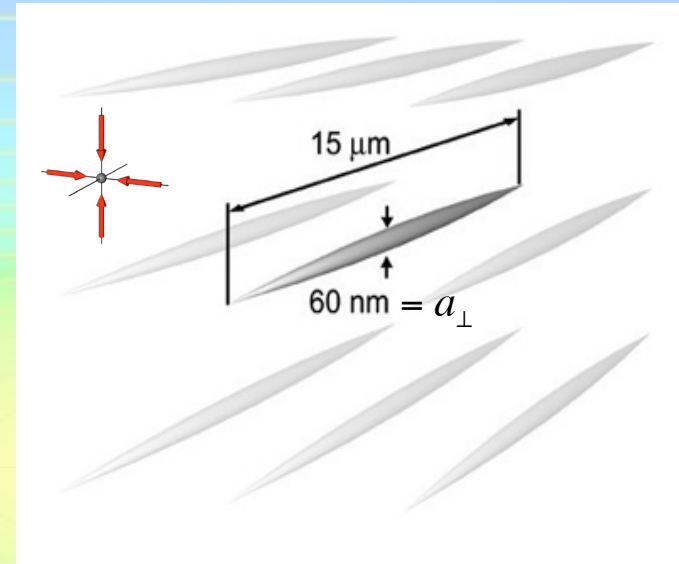
TABLE I. Groundstate properties of two slab systems under different approximations. Energies are in mHa/ e^- and distance are in Bohr radii. ‡ from Ref. 24, § is guessed from Refs. 20 and 23 taking into account estimated error bars.

Planned applications

Periodic system: Replace bands of single-particle excitations by bands of collective modes



Luttinger liquid in a harmonic trap



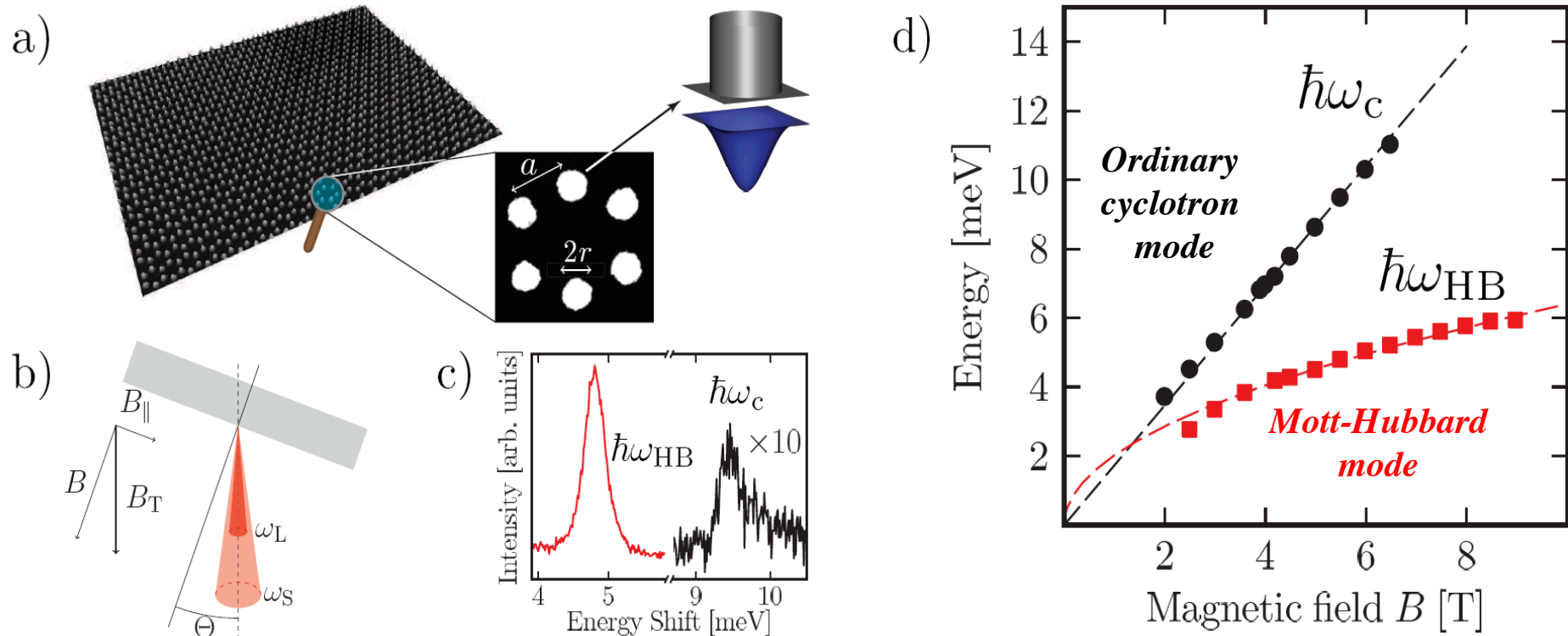
$$\hat{\mathcal{H}} = \sum_i \frac{\hat{p}_i^2}{2m} + g_{1D} \sum_{i<j} \delta(\hat{x}_i - \hat{x}_j) + \text{external potential}$$

$$g_{1D} = \frac{2\hbar^2 a_{3D}}{m a_{\perp}^2}$$

← 3D scattering length
 ← radius of tube

Two-dimensional Mott-Hubbard electrons in an artificial honeycomb lattice

A. Singha *et al.* Science **332**, 1176 (2011)



Generalization of QCM to systems in magnetic field:
Pittalis, Tokatly and Vignale, 2011

QCM in a Magnetic Field

S. Pittalis, G. V. and I. V. Tokatly, arXiv 1109.3644

- Current density does not vanish at equilibrium: $\mathbf{j}_0 \neq 0$.
- Elastic approximation formulated in a generalized co-moving frame in which $n = n_0$ and $\mathbf{j} = \mathbf{j}_0$ at all times
- Relation between current and displacement changes to

$$\mathbf{j} = \mathbf{j}_0 + n_0 \dot{\mathbf{u}} + \nabla \times (\mathbf{j}_0 \times \mathbf{u})$$

- Time derivative is replaced by convective derivative

$$D_t = \partial_t + \mathbf{v}_0 \cdot \nabla$$

- Lorentz force term+ subtle changes to the kinetic energy

$$D_t^2 \mathbf{u} + D_t \mathbf{u} \times \mathbf{B}_0 + (\mathbf{u} \cdot \nabla) \nabla V_0 + \mathbf{v}_0 \times (\mathbf{u} \cdot \nabla) \mathbf{B}_0 = n_0^{-1} \mathbf{F}_{el} - \nabla V_1$$

Conclusions and speculations I

1. Quantum Continuum Mechanics in the elastic approximation is a direct extension of the collective approximation for the homogeneous electron gas to inhomogeneous quantum systems. We expect it to be useful for
 - Theory of dispersive Van derWaals forces, especially in complex geometries (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

2. 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)]

$$E_{xc}[\mathbf{u}] = \frac{1}{2} \int d\mathbf{r} \left\{ T_{\mu\nu}^{xc} \left[4u_{\mu\alpha} u_{\nu\alpha} - \partial_{\mu} u_{\alpha} \partial_{\nu} u_{\alpha} \right] - n_0 u_{\mu} u_{\nu} \partial_{\mu} \partial_{\nu} V_{xc} \right\} \\ + \frac{1}{4} \int d\mathbf{r} \int d\mathbf{r}' \left[u_{\mu}(\mathbf{r}) - u_{\nu}(\mathbf{r}) \right] K_{\mu\nu}(\mathbf{r}, \mathbf{r}') \left[u_{\mu}(\mathbf{r}') - u_{\nu}(\mathbf{r}') \right]$$

$$T_{\mu\nu}^{xc}(\mathbf{r}) = \frac{1}{2m} \left(\partial_{\mu} \partial'_{\nu} + \partial'_{\mu} \partial_{\nu} \right) \left[\rho_1(\mathbf{r}, \mathbf{r}') - \rho_{1,s}(\mathbf{r}, \mathbf{r}') \right]_{\mathbf{r}=\mathbf{r}'}$$

$$K_{\mu\nu}^{xc}(\mathbf{r}, \mathbf{r}') = n_0(\mathbf{r}) n_0(\mathbf{r}') \left[g(\mathbf{r}, \mathbf{r}') - 1 \right] \partial_{\mu} \partial_{\nu} V_C(|\mathbf{r} - \mathbf{r}'|)$$

3. Time-dependent DFT offers a natural way to improve upon the elastic approximation