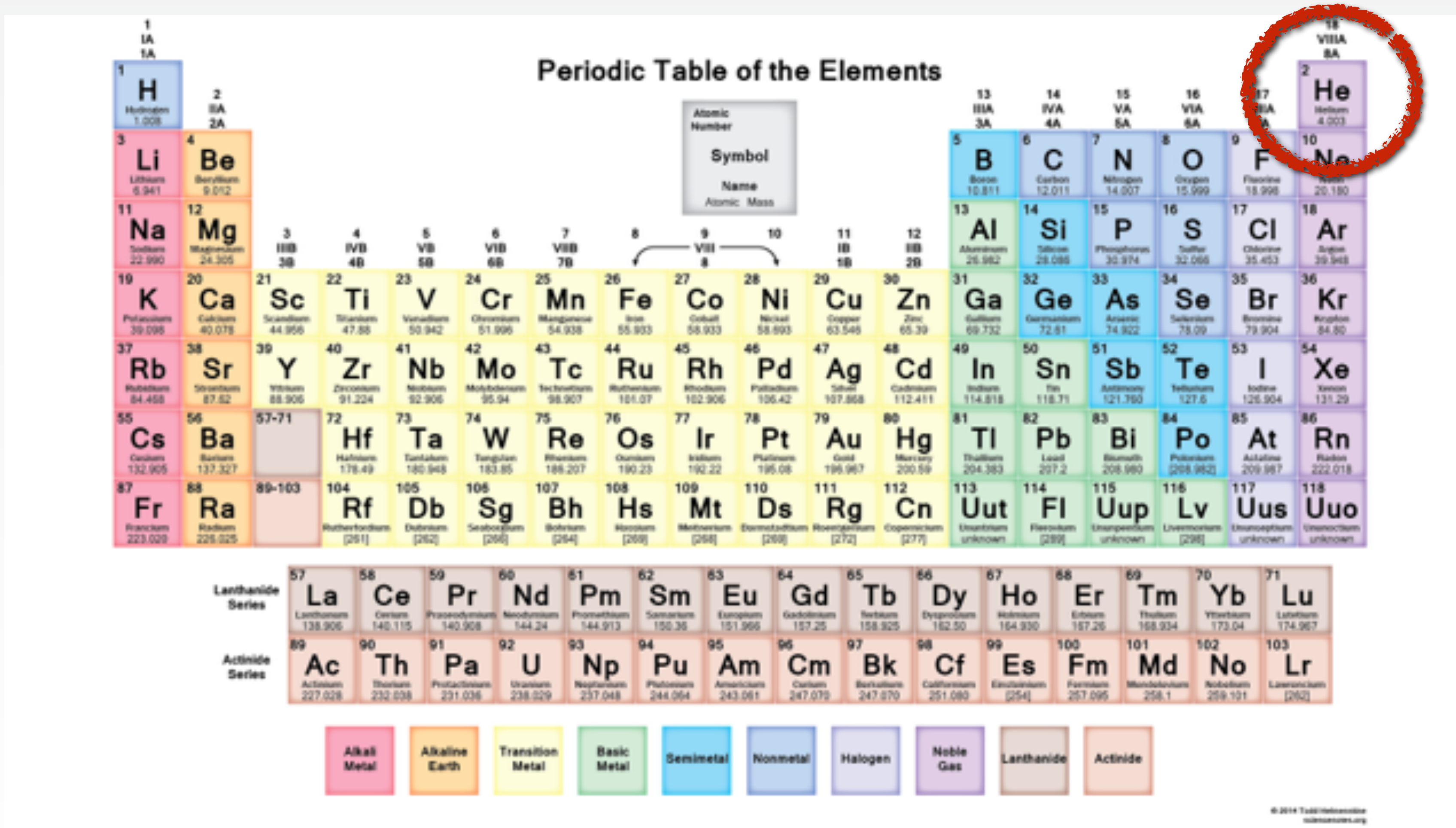
Excitations of a quantum solid

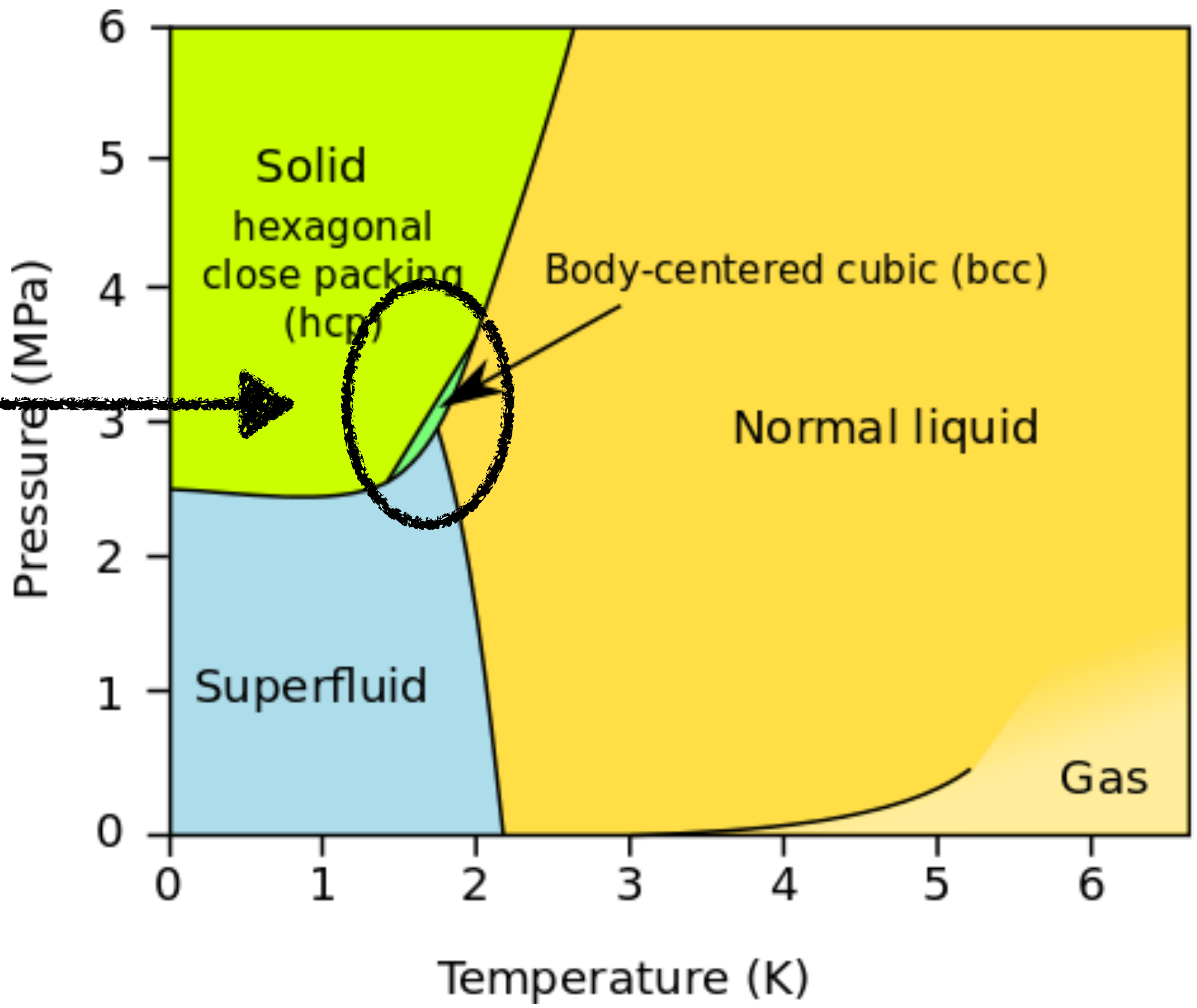
Daniel Podolsky



Collaborators: S. Gazit, H. Nonne, A. Auerbach, D. Arovas

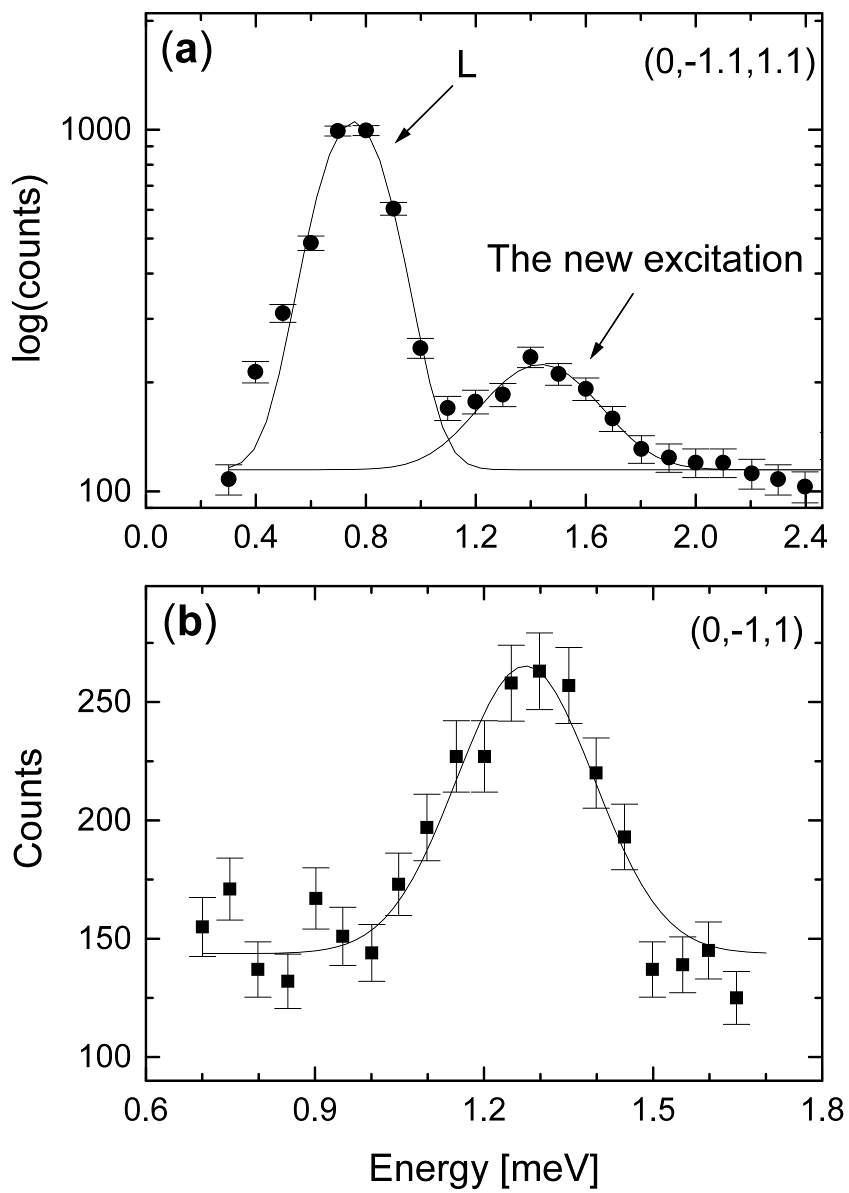
Technion
Israel Institute of Technology

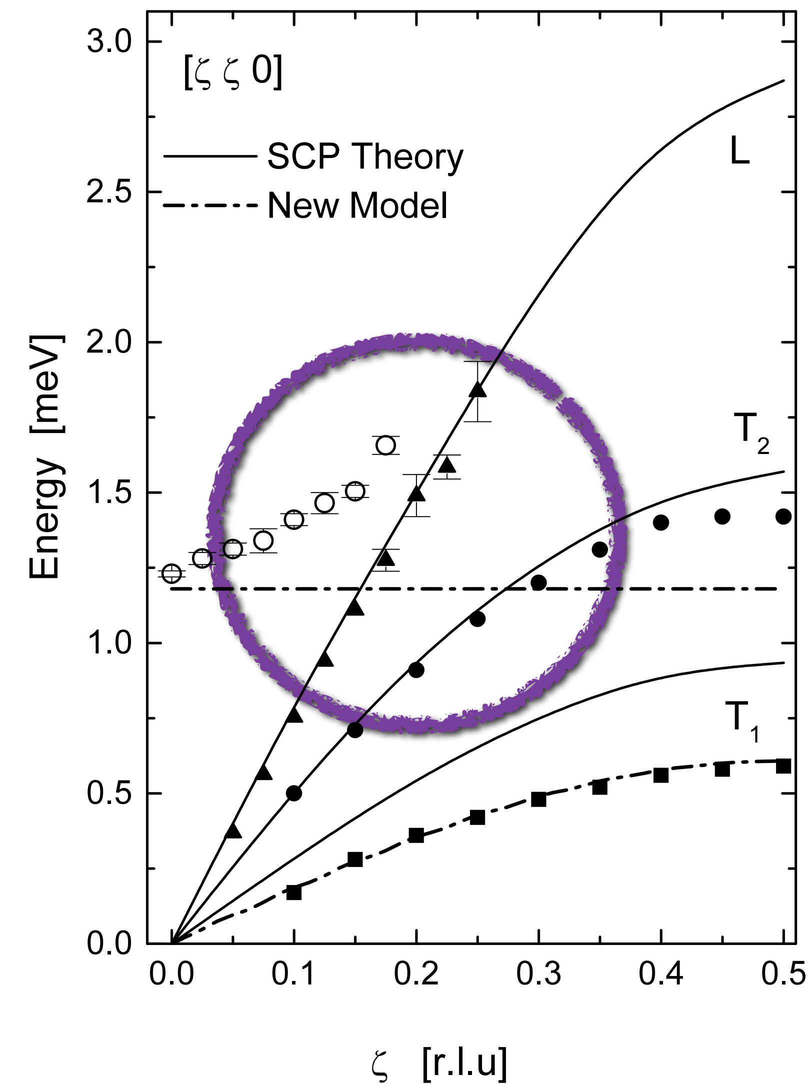
Helium 4 - Phase diagram



Inelastic neutron scattering

Optical mode observed!

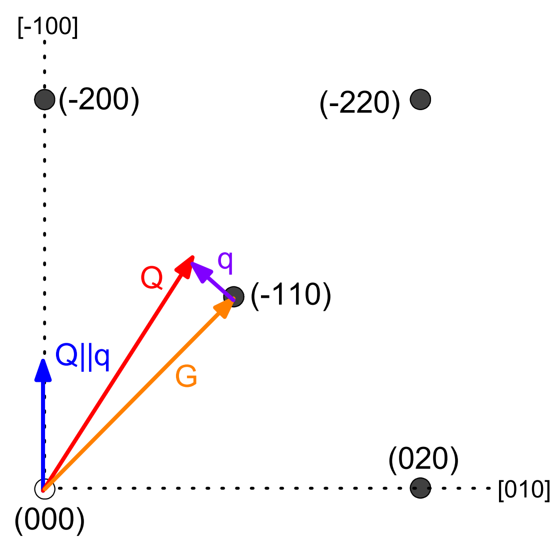




Markovic et al., PRL **88**, 195301 ('02)

Multiple optical modes?

Look at different directions and polarizations



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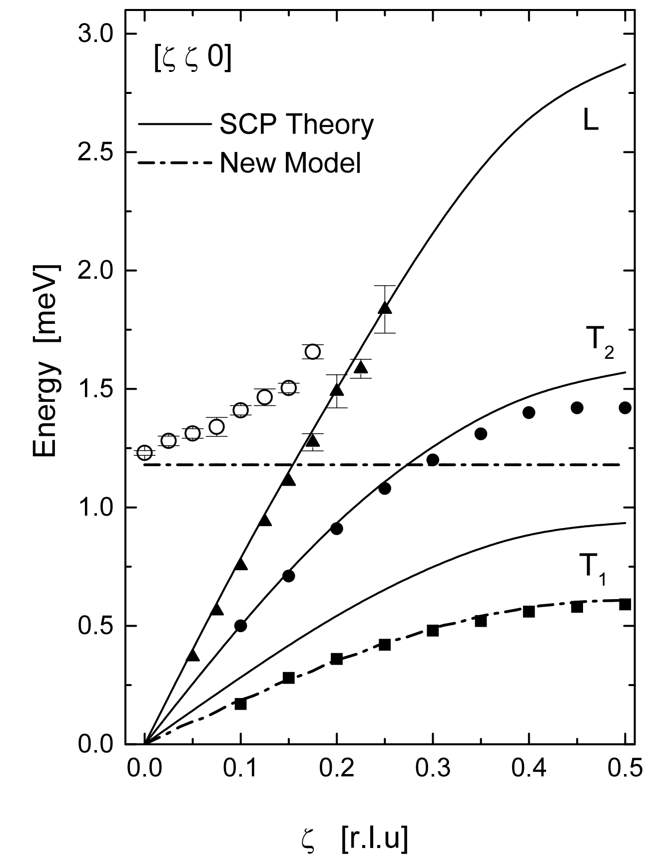
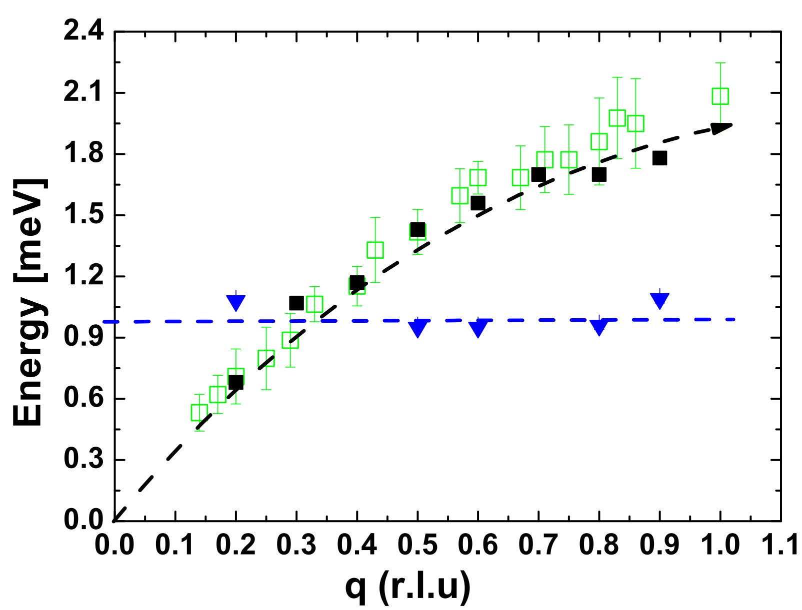


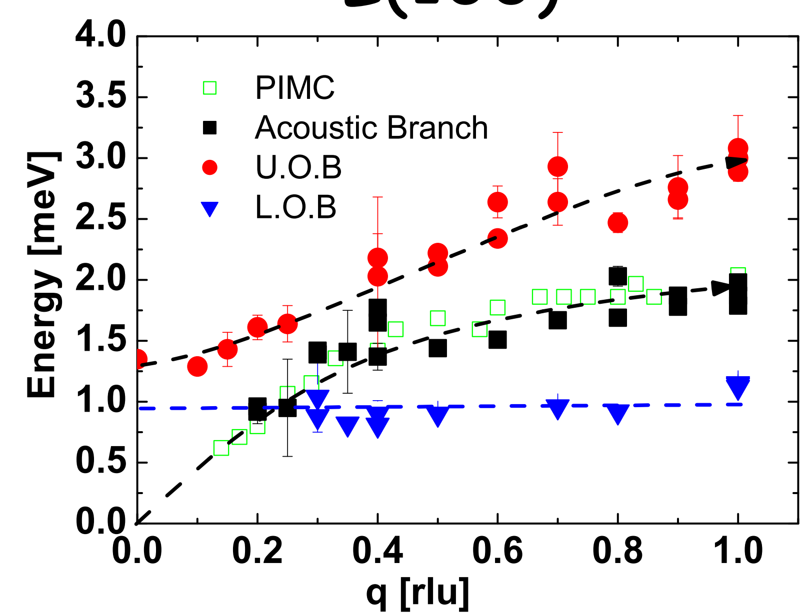
Markovic et al., PRL **88**, 195301 ('02)

T(100)



Pelleg et al, PRB **73**, 180301R ('06)

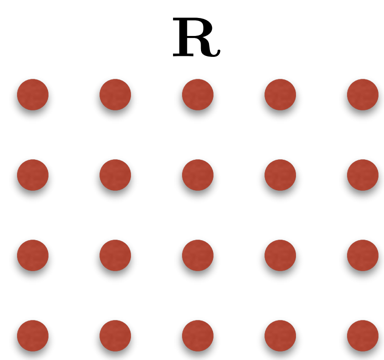
L(100)



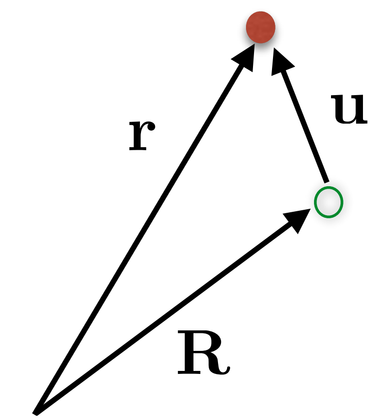
Pelleg et al., JLTP **151**, 1164 ('08)

Harmonic theory of solids

Equilibrium:



Fluctuations:



$$\mathbf{r}(\mathbf{R}) = \mathbf{R} + \mathbf{u}(\mathbf{R})$$

Small fluctuations $\quad \sqrt{\langle \mathbf{u}^2 \rangle} \ll \Delta R$

$$U_{\rm harm} = \frac{1}{2} \sum_{\mathbf{R}\mathbf{R}'} \sum_{\mu\nu} u_\mu(\mathbf{R}) D_{\mu\nu}(\mathbf{R} - \mathbf{R}') u_\nu(\mathbf{R}')$$

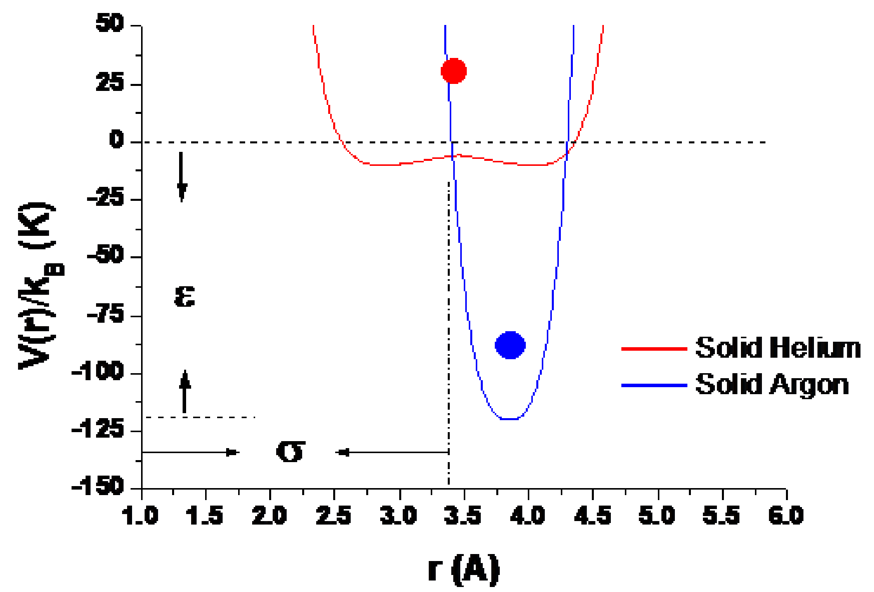
Monatomic Bravais lattice ⇨ acoustic phonons only

Corrections to harmonic theory: $\quad U_{\rm anh} \sim u^3 + u^4 + \ldots$

Lindemann criterion: $\quad \sqrt{\langle \mathbf{u}^2 \rangle} = 0.1\, \Delta R \quad$ ⇨ melting

Helium – A quantum solid

Atoms do not sit at minimum of V:



Large zero point motion:

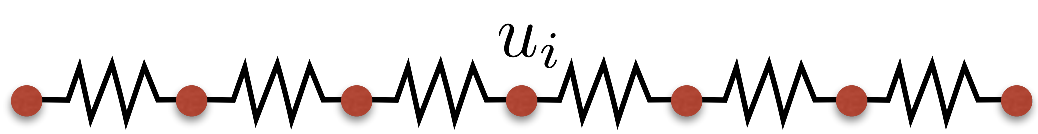
H. Glyde, "Helium, Solid"

Rare-gas crystal	Debye temperature θ_D (K)	Melting temperature T_M(K)	Debye zero point energy $E_{ZD} = \frac{9}{8}\theta_D$	Lindemann parameter $\delta = \langle u^2 \rangle^{1/2}/R$
^{3}He(bcc)	19	0.65	21	0.368
^{4}He(bcc)	25	1.6	28	0.292
Ne	66	24.6	74	0.091
Ar	84	83.8	95	0.048
Kr	64	161.4	72	0.036
Xe	55	202.0	62	0.028

Harmonic theory does not give correct acoustic phonon velocities

Large quantum fluctuations

⇨ restoring force is non-linear



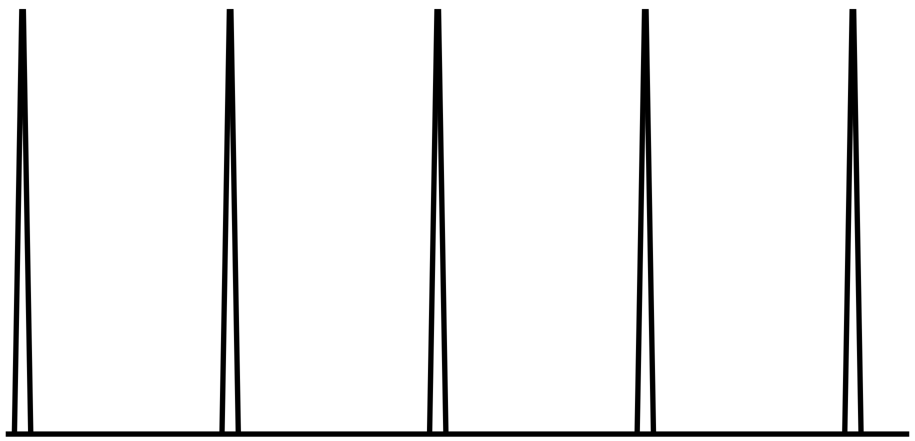
$$m\ddot{u}_i = -\kappa(u_i - u_{i+1}) - \kappa(u_i - u_{i-1}) + \gamma(u_i - u_{i+1})^2 + \gamma(u_i - u_{i-1})^2 + \cdots$$

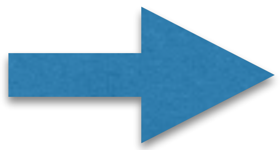
⇨ Non-linear equations can in principle give multiple solutions (more phonons than number of degrees of freedom)

⇨ How to construct a linear theory for optical modes?

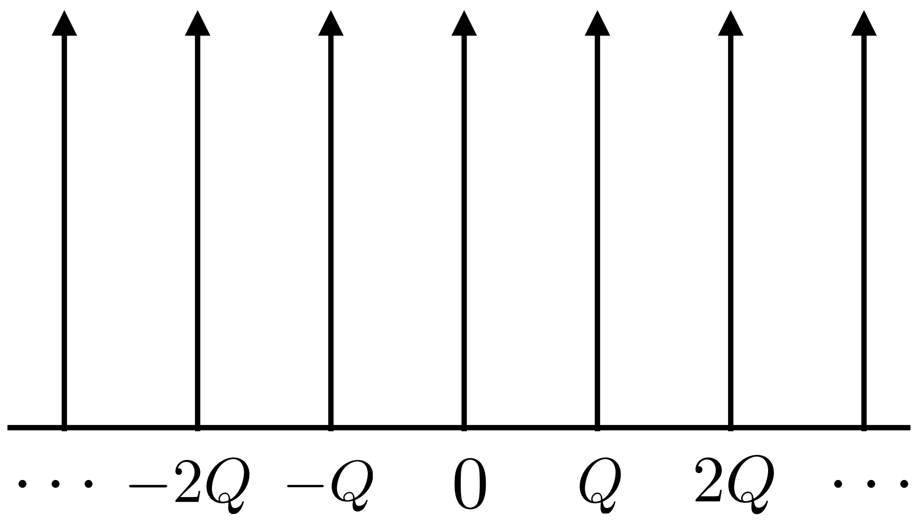
A different point of view

Idealized crystal:



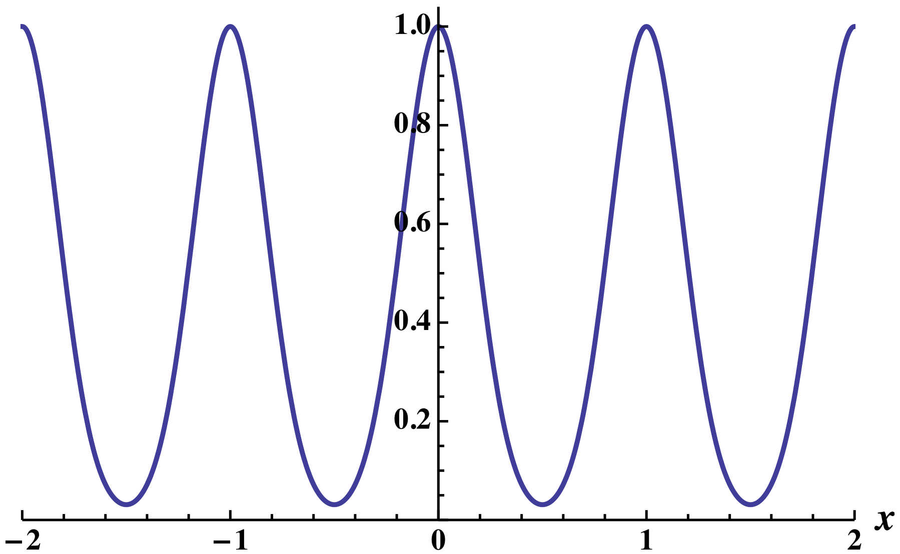


Bragg peaks:



A different point of view

Helium:



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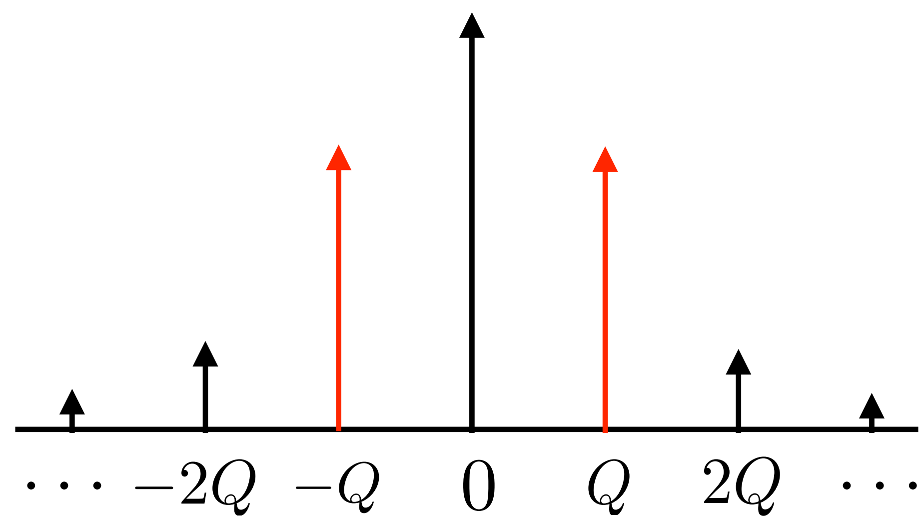
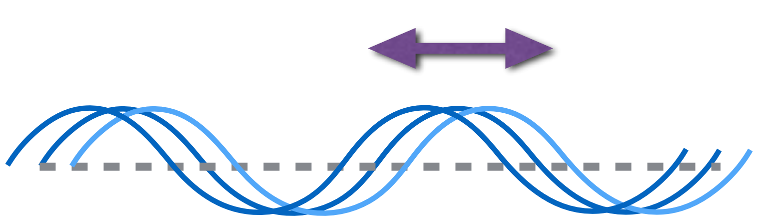


Focus on dynamics of principal Bragg vectors

Can we think of solid He-4 as a charge density wave (CDW)?

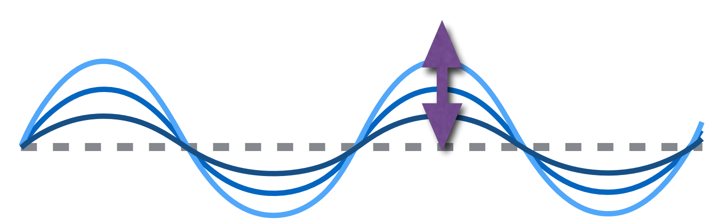
A CDW allows naturally for gapped modes:

"phason"



$$\omega \sim cq$$

"amplitudon"



$$\omega \sim \sqrt{m^2 + c^2 q^2}$$

Ginzburg-Landau theory for 3D CDW

Density modulation: $\rho(\mathbf{r}) = n(\mathbf{r}) - n_0$

Assume order parameter is small (large fluctuations):

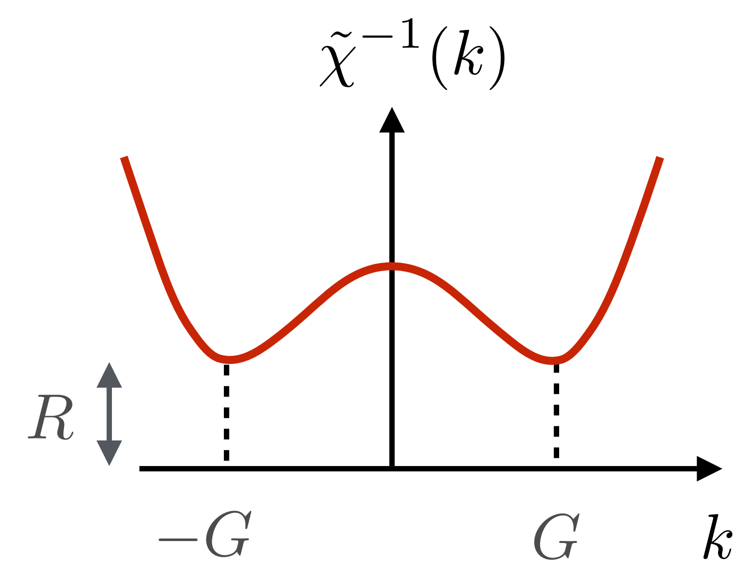
$$F_{\mathrm{GL}} = \frac{1}{2}\int d\mathbf{r}_1 d\mathbf{r}_2\, \rho(\mathbf{r}_1)\chi^{-1}(\mathbf{r}_1 - \mathbf{r}_2)\rho(\mathbf{r}_2) - B\int d\mathbf{r}\, \rho(\mathbf{r})^3 + C\int d\mathbf{r}\, \rho(\mathbf{r})^4$$

In Fourier space:

$$F_{\mathrm{GL}} = \frac{1}{2}\int d\mathbf{k}\, \frac{1}{\tilde{\chi}(\mathbf{k})}\left|\rho(\mathbf{k})\right|^2 - B\int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3\, \rho(\mathbf{k}_1)\rho(\mathbf{k}_2)\rho(\mathbf{k}_3)\delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3)$$
$$+ C\int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3 d\mathbf{k}_4 \rho(\mathbf{k}_1)\rho(\mathbf{k}_2)\rho(\mathbf{k}_3)\rho(\mathbf{k}_4))\delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4)$$

Static susceptibility:

$$\tilde{\chi}^{-1}(\mathbf{k}) = R + a\,(\mathbf{k}^2 - G^2)^2$$



"Should all crystals be BCC?"

Alexander and McTague, PRL **41**, 702 (1978)

Baym, Bethe, and Pethick, Nuc. Phys. A**175**, 225 (1971)

Minimize F_{GL}, order by order:

$$F_{\rm GL} = \frac{1}{2}\int d\mathbf{k}\,\frac{1}{\tilde{\chi}(\mathbf{k})}\,|\rho(\mathbf{k})|^2 - B\int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3\,\rho(\mathbf{k}_1)\rho(\mathbf{k}_2)\rho(\mathbf{k}_3)\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3)$$
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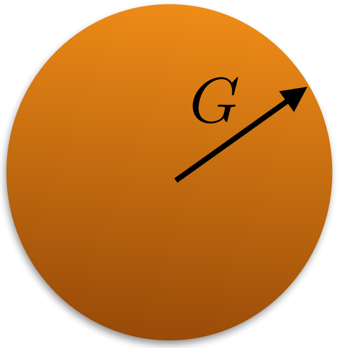
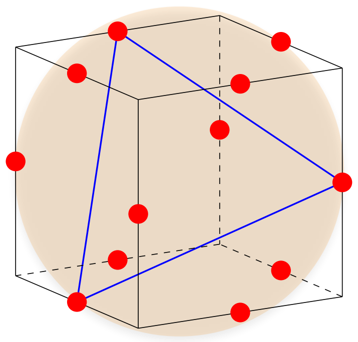
1. "Condense" on sphere k=G

$\rho(\mathbf{k}) \neq 0 \qquad |\mathbf{k}| = G$



2. Maximize number of triangles with zero total momentum



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$$+\,C\int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3 d\mathbf{k}_4 \rho(\mathbf{k}_1)\rho(\mathbf{k}_2)\rho(\mathbf{k}_3)\rho(\mathbf{k}_4))\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4)$$

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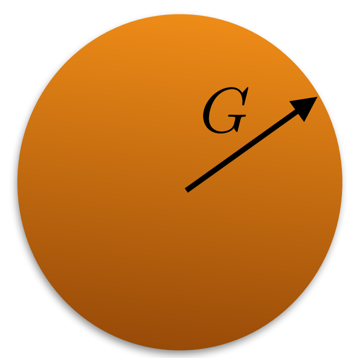

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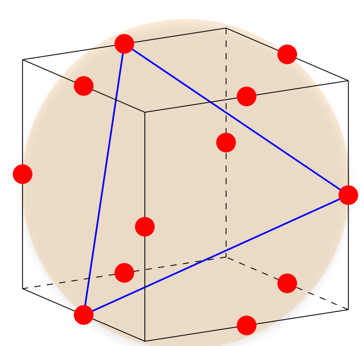
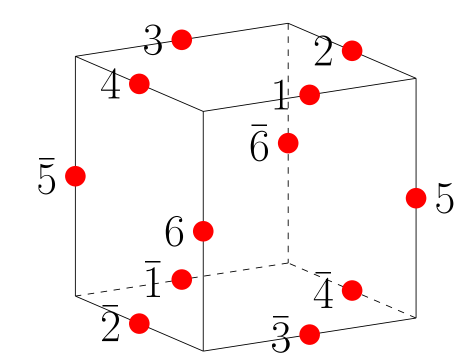


BCC wins:



Collective modes

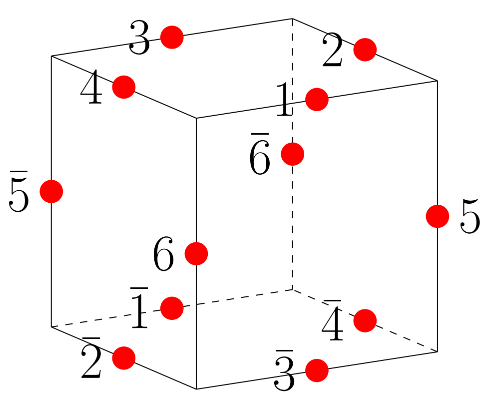
Dynamical Ginzburg-Landau:

$$L = \frac{1}{2}\int d^3r \left(\frac{\partial \rho}{\partial t}\right)^2 - F_{\mathrm{GL}}$$

Fluctuations about mean-field:

$$\rho(\mathbf{r},t) = \sum_i (\bar{\rho}_i + \psi_i(\mathbf{r},t)) e^{i\mathbf{G}_i\cdot\mathbf{r}}$$

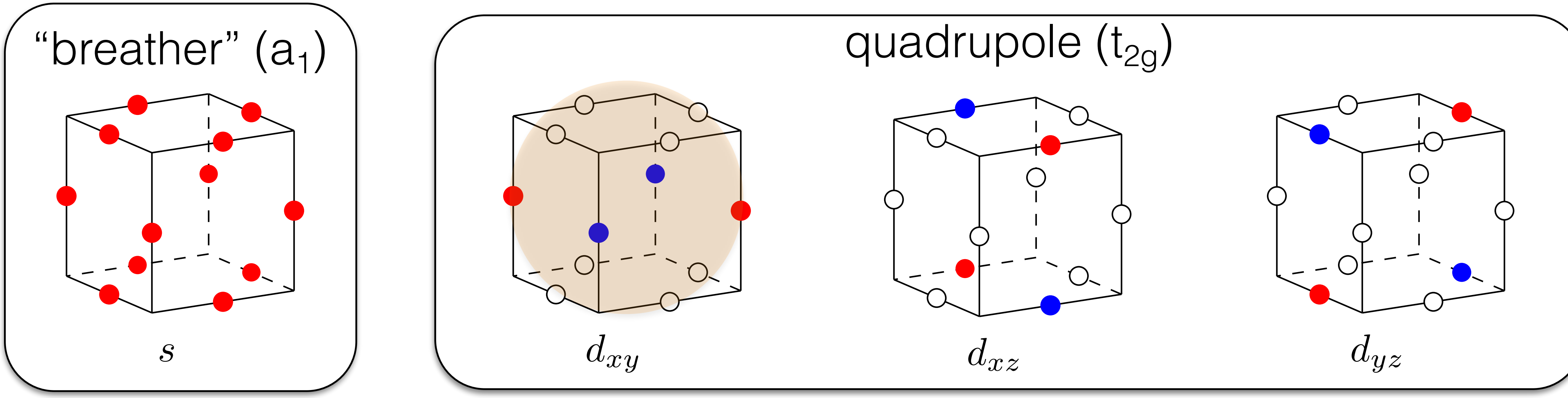
$$\psi_i(\mathbf{r},t) = \psi^*_{-i}(\mathbf{r},t)$$

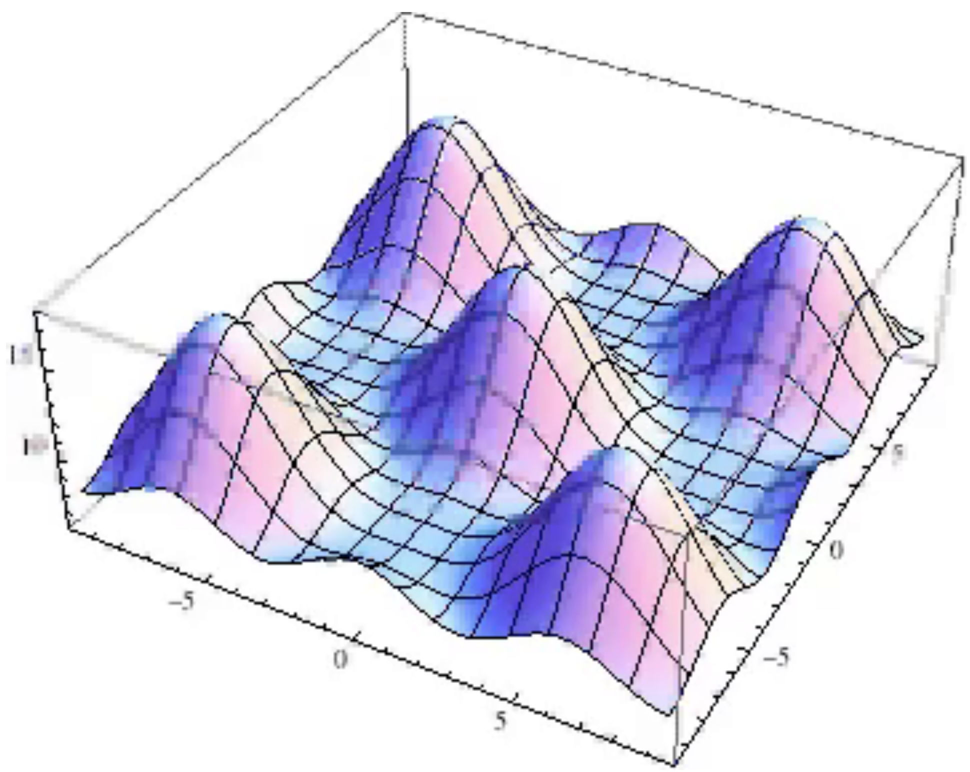


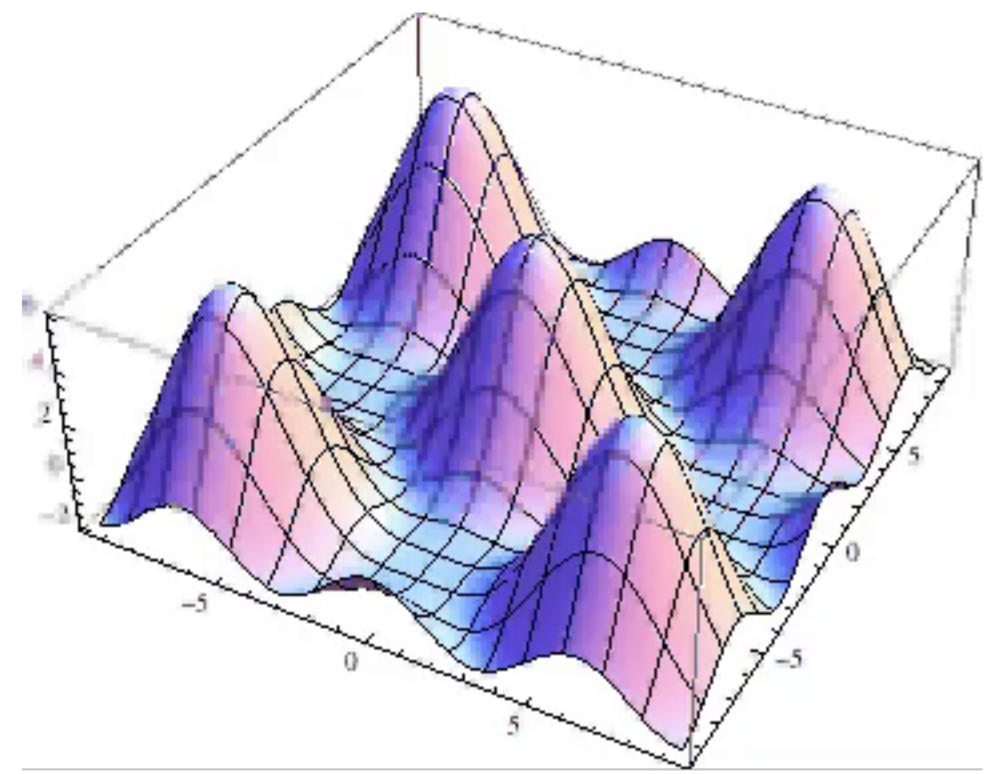
Linearize Euler-Lagrange equations

6 pairs of reciprocal lattice vectors ⇨ 12 modes

Visualizing the optical modes



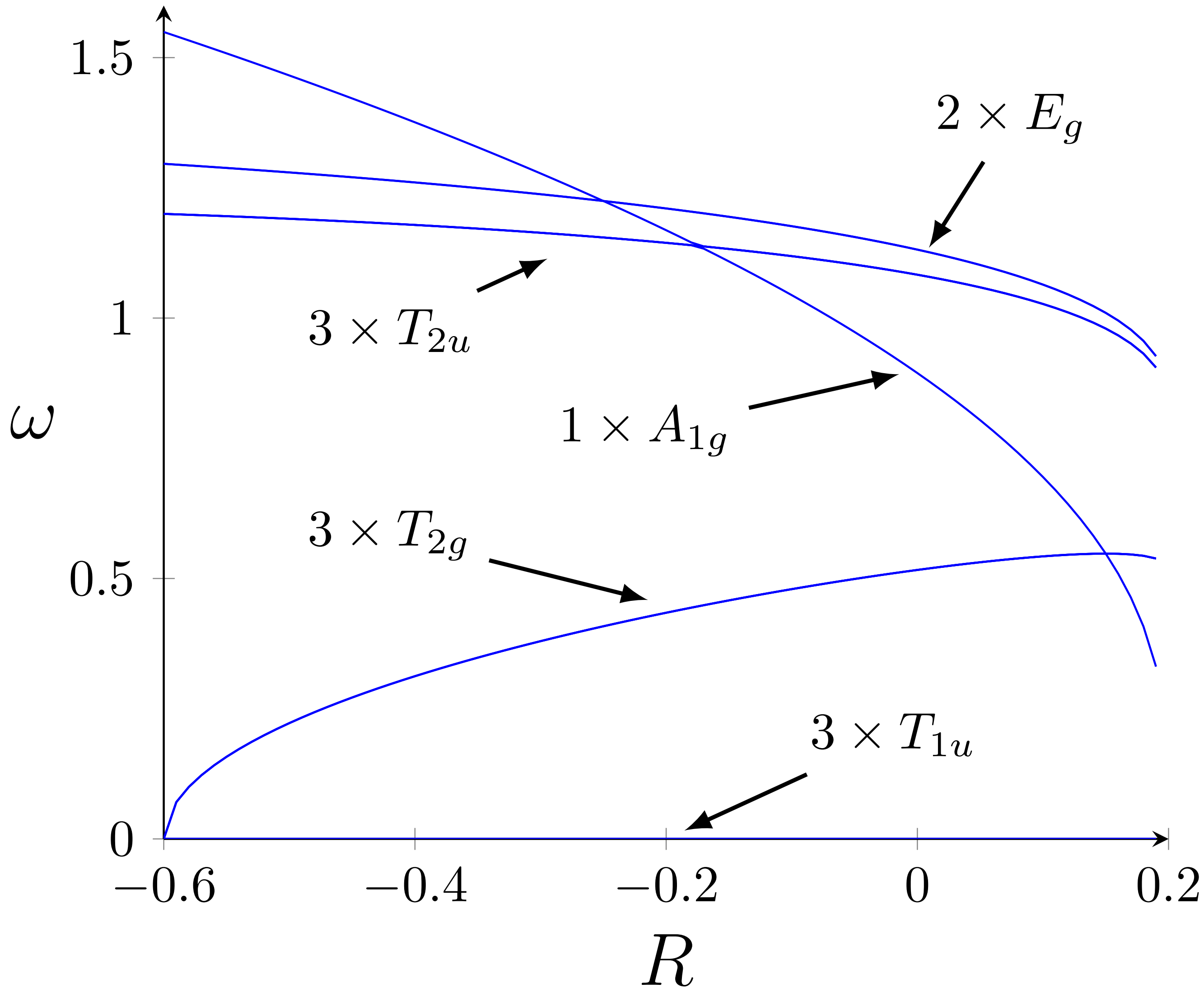




d_{xy} "quadrupolon" has vanishing z-axis spring constant ⇨ flat band

Which gapped mode is lowest?

Breather or quadruplon, depends on GL parameters:



Neutron scattering

Dynamical structure factor: $S(\mathbf{q},\omega) = \mathrm{Im}\left\{\langle \delta\rho_{\mathbf{G}}(\mathbf{q},\omega)\delta\rho_{-\mathbf{G}}(-\mathbf{q},-\omega)\rangle\right\}$

Compute by quantizing Ginzburg-Landau action. Result:

$$S(\mathbf{G}+\mathbf{q},\omega) = \sum_{\alpha} \frac{M_{\mathbf{G},\alpha}(\mathbf{q})}{2\omega_\alpha(\mathbf{q})}\left[(1+n_B(\omega_\alpha))\delta\left(\omega-\omega_\alpha(\mathbf{q})\right) - n_B(\omega_\alpha)\delta\left(\omega+\omega_\alpha(\mathbf{q})\right)\right]$$

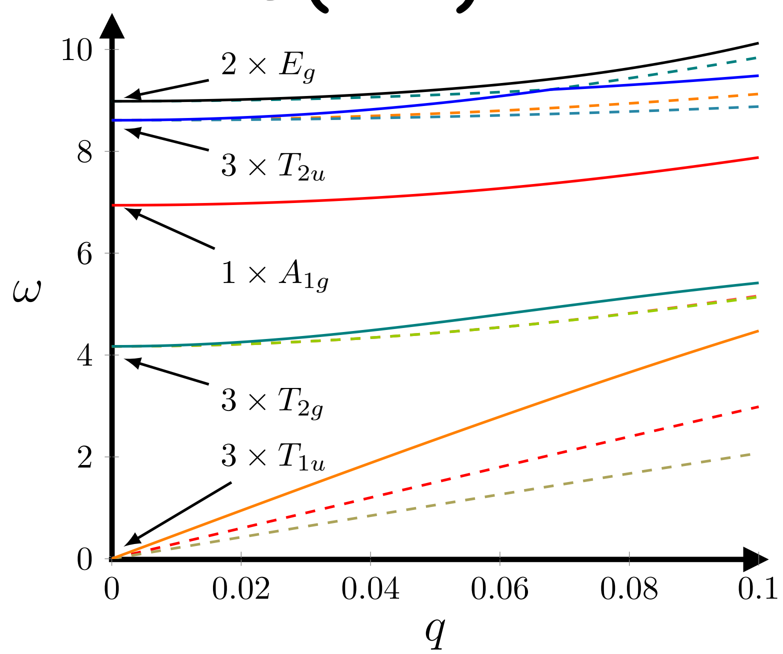
Note — sum rule is satisfied:

$$\int_{-\infty}^{\infty} d\omega\, \omega\, S(\mathbf{G}+\mathbf{q},\omega) = 1$$

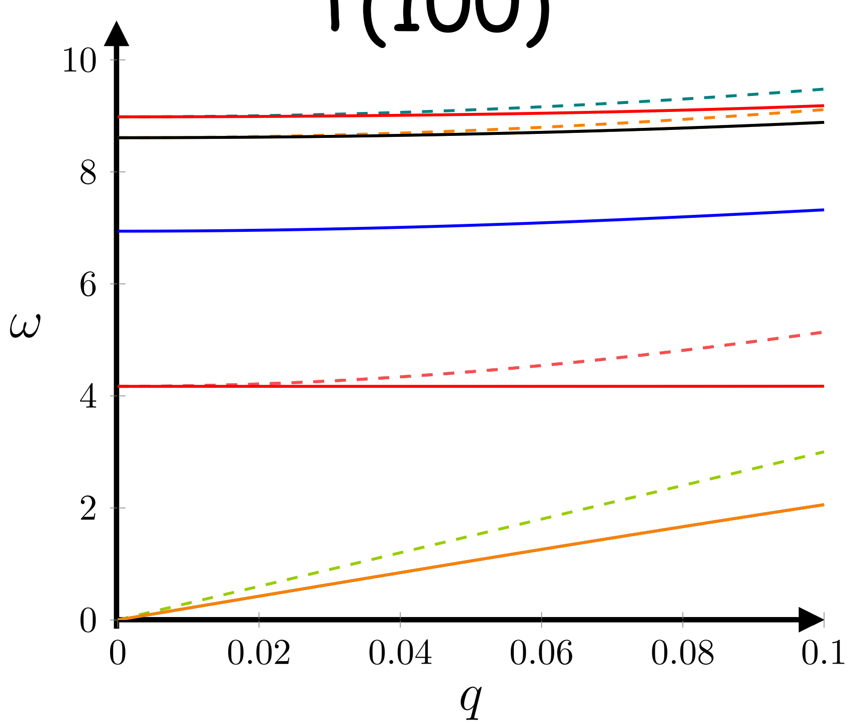
Hence, despite having more phonons than predicted by harmonic theory, the overall spectral weight remains the same. We have not introduced spurious degrees of freedom.

Comparison to experiment

L(110)



T(100)



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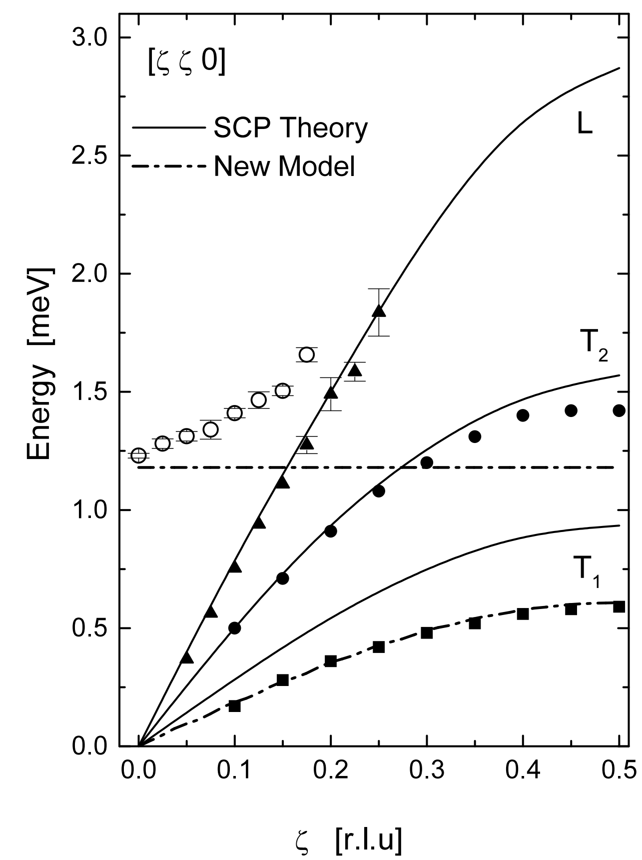

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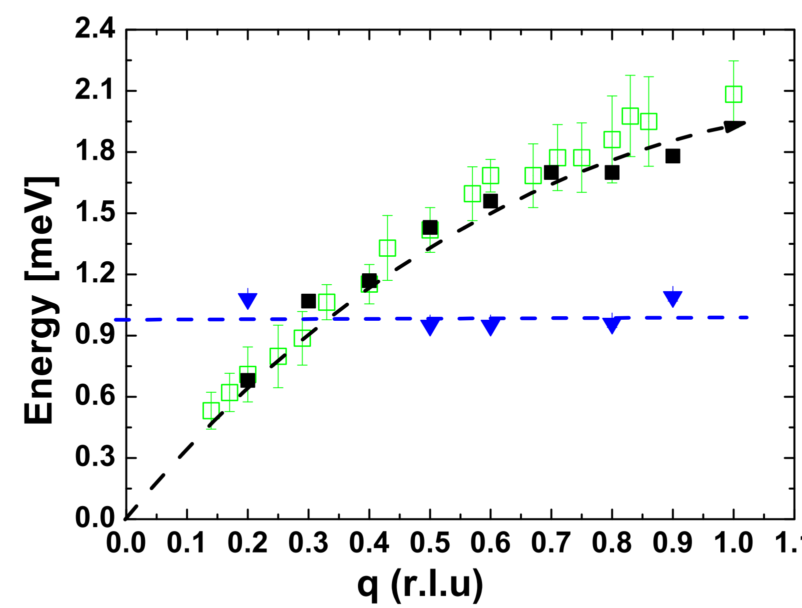
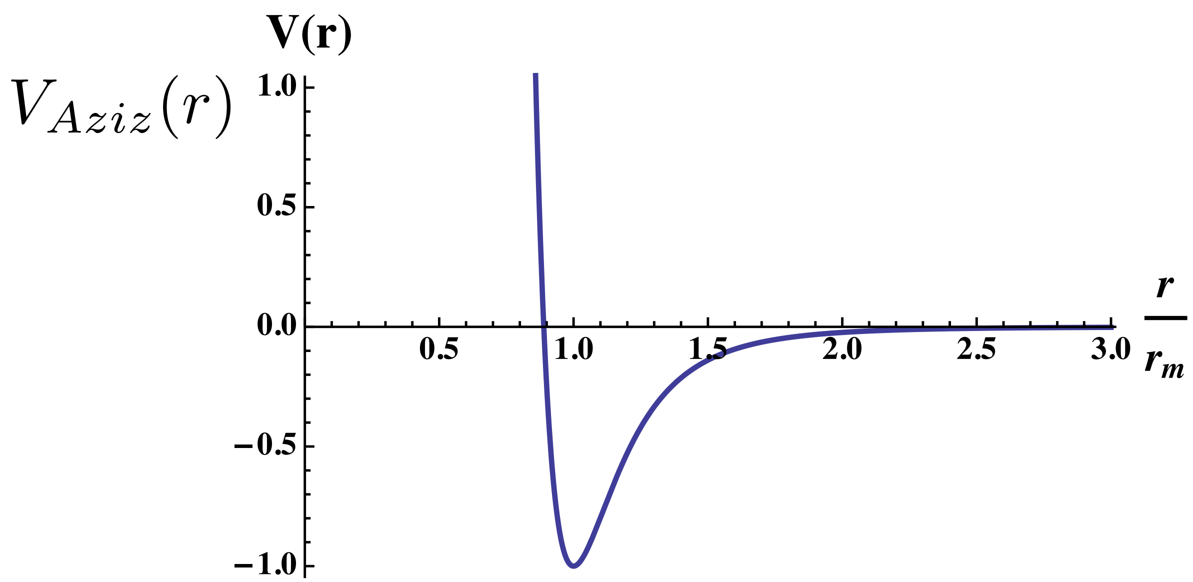


Pelleg et al, PRB **73**, 180301R ('06)

Quantum Monte Carlo

AB-initio simulations



$$H = -\frac{1}{2m}\sum_{i=i}^{N}\nabla_i^2 + \sum_{i<j} V_{Aziz}(r_i - r_j)$$

$$n_0 = 0.02854\,\mathring{A}^{-3}$$

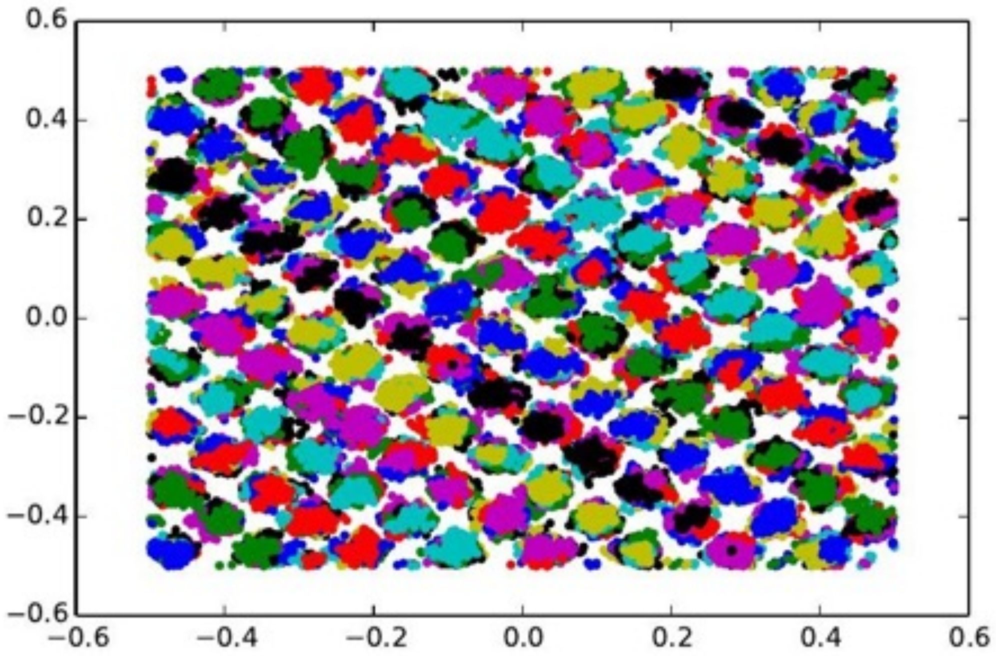
$$T = 1.6\,K$$

Place 2000 atoms in a box with periodic BC

Simulate using continuous space path integral QMC

Quantum Monte Carlo

2000 He4 Atoms



BCC phase

large zero point motion

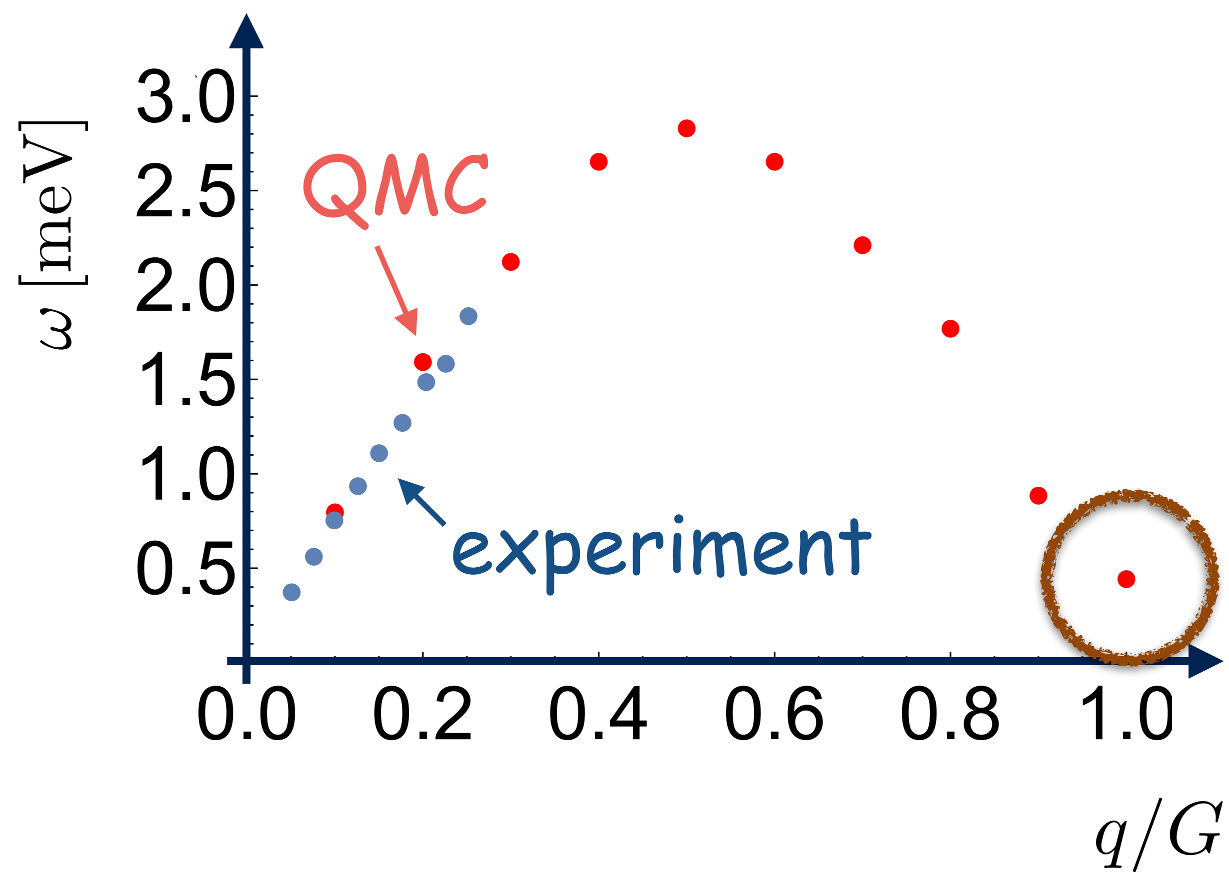
Structure factor:

$$S(\mathbf{q},\omega) = \langle \rho(\mathbf{q},\omega)\rho(-\mathbf{q},-\omega)\rangle \qquad \rho(\mathbf{q},t) = \sum_n e^{i\mathbf{q}\cdot\mathbf{r}_n(t)}$$

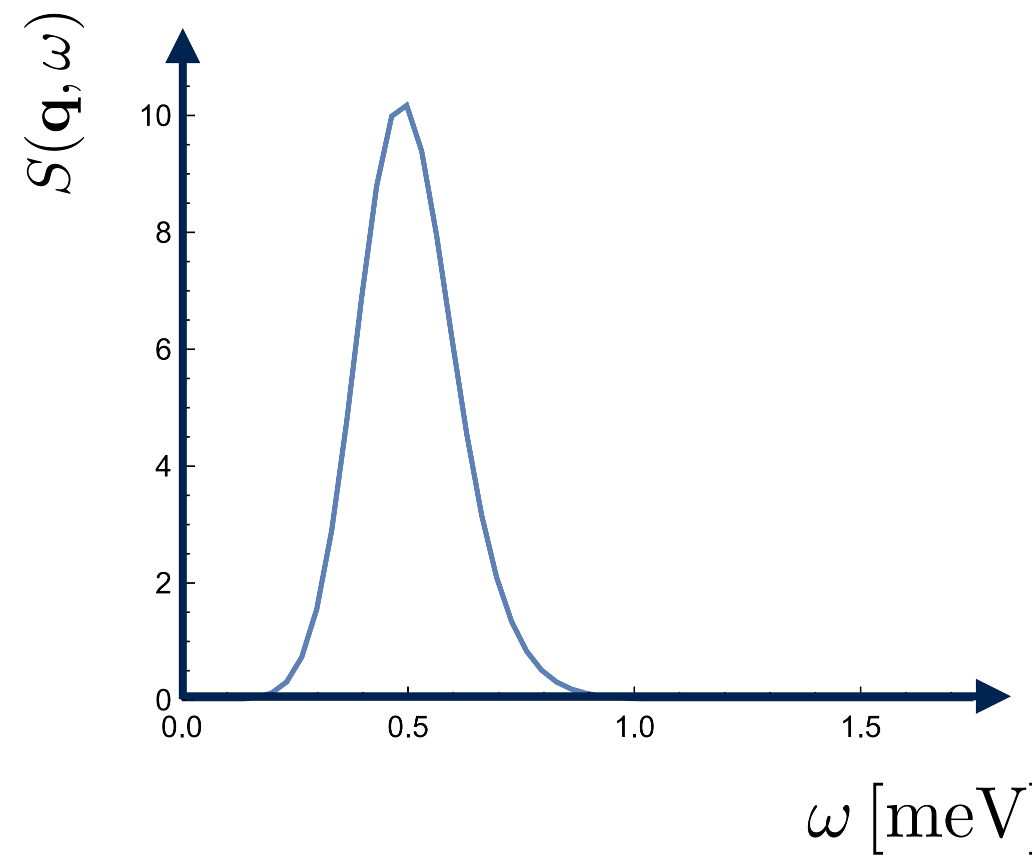
QMC simulations are performed along the imaginary time axis, perform numerical analytical continuation to real time.

QMC results

L(110) dispersion



At Bragg vector:



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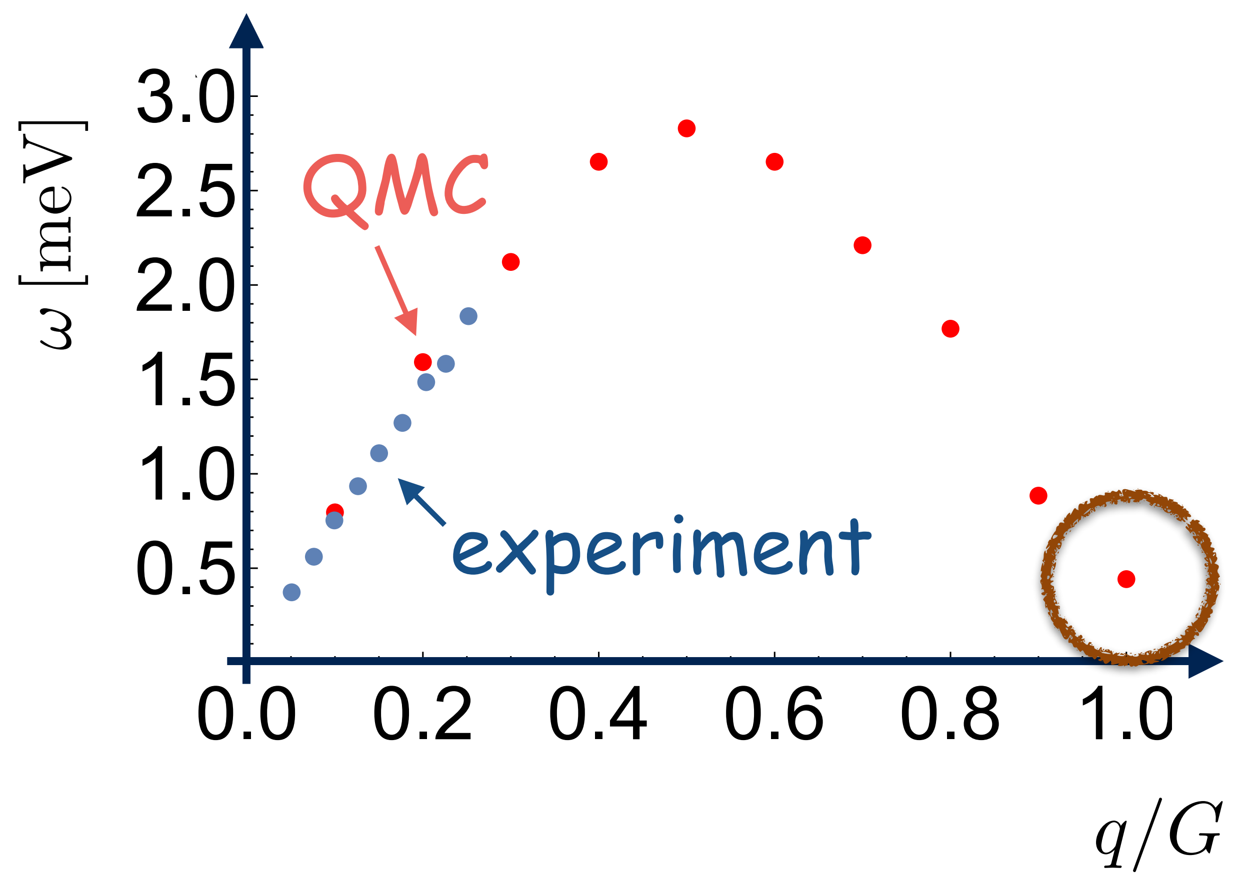

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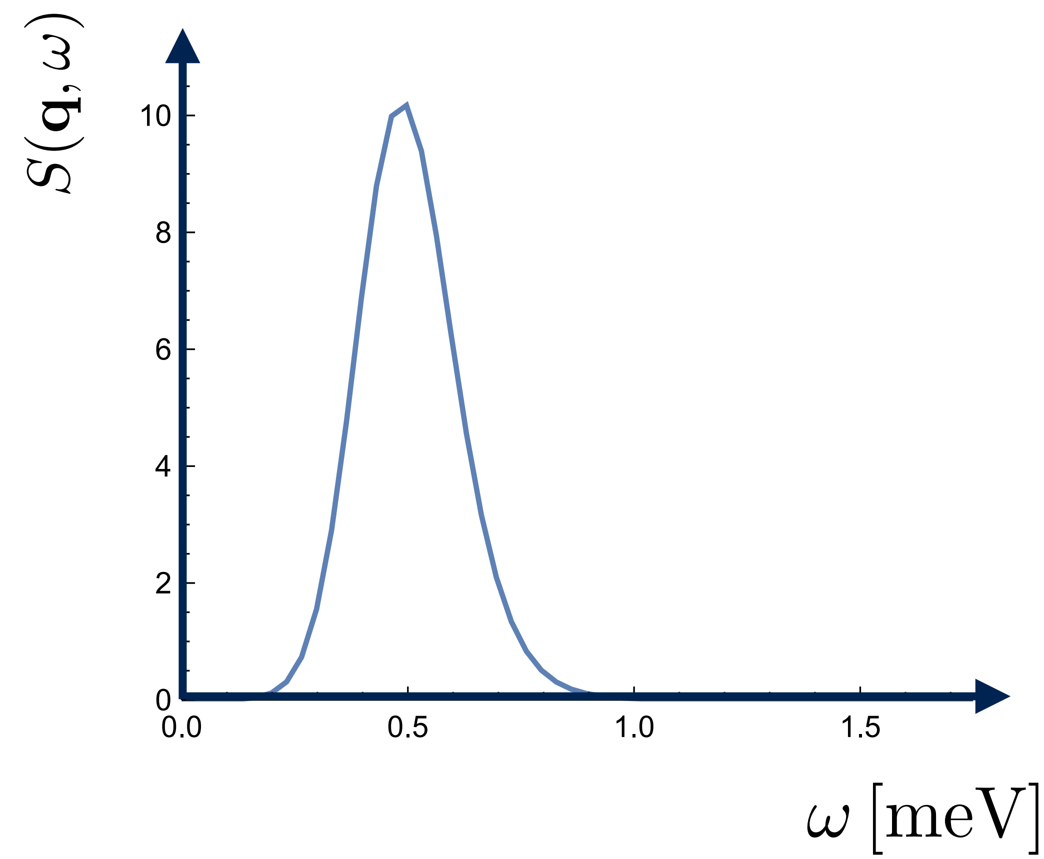

Confirms presence of optical mode (e.g. not due to crystal domains).

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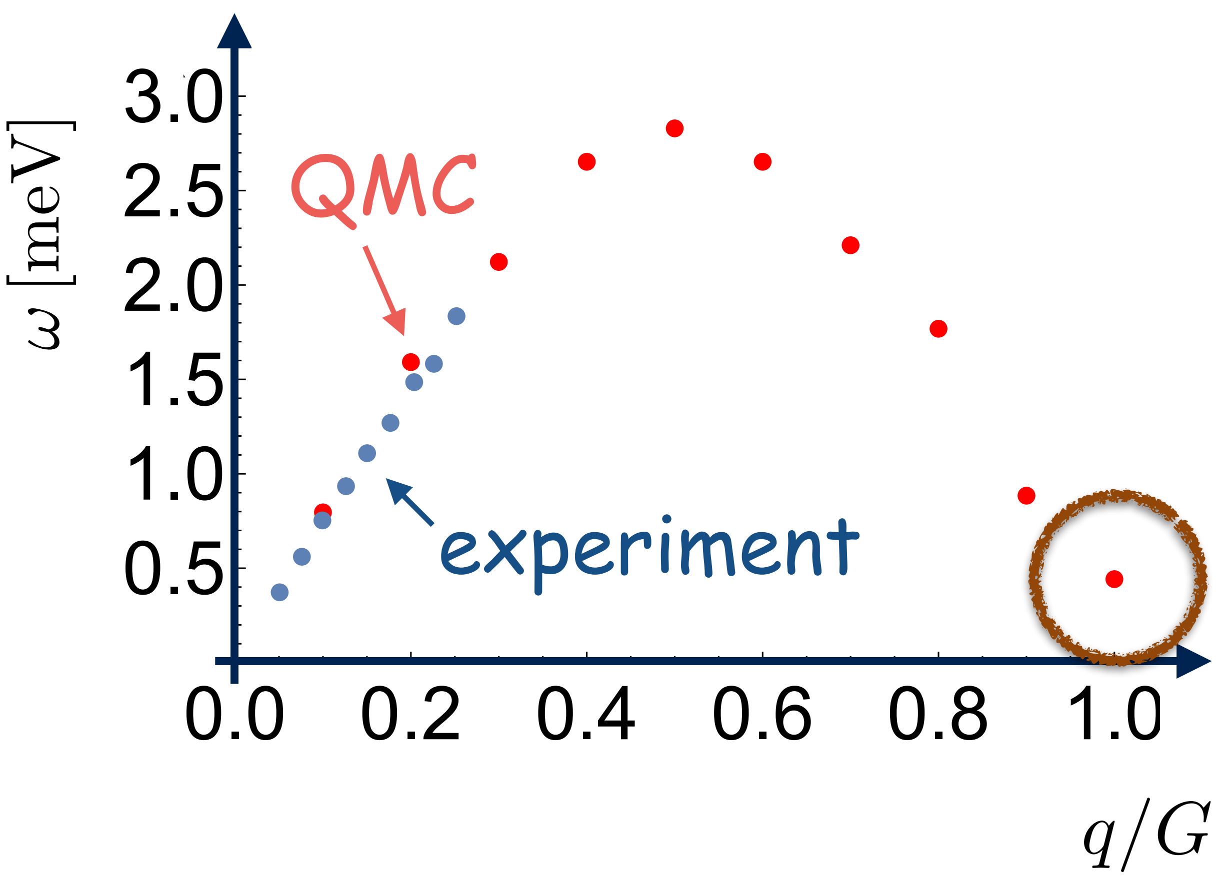

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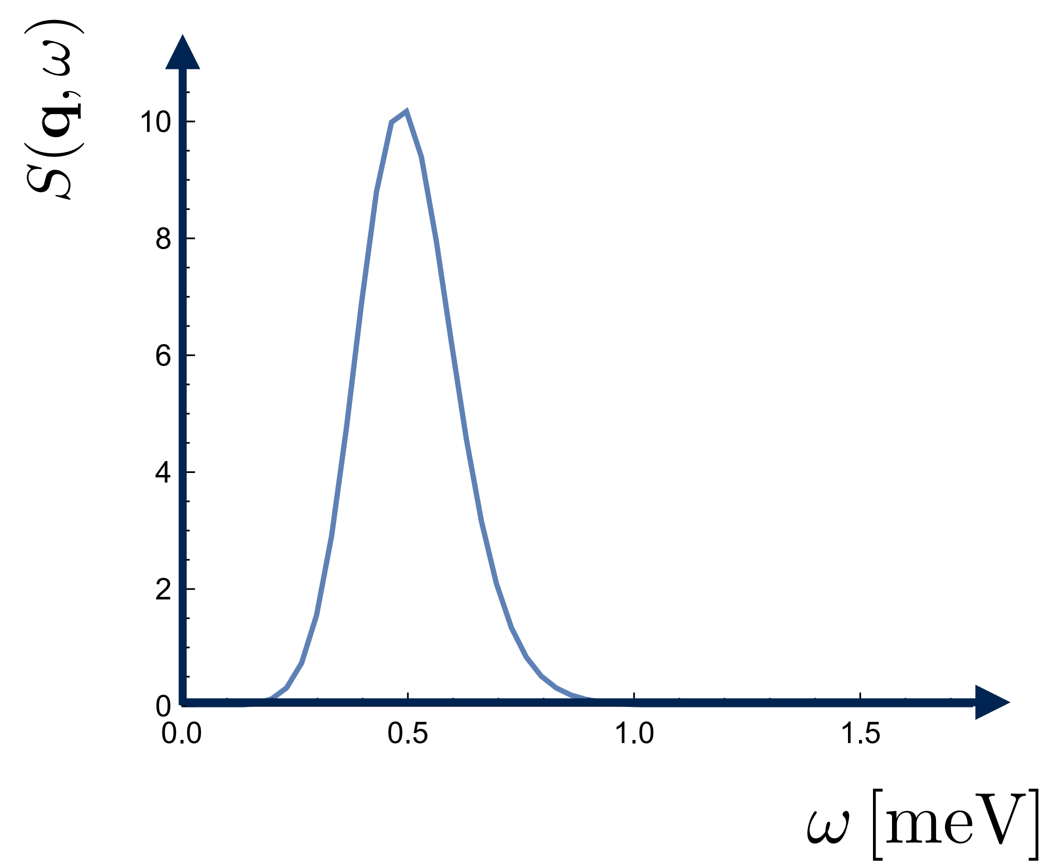

Confirms presence of optical mode (e.g. not due to crystal domains).

Small energy. Difficulty with analytical continuation?
Lowest optical mode missed by experiment?

Summary:

* In Helium, harmonic theory fails due to large zero point motion

* New "harmonic theory" for the optical modes

* QMC finds low energy optical mode — could it be there?

* Prediction: such modes should appear in other quantum solids (solid Helium-3, 2d and 3d CDWs, etc)