Excitations in Strongly Interacting BECs

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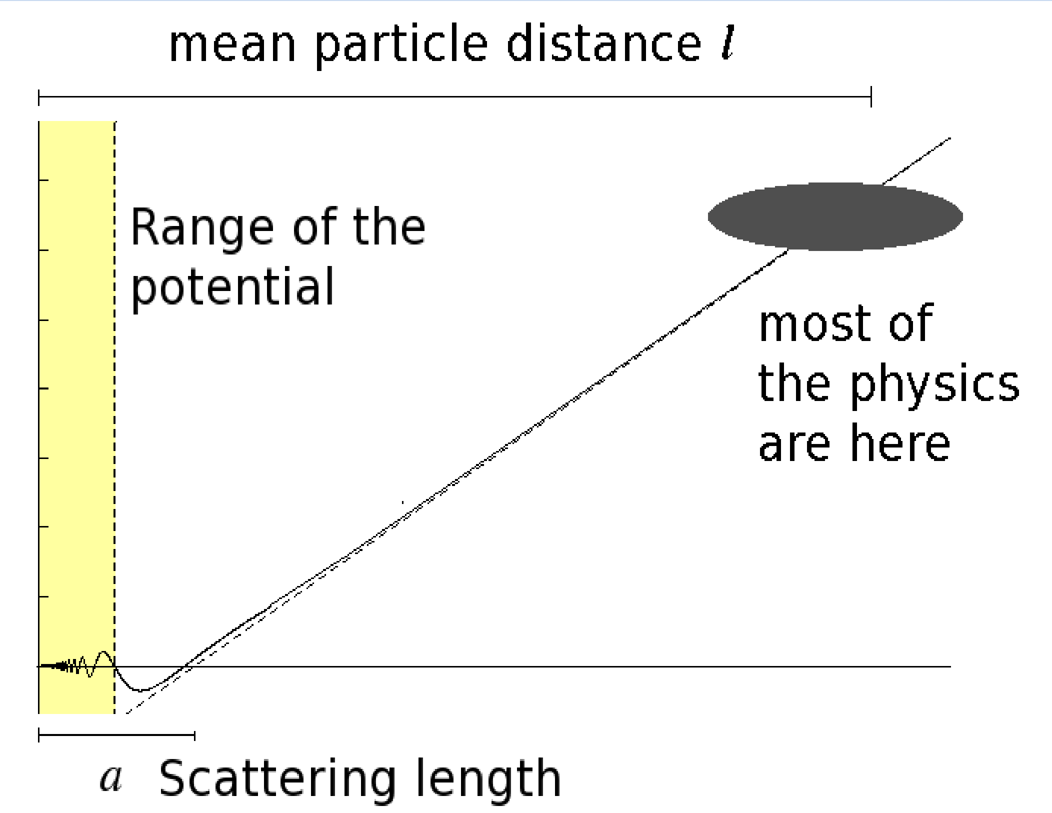
Excitations in Strongly Interacting BECs

Weakly Interacting Systems and Universal Regime

Very dilute systems dominated by two-body correlations

System in gaseous phase



Mean interparticle distance

$$d = \rho^{-1/3} \text{ large}$$

Low energy two-body processes

$$E = \frac{\hbar^2 k^2}{2m} \quad \rightarrow \quad \tan \delta_l(k) \rightarrow k^{2l+1}$$

only s-wave scattering (*l=0*)

$$\cot \delta_0 = -\frac{1}{ka} + \frac{1}{2} k r_0 + \cdots$$

a = scattering length

only the s-wave scattering length is relevant when $ka \rightarrow 0$

Universal regime at T=0 $\quad \rho a^3 \longrightarrow 0 \qquad ka \longrightarrow 0$

Excitations in Strongly Interacting BECs

Hard Core Potential

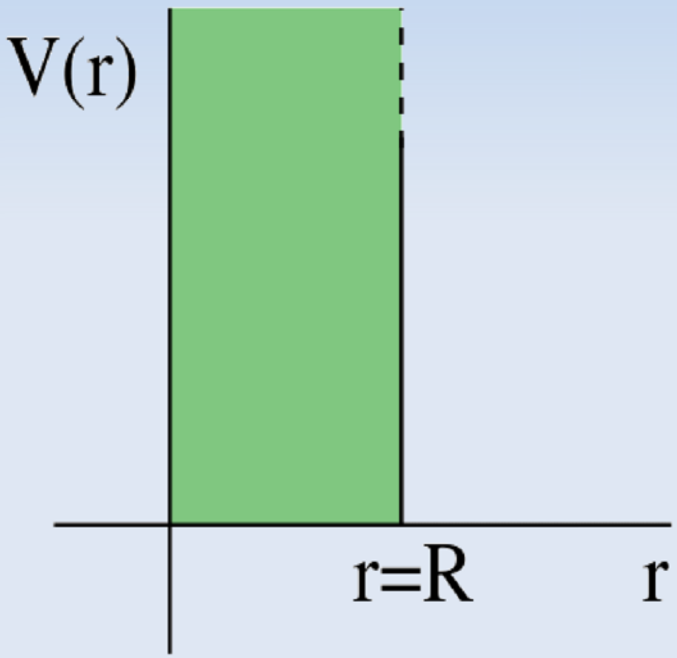
We want to solve the many-body Schroëdinger equation

$$-\frac{\hbar^2}{2m}\sum_{j=1}^{N}\nabla_j^2\Psi_0+\sum_{i<j}^{N}V(r_{ij})\Psi_0=E\,\Psi_0$$

for the wave function (or related quantities)

$$\Psi_0=\Psi_0(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\ldots,\mathbf{r}_N)$$

Starting from a suitable model potential.
Several choices are available:



Hard Core Potential

A system of N spinless bosons of mass *m* interacting through a purely repulsive and infinite potential of radius *R*

$$V(r)=\begin{cases}\infty & r\leq R\\ 0 & r>R\end{cases}$$

with R=a the Scattering Length

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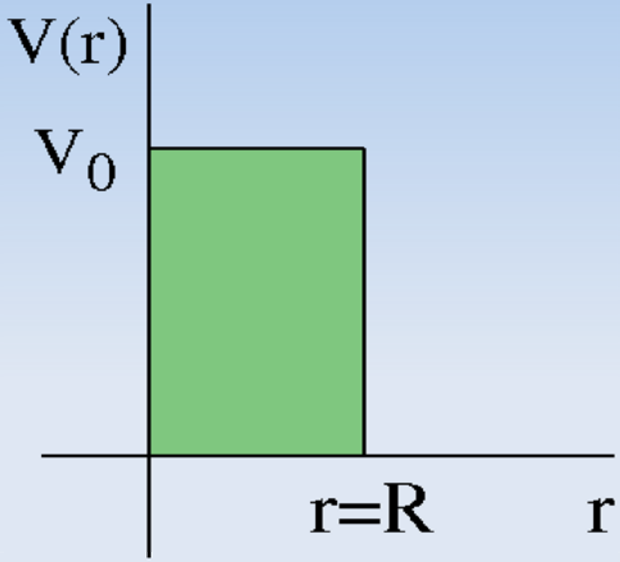
Repulsive Soft Core Potential

Soft Core Potential

A system of N spinless bosons of mass *m* interacting through a purely repulsive but finite potential of radius *R*

$$V(r) = \begin{cases} V_0 > 0 & r \leq R \\ 0 & r > R \end{cases}$$

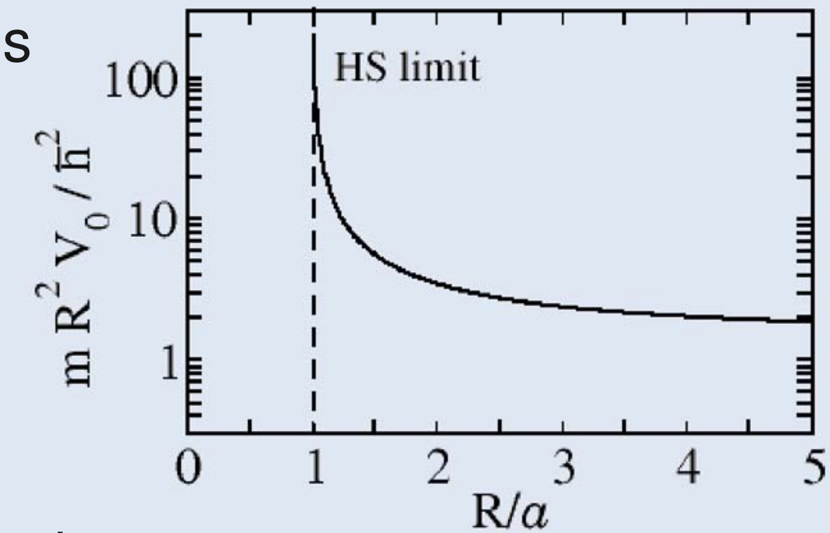


with V_0= height of the potential

The corresponding scattering length is given by the expression

$$a = R\left[1 - \frac{\tanh(K_0 R)}{K_0 R}\right]$$

with the constant $K_0^2 = \frac{m}{\hbar^2} V_0$



This potential is defined by two parameters

Excitations in Strongly Interacting BECs

The Euler-Lagrange Problem

Variational Energy: $$\frac{E}{N} = \frac{1}{2}\rho \int d\mathbf{r}_{12}\, g(r_{12}) \left[V(r_{12}) - \frac{\hbar^2}{2m}\nabla^2 \ln f_2(r_{12}) \right]$$

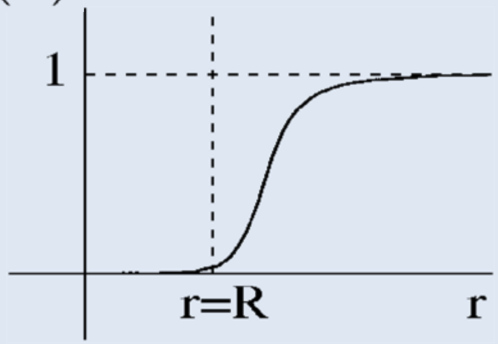
We want to solve the Optimal Variational Problem

$$\frac{\delta E[f]}{\delta f(r)} = 0 \qquad \text{with} \qquad E[f] = \frac{\langle \Psi_0 \mid H \mid \Psi_0 \rangle}{\langle \Psi_0 \mid \Psi_0 \rangle}$$

For the simple Jastrow *ansatz*, valid at low densities

$$\Psi_0 = \Psi_0(\mathbf{r_1}, \mathbf{r_2}, \mathbf{r_3}, \ldots, \mathbf{r_N}) = \prod_{i<j} f(r_{ij})$$

where $f(r)$ Is the two-body correlation factor with the general structure



- Is zero inside the core
- Goes to 1 at large distance
- Is non-negative

Equivalently: $g = g[f]$

$$g(r_{12}) = \frac{N(N-1)}{\rho^2} \frac{\int d\mathbf{r_3} d\mathbf{r_4} \cdots d\mathbf{r_N} \; |\Psi_0|^2}{\int d\mathbf{r_1} d\mathbf{r_2} \cdots d\mathbf{r_N} \; |\Psi_0|^2} \qquad \longrightarrow \qquad \frac{\delta E[f]}{\delta g(r)} = 0$$

Excitations in Strongly Interacting BECs

The Euler-Lagrange Problem

In terms of the Staic Structure Factor

$$S(q) = 1 + \rho \int d\mathbf{r}\, e^{i\mathbf{q}\cdot\mathbf{r}}\,[g(r) - 1]$$

The solution of the Optimization problem reads

$$S(q) = \frac{t(q)}{\sqrt{t^2(q) + 2t(q)V_{ph}(q)}}$$

with $t(q) = \dfrac{\hbar^2 q^2}{2m}$ and the *simplified* Particle-Hole potential

$$V_{ph}(r) = g(r)V(r) + \frac{\hbar^2}{m}\,|\nabla\sqrt{g(r)}\,|^2 + [g(r) - 1]\omega_I(r)$$

written in terms of the Induced Interaction

$$\omega_I(q) = \frac{1}{2}t(q)\frac{(2S(q)+1)(S(q)-1)^2}{S^2(q)}$$

→ Solve the problem iteratively

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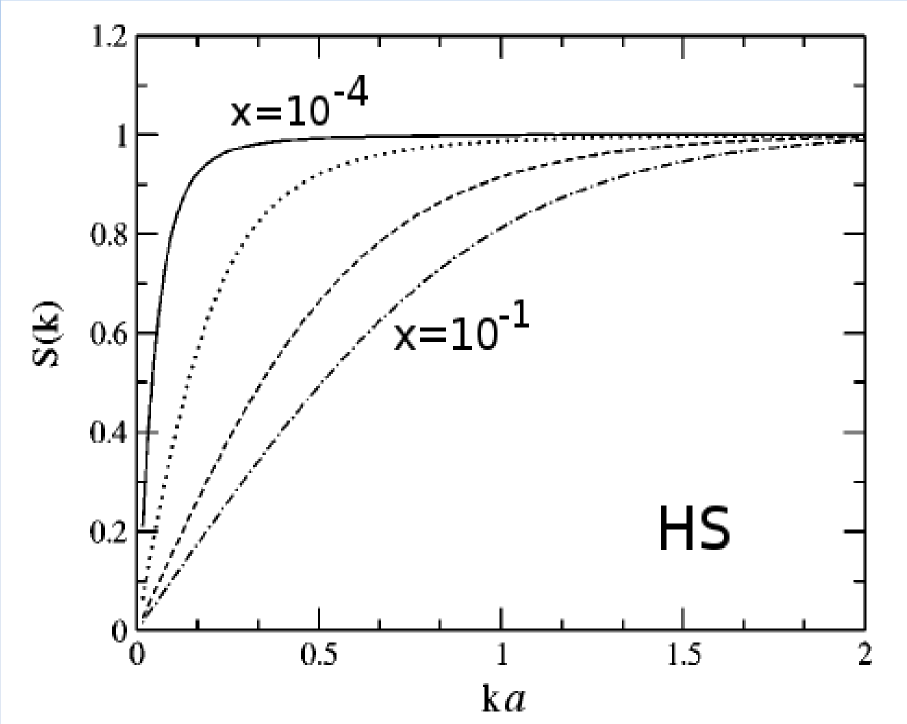
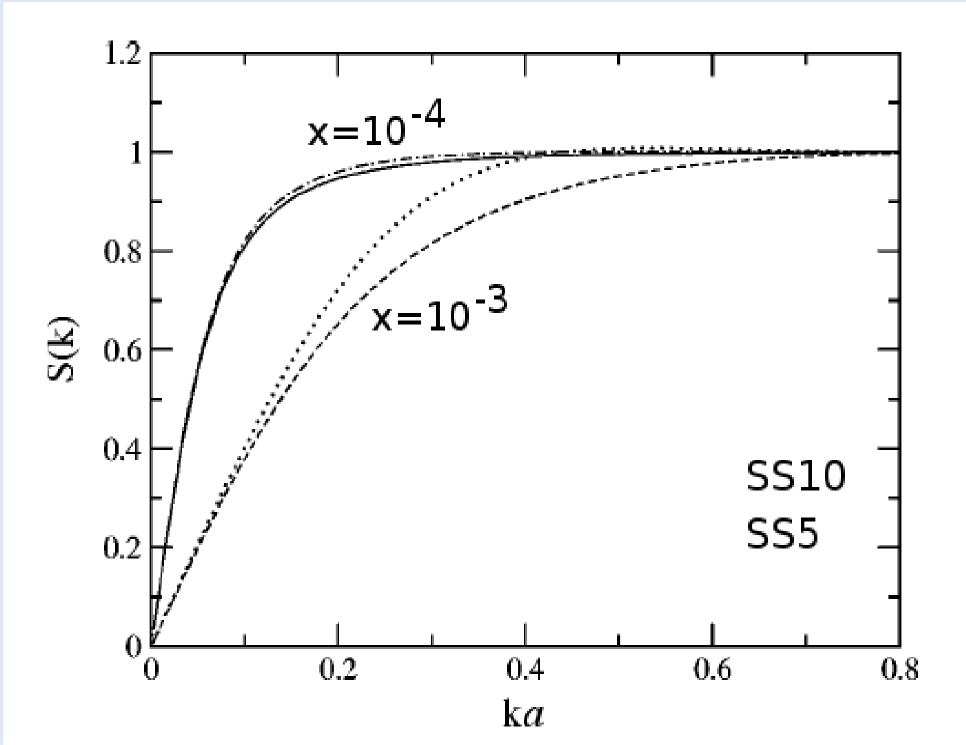
HNC/EL Results for S(k)



S(k) for Hard Spheres at several values of the gas parameter $x=10^{-4}$, 10^{-3}, 10^{-2} and 10^{-1}

S(k) for Soft Spheres at two values of the gas parameter $x=10^{-4}$ and 10^{-3}, for R=10a (SS10) and R=5a (SS5) (upper and lower curves in each case)



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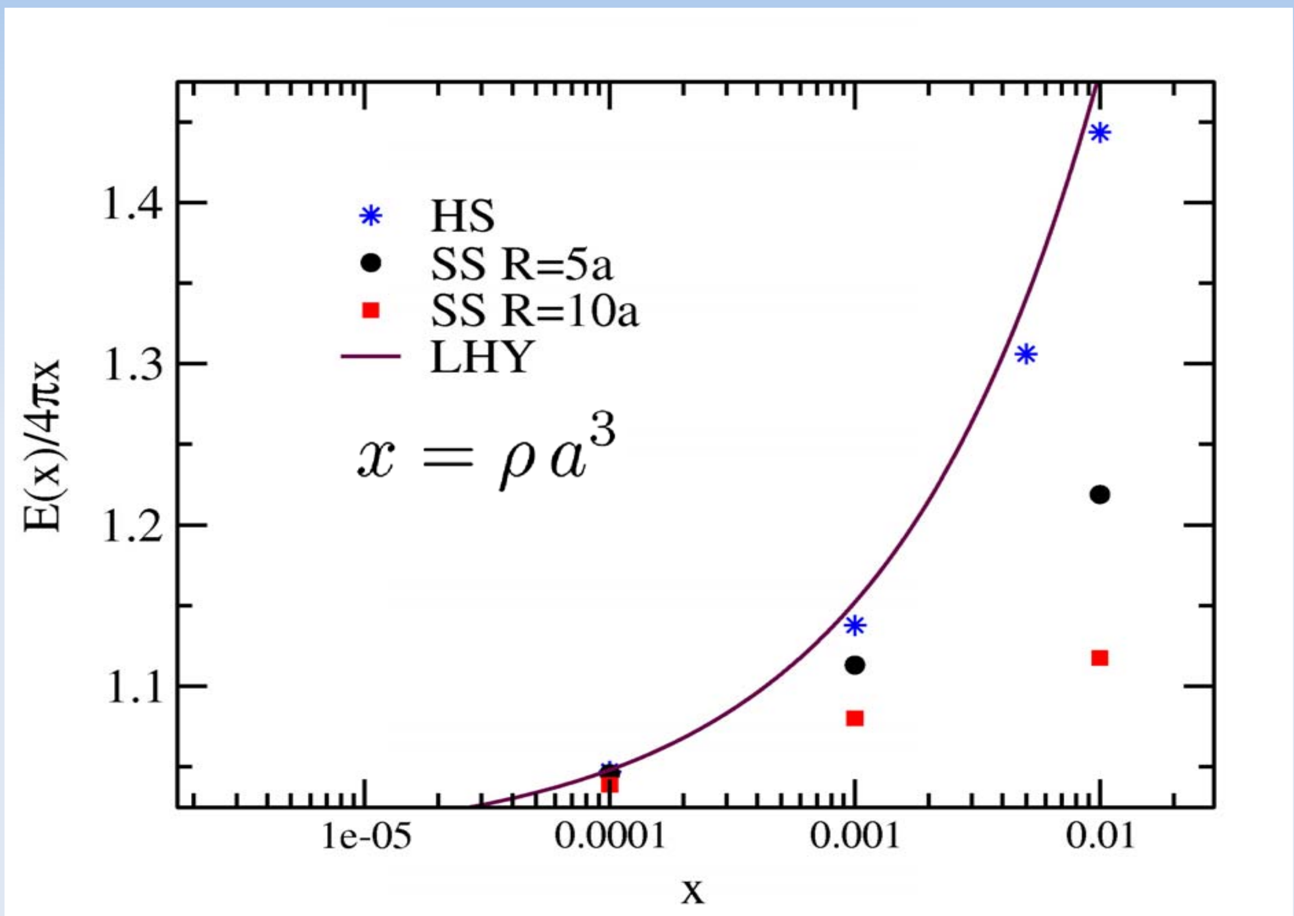
Results for the Ground State Energy



Comparison to DMC energies for HS

x	$\bar{E}_{DMC}/N$	$\bar{E}_{EL}/N$
10^{-6}	$1.262 \cdot 10^{-5}$	$1.264 \cdot 10^{-5}$
10^{-5}	$1.274 \cdot 10^{-4}$	$1.279 \cdot 10^{-4}$
10^{-4}	$1.311 \cdot 10^{-3}$	$1.316 \cdot 10^{-3}$
10^{-3}	$1.424 \cdot 10^{-2}$	$1.430 \cdot 10^{-2}$
$5 \cdot 10^{-3}$	$8.155 \cdot 10^{-2}$	$8.206 \cdot 10^{-2}$
10^{-2}	$1.796 \cdot 10^{-1}$	$1.814 \cdot 10^{-1}$
$5 \cdot 10^{-2}$	1.338	1.383

Lee-Huang-Yang energy $$\frac{E}{N} = \left(\frac{\hbar^2}{2ma^2}\right) 4\pi x \left[1 + \frac{128}{15}\sqrt{\frac{x}{\pi}}\right]$$

Hard Spheres follow the Lee-Huang-Yang law most closely

Excitations in Strongly Interacting BECs

Excitation Spectrum in Bogoliubov Approximation

Bogoliubov model of elementary excitations, valid at low densities when the scattering length dominates

$$\omega(k) = \sqrt{\left(\frac{\hbar^2 k^2}{2m}\right)^2 + \frac{8\pi\hbar^2\rho a}{m}\frac{\hbar^2 k^2}{2m}}$$

Expand for low a at fixed momentum k

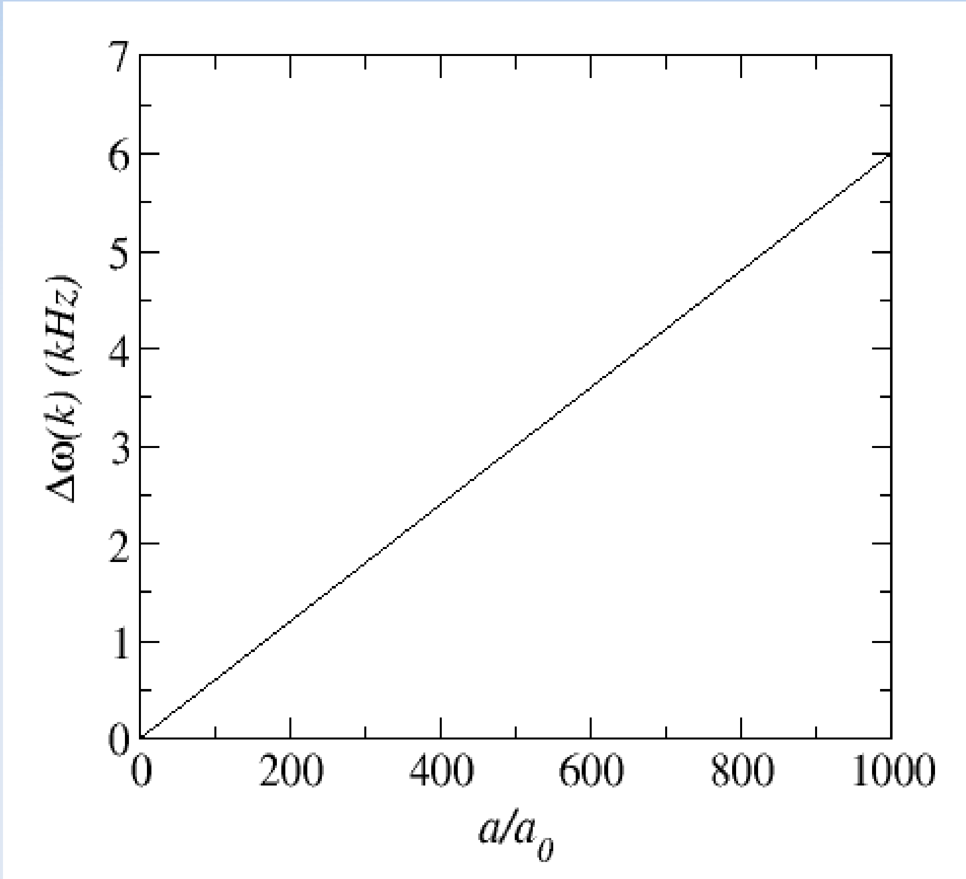
$$\Delta\omega(k) = \omega(k) - \frac{\hbar^2 k^2}{2m} \approx \frac{4\pi\hbar^2\rho}{m}\, a$$

→ Linear dependence on a

Ex: experimental conditions on a BEC of ^{85}Rb atoms

$$\frac{1}{2\pi}\frac{\hbar k^2}{2m} = 15.423\,\mathrm{kHz} \qquad k = \frac{4\pi}{780}\, nm^{-1}$$

$$\rho = 7.6\cdot 10^{13}\, cm^{-3}$$



$a_0 = 0.529$ Å Bohr radius

Excitations in Strongly Interacting BECs

Experimental measurements for a BEC of ^{85}Rb atoms

Experimental measurements
Papp et al. PRL**101**, 135301 (2008)

Gas of ^{85}Rb atoms in an F=2, M=-2 state
Experimental conditions:

$$k = \frac{4\pi}{780}\, nm^{-1} \qquad \rho = 7.6\cdot 10^{13}\, cm^{-3}$$

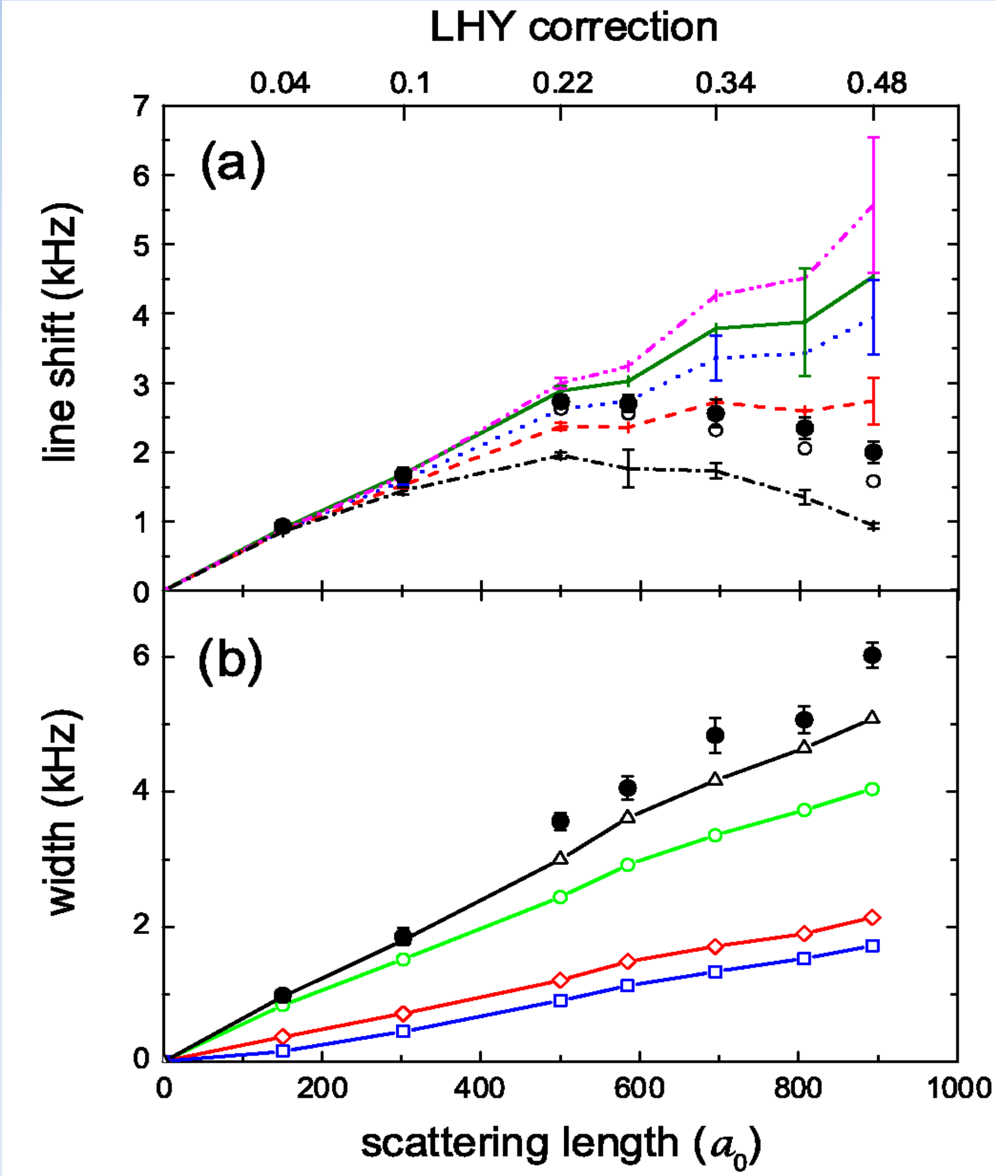
such that $\frac{1}{2\pi}\frac{\hbar k^2}{2m} = 15.423\,\mathrm{kHz}$

Black circles in upper panel: measured line shifts (black circles)

$$\Delta\omega(k) = \omega(k) - \frac{1}{2\pi}\frac{\hbar k^2}{2m}$$

Lower panel: measured width (sigma) of the experimental peak (black circles)

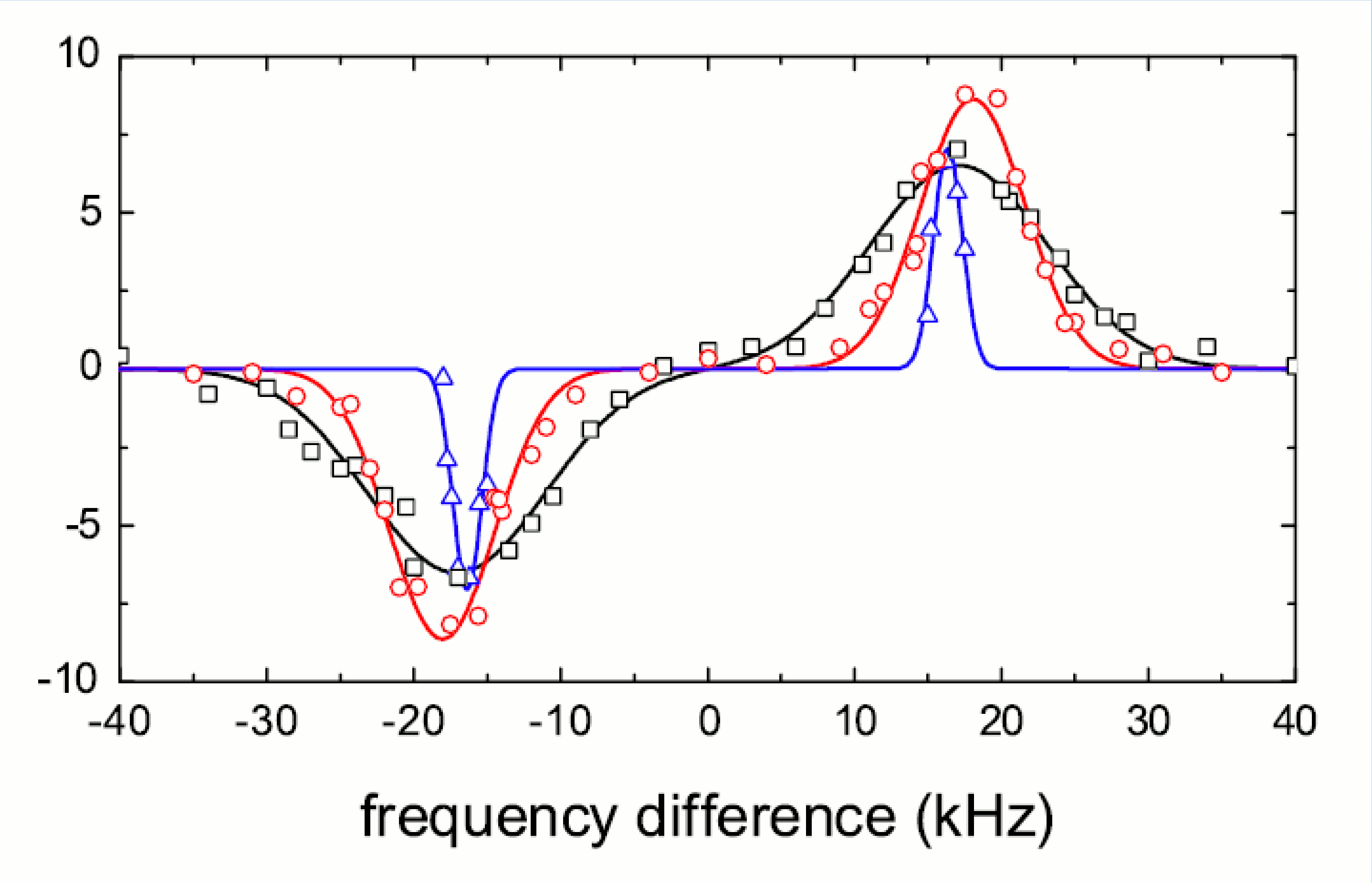
→ Can we repreduce this from S(k,ω) ?



Excitations in Strongly Interacting BECs

Experimental measurements for a BEC of ^{85}Rb atoms

Experimental Bragg scattering data



Blue line: a/a_o=100 Red line: a/a_o=585 Back line: a/a_o=890

Excitations in Strongly Interacting BECs

Response function in the CBF approximation

$S(k,w)$ is the imaginary part of the density-density response induced by a time-dependent perturbation

$$S(k,\omega) = -\frac{1}{\pi} Im\chi(k,\omega) \equiv -\frac{1}{\pi} Im\left[\frac{\delta\rho_1(k,\omega)}{\rho_0 U_{ext}(k,\omega)}\right]$$

Variational wave function: $\Psi = \dfrac{1}{\sqrt{\mathcal{N}(t)}} e^{\delta U(t)} e^{-iE_0 t/\hbar} \Psi_0$

with time-dependent correlations

$$\delta U = \sum_j \delta u_1(\mathbf{r}_j;t) + \sum_{i<j} \delta u_2(\mathbf{r}_i,\mathbf{r}_j;t) + \cdots$$

and the minimization of the action integral

$$\delta S = \delta \int_{t_0}^{t} dt \, \langle \Psi \mid H - i\hbar\frac{\partial}{\partial t} \mid \Psi \rangle \equiv 0$$

Setting $\delta u_n = 0 \ \forall n > 1$ leads to the Feynman approximation

$$S(k,\omega) = S(k)\delta(\omega - \epsilon_F(k)) \quad , \quad \epsilon_F(k) = \frac{\hbar^2 k^2}{S(k)}$$

Excitations in Strongly Interacting BECs

Response function in the CBF approximation

Keeping δu_2 improves over that. Use continuity equations for the one- and two-particle densities and currents to isolate δu_1 and δu_2 In terms of one- and two-body density fluctuations.
Disregarding triplet correlations one arrives to

$$\chi(k,\omega) = \frac{S(k)}{\hbar\omega - \epsilon_F(k) - \Sigma(k,\omega)} - \frac{S(k)}{\hbar\omega + \epsilon_F(k) + \Sigma^*(k,\omega)}$$

with the Self-Energy

$$\Sigma(k,\omega) = \frac{1}{2}\int \frac{d\mathbf{p}\, d\mathbf{q}}{(2\pi)^3\rho}\delta(\mathbf{k}+\mathbf{p}+\mathbf{q})\frac{|V_3(\mathbf{k};\mathbf{p},\mathbf{q})|^2}{\hbar\omega - \epsilon_F(p) - \epsilon_F(q)}$$

and the three-phonon coupling vertex

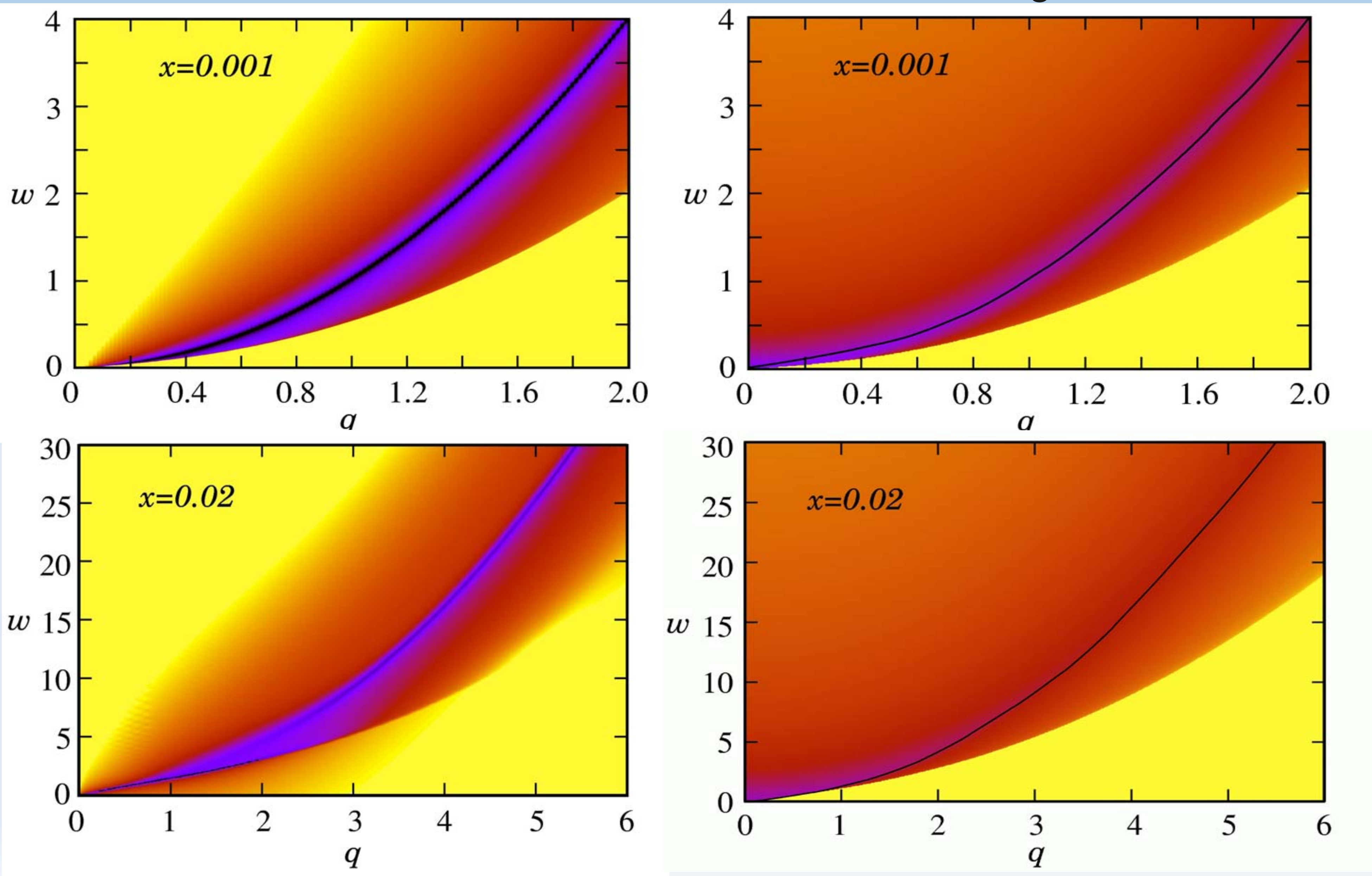
$$V_3(\mathbf{k};\mathbf{p},\mathbf{q}) = \frac{\hbar^2}{2m}\sqrt{\frac{S(p)S(q)}{S(k)}}\left[\mathbf{k}\cdot\mathbf{p}X(p) + \mathbf{k}\cdot\mathbf{q}X(q) - k^2 u_3(\mathbf{k};\mathbf{p},\mathbf{q})\right]$$

Written in terms of S(k) through $X(p) = 1 - 1/S(p)$

Excitations in Strongly Interacting BECs

Response function for HS in the CBF approximation

CBF | Bogoliubov



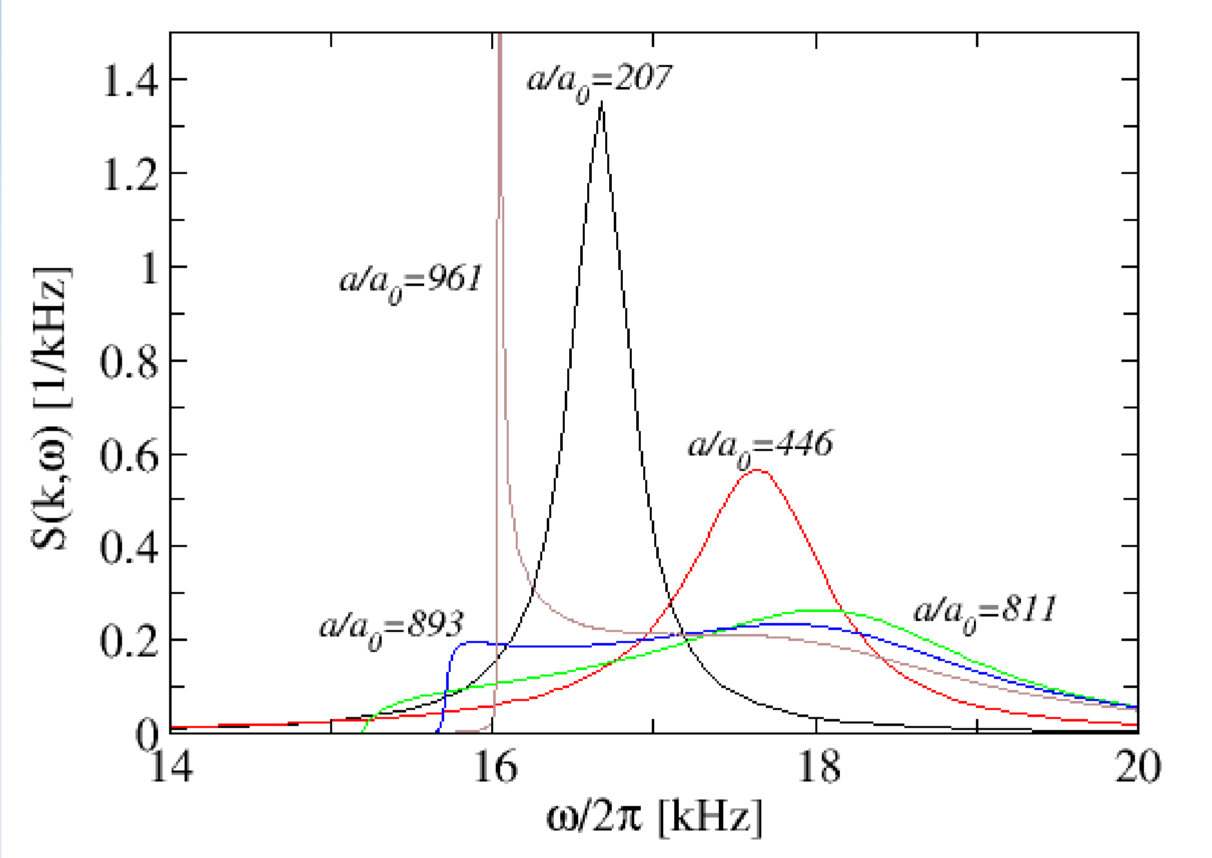
Excitations in Strongly Interacting BECs

CBF results for Soft Spheres S(k,w) with R=3.5a

$$k = \frac{4\pi}{780}\, nm^{-1}$$

$$\rho = 7.6 \cdot 10^{13}\, cm^{-3}$$

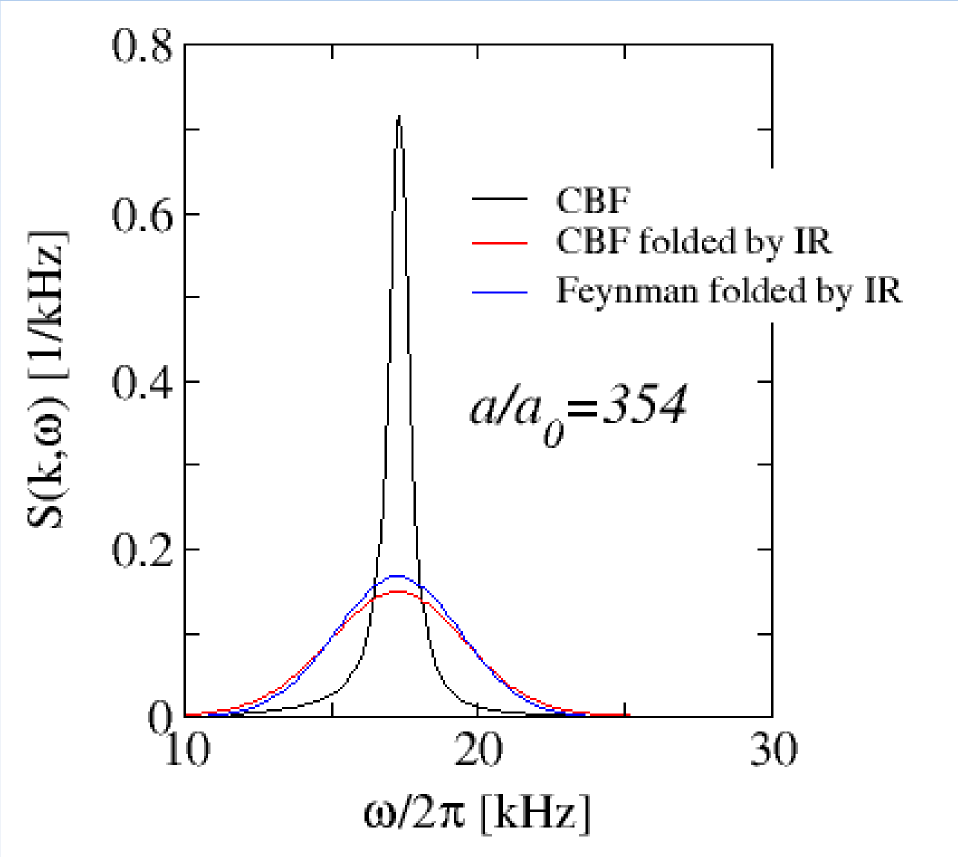
Soft Spheres with R=3.5a for different values of the scattering length

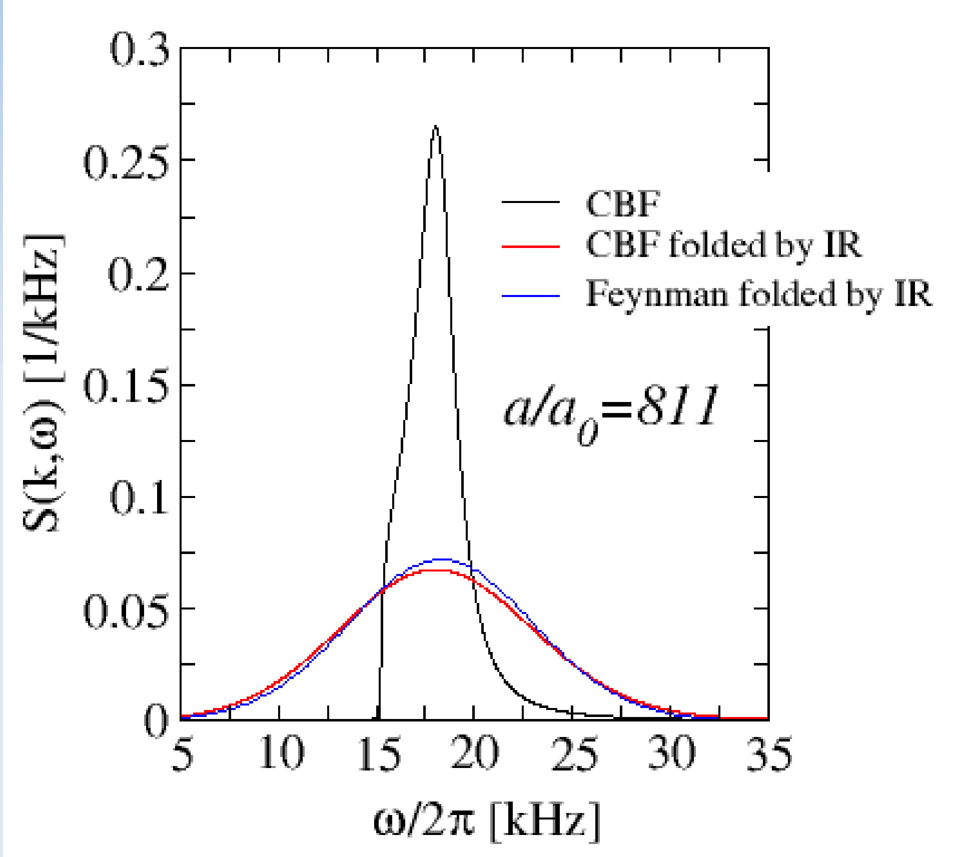


The position of the peak moves to higher energies with increasing scattering length, then disapperas, and finally shifts to lowe energies at even higher values of a

Excitations in Strongly Interacting BECs

Impact of the Instrumental Resolution Effects for SS with R=3.5a



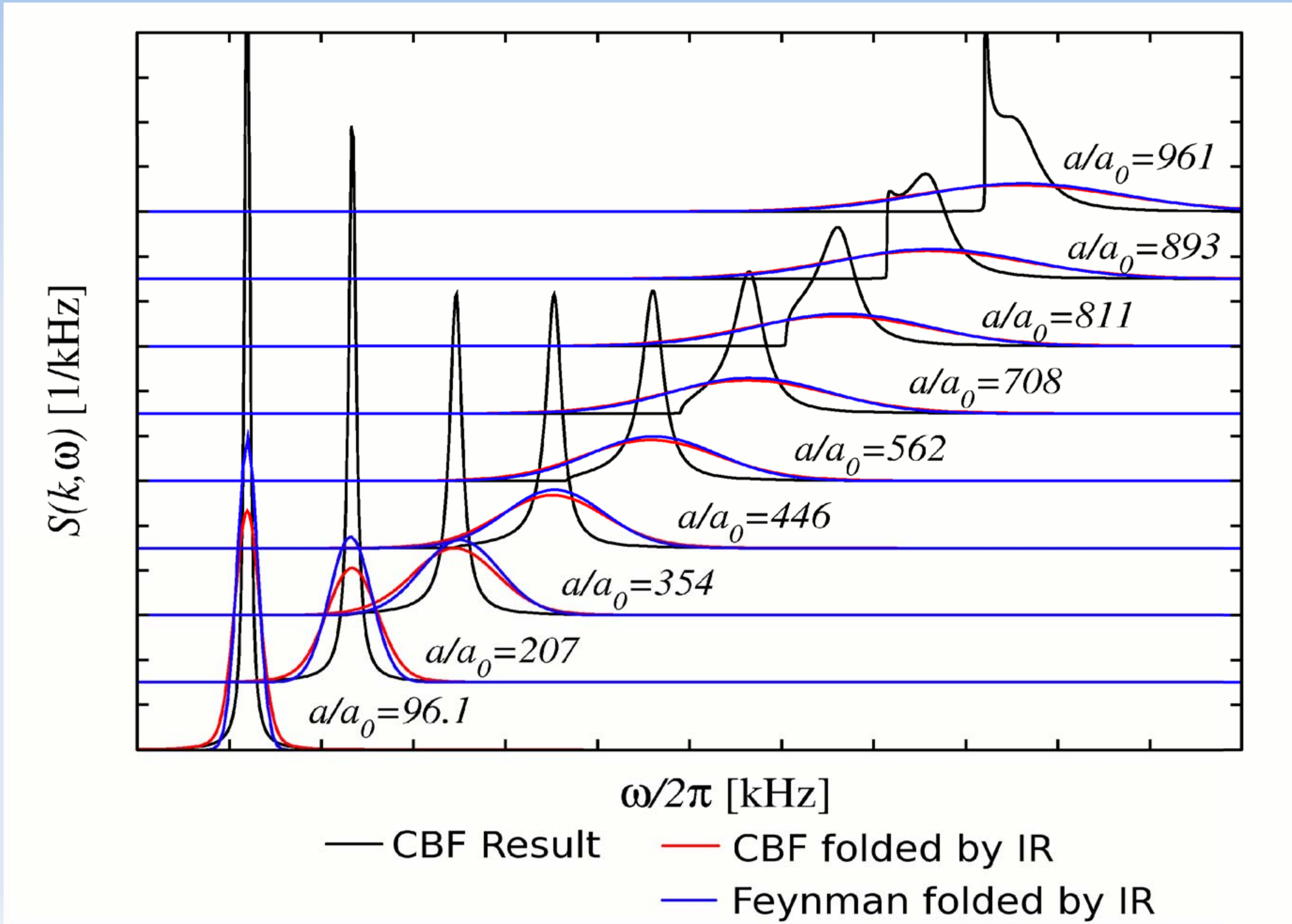


Instrumental Resolution Effects do kill all features in the response, leaving only a gaussian-like function that is almost identical to the Feynamn approximation folded by the same function

Max. Differences between folded Feynman and folded CBF ~ 0.4 kHz

Excitations in Strongly Interacting BECs

Impact of the Instrumental Resolution Effects for SS with R=3.5a



Excitations in Strongly Interacting BECs

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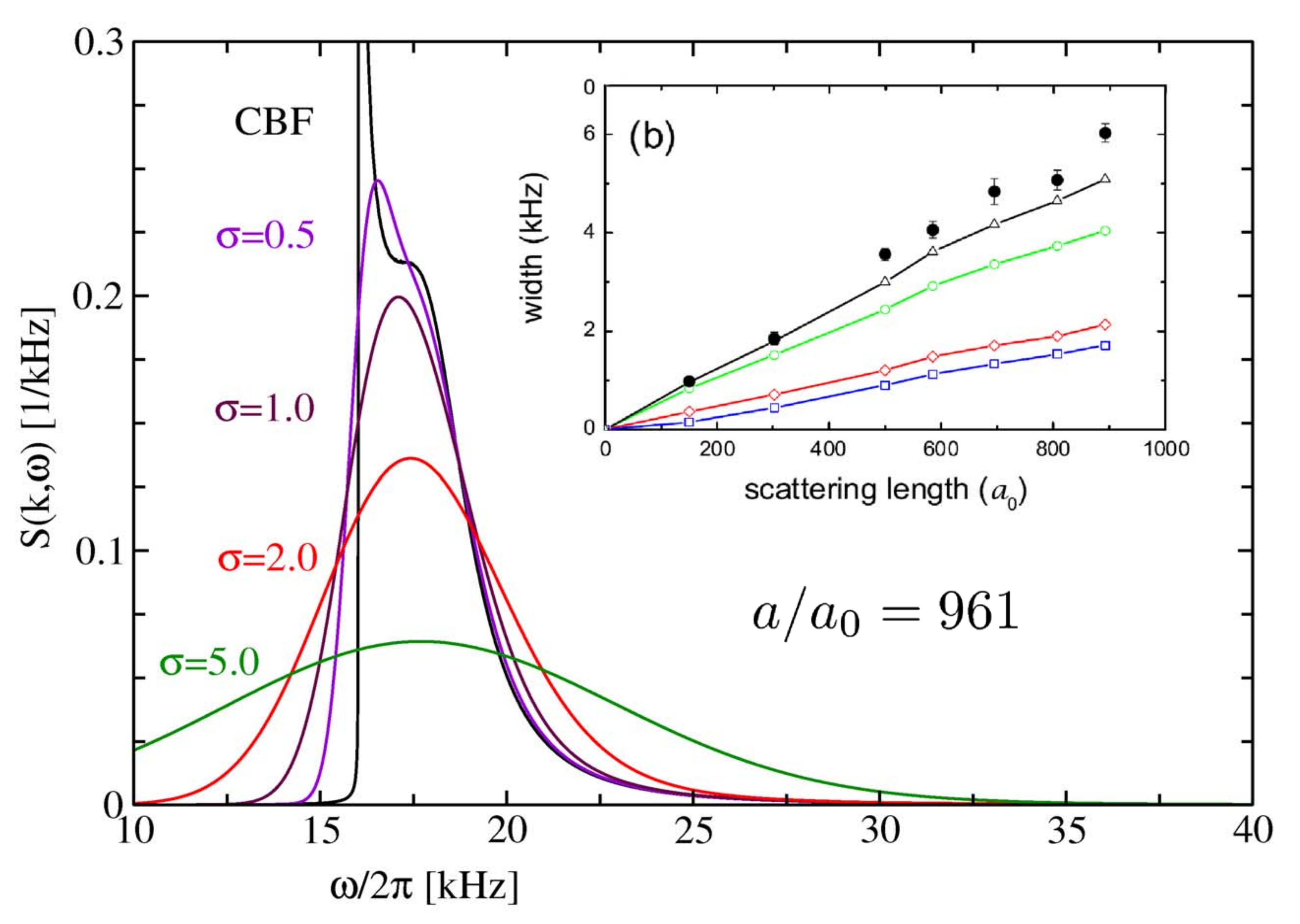
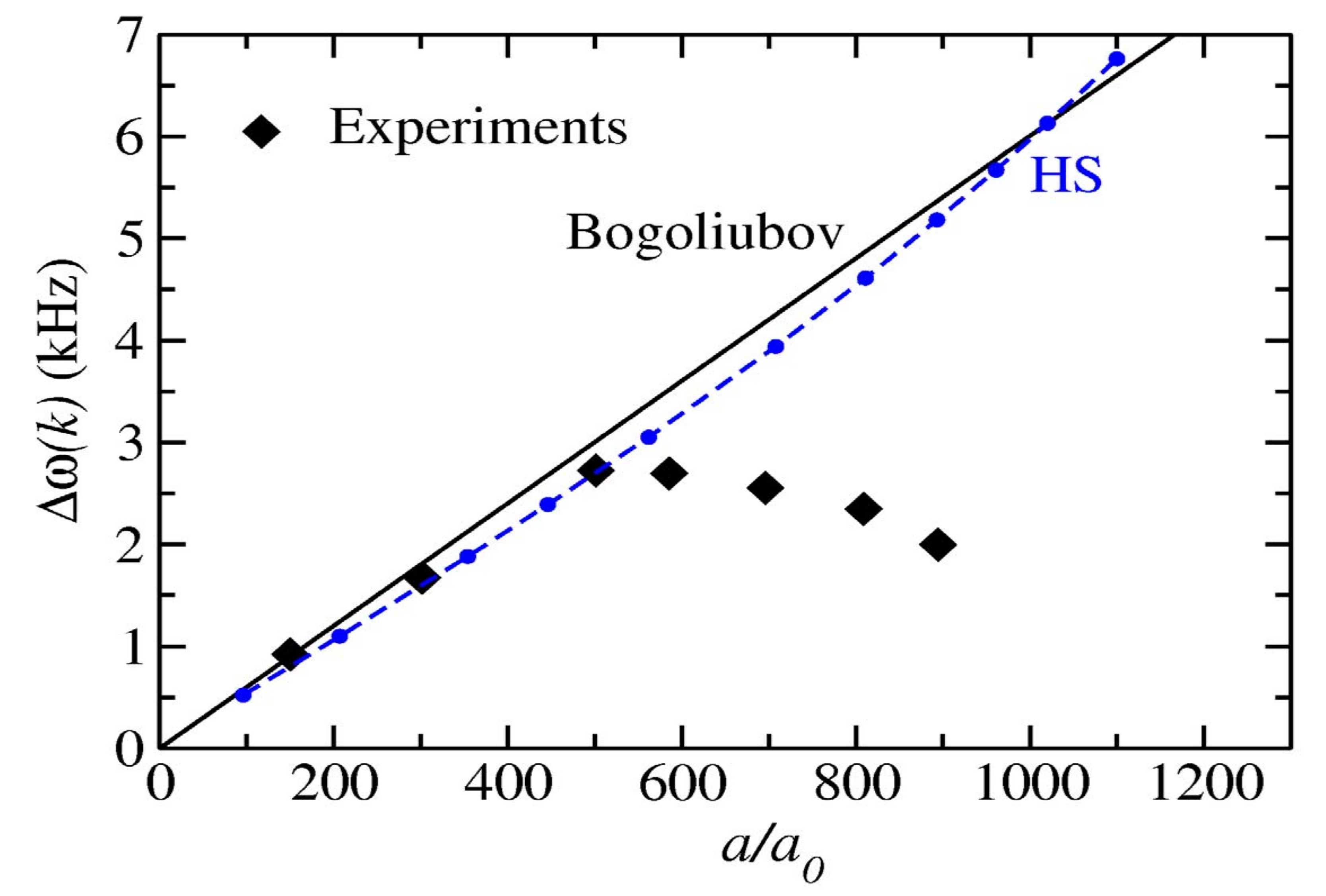


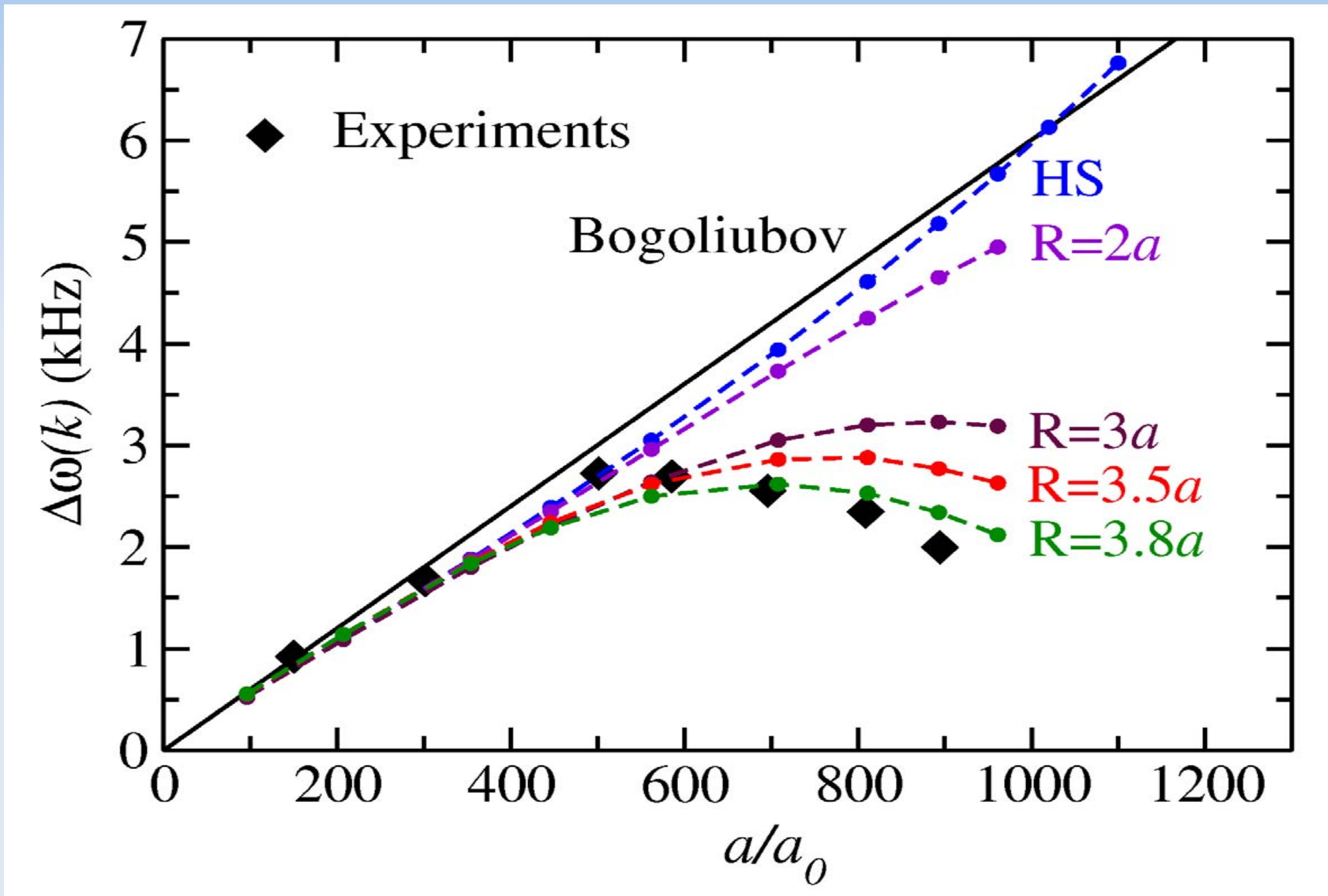
Excitations in Strongly Interacting BECs

Results for Hard Spheres and Soft Spheres



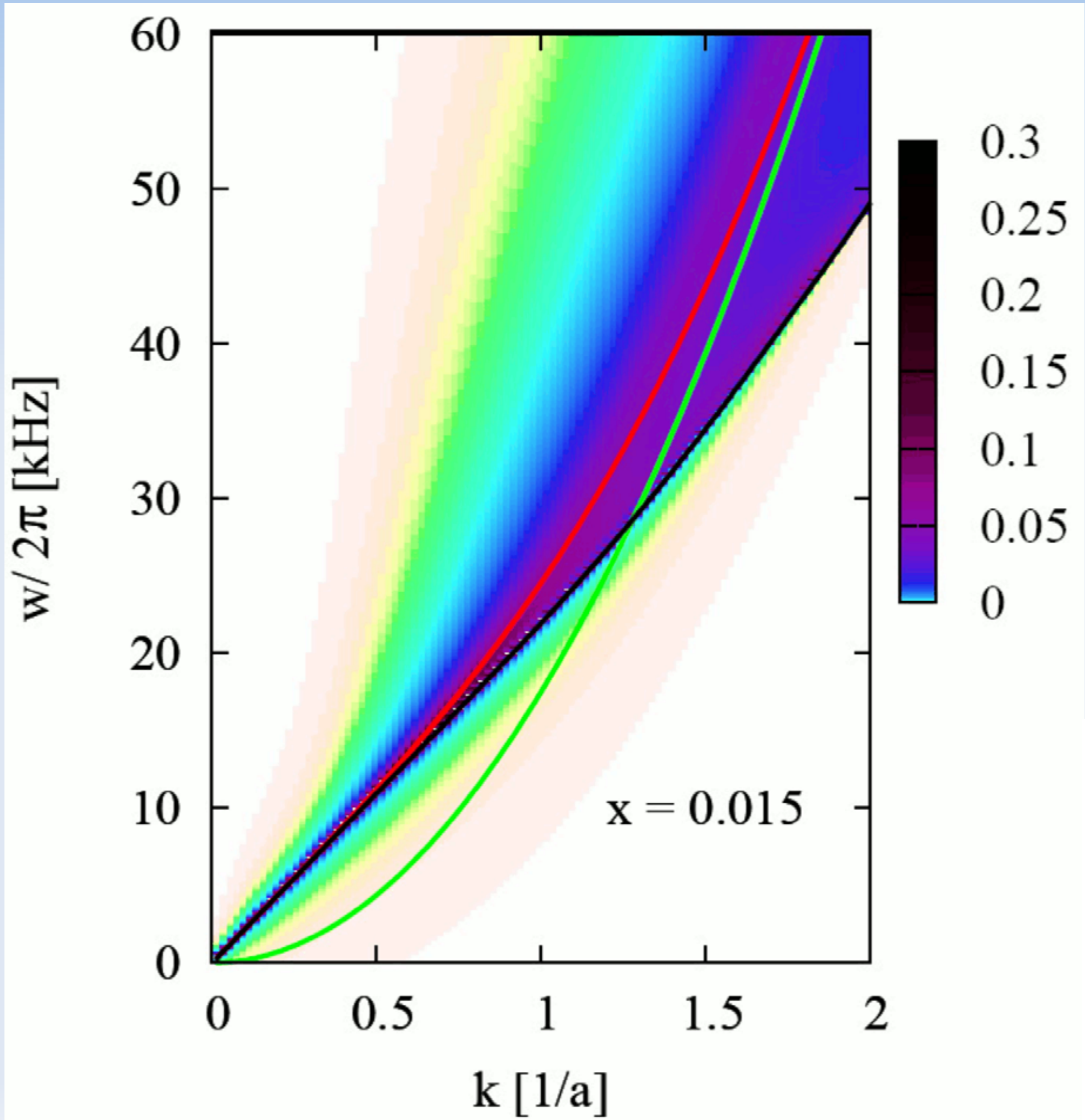
Excitations in Strongly Interacting BECs

Results for Hard Spheres and Soft Spheres



Excitations in Strongly Interacting BECs

S(k,ω) for Soft Spheres

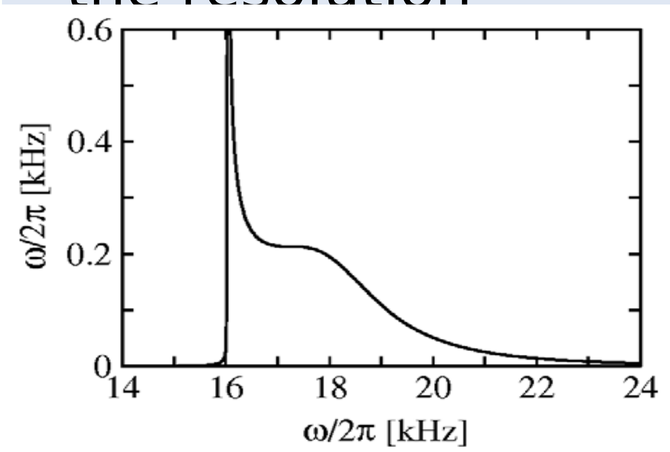


S(k,ω) map for a somewhat larger value of x.

Green line: free

Red line: Feynman

Wider structures develop with increasing energy ω,which could be seen increasing the resolution



Excitations in Strongly Interacting BECs

More realistic potentials (?)

More realistically, Rb atoms interact through a Van der Waals forces. However, only the long range part of *V(r)* is relevant at low densities

$$V(r \gg r_0) = V_0 \left[\left(\frac{r_0}{r}\right)^{12} - \left(\frac{r_0}{r}\right)^{6} \right] \approx -V_0 \left(\frac{r_0}{r}\right)^{6} = -\frac{C_6}{r^6}$$

Molecular dynamics simulations yield energy curves that directly provide values of V_0, r_0 and C_6 Krauss & Stevens, *J.Chem.Phys.***93**,4236(1990)

Actually several choices are available for ^{85}Rb atoms:

- Krauss & Stevens: $C_6 \sim 5700$ a.u.
- Geltman *et al.* $4619 \lesssim C_6 \lesssim 4635$ a.u.
- Van Kampen *et al.* $4698 \lesssim C_6 \lesssim 4710$ a.u.
- J.Pade: $C_6 \sim 4698$ a.u. & $C_6 \sim 5295$ a.u.

All these yield negative values for the scattering length in a broad range

$$-480 \lesssim a \lesssim -255$$

Experiments of ^{85}Rb BECS change a exploting Feschbach resonances

Excitations in Strongly Interacting BECs

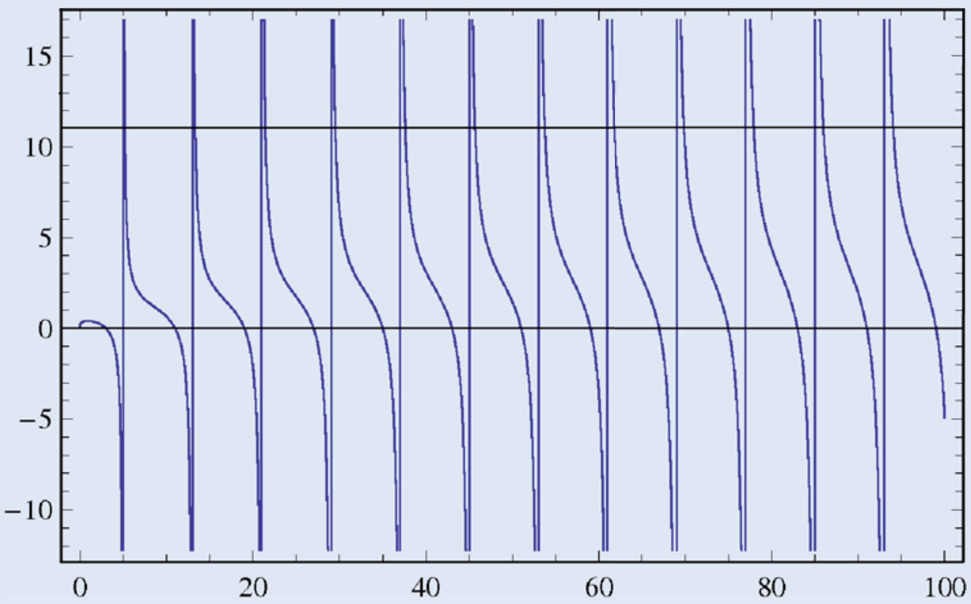
More realistic potentials (?)

We set C_6 = 4700 a.u. and use the (2n-2,n)-LJ Pade's potential with n=6

$$V(r) = V_0 \left[\left(\frac{r_0}{r}\right)^{10} - \left(\frac{r_0}{r}\right)^{6} \right]$$

since this one has an anlytic expression for the scattering length

$$a = r_0 \left(\frac{x}{2}\right)^{\frac{1}{4}} \frac{\Gamma\left(\frac{5-x}{8}\right)\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{3-x}{8}\right)\Gamma\left(\frac{5}{4}\right)} \quad \text{with} \quad x = r_0\sqrt{\frac{mV_0}{\hbar^2}}$$

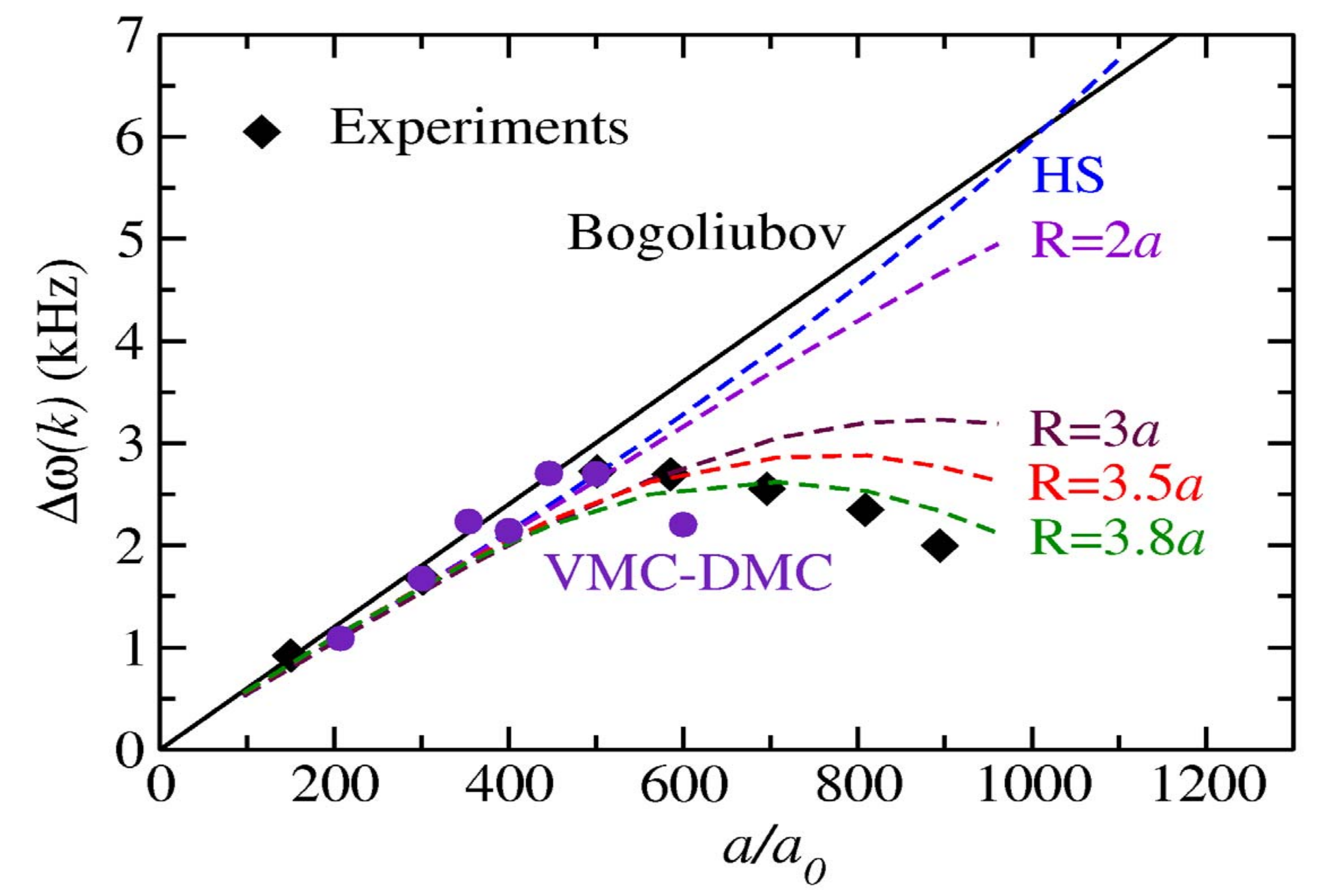


- Many combinations of r_0 and V_0 yield the same a
- Slight changes in r_0 and V_0 yield large changes in a when a/r_0 is large

The systems has a very weakly-bound state for large a

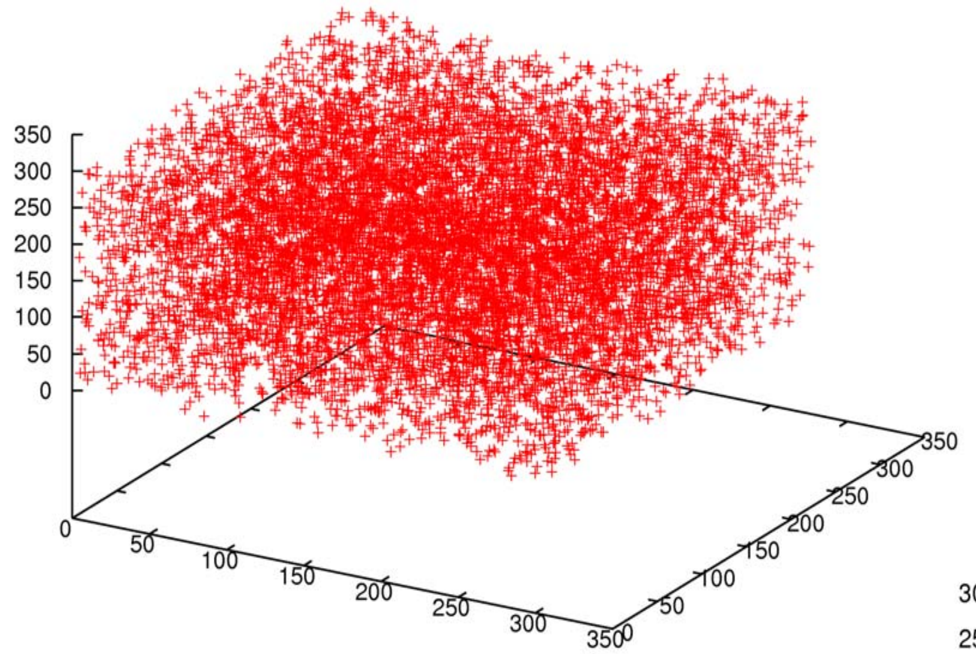
Excitations in Strongly Interacting BECs

Results for Hard and Soft Spheres, and Monte Carlo



Excitations in Strongly Interacting BECs

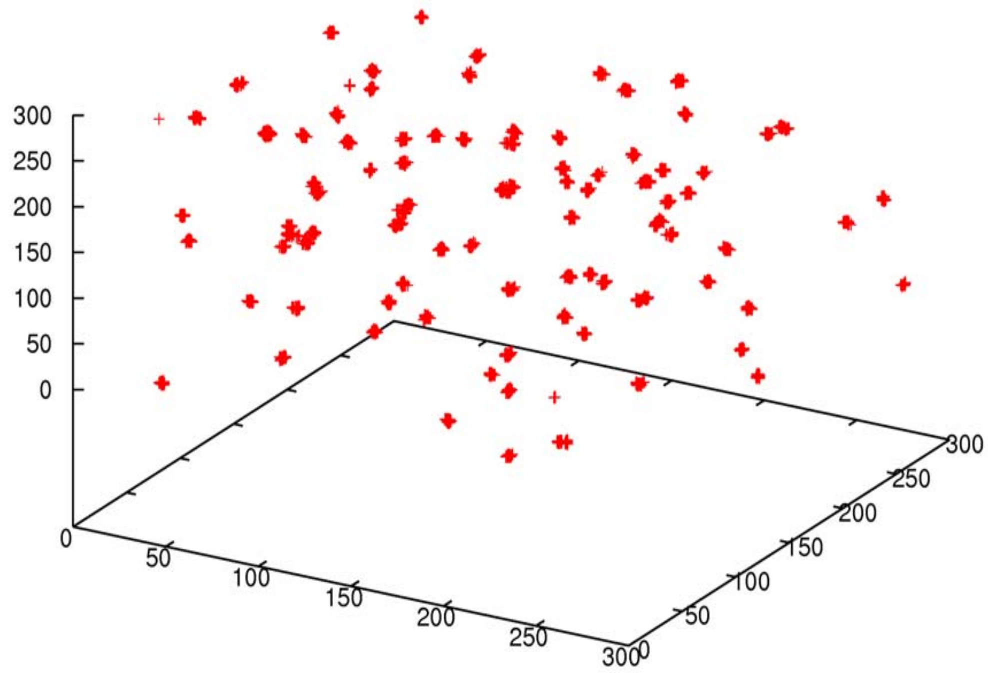
Monte Carlo Results for the (10,6)LJ potential



Particle coordinates for several different realizations of the system

⇦ Small scattering lengths
Universal regime
a gas

Large scattering lengths
out of the Universal regime
clusters ⇨



Excitations in Strongly Interacting BECs

Summary and Conclusions:

We can use simple HNC/EL and CBF to describe quantum gases at the experimental values of x nowadays available, showing the departure from the universal regime.

At least a two-parameter potential is required to get qualitative agreement with the experimental data for the excitation spectrum.

Experiments have to improve considerably the resolution in order to see any detailed structure that goes beyond the Feynman approximation.

Realistic potentials are not easy to deal with. One has to describe the system in a metastable state. *Work is being done along this line...*