# Sum-Rule Approach for Collective Excitations of Ultracold Quantum Gases

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# Outline

# Introduction

## Ultracold Quantum Gases

- Bose–Einstein codensate in 1995: New playground for quantum physics
- Phase transition at $T_C$: New phase
- Macroscopic occupation of ground state: Quantum fluctuations

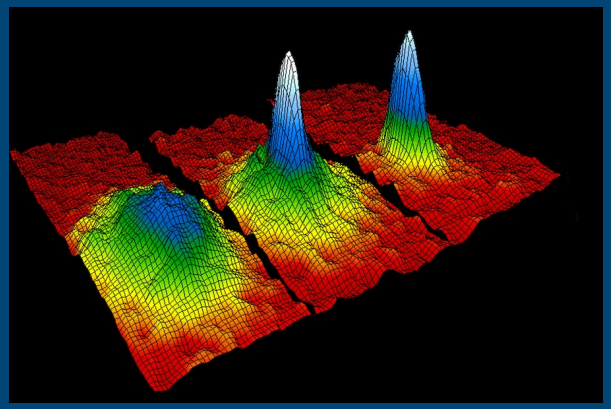


Fig.: Formation of a BEC (NIST)

## Experimental Observation

- Comparing experimental and theoretical results for collective excitation frequencies

# I. Linear Response

$$H_t = H^{(0)} + H_t^{(1)} = H^{(0)} + f(t)\, B$$

## Interaction Picture

Evolution for systems with time-independent Hamiltonian

$$U_0(t-t_0) = \mathrm{e}^{-\mathrm{i}H^{(0)}(t-t_0)/\hbar}$$

General time evolution

$$U(t,t_0) = U_0(t-t_0)\, U_1(t,t_0)$$

Splitting of time dependence (Interaction picture)

$$|\psi(t)\rangle = U_1(t,t_0)\,|\psi\rangle$$
$$G(t) = U_0^\dagger(t-t_0)\, G\, U_0(t-t_0)$$

First-order approximation

$$U_1(t,t_0) = 1 - \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} H_t^{(1)}(t')\,\mathrm{d}t' + \mathcal{O}\left(H_t^{(1)^2}\right)$$

## System Hamiltonian

$$H_t = H^{(0)} + H_t^{(1)} = H^{(0)} + f(t)\, B$$

$B$ Modulated operator

$f(t)$ Modulation in time ('field', 'force')

## Effects of the Pertubation

$$\delta\langle A(t)\rangle = \langle A(t)\rangle_{H_t} - \langle A(t)\rangle_{H^{(0)}}$$

$A$ Observed operator

$\delta\langle A(t)\rangle$ Deviation from equilibrium

$$\delta\langle A(t)\rangle = \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} \big\langle \big[A(t), B(t')\big]\big\rangle\, f(t')\,\mathrm{d}t' + \dots$$

$\langle A(t)\rangle$ Equilibrium average, short notation for $\langle A(t)\rangle_{H^{(0)}}$

## Response Functions

Deviation in first-order approximation (Kubo 1957)

$$\delta\langle A(t)\rangle = 2\mathrm{i}\int_{t_0}^{t} \chi''_{AB}(t,t')\, f(t')\,\mathrm{d}t'$$

$$\chi''_{AB}(t,t') = \frac{1}{2\hbar}\left\langle\left[A(t), B(t')\right]\right\rangle = \frac{1}{2\hbar}\left\langle\left[A(t-t'), B\right]\right\rangle$$

$\chi''_{AB}$ Time domain response function

Fourier transform

$$\tilde{\chi}''_{AB}(\omega) = \mathcal{F}\left[\chi''_{AB}\right](\omega)$$

$\tilde{\chi}''_{AB}$ Frequency domain response function

## Dynamic Susceptibility

Implementation of causality

$$\chi_{AB}(t-t') = 2\mathrm{i}\,\theta(t-t')\,\chi''_{AB}(t-t')$$

$\chi_{AB}$ Dynamic Susceptibility

Deviation from equilibrium in time

$$\delta\langle A(t)\rangle = \int_{-\infty}^{\infty} \chi_{AB}(t-t')\,f(t')\,\mathrm{d}t' = \big(\chi_{AB} * f\big)(t)$$

Deviation from equilibirum in frequency

$$\tilde{\delta}\langle A(\omega)\rangle = \mathcal{F}\big[\chi_{AB} * f\big](\omega) = \tilde{\chi}_{AB}(\omega)\,\tilde{f}(\omega)$$

# II. Correlation Functions

$$c_{AB}(t-t') = \langle A(t)\, B(t') \rangle = \langle A(t-t')\, B \rangle$$

## Correlation Functions

$$c_{AB}(t-t') = \left\langle A(t-t')\, B \right\rangle = \left\langle A\, B(t'-t) \right\rangle$$

$$\begin{aligned}\tilde{c}_{AB}(\omega) &= \mathcal{F}\big[c_{AB}\big](\omega) \\ &= 2\pi \sum_{i,j} p_j \, \langle i|A|j\rangle \, \langle j|B|i\rangle \, \delta(\omega - \omega_{ji})\end{aligned}$$

## Relation to Response Functions: Fluctuation-Dissipation Theorem

$$\chi''_{AB}(t-t') = \frac{1}{2\hbar}\left[c_{AB}(t-t') - c_{BA}(t'-t)\right]$$

$$\tilde{\chi}''_{AB}(\omega) = \frac{1-\mathrm{e}^{-\hbar\beta\omega}}{2\hbar}\tilde{c}_{AB}(\omega)$$

## Moments of Correlation Functions

$$m_{AB}^{(n)} = \frac{1}{2\pi}\int_{-\infty}^{\infty} (\hbar\omega)^n\, \tilde{c}_{AB}(\omega)\,\mathrm{d}\omega = \sum_{i,j} (\hbar\omega_{ij})^n\, p_j\, \langle i \,|\, A \,|\, j\rangle \langle j \,|\, B \,|\, i\rangle$$

## Sum Rules

Replacing $\omega^n = \mathrm{i}^n \frac{\mathrm{d}^n}{\mathrm{d}t^n} \mathrm{e}^{-\mathrm{i}\omega t}\Big|_{t=0}$

$$\begin{aligned} m_{AB}^{(n)} &= \frac{\mathrm{i}^n \hbar^n}{2\pi} \frac{\mathrm{d}^n}{\mathrm{d}t^n} \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\omega t}\, \tilde{c}_{AB}(\omega)\,\mathrm{d}\omega \Bigg|_{t=0} \\ &= \mathrm{i}^n \hbar^n \frac{\mathrm{d}^n}{\mathrm{d}t^n} c_{AB}(t) \Bigg|_{t=0} \\ &= \mathrm{i}^n \hbar^n \left\langle \frac{\mathrm{d}^n A}{\mathrm{d}t^n}(0)\, B \right\rangle \end{aligned}$$

## Sum Rules II

Inserting Heisenberg equation of motion

$$
\begin{aligned}
m_{AB}^{(n)} &= \mathrm{i}^n \hbar^n \left\langle \frac{\mathrm{d}^n A}{\mathrm{d}t^n}(0)\, B \right\rangle \\
&= \left\langle \left[ \cdots \left[ \cdots [A(t), H^{(0)}] \cdots , H^{(0)} \right] \cdots , H^{(0)} \right] B \right\rangle_{t=0} \\
&= \langle \mathcal{H}^n [A(t)]\, B \rangle = (-1)^k \left\langle \left( \mathcal{H}^j A \right) \left( \mathcal{H}^k B \right) \right\rangle
\end{aligned}
$$

where $\mathcal{H}[G] = [G(t), H]\,(0)$

## Sum Rules for Self-Correlation Functions (Bohigas et al. 1979)

$$
m_A^{(n)} = \frac{1}{2}(-1)^k \begin{cases} \langle [\mathcal{H}^j A, \mathcal{H}^k A] \rangle & n \text{ odd} \\ \langle \{\mathcal{H}^j A, \mathcal{H}^k A\} \rangle & n \text{ even} \end{cases} \qquad n = j + k
$$

## Estimates at Zero Temperature

Macroscopic occupation of ground state: $\rho \approx |0\rangle\langle 0|$

$$m_A^{(n)} = \sum_{i,j} (\hbar\omega_{ij})^n \, p_j \, |\langle i \,|\, A \,|\, j\rangle|^2$$
$$\approx \sum_i (\hbar\omega_{i0})^n \, |\langle i \,|\, A \,|\, 0\rangle|^2$$

- Interested in lowest contributing $\omega_{i0}$
- One summand $\Leftrightarrow$ only one excitation: $\hbar\omega_{2,0} = m_A^{(2)} \Big/ m_A^{(1)}$
- More summands:

$$(\hbar\omega_{\min})^k \underbrace{\sum_i (\hbar\omega_{i0})^j \, |\langle i \,|\, A \,|\, 0\rangle|^2}_{=m_A^{(j)}} \leq \underbrace{\sum_i (\hbar\omega_{i0})^n \, |\langle i \,|\, A \,|\, 0\rangle|^2}_{=m_A^{(n)}}$$

## Estimates at Zero Temperature – Résumé

- Estimates for lowest excitation frequency

$$(\hbar\omega_{\min})^k \leq m_A^{(j)} \Big/ m_A^{(n)} \qquad \text{with } k+j=n$$

- Estimate exact if only one excitation frequency exists
- Moments given via sum rules

$$m_A^{(j+k)} = \frac{1}{2}(-1)^k \begin{cases} \langle [\mathcal{H}^j A, \mathcal{H}^k A] \rangle & j+k \text{ odd} \\ \langle \{\mathcal{H}^j A, \mathcal{H}^k A\} \rangle & j+k \text{ even} \end{cases}$$

# III. Application to Ultracold Quantum Gases

$$H^{(0)} = H_{\text{kin}} + H_{\text{trap}} + H_{\text{int}}$$

$$H_{\text{kin}} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_i\,, \quad H_{\text{trap}} = \sum_{i=1}^{N} V(\mathbf{r}_i)\,, \quad H_{\text{int}} = \sum_{i=1}^{N}\sum_{j\,(>i)}^{N} U(\mathbf{r}_i - \mathbf{r}_j)$$

## Breathing Mode

Isotropic harmonic trap

$$V(\mathbf{r}_i) = \frac{1}{2} m \Omega_{\text{ho}}^2 \mathbf{r}_i^2$$

Modulation of trapping frequency

$$H_t^{(1)} = \frac{1}{2} m\, \Omega^2(t) \sum_{i=1}^{N} \mathbf{r}_i^2 = -f(t) M$$

## First Moment

$$m_M^{(1)} = \frac{1}{2} \left\langle \left[ \left[ M, H^{(0)} \right], M \right] \right\rangle \sim \left\langle \mathbf{r}^2 \right\rangle \sim \left\langle H_{\text{trap}} \right\rangle = E_{\text{trap}}$$

## Further moments

0. Moment $\sim \langle \mathbf{r}^4 \rangle$
1. *Moment* $\sim E_{\text{trap}}$
2. Moment $\sim 1 + \langle \mathbf{r} \cdot \boldsymbol{\nabla} \rangle + \langle (\mathbf{r} \cdot \boldsymbol{\nabla})^2 \rangle$
3. Moment Depends on interaction potential $U(\mathbf{r}_{ij})$

## Third Moment: Interaction Potentials

Consider interaction potentials $U(\mathbf{r}_{ij})$ :

$$U(\lambda \mathbf{r}_{ij}) = \lambda^n U(\mathbf{r}_{ij}) \quad \forall \lambda > 0 \qquad \text{(positive homogeneity)}$$

Examples

delta interaction $(n = -\mathcal{D})$ $U_\delta(\mathbf{r}_{ij}) = g\delta(\mathbf{r}_{ij})$

dipole-dipole interaction $(n = 3)$ $U_{\text{dd}}(\mathbf{r}_{ij}) = \mathbf{D}^2/\mathbf{r}_{ij}^3 - (\mathbf{D} \cdot \mathbf{r}_{ij})^2 / \mathbf{r}_{ij}^5$

## Third Moment: Result

For interaction potential positive homogenous of degree $n$

$$m_M^{(3)} = \frac{1}{2}\left\langle\left[\left[[A, H^{(0)}], H^{(0)}\right], [H^{(0)}, A]\right]\right\rangle \sim 4E_{\text{kin}} + 4E_{\text{trap}} + n^2 E_{\text{int}}$$

## Upper Bound for Breathing Mode Frequency

General result regarding contact and dipole-dipole interaction

$$(\hbar\omega_{\text{min}})^2 \leq m_M^{(3)} \Big/ m_M^{(1)} = \hbar^2\Omega_{\text{ho}}^2 \frac{4E_{\text{kin}} + 4E_{\text{trap}} + \mathcal{D}^2 E_\delta + 9E_{\text{dd}}}{2E_{\text{trap}}}$$

- Independent of underlying statistics (bosons, fermions, ...)
- Independent of modulation form $f(t)$
- Further simplification using virial identity
  $2E_{\text{kin}} - 2E_{\text{trap}} + \mathcal{D}E_\delta + 3E_{\text{dd}} = 0$

## Breathing Mode Frequency: Exact Limit

- Recall: Frequency estimate exact if $\langle j|M|0\rangle \neq 0$ for only one $j$
- Direct calculation of matrix element for bosons and fermions with $H_{\text{int}} = 0$ verifies that

Results are exact in the non-interacting case!

## Bose Gas: Breathing Mode Frequency

Using virial identity the upper bound $\tilde{\omega}$ reads

$$\omega_{\text{min}}/\Omega_{\text{ho}} \leq \sqrt{5 - E_{\text{kin}}/E_{\text{trap}}} = \tilde{\omega}$$

Interested in dependence on interaction strength $P$. Limits:

$P \to 0$ Then $E_{\text{kin}} = E_{\text{trap}}$ and $\tilde{\omega} = 2$

$P \gg 1$ Then $E_{\text{kin}} \to 0$ and $\tilde{\omega} = \sqrt{5}$ (Thomas–Fermi limit)

## Bose Gas: Mean-Field Approach

- Gross–Pitaevskii equation, obtained by minimizing Langrange density $\mathcal{L}(|\Psi|^2) = -E(|\Psi|^2)$
- Variational approach: Approximative solution from minimizing $\mathcal{L}$ with Gaussian trial function with width parameter $\xi$
- Also suited to implement time dependence

## Bose Gas: Breathing Mode Frequency

Variational approach gives expressions for $E_{\text{kin}}$ and $E_{\text{trap}}$

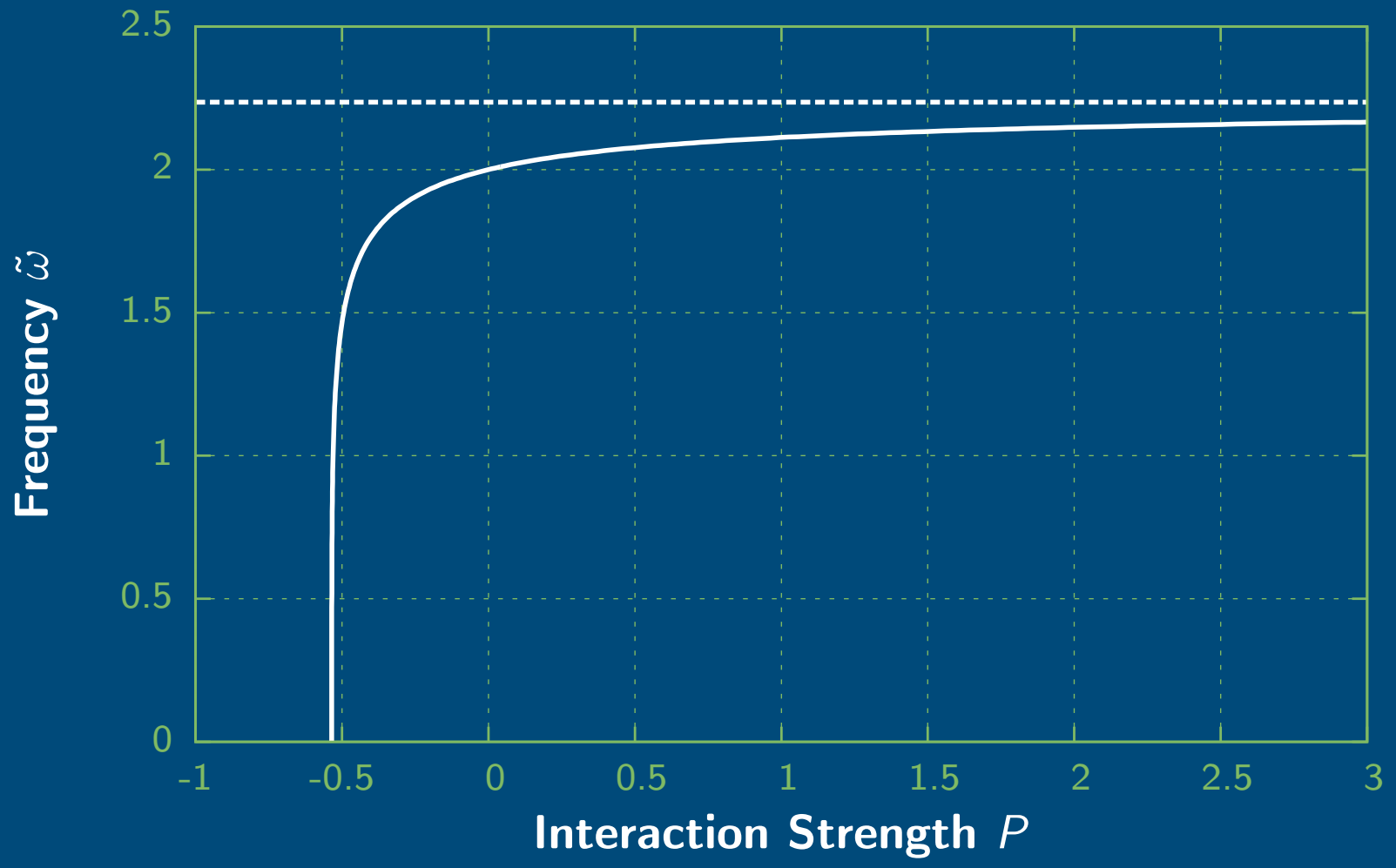
$$\tilde{\omega} = \sqrt{5 - E_{\text{kin}}/E_{\text{trap}}} = \sqrt{5 - \xi^{-4}}$$

Minimization gives defining equation for $\xi$:

$$\xi^2 - \xi^{-2} - P\xi^{-3} = 0 \qquad (\star)$$

- Equation $(\star)$ is equivalent to virial identity
- Same result as with time dependent variational approach

# Bose Gas: Breathing Mode Frequency (Stringari 1996)



## Dipolar Fermi Gas: Breathing Mode Frequency

- Variational ansatz with Heaviside theta as Wigner function
- Variational parameters $R_{x,z}$ and $K_{x,z}$ for density and momentum distribution

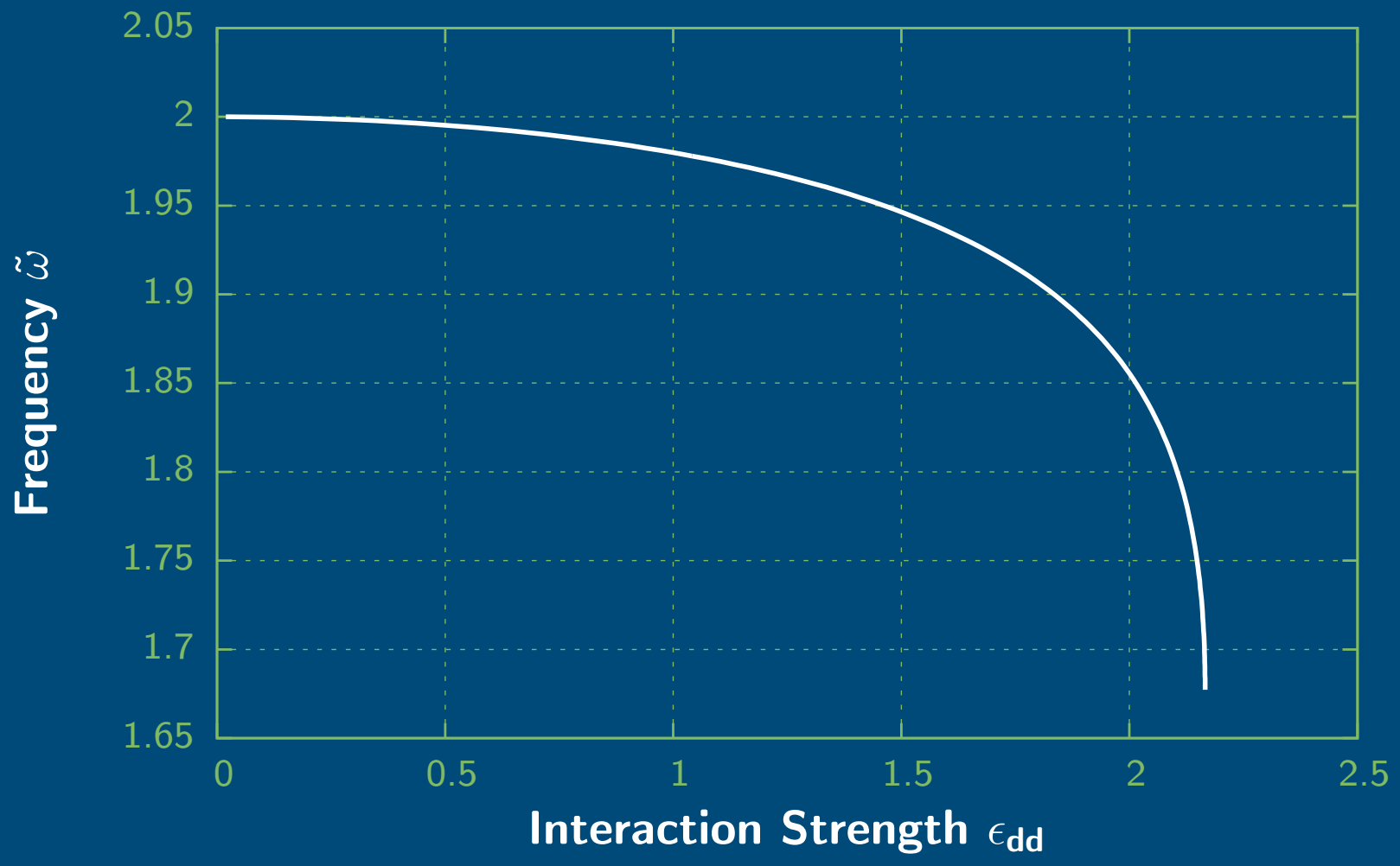
(Lima and Pelster 2010)

$$\nu_0(\mathbf{x}, \mathbf{k}) = \Theta\left(1 - \sum_{j=1}^{\mathcal{D}} \frac{x_j^2}{R_j^2} - \sum_{j=1}^{\mathcal{D}} \frac{k_j^2}{K_j^2}\right)$$

With expressions for $E_{\text{kin}}$ and $E_{\text{trap}}$ (Sogo et al. 2009)

$$\tilde{\omega} = \sqrt{5 - E_{\text{kin}}/E_{\text{trap}}} = \sqrt{5 - \frac{K_x^2\left[2 + (K_z/K_x)^2\right]}{R_z^2\left[1 + 2(R_x/R_z)^2\right]}}$$

# Fermi Gas: Breathing Mode Frequency



## Outlook

- Different excitation modes
- Anisotropic trapping potentials
- Collective modes for modulated interaction strength (Pollack et al. 2010)
- Boson-fermion mixed condensate (Miyakawa et al. 2000)
- Spin-orbit coupled quantum gas (Li et al. 2012)

**Thank you for your attention**

**Questions?**

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