Soft-Potential supersolids.

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Outline

- Soft Disk (SD) bosons:

  a) Methodology

  b) Motivation

  c) Qualitative phase diagram, incl. supersolidity.

  d) Excitation spectrum
- Conclusions

Path Integral Monte Carlo

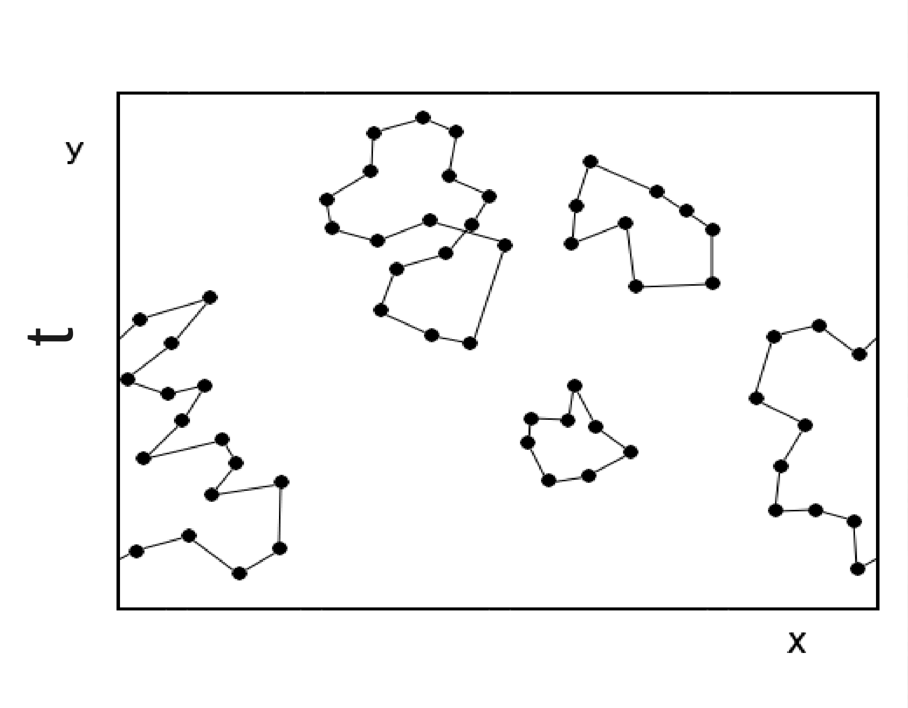
$$\langle O\rangle=\frac{Tr(\rho O)}{Tr(\rho)} \qquad R_i=(\boldsymbol{r}_i^1,\boldsymbol{r}_i^2,\dots,\boldsymbol{r}_i^N) \qquad \lambda=\frac{\hbar^2}{2\mathrm{m}} \quad \beta=\frac{1}{K_b T} \quad \tau=\frac{\beta}{M}$$

$$\rho(R_0,R_M;\beta)=\langle R_0|e^{-\beta H}|R_M\rangle=\lim_{M\to\infty}\int dR_1,\dots,dR_{M-1}\,A(R_0,\dots,R_M,\tau)$$

$$A(R_0,\dots,R_M,\tau)=(4\pi\lambda\tau)^{-3\mathrm{NM}/2}\exp\left(-\sum_{m=1}^{M}\left[\frac{(R_{m-1}-R_m)^2}{4\lambda\tau}+\tau U(R_m)\right]\right)$$

- Most properties can be extracted fixing $R_0=R_M=R$
- Sampling through Metropolis Algorithm.

$$\rho_B(R_0,R_M;\beta)=\frac{1}{N!}\sum_P \rho(R_0,P(R_M);\beta)$$



DM Ceperley - Reviews of Modern Physics, 1995

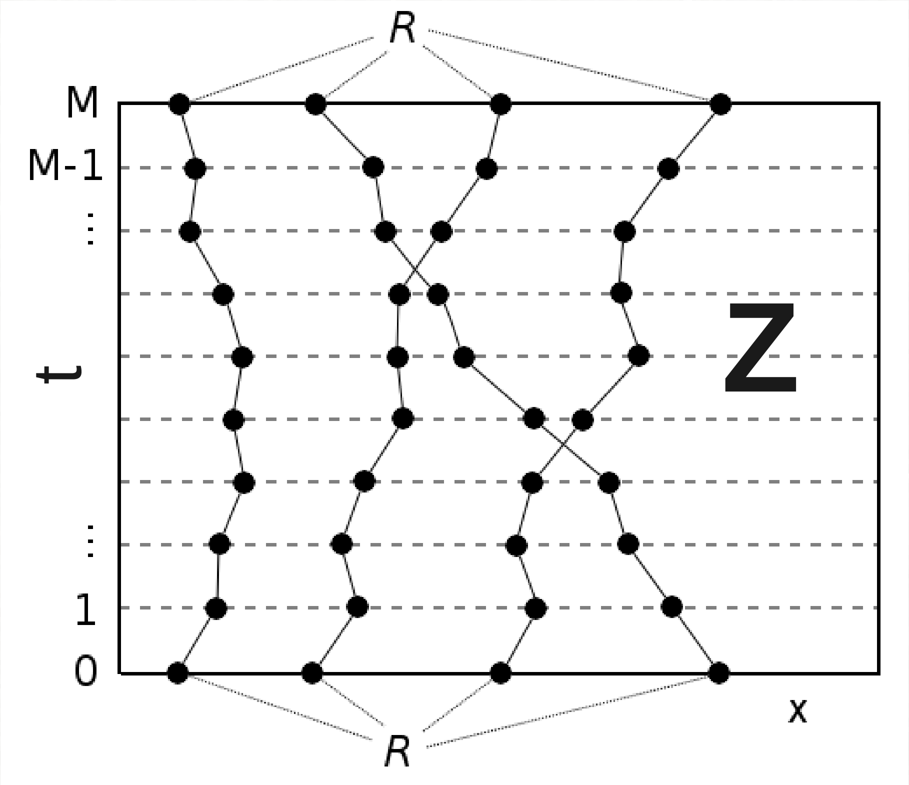
Worm Algorithm

- Path integral Monte Carlo living in an extended space:

  Z sector: closed configurations.

  G sector: one open world line (worm).

- Permutations are sampled through G sector.



M. Boninsegni, N. V. Prokof’ev, and B. V. Svistunov, Phys. Rev. E, 74, 036701, 2006.

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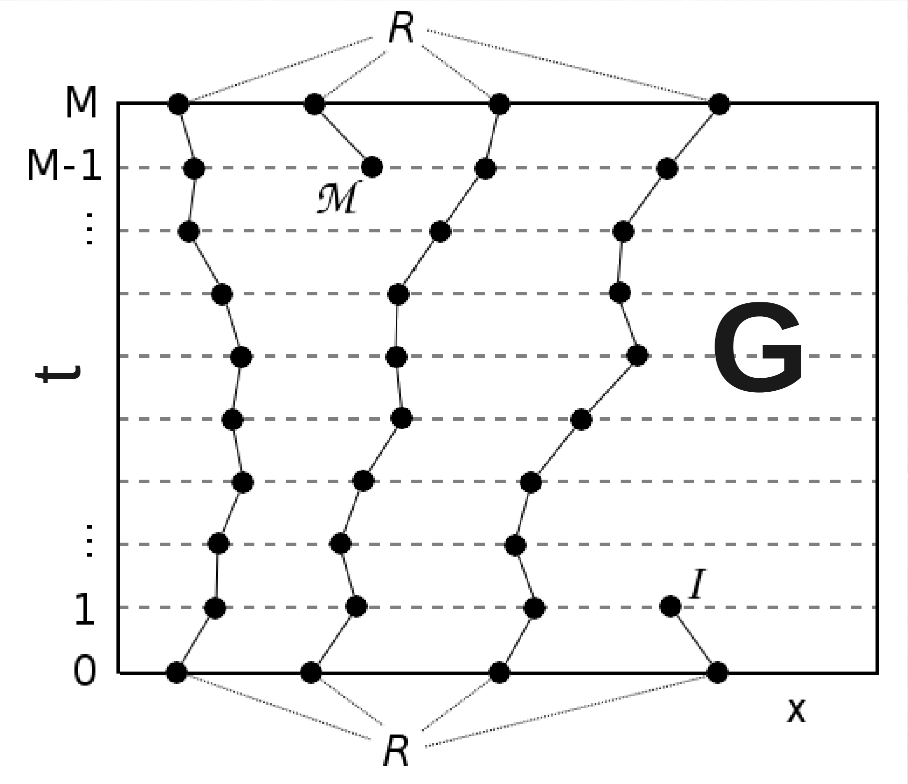


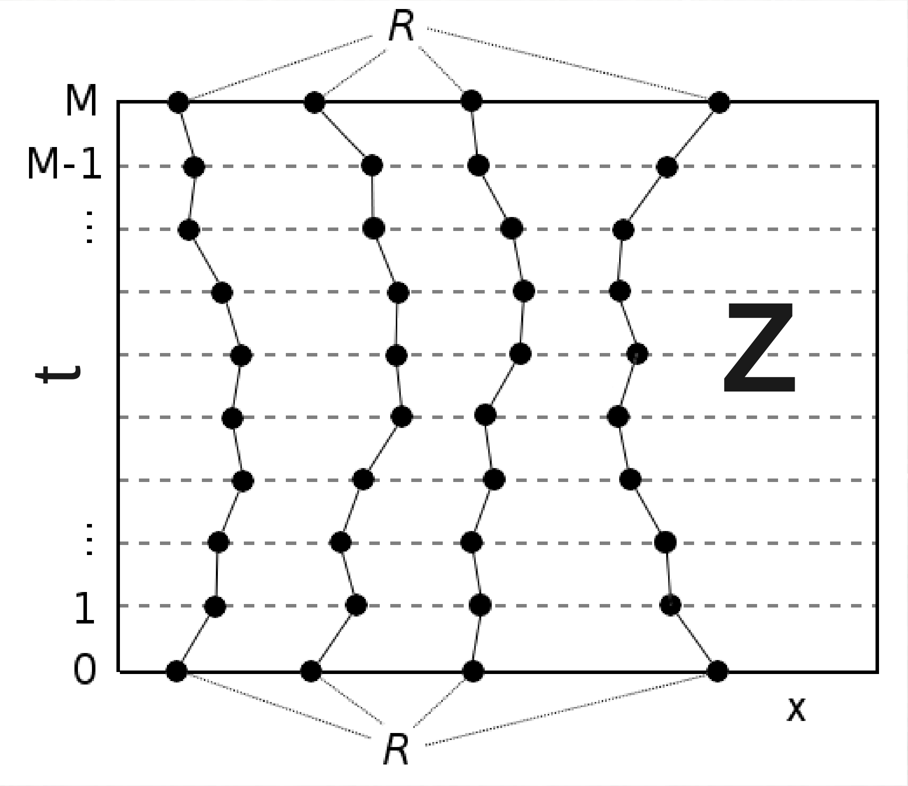
M. Boninsegni, N. V. Prokof’ev, and B. V. Svistunov, Phys. Rev. E, 74, 036701, 2006.

Worm Algorithm

- Defined in the grand canonical ensemble:

$$A(R_0,\ldots,R_M,\tau)=(4\pi\lambda\tau)^{-3NM/2}\exp\left(-\sum_{m=1}^{M}\left[\frac{(R_{m-1}-R_m)^2}{4\lambda\tau}+\tau(U(R_m)-\mu N_m)\right]\right)$$

- Set of local Metropolis MC moves acting mainly on I and $\mathcal{M}$.



M. Boninsegni, N. V. Prokof’ev, and B. V. Svistunov, Phys. Rev. E, 74, 036701, 2006.

Worm Algorithm

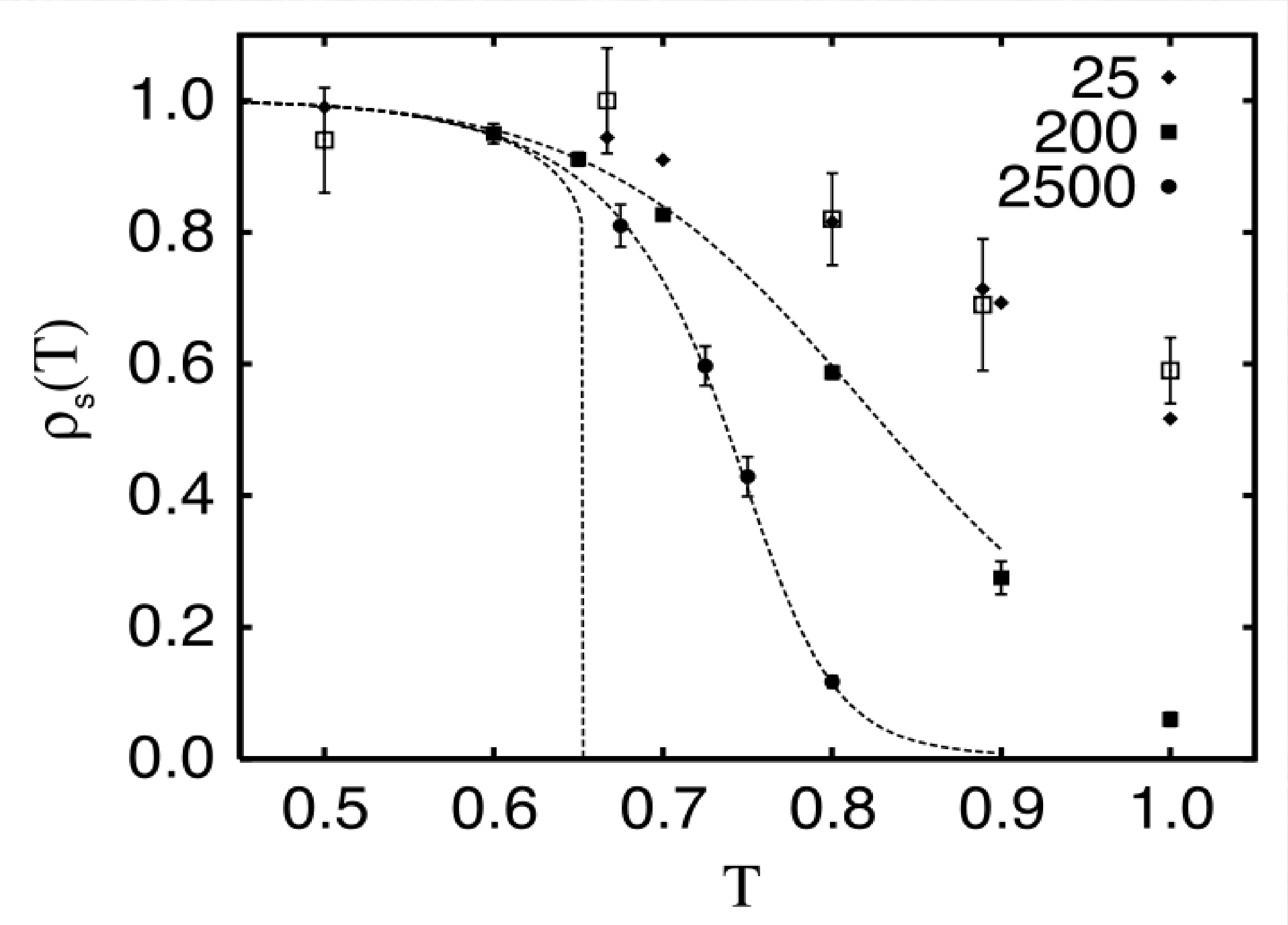
Much more efficient permutation sampling.

$$\rho_s = \frac{m}{\hbar^2} \frac{\langle |\boldsymbol{W}|^2 \rangle L^{2-d}}{\rho^2 \beta d}$$

Dimensionality: d.

Cell side: L.

Winding number: $\boldsymbol{W}=(W_1,..,W_d)$.



M. Boninsegni, N. V. Prokof'ev, and B. V. Svistunov, Phys. Rev. E, 74, 036701, 2006.

Supersolidity

- Order parameters:

Solidity

$$\rho_{\boldsymbol{k}}=\sum_{i<N} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_i} \qquad S(\boldsymbol{k})=\frac{1}{2\pi N}\langle\rho_{\boldsymbol{k}}\rho_{-\boldsymbol{k}}\rangle$$

Superfluid fraction

$$\rho_s=1-\frac{I_e}{I_c}$$

Penrose, O., and L. Onsager, 1956, Phys. Rev. 104, 576.

Gross, E. P., 1957, Phys. Rev. B 106, 161.

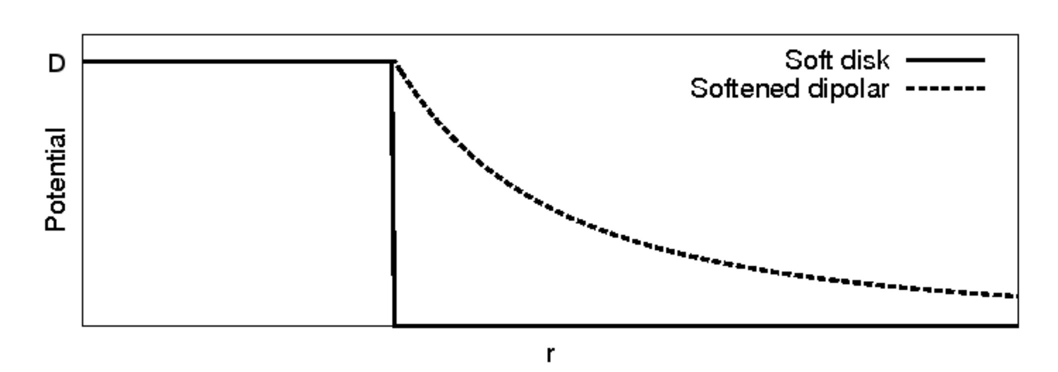
Leggett, A. J., 1970, Phys. Rev. Lett. 25, 1543.

Kim, E., and M. H. W. Chan, 2004a, Nature 427, 225.

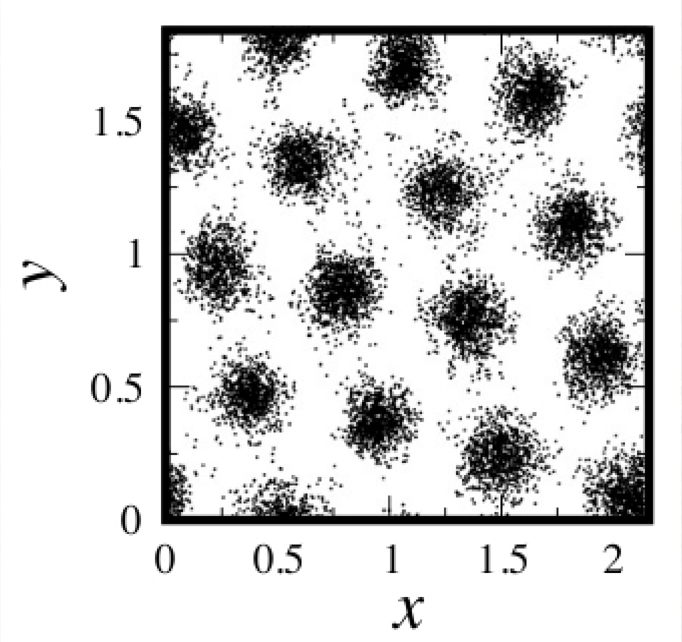
Lattice models

Soft Disks: motivation

Prototype for a class of systems displaying supersolidity.



F. Cinti et al., Phys. Rev. Lett., 105, 135301, 2010.



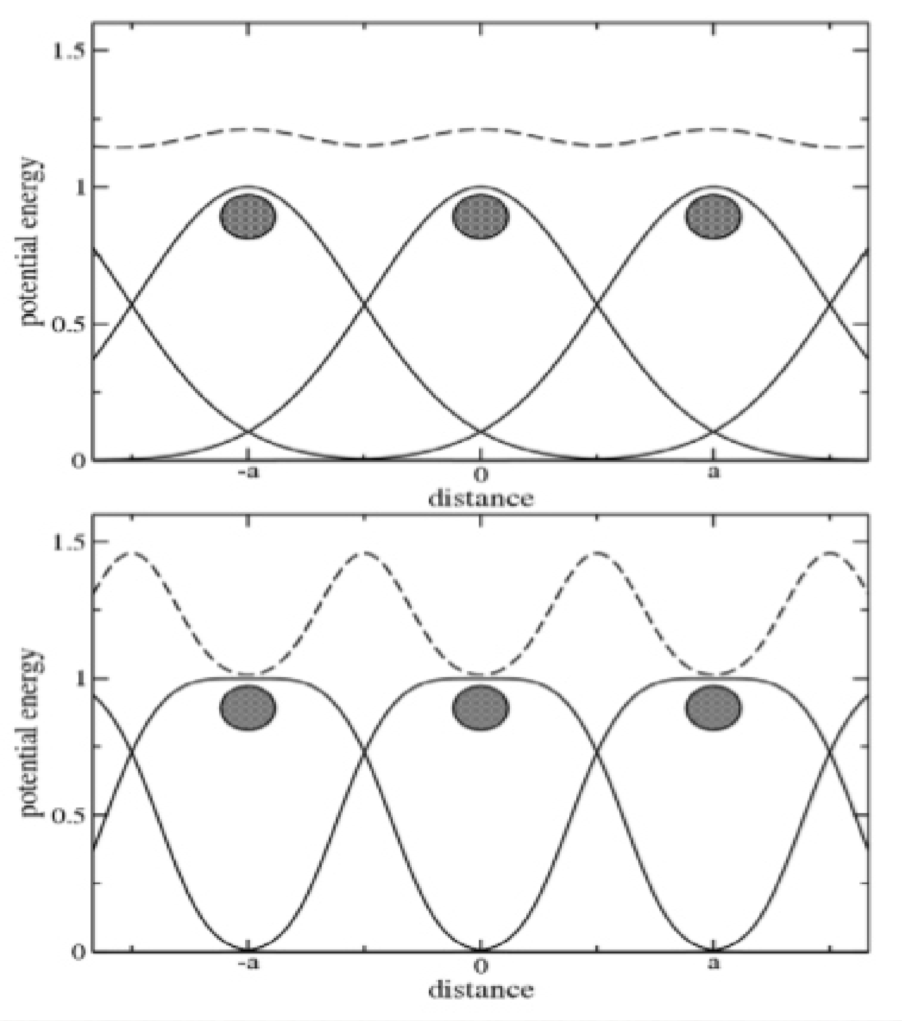
Quantum version of classical systems displaying cluster phases.

Bianca M Mladek et all. Phys. Rev. Lett., 99, 235702, 2007.

Bianca M Mladek et al., J. Phys.: Condens. Matter 20 (2008) 49424

C. N. Likos et al., Phys. Rev. E, 63,031206, 20015

Clustering



- System develops a barrier between clusters due to overlapping potentials *V*(***r***).

Bianca M Mladek et al., J. Phys.: Condens. Matter 20 (2008) 494245

- Clustering at high density if *V*(***q***)<*0* for some ***q***.

C. N. Likos et al. Phys. Rev. E, 63,031206, 2001

Soft Disks: Simulations

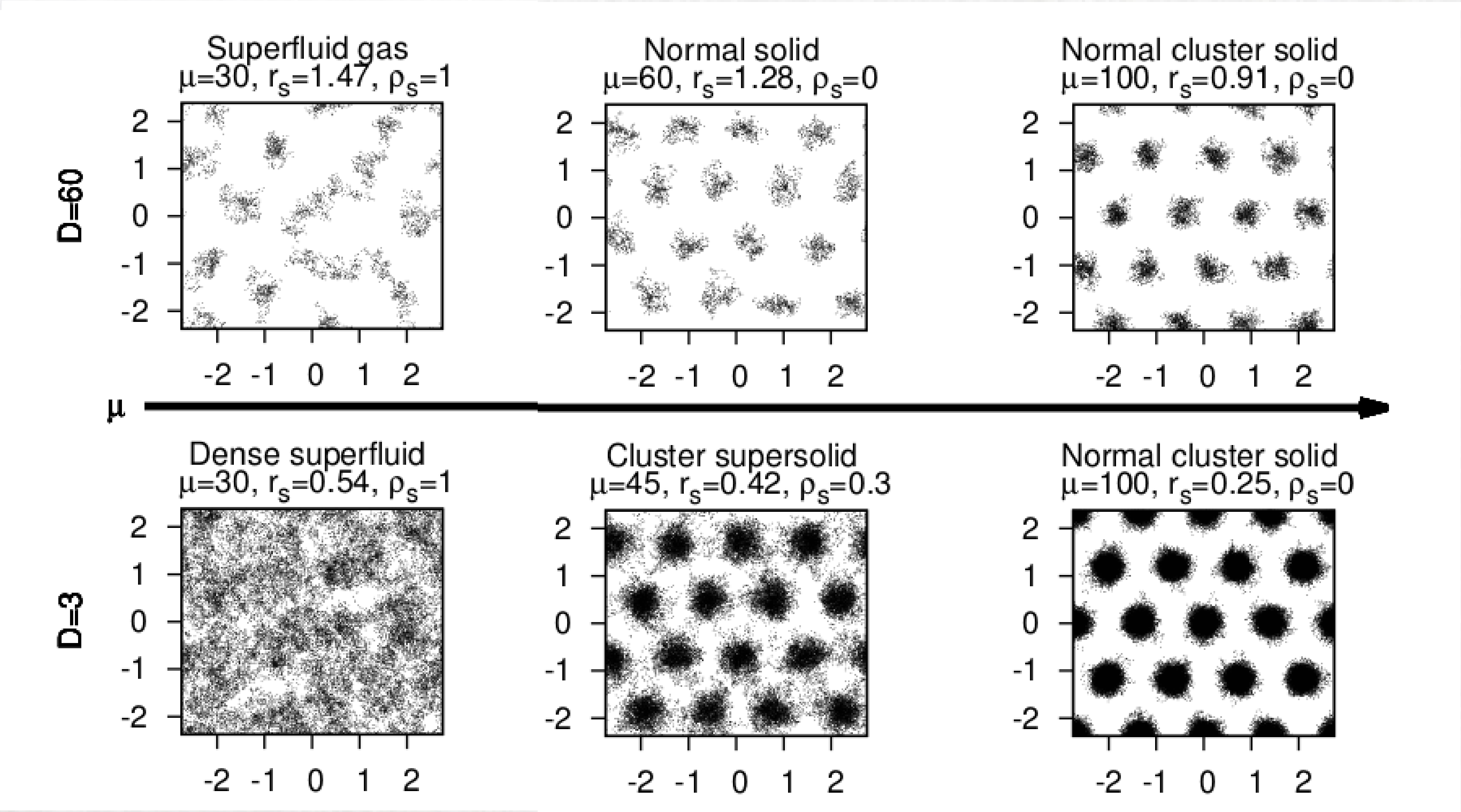
$$H = -\frac{\hbar^2}{2\mathrm{m}} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j} v(\boldsymbol{r_{ij}})$$

$$v(\boldsymbol{r_{ij}}) = \begin{cases} D & if \;\; r \leqslant 1 \\ 0 & if \;\; r > 1 \end{cases}$$

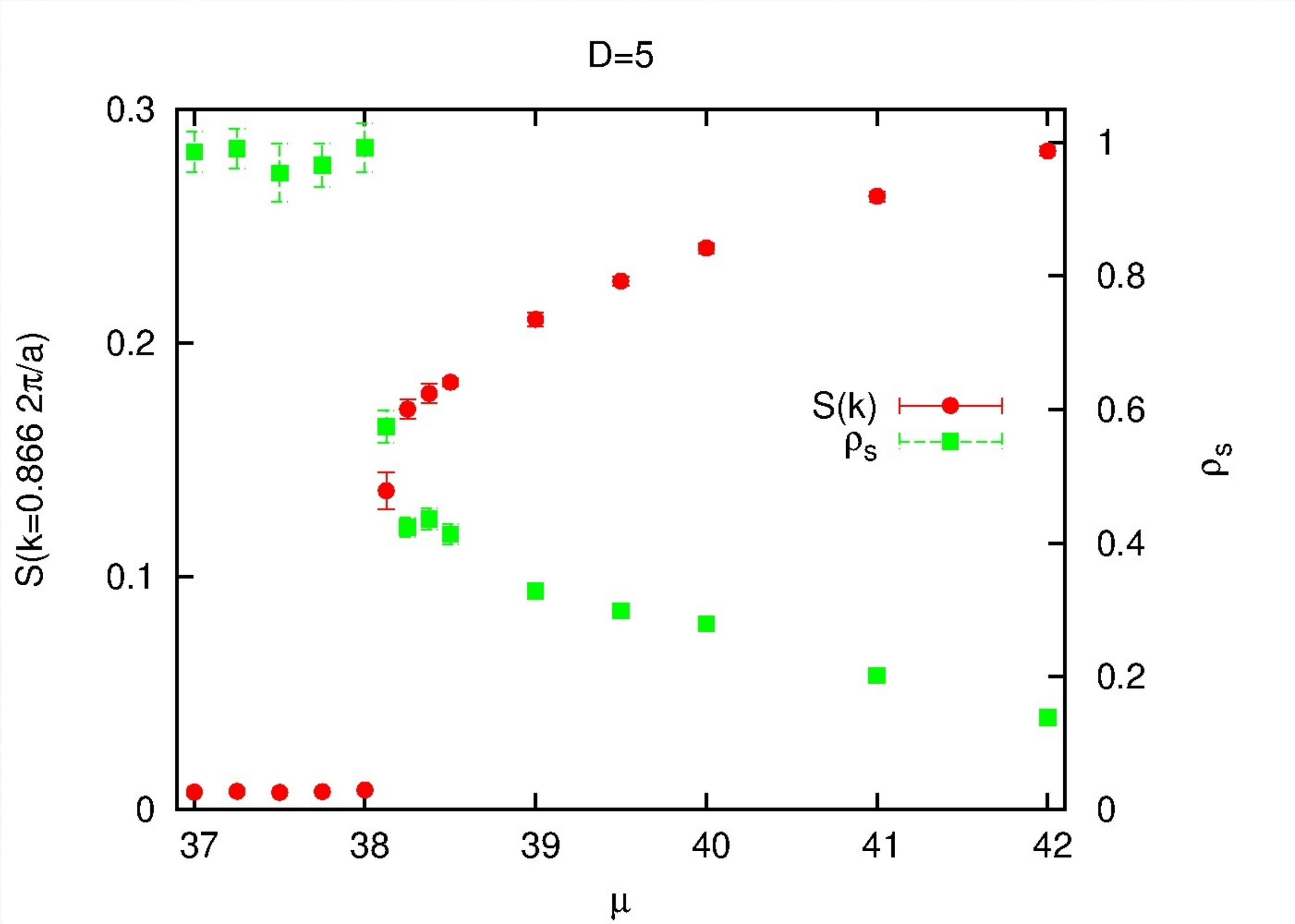
$$\frac{\hbar^2}{m} = 1$$

- Simulations performed using worm algorithm, a finite T, exact QMC technique.
- PBC, in a cell $L(1, \sqrt{3}/2)$.
- Grand-canonical (T,V,μ) ensemble.

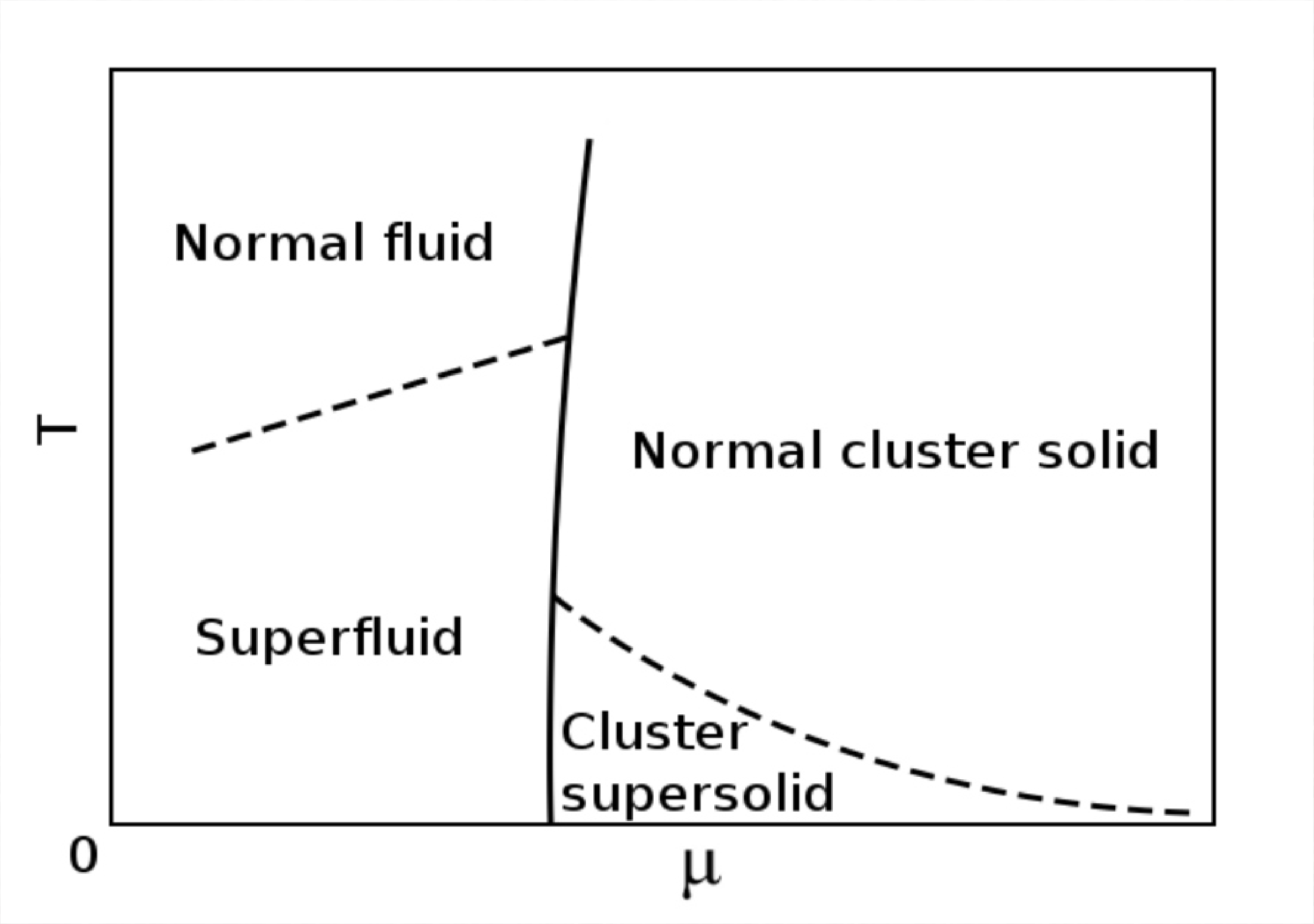
Soft Disk: low T



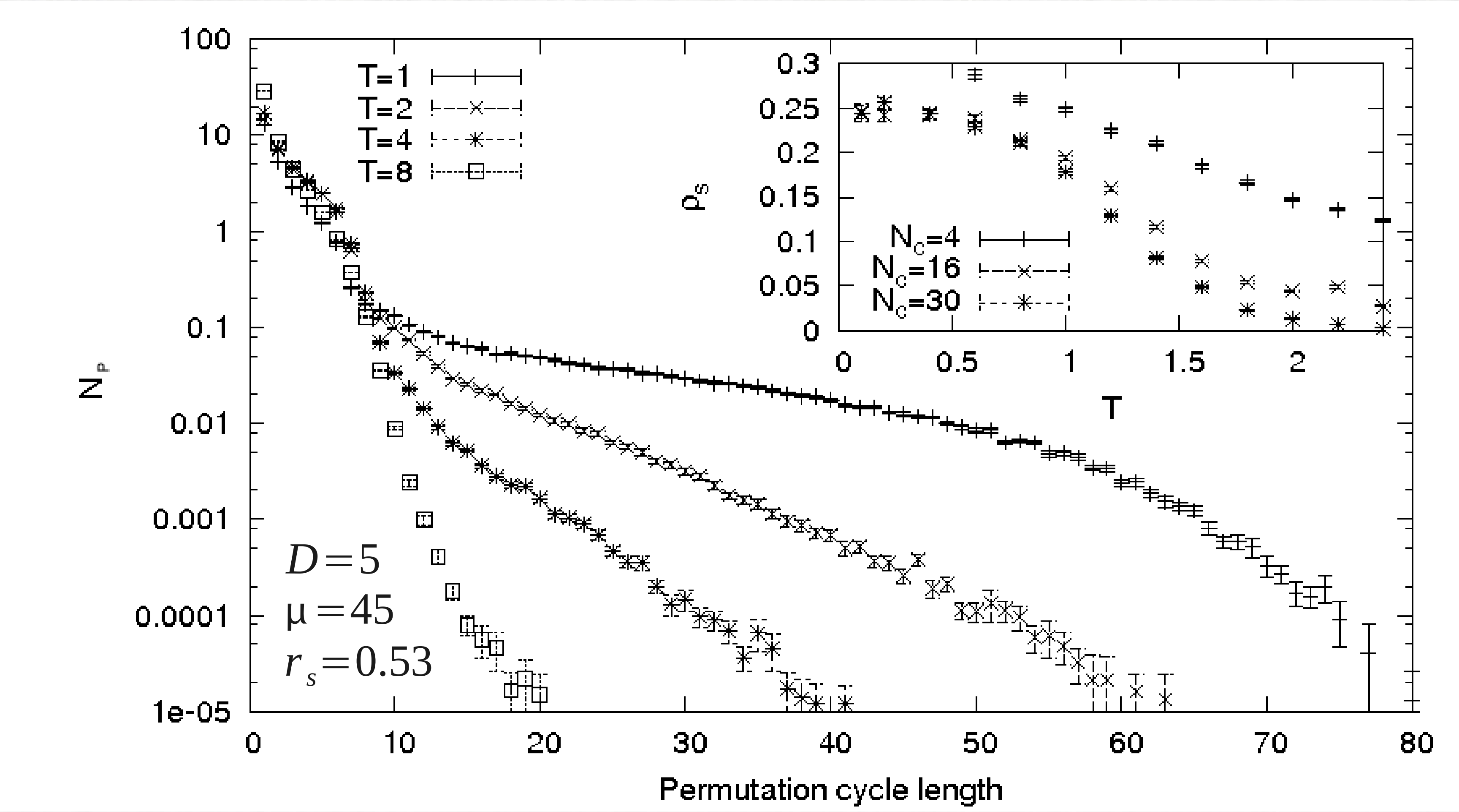
Order parameters



Soft Disk: Low D phase diagram



Supersolidity: exchange cycles



Excitation Spectrum: Quantum case

- Calculated from imaginary time density-density correlation function.

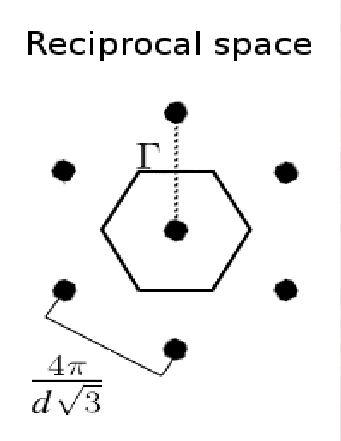
$$F(\boldsymbol{k},t)=\frac{Tr\left(\rho_{-\boldsymbol{k}}e^{-tH}\rho_{\boldsymbol{k}}e^{-(\beta-t)H}\right)}{N\,Tr(\rho)} \qquad \rho_{\boldsymbol{k}}=\sum_{i<N}e^{i\boldsymbol{k}\cdot\boldsymbol{r}_i} \qquad F(\boldsymbol{k},t)=\int_{-\infty}^{\infty}d\omega\, e^{-t\omega}S(\boldsymbol{k},\omega)$$

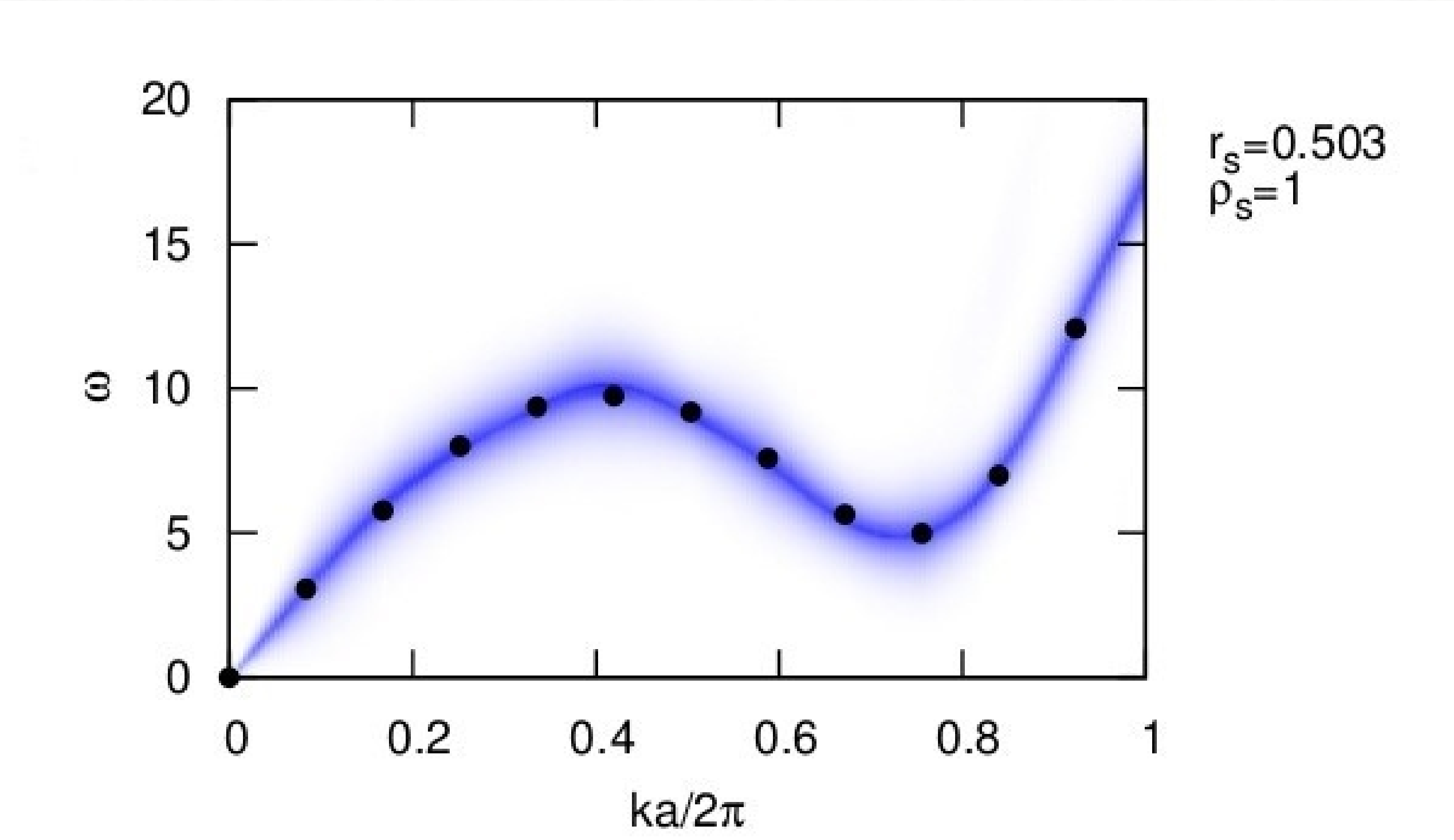
- The inverse Laplace is an ill-conditioned problem.
- Inversion performed using GIFT algorithm.

E. Vitali, M. Rossi, L. Reatto, and D. E. Galli, Phys. Rev. B 82, 174510

Excitation Spectrum

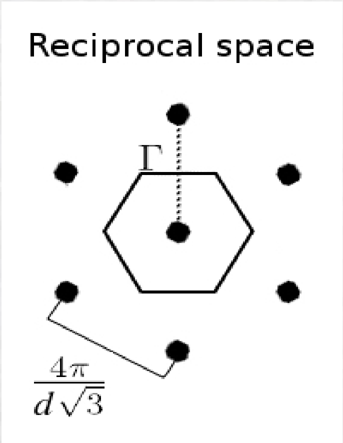
Superfuid

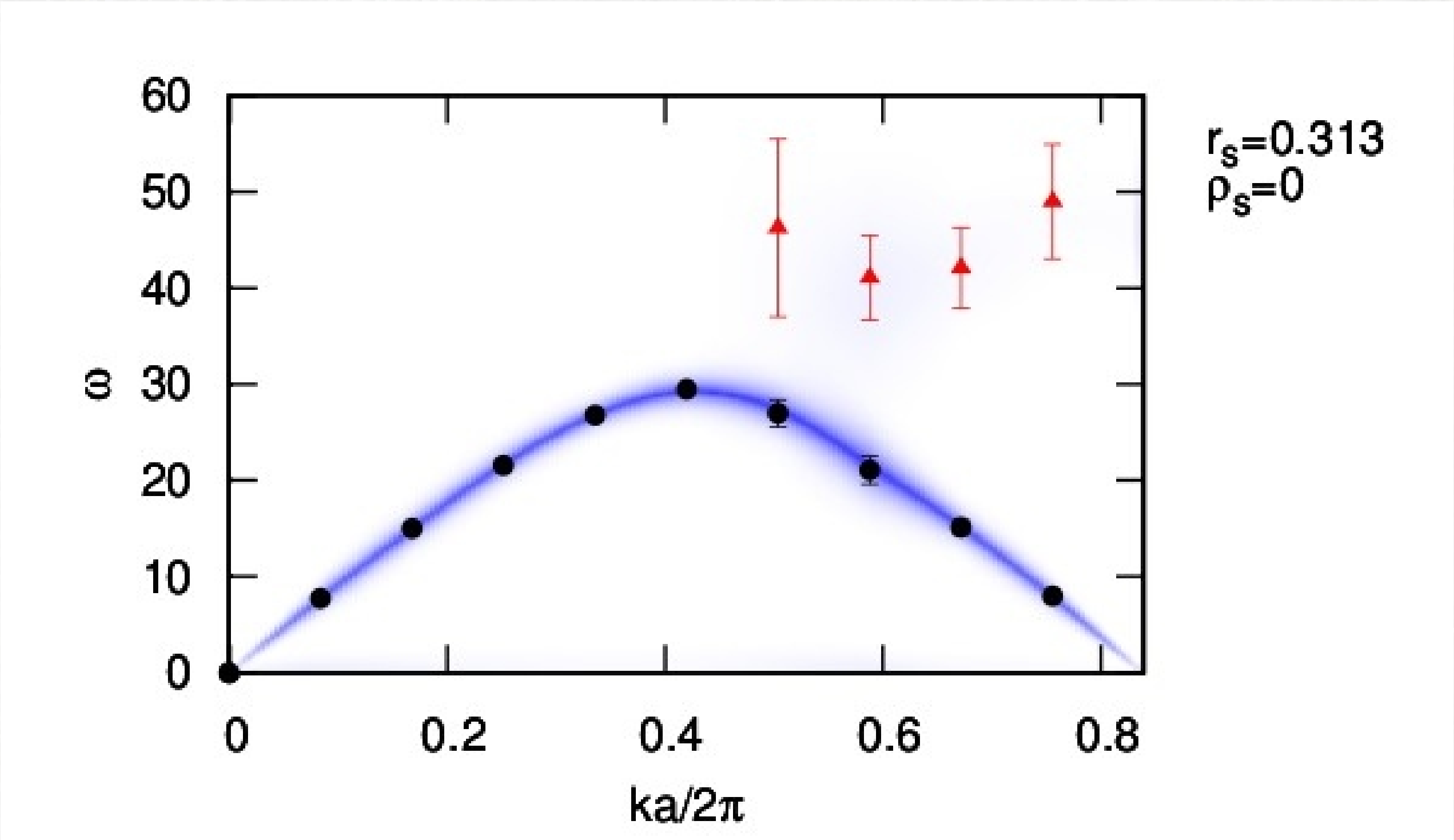




Excitation Spectrum

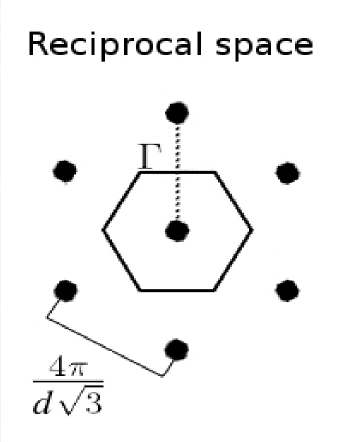
Normal cluster solid

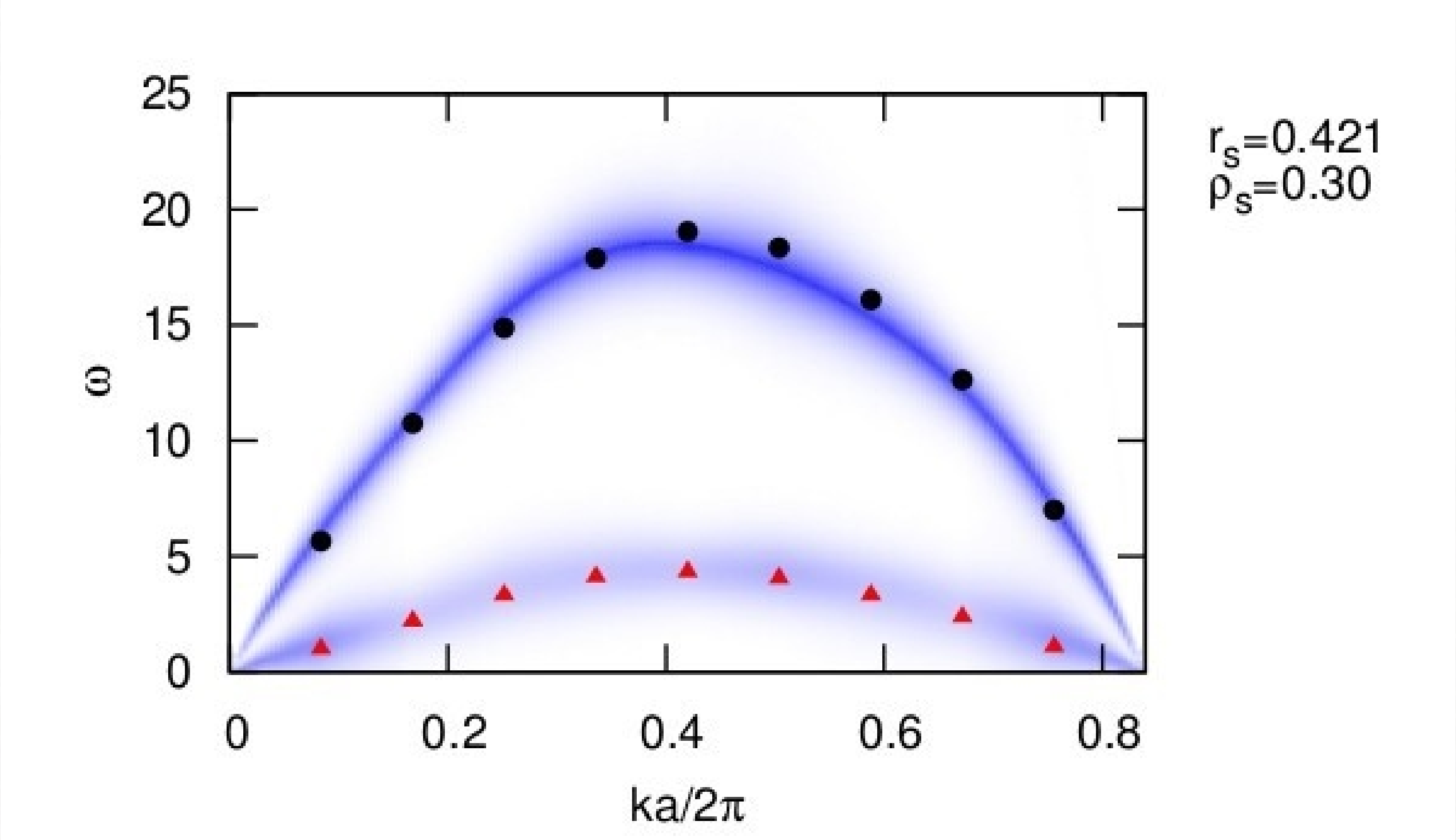




Excitation Spectrum

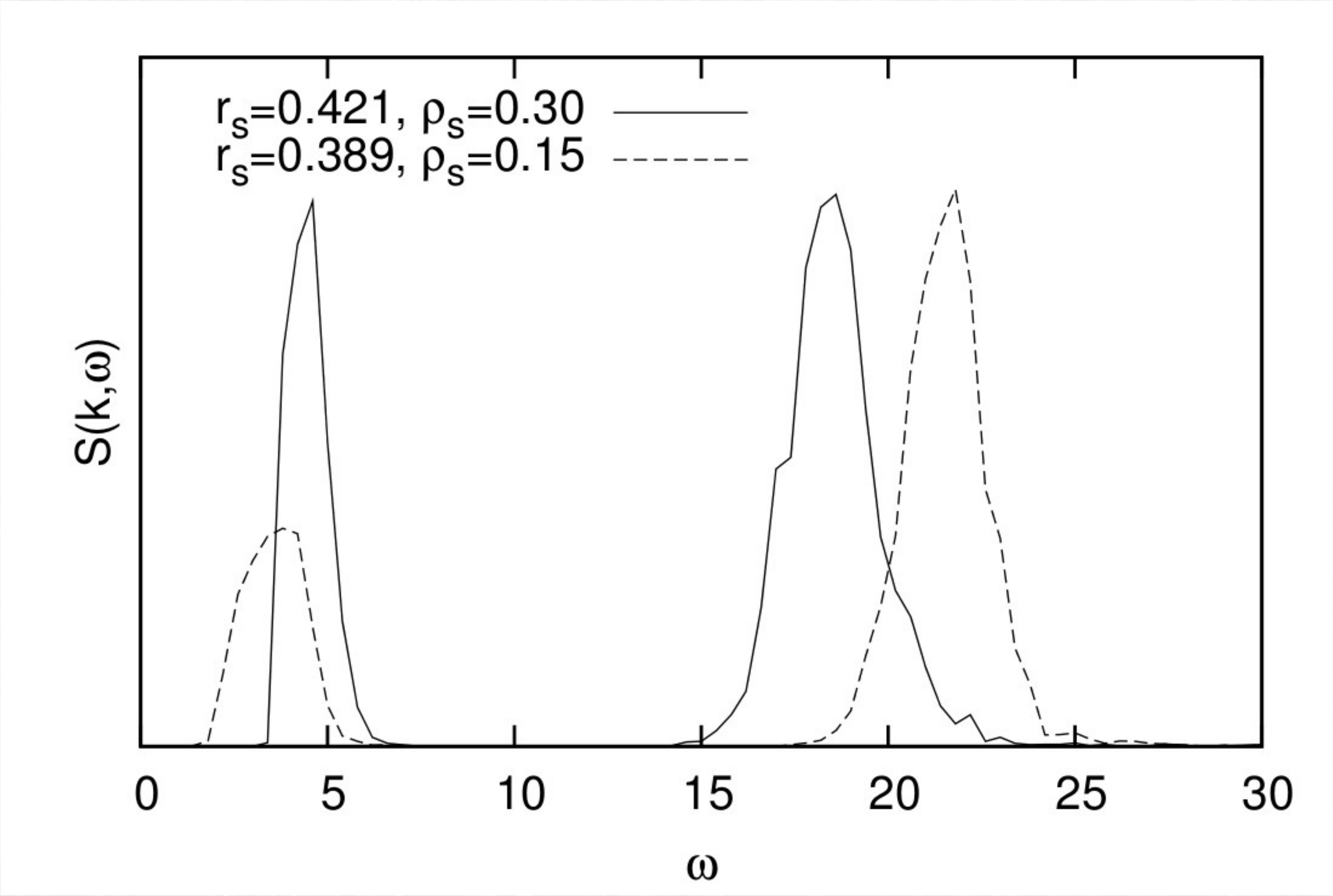
Supersolid





Excitation Spectrum

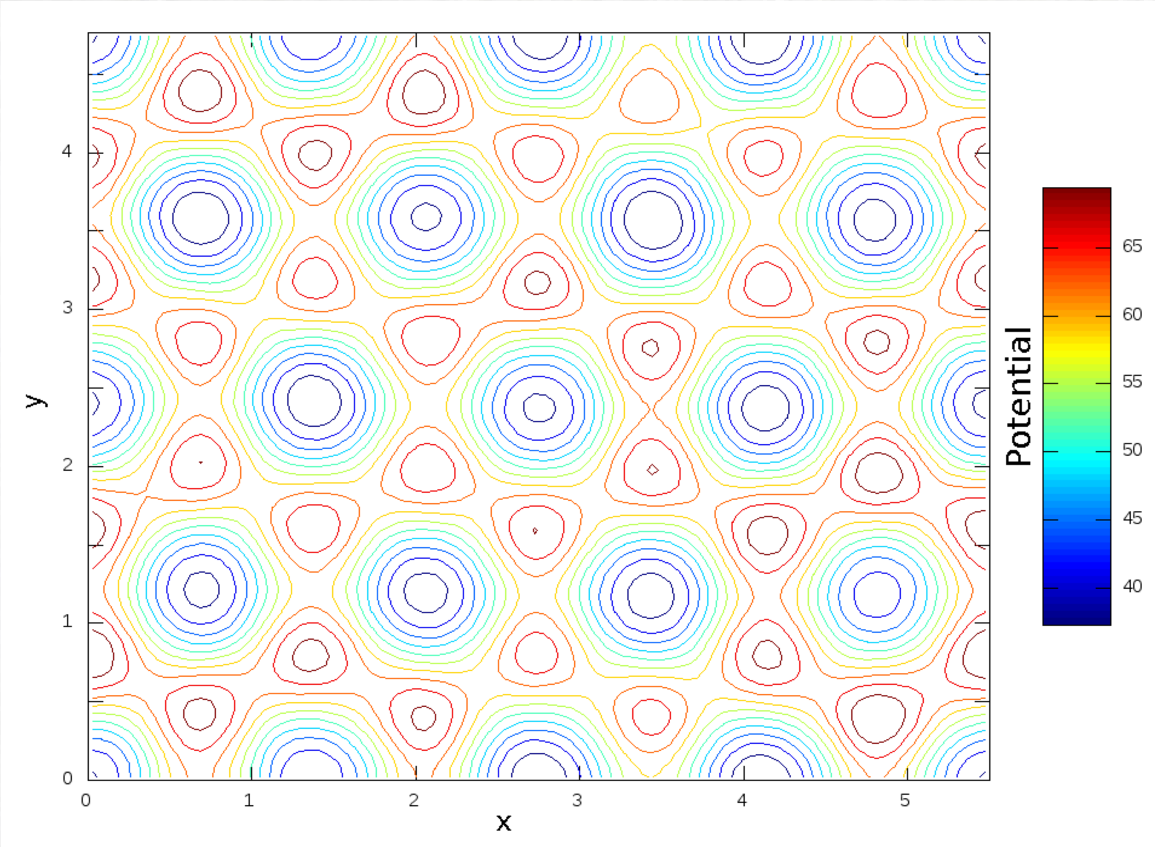
Supersolid peak shifts toward lower energies as superfluidity decreases.

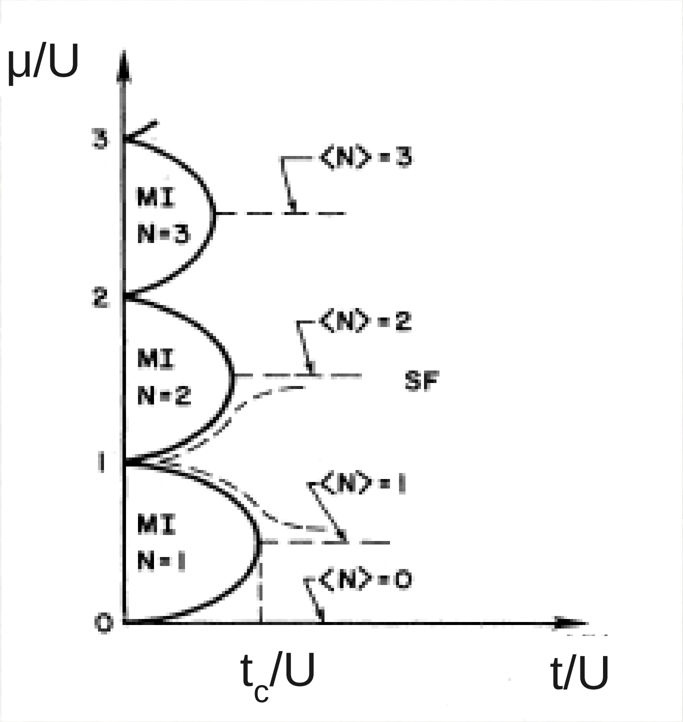


Lattice model

- Interacting bosons on a lattice: BH model.

$$H = -t \sum_{\langle i,j \rangle} \left(b_i^\dagger b_j + b_j^\dagger b_i \right) + \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right) - \mu \sum_i \hat{n}_i$$





Matthew P. A. Fisher et al., Phys. Rev. B 40, 546 (1989)

Conclusions

- A soft core bosons system in 2D has been characterized.
- A supersolid phase was observed.
- Excitation spectrum of the system was investigated.

Outlook

- Investigate properties of the system at intermediate D.
- Hard core.

Thank you for the attention

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•F. Cinti, P. Jain, M. Boninsegni, A. Micheli, P. Zoller, and G. Pupillo. Phys. Rev. Lett., 105, 135301, 2010.

•Bianca M Mladek, Patrick Charbonneau, and Daan Frenkel. Phys. Rev. Lett., 99, 235702, 2007.

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•C. N. Likos, A. Lang, M. Watzlawek, and H. L uwen. Phys. Rev. E, 63,031206, 2001

•A. J. Leggett, Phys. Rev. Lett. 25, 1543, 1970

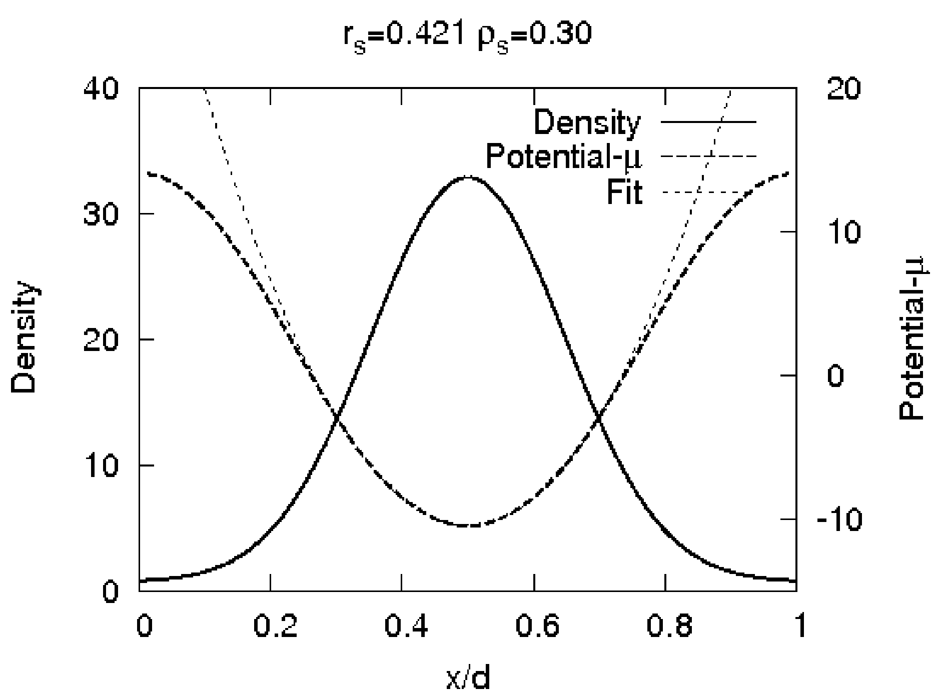
•E. Vitali, M. Rossi, L. Reatto, and D. E. Galli, Phys. Rev. B 82, 174510

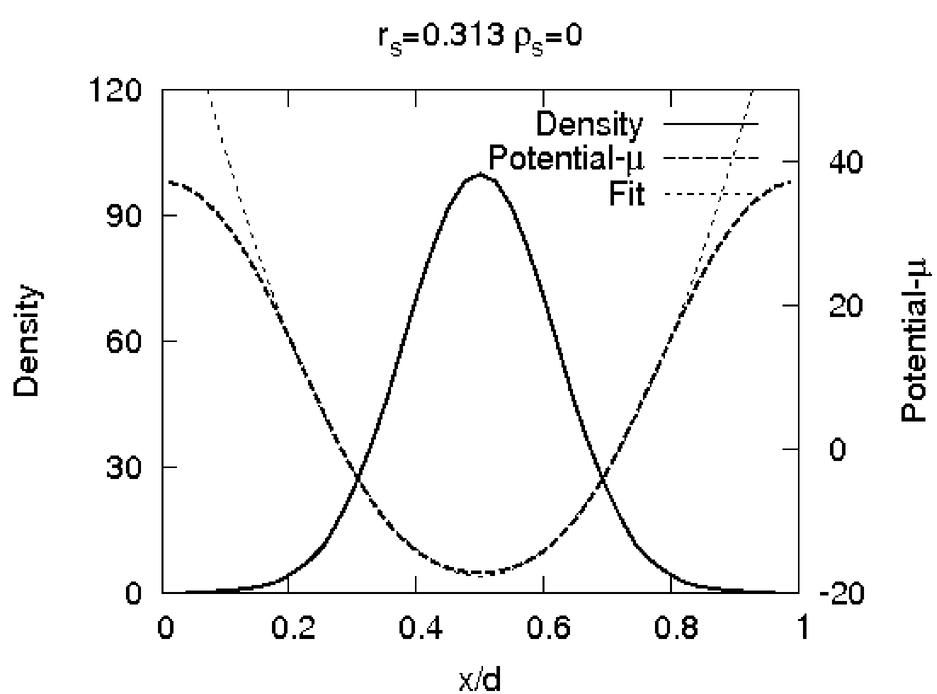
•Tim Neuhaus, Christos N. Likos, J. Phys.: Condens. Matter, 23, 234112 (2011).

•Matthew P. A. Fisher et al., Phys. Rev. B 40, 546 (1989)

Density and Potential

Felt by a test particle added to the system.





Density profile

Legget bound relates the density to superfluid fraction.

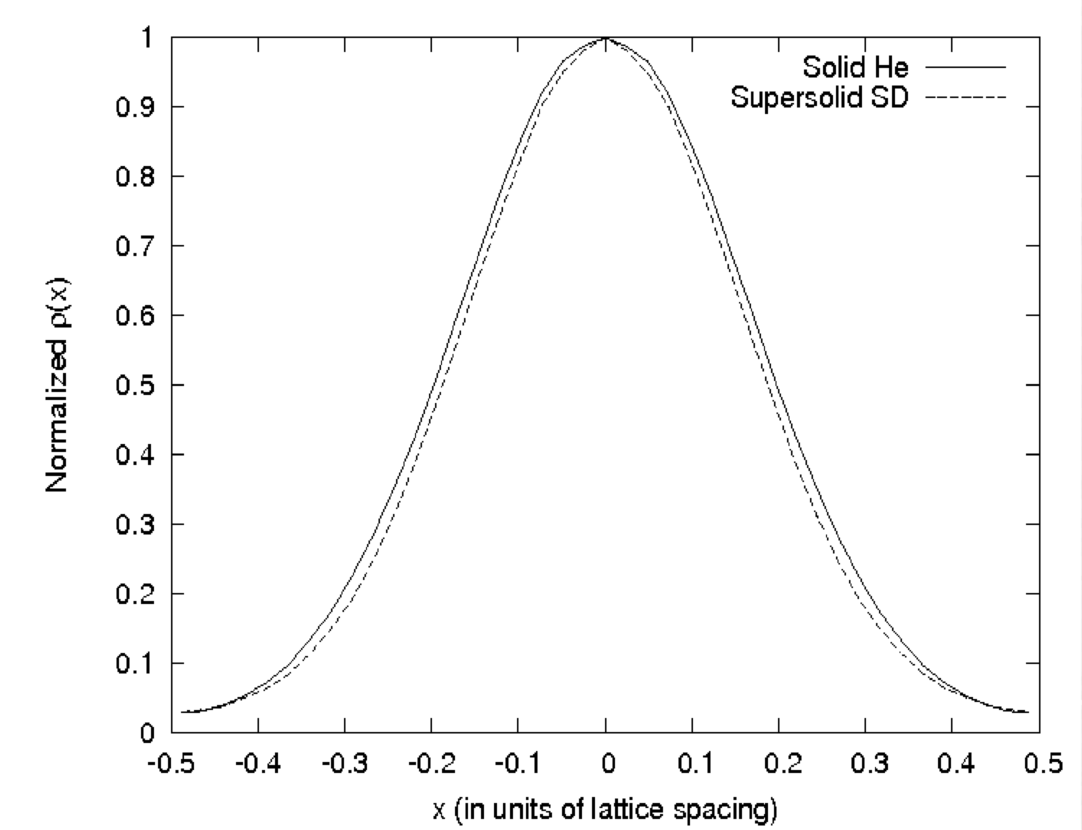
$$\rho_s \leqslant \min_{v_s(\boldsymbol{r})} \frac{1}{V\,\rho\,v_0^2} \int \rho(\boldsymbol{r}) |\boldsymbol{v}_s(\boldsymbol{r})|^2 \, d\boldsymbol{r}$$

$$\boldsymbol{v}_s(\boldsymbol{r}) = \left(\frac{\hbar}{m}\right) \nabla \varphi(\boldsymbol{r})$$

$$\varphi(\boldsymbol{r}+\boldsymbol{L}) = \varphi(\boldsymbol{r}) + 2\pi n$$

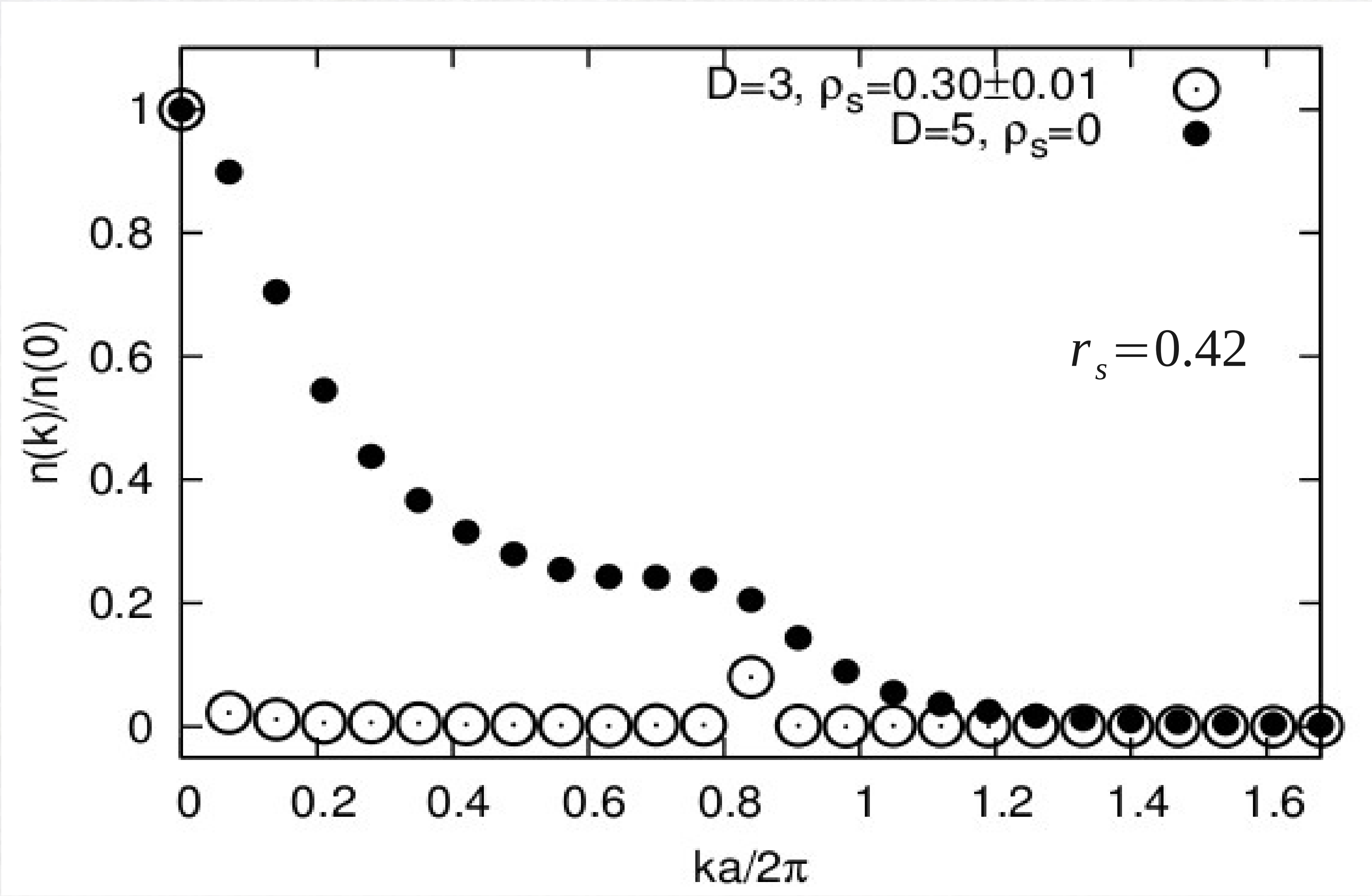
$$v_0 = \langle \boldsymbol{v}_s(\boldsymbol{r}) \rangle_V$$

$$\rho = \langle \rho(\boldsymbol{r}) \rangle_V$$

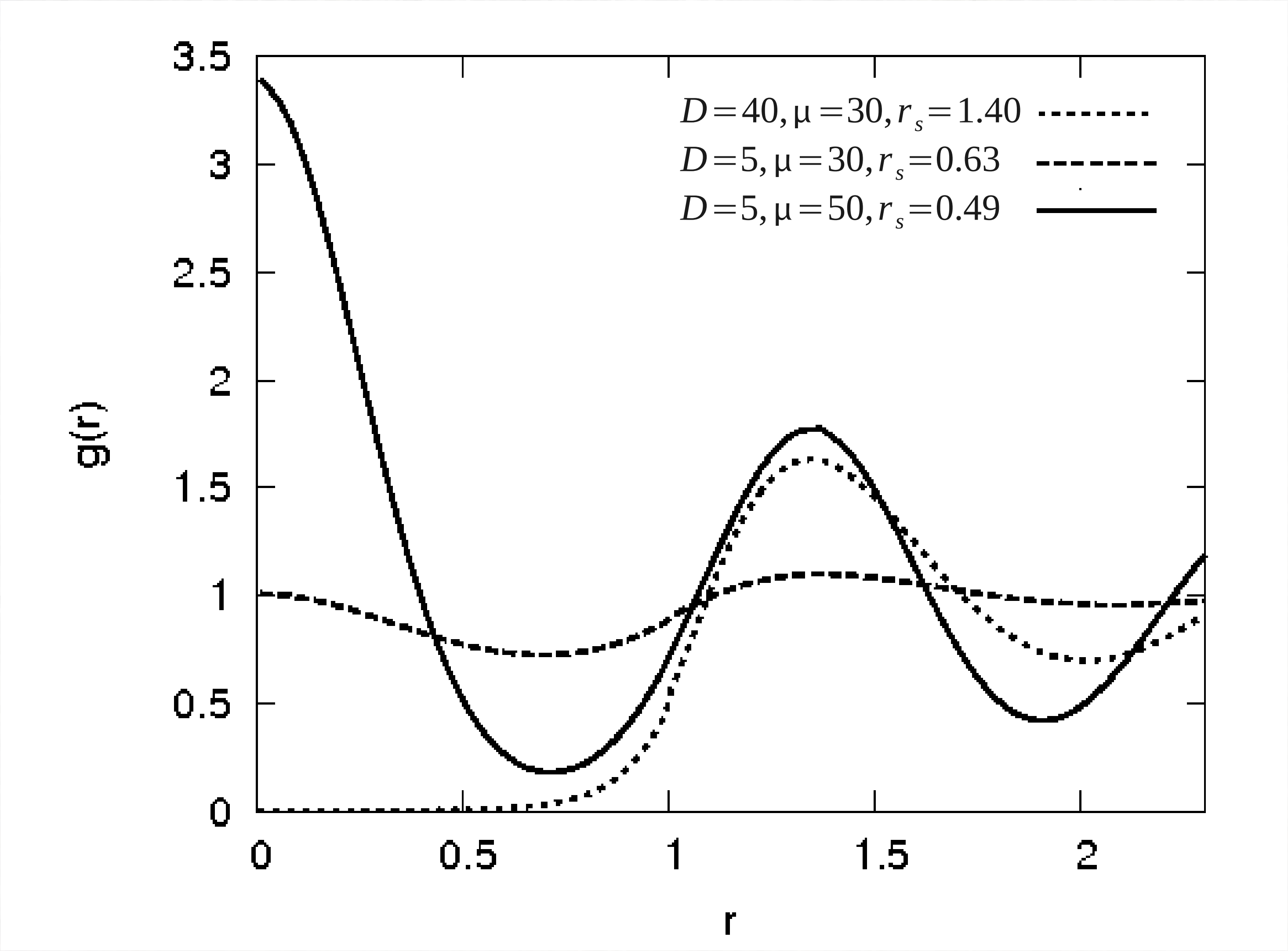


A. J. Leggett, Phys. Rev. Lett. 25, 1543, 1970

Momentum distribution

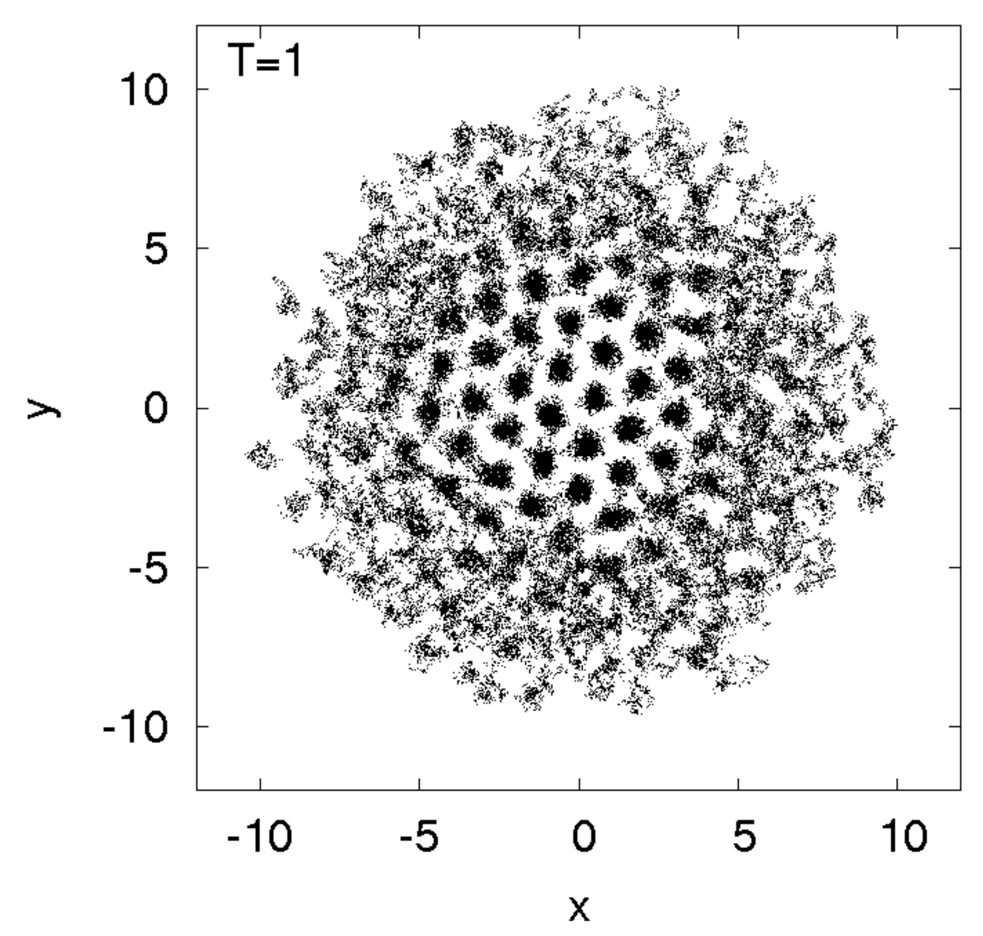


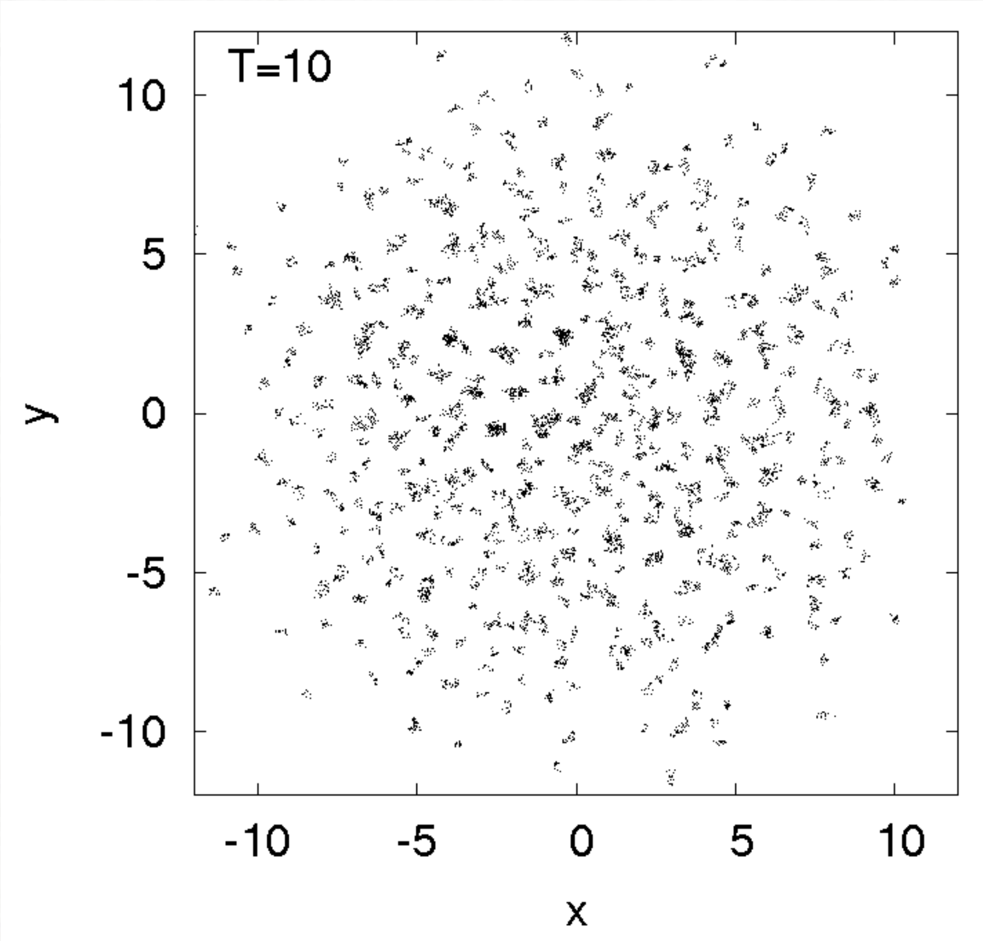
Pair correlation function



Trapped system

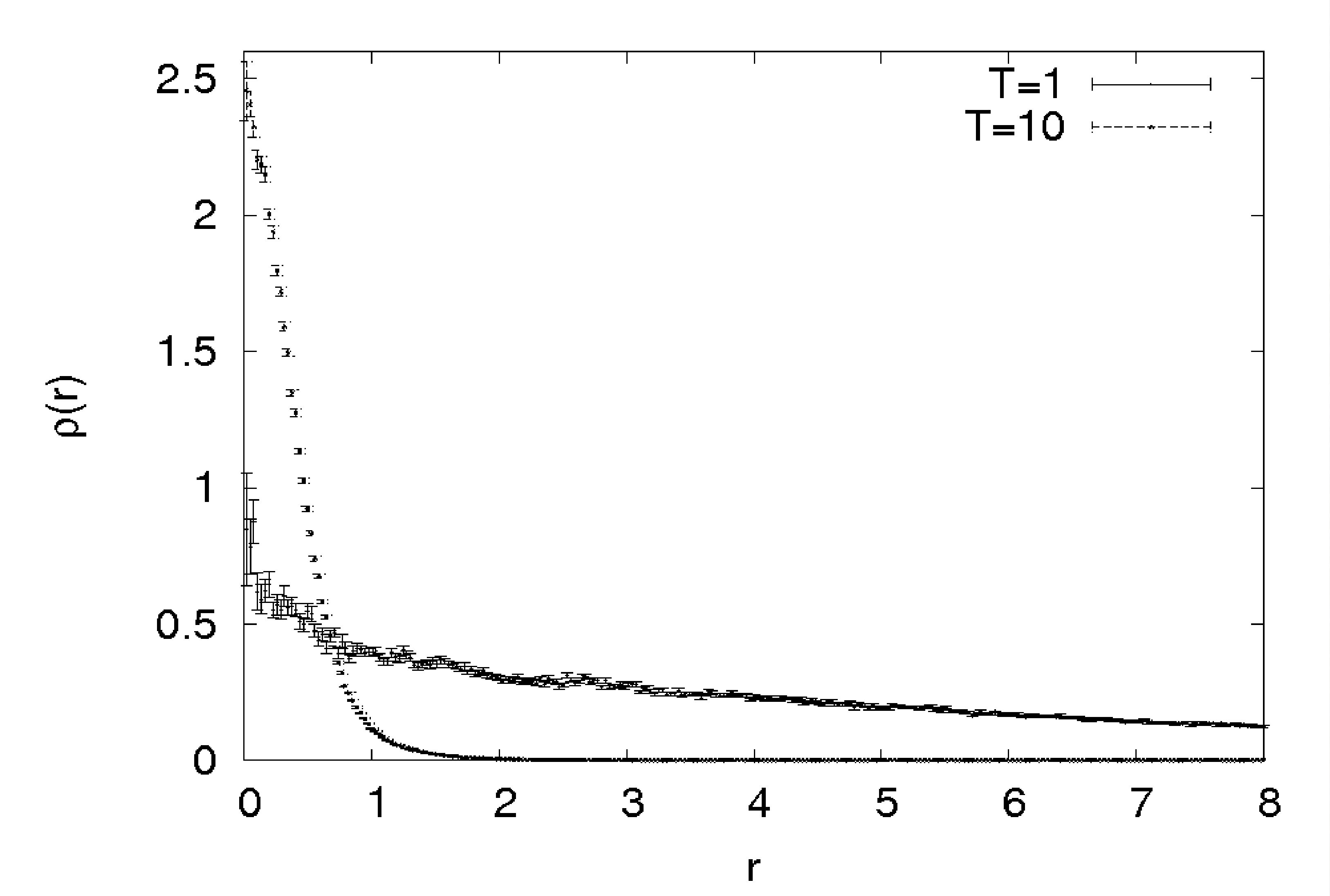
Confining harmonic potential, D=5, μ=50





One body density matrix

Confining harmonic potential, D=5, μ=50



Close

Add a $\bar{M}$ long wold line, connecting $r_0 = \mathcal{I}$ and $r_{\bar{M}} = \mathcal{M}$ generated with distribution (not normalized):

$$\rho_0(\boldsymbol{r_0}, \boldsymbol{r_{\bar{M}}}; \beta) = \int d\boldsymbol{r_1}, \ldots, d\boldsymbol{r_{\bar{M}-1}} (4\pi\lambda\tau)^{-3NM/2} \exp\left(-\sum_{m=1}^{\bar{M}} \left[\frac{(\boldsymbol{r_{m-1}} - \boldsymbol{r_m})^2}{4\lambda\tau}\right]\right), \quad \bar{M} < P < M$$

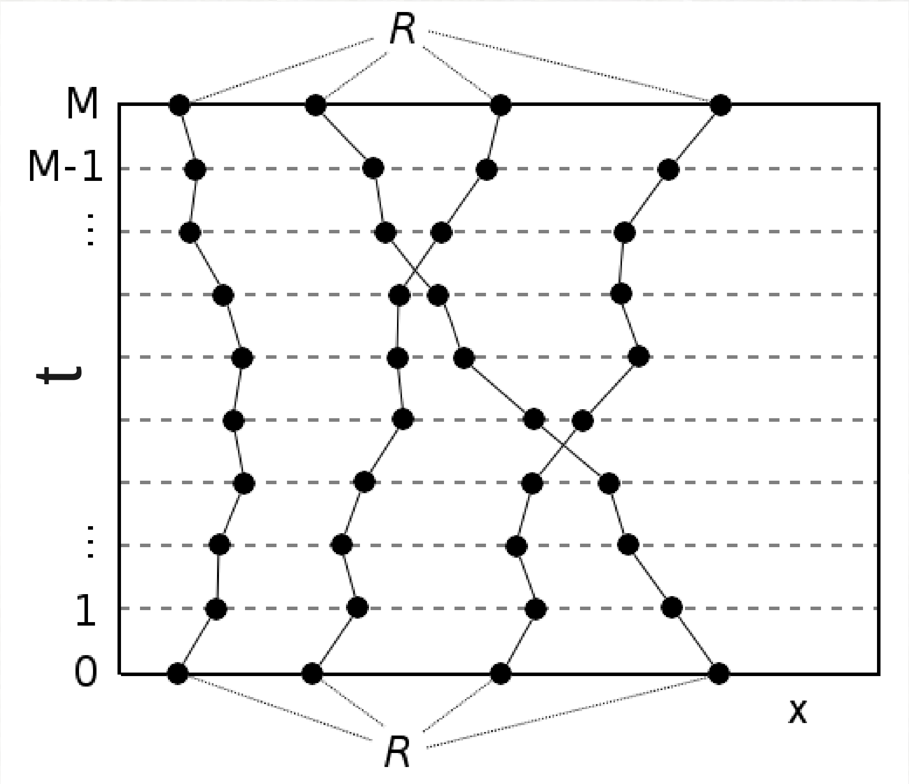
$$P_{cl} = min\left(1, \rho_0(\boldsymbol{r_0}, \boldsymbol{r_{\bar{M}}}, \bar{M}\tau) \frac{e^{\Delta U + \mu \bar{M}\tau}}{CPNM}\right)$$

Open

Remove a $\bar{M}$ long piece of world line, creating the worm.

$$\bar{M} < P < M$$

$$P_{op} = min\left(1, CPNM \frac{e^{\Delta U - \mu \bar{M}\tau}}{\rho_0(\boldsymbol{r_0}, \boldsymbol{r_{\bar{M}}}, \bar{M}\tau)}\right)$$



Insert

Add a $\bar{M}$ long worm, generated with distribution:

$$\rho_0(\boldsymbol{r}_0, \boldsymbol{r}_{\bar{M}}; \beta) = \int d\boldsymbol{r}_1, \ldots, d\boldsymbol{r}_{\bar{M}-1} (4\pi\lambda\tau)^{-3NM/2} \exp\left(-\sum_{m=1}^{\bar{M}} \left[\frac{(\boldsymbol{r}_{m-1} - \boldsymbol{r}_m)^2}{4\lambda\tau}\right]\right), \quad \bar{M} < P < M$$

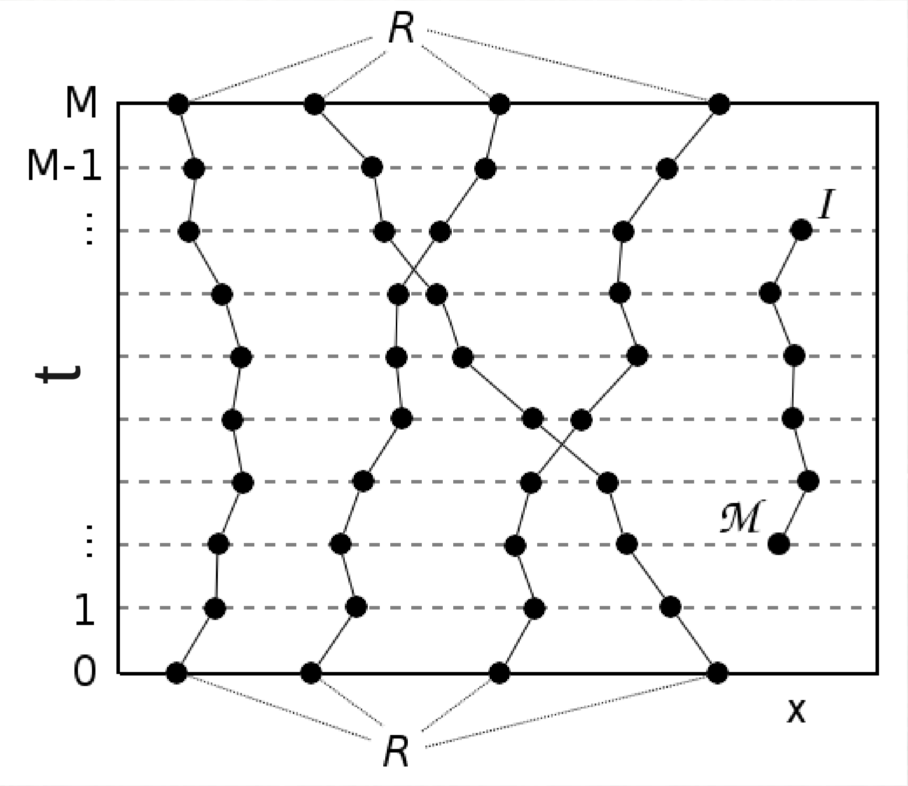
$$P_{in} = min\left(1, CVMPe^{\Delta U + \mu \bar{M} \tau}\right)$$

Remove

Remove (if possible) a $\bar{M}$ long piece of world line connected to I.

$$\bar{M} < P < M$$

$$P_{re} = min\left(1, e^{\Delta U - \mu \bar{M} \tau} / CVMP\right)$$



Advance

Add a $\bar{\text{M}}$ long piece of world line connected to I.

The new world line is generated with distribution:

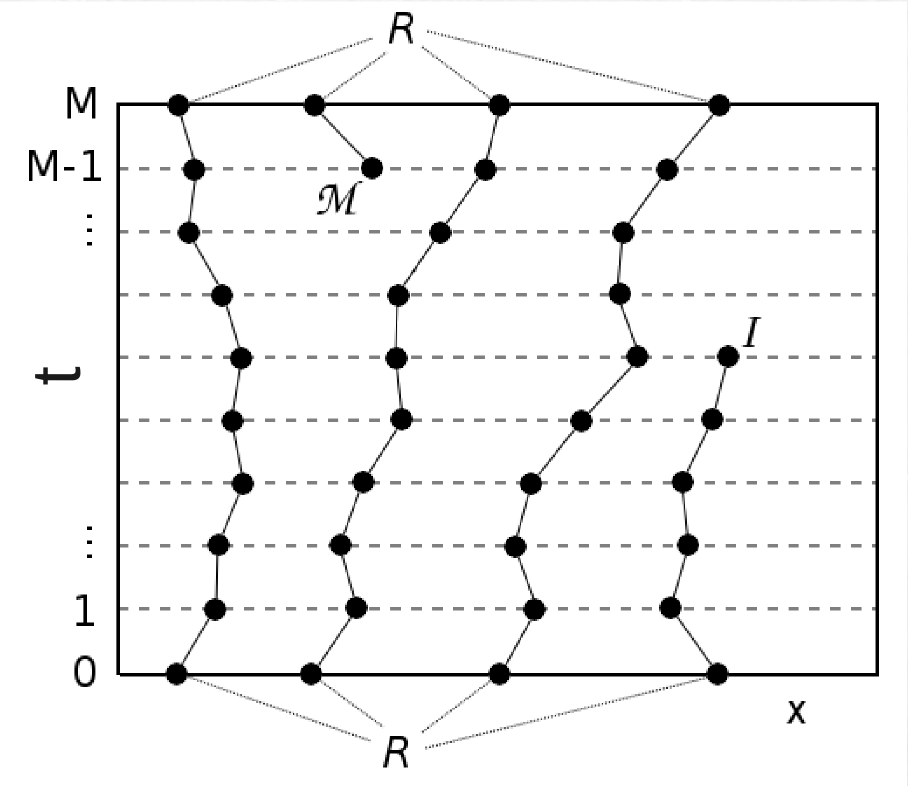
$$\rho_0(\boldsymbol{r_0},\boldsymbol{r_{\bar{M}}};\beta)=\int d\boldsymbol{r_1},\ldots,d\boldsymbol{r_{\bar{M}-1}}(4\pi\lambda\tau)^{-3NM/2}\exp\left(-\sum_{m=1}^{\bar{M}}\left[\frac{(\boldsymbol{r_{m-1}}-\boldsymbol{r_m})^2}{4\lambda\tau}\right]\right),\ \ \bar{M}<P<M$$

$$P_{ad}=min\left(1,e^{\Delta U+\mu M\tau}\right)$$

Recede

Remove a $\bar{\text{M}}$ long piece of world line connected to I.

$$P_{re}=min\left(1,e^{\Delta U-\mu\bar{M}\tau}\right)\qquad \bar{M}<P<M$$



Swap

Choose a bead $\boldsymbol{r}_\alpha$ at time $\beta(I+\bar{M})$ with distribution:

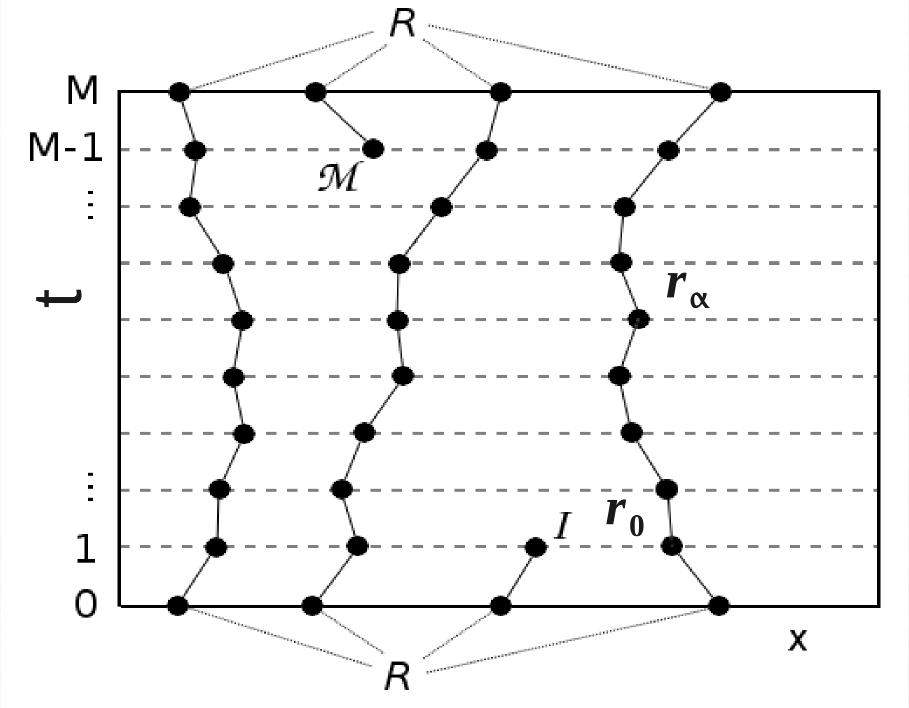
$$P_\alpha = \rho_0(\boldsymbol{r_0}, \boldsymbol{r_\alpha}, \bar{M}\tau)/E_1, \quad E_1 = \sum_{\alpha\in\beta(I+\bar{M})} \rho_0(\boldsymbol{r_0}, \boldsymbol{r_\alpha}, \bar{M}\tau) \qquad \bar{M} < P < M$$

Where $\boldsymbol{r}_0 = I$. Generate a $\bar{M}$ long wold line, connecting $\boldsymbol{r}_0$ and $\boldsymbol{r}_\alpha$ generated with distribution (not normalized):

$$\rho_0(\boldsymbol{r_0}, \boldsymbol{r_{\bar{M}}}; \beta) = \int d\,\boldsymbol{r_1}, \ldots, d\,\boldsymbol{r_{\bar{M}-1}} (4\pi\lambda\tau)^{-3NM/2} \exp\left(-\sum_{m=1}^{\bar{M}} \left[\frac{(\boldsymbol{r_{m-1}} - \boldsymbol{r_m})^2}{4\lambda\tau}\right]\right)$$

$$P_{sw} = min\left(1, e^{\Delta U\, E_1/E_2}\right)$$

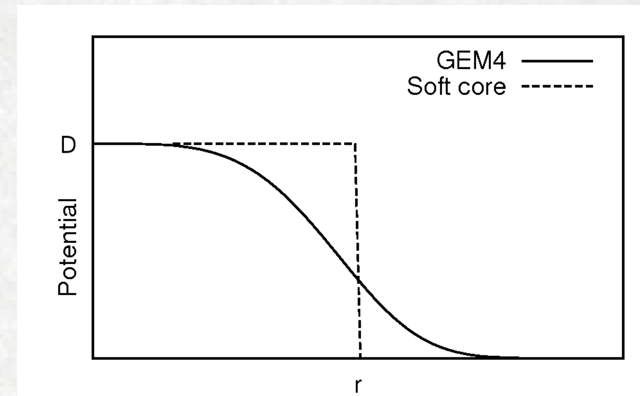
$$E_2 = \sum_{\gamma\in\beta(I)} \rho_0(\boldsymbol{r_\gamma}, \boldsymbol{r_\alpha}, \bar{M}\tau)$$

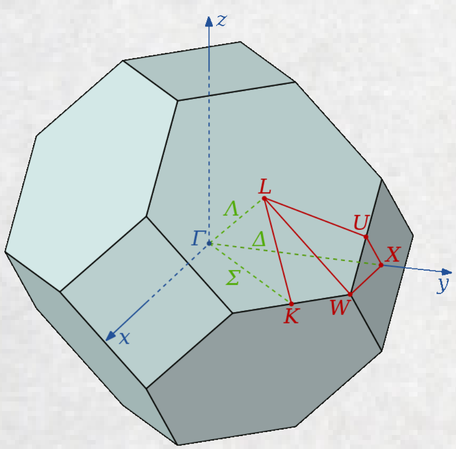


Excitation Spectrum: Classical case (FCC)

Classical cluster solid dispersion, shows 3(K-1) degenerate, k-indipendent optical modes.

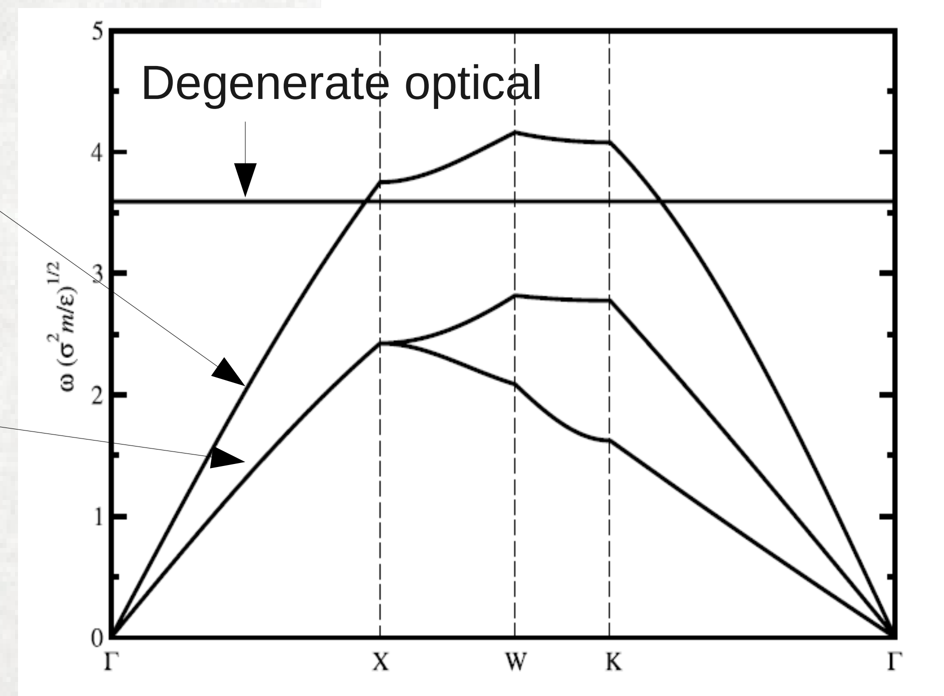
GEM4 $v(r)=D\, e^{(-(r/\sigma)^4)}$





Longitudinal acoustic

Transverse acoustic



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