Bound States in Multilayers of Cold Dipolar Molecules

Jeremy Armstrong

Collaborators:
Nikolaj Zinner, Dmitri Fedorov,
Aksel Jensen, Artem Volosniev

Aarhus University, Denmark

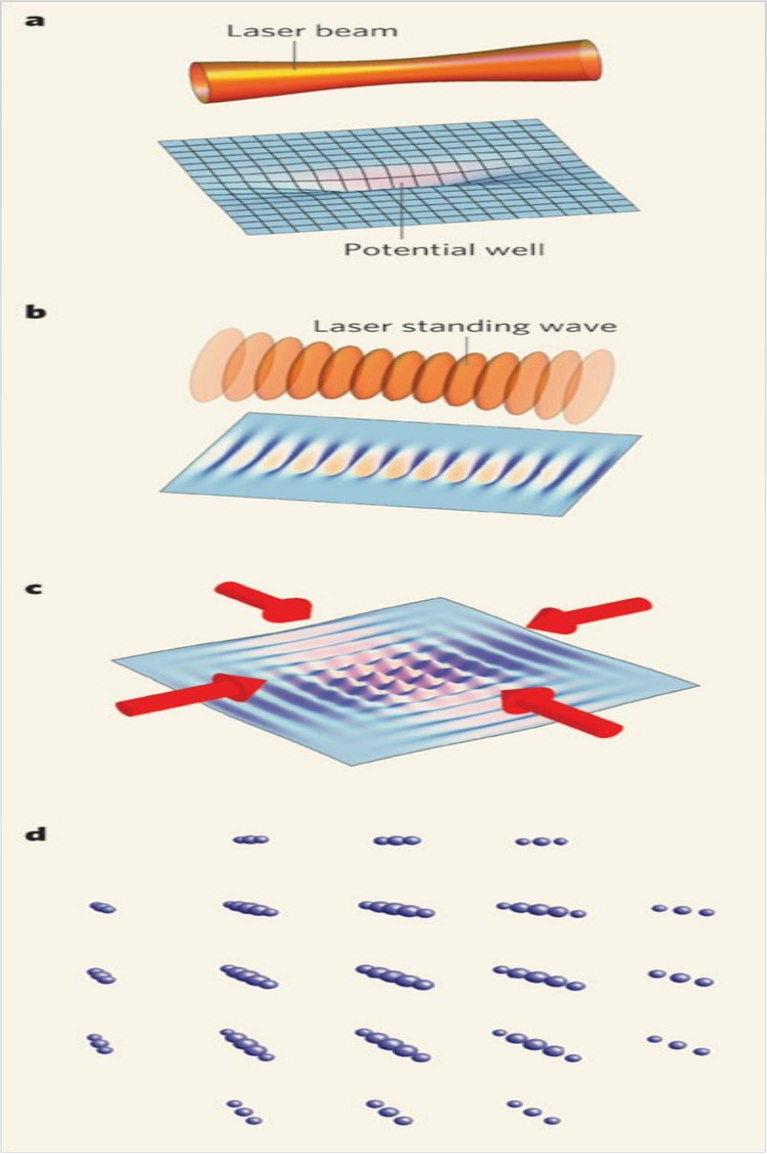
Outline

- Introduction
- Oscillator “Simulation”
- Multilayers
- Thermodynamics
- Conclusion & outlook

Cold Dipolar Gases

- Long range, anisotropic force
  - Magnetic dipoles (^{52}Cr) and electric dipoles of alkali molecules (KRb, LiK)
- Search for new quantum phases
- Ultracold chemistry

Setup



Greiner & Fölling, *Nature* **453** (2008) 736

Multilayer System

- Dipoles confined in adjacent layers
- External electric field polarizes and aligns dipoles
- Attractive inter-layer interaction and repulsive intra-layer interaction

$$V_{dip}(r) = D^2 \frac{r^2 - 2\mathrm{d}^2}{(r^2 + d^2)^{5/2}}$$

Simulation of Potentials

- Harmonic oscillator used to simulate other interactions
- Analytically solveable for any combination of masses, interaction frequencies, and one body fields

$$H_x = -\sum_{k=1}^{N} \frac{\hbar^2}{2\mathrm{m}_k} \frac{\partial^2}{\partial x^2} + \frac{1}{4} \sum_{i,k}^{N} \mu_{ik} \omega_{ik}^2 \left(x_i - x_k + x_{ik,0} \right)^2 + \frac{1}{2} \sum_{k=1}^{N} m_k \omega_k^2 \left(x_k - x_{k,0} \right)^2$$

- Armstrong, *et. al.*, J. Phys. B: At. Mol. Opt. Phys. **44** (2011) 055303

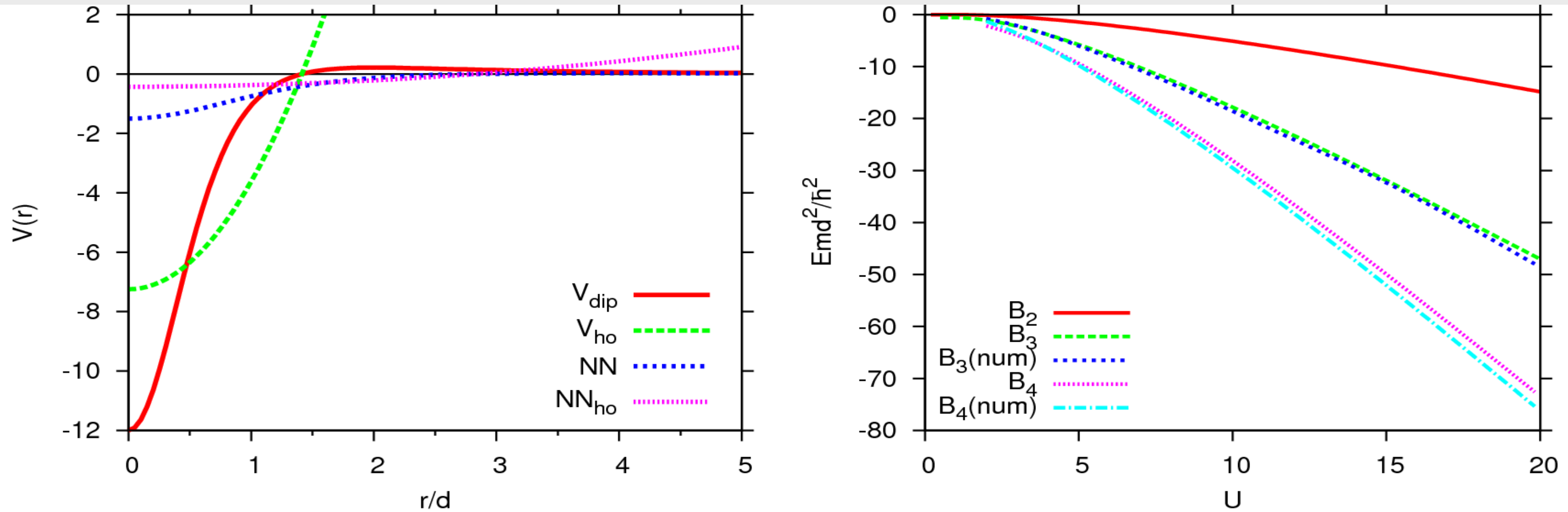
Determination of Parameters

- Need to determine ω_{ik}, V_0, $x_{ik,0}$, ω_k, $x_{k,0}$
  - Choose: $x_{ik,0}=\omega_k=x_{k,0}=0$
  - $V_{ho}(r_i-r_k)=V_0\left(\frac{(r_i-r_k)^2}{2(nd)^2}-1\right)$ $\quad \omega_{ik}^2=\frac{V_0}{\mu(nd)^2}$
  - Binding energy of two-particle system determines V_0
- Repulsion: $V_{rep}(r_i-r_k)=-\frac{1}{2}\mu_{ik}\omega_r^2(r_i-r_k)^2+V_{0,r}$

Solution

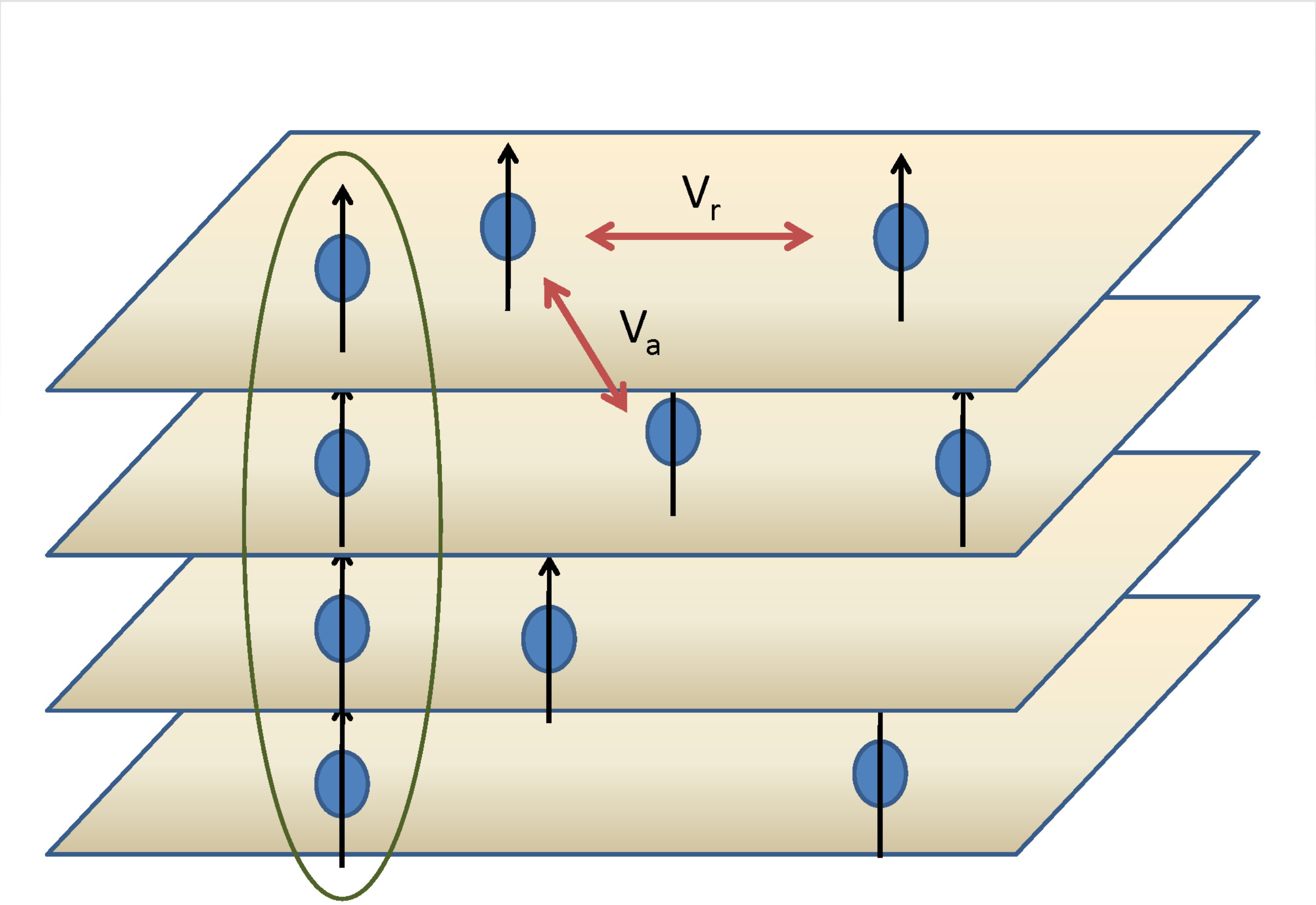
- Parameters set separately for each pair
- Oscillator system solved by coordinate transformation
- Produces new oscillator frequencies in diagonal coordinates
- New frequencies correspond to normal mode excitations

Dipole-Dipole Simulation



- Further Comments: N. T. Zinner, *et al*. arXiv: 1105.6264(2011)

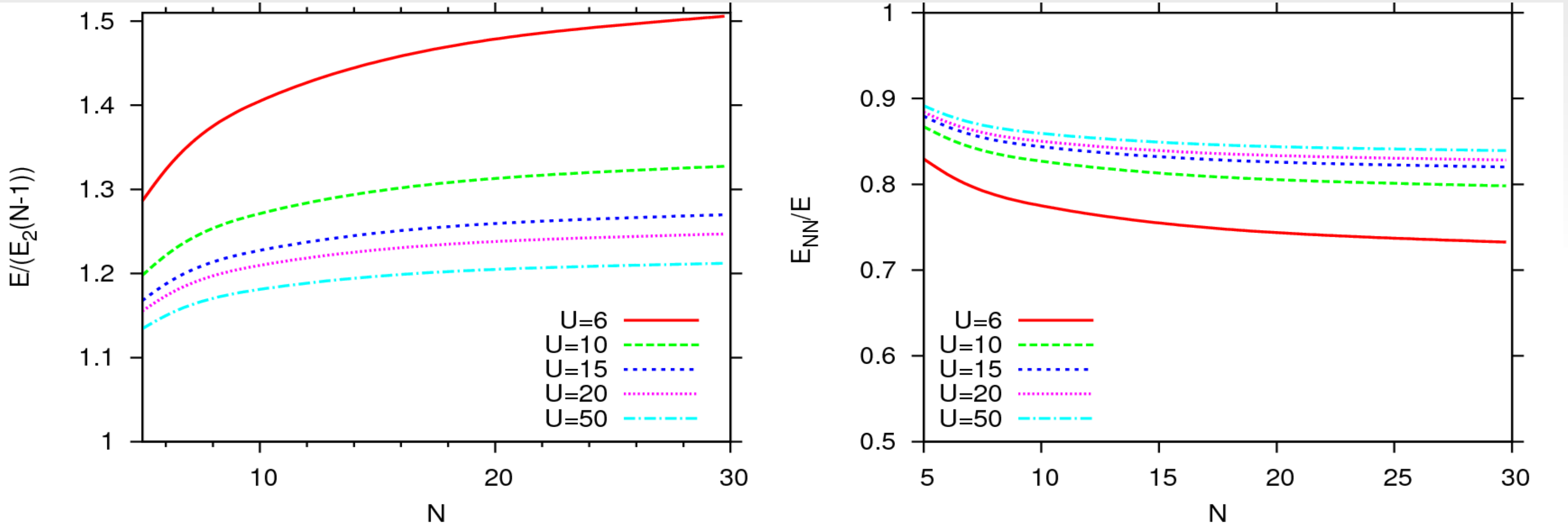
Multilayer System



Armstrong, *et al*., arXiv: 1106.2102(2011)

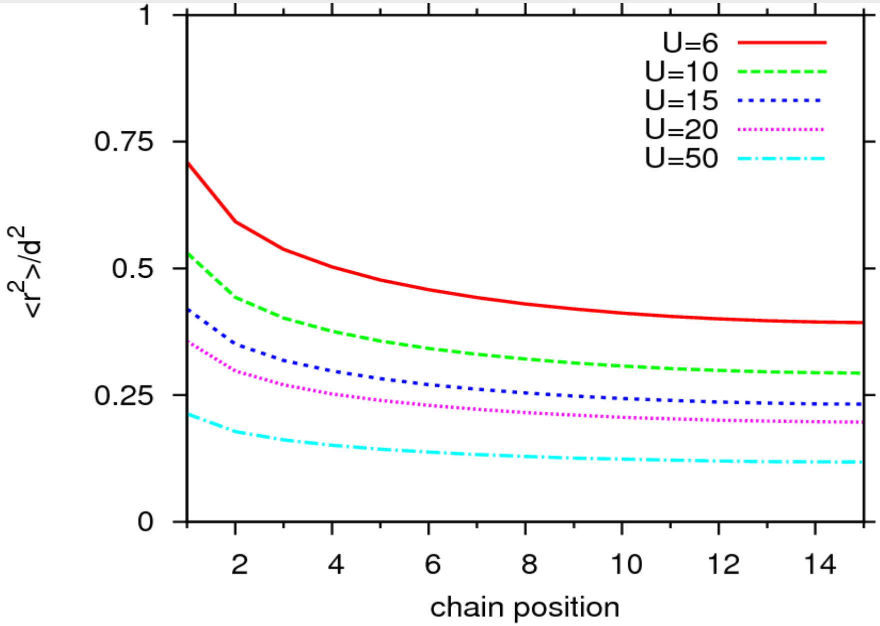
Results—Single String

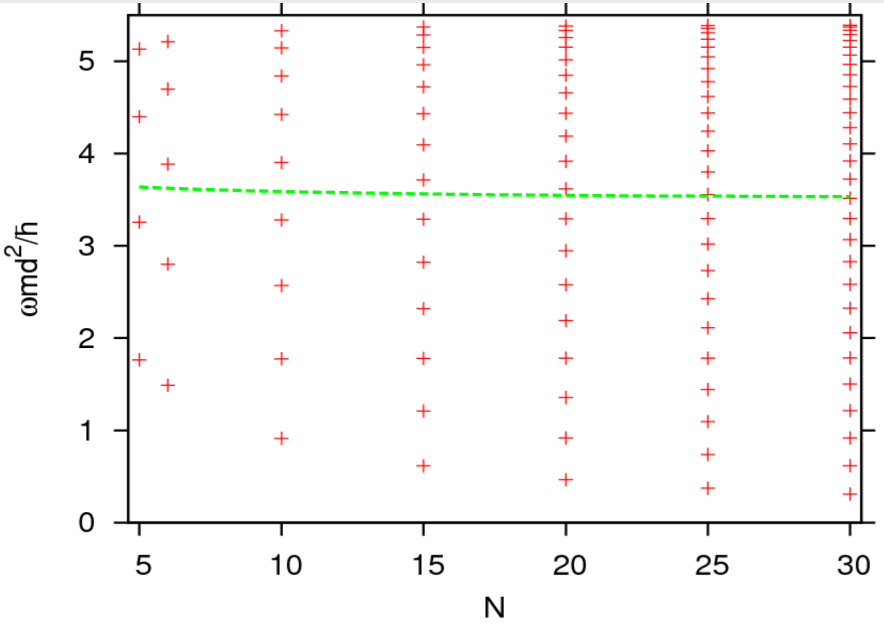
Energies



Results—Single String

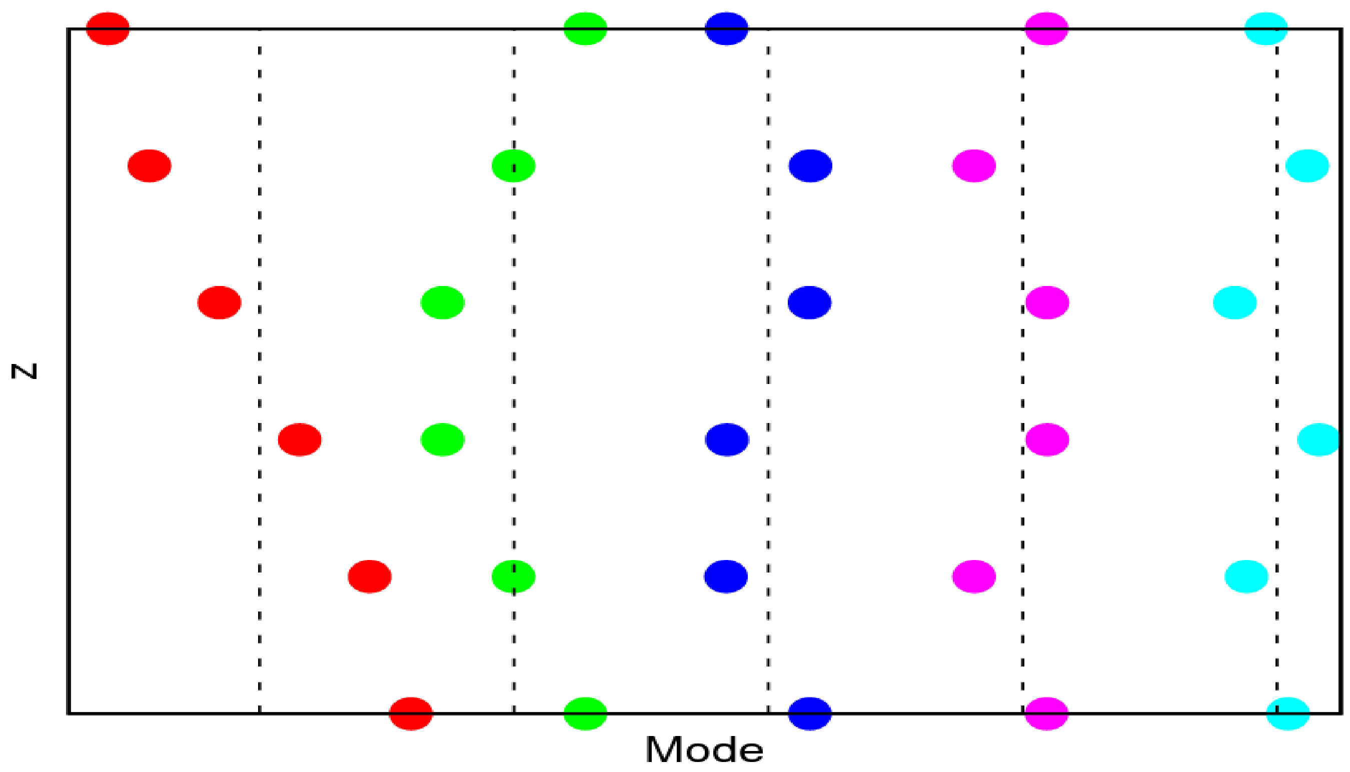
Radii & frequencies





Results—Single String

Normal Modes



ω_i=2.00 3.77 5.23 6.34 7.03

Multiple “Strings”

- Intralayer repulsion introduced

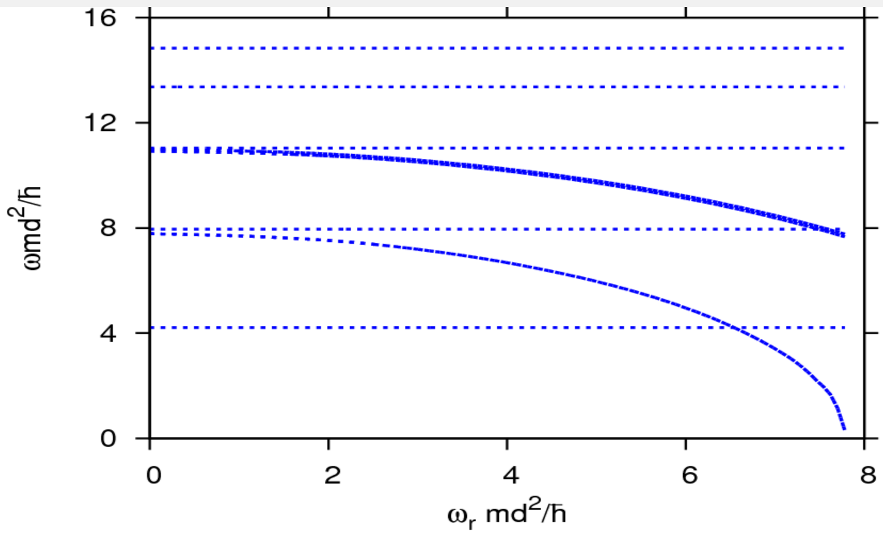
$$V_r(r_{ij}) = -.\frac{1}{2}\mu_{ij}\omega_r^2 r_{ij}^2 + \frac{1}{2}\mu_{ij}\omega_r^2\alpha^2 d^2$$

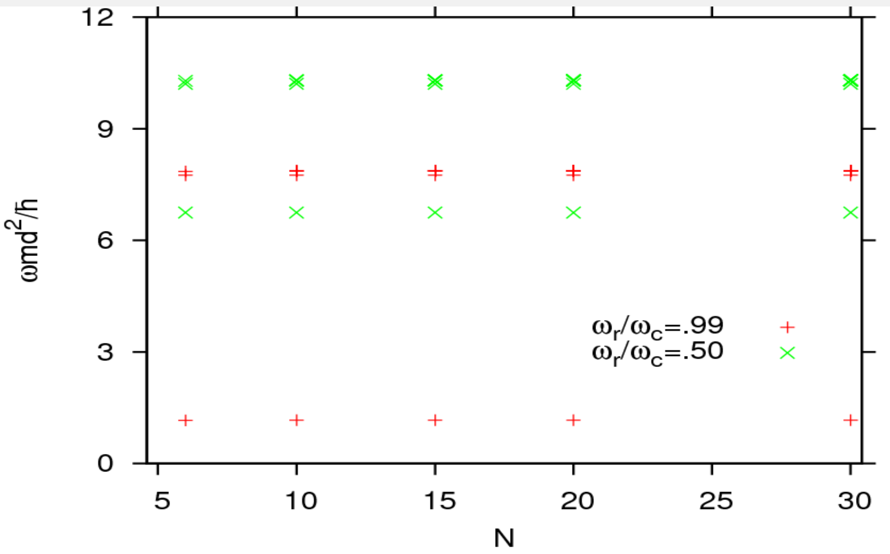
- Actual repulsion: $V_r(r_{ij}) = \frac{\lambda}{r^3}, r > w; -3\frac{\lambda}{w^3}\ln(\frac{r}{we^{1/3}}), r < w$
- Repulsive frequency “excludes” bound states

$$\frac{md^2}{\hbar}\omega_r = \frac{6}{\alpha^2}\sqrt{\frac{m\lambda}{\hbar^2 w}}$$

Results—Multiple Strings

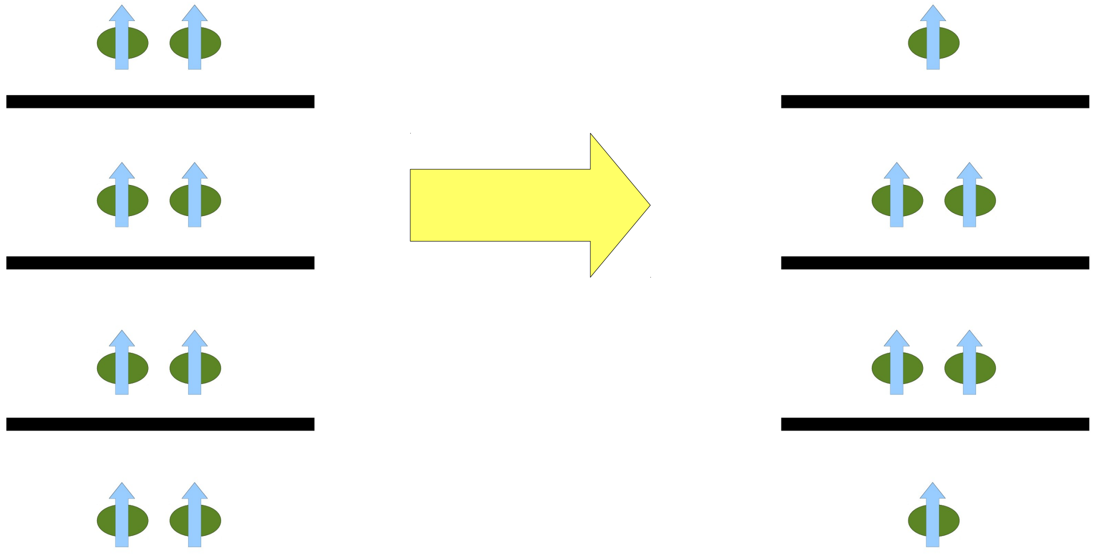
Frequencies





Multiple Strings—Critical Stability

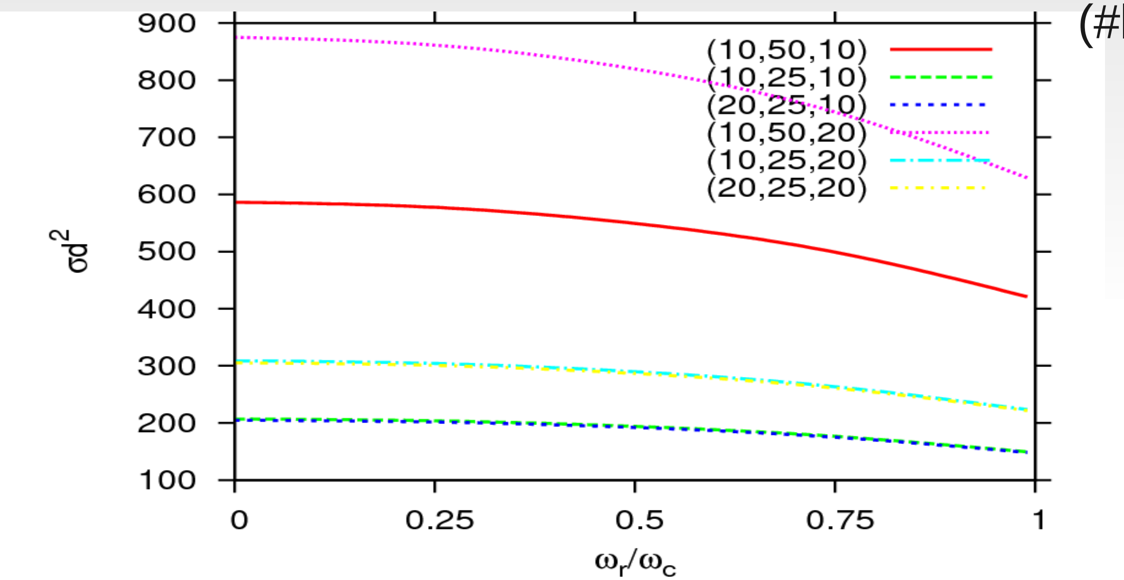
- At critical repulsion, normal mode frequencies become imaginary
- Large amplitude of <r^2> and norm. modes indicate breaking mode



Results—Multiple Strings

Density relations

(#layers, #ptcls/layer, U)



Multiple Strings?

- Can we have more than one particle per layer?
- D^2=20, ω_c=7.78; α~1.92

$$\frac{md^2}{\hbar}\omega_r=\frac{6}{\alpha^2}\sqrt{\frac{mD^2}{\hbar^2 w}} \qquad \alpha=2.78$$

- Multiple strings appear unstable

Conclusions(I)

- Crystal-like behavior in excitations
- Speed of sound
- Single strings prevalent under most conditions
- Stability increases towards the central layers

Thermodynamics

- Particles in separate layers are distinguishable
- Partition function factorizes

$$Z = Z_{sep} Z_{f/b}; Z_{sep} = \prod_{j}^{W-1} \left(\frac{\exp[-\Theta_j/(2T)]}{1-\exp[-\Theta_j/T]} \right)^2 ; \Theta_j = \frac{\hbar \omega_j}{k_B}$$

- Multiple Strings require boson or fermion partition function

Identical Particles

- Partition function for two fermions or bosons is analytic and closed:

$$Z_f = 2^W \prod_j^W \frac{\exp[-2\Theta_j/T]}{(1-\exp[-2\Theta_j/T])^2}$$

$$Z_b = \prod_j^W \frac{\exp[-\Theta_j/T] + \exp[-3\Theta_j/T]}{(1-\exp[-2\Theta_j/T])^2}$$

- More than two particles:

$$Z_{f/b} = \prod_j^W \left(\sum_{k=0} g_k \exp[-(k+M-1)\Theta_j/T] \right)$$

Counting States

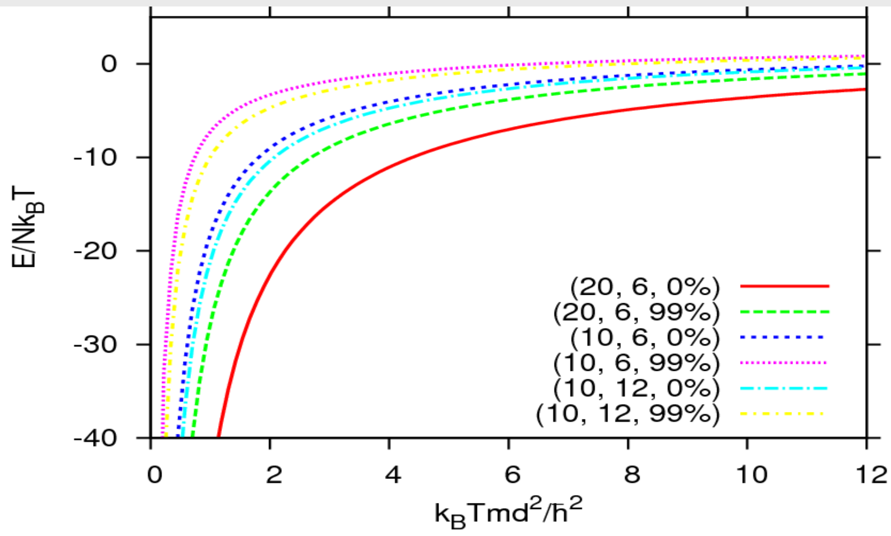
- Start with mean field picture
- Ground state has the mean field number of states
- Excitations exclude center of mass excitations

$$g_j = g_{MF,j} - \sum_{k=0}^{j-1} g_k d(j-k)$$

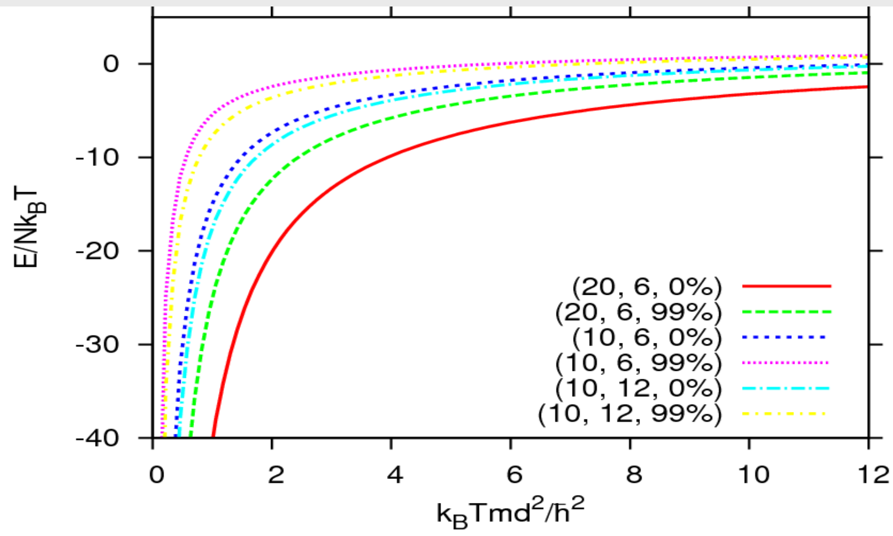
$$d(j-k)_{2D} = (j-k+1)$$

$$d(j-k)_{3D} = (j-k+1)(j-k+2)/2$$

Energy



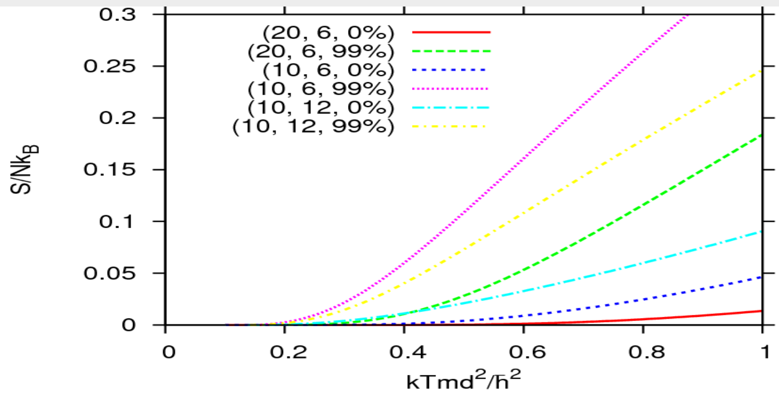
bosons

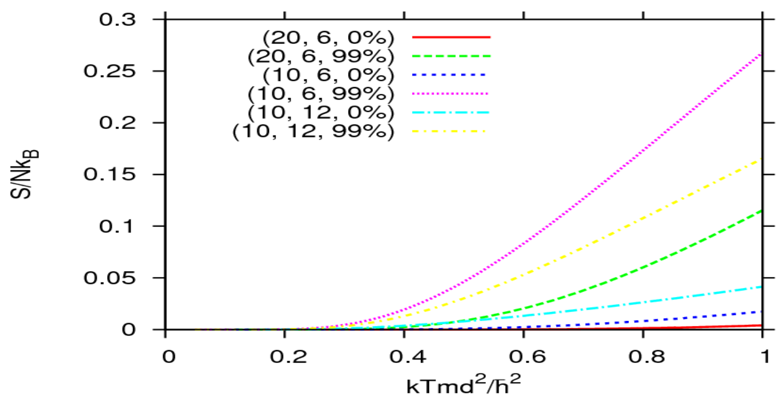


fermions

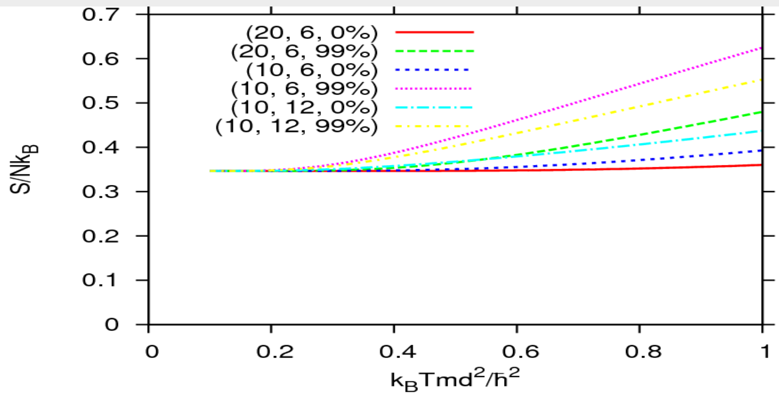
Entropy

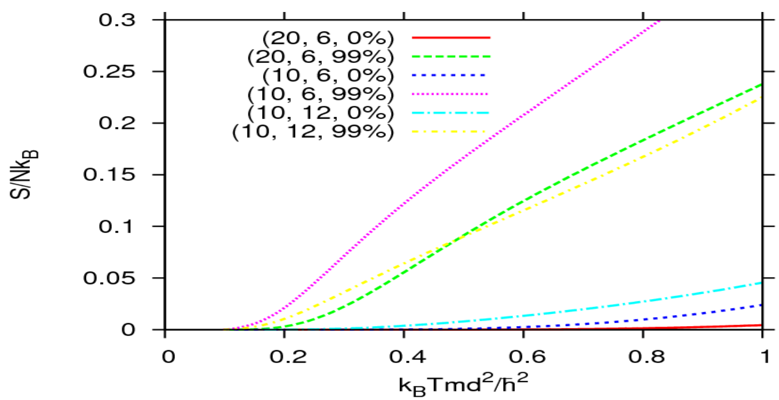
bosons





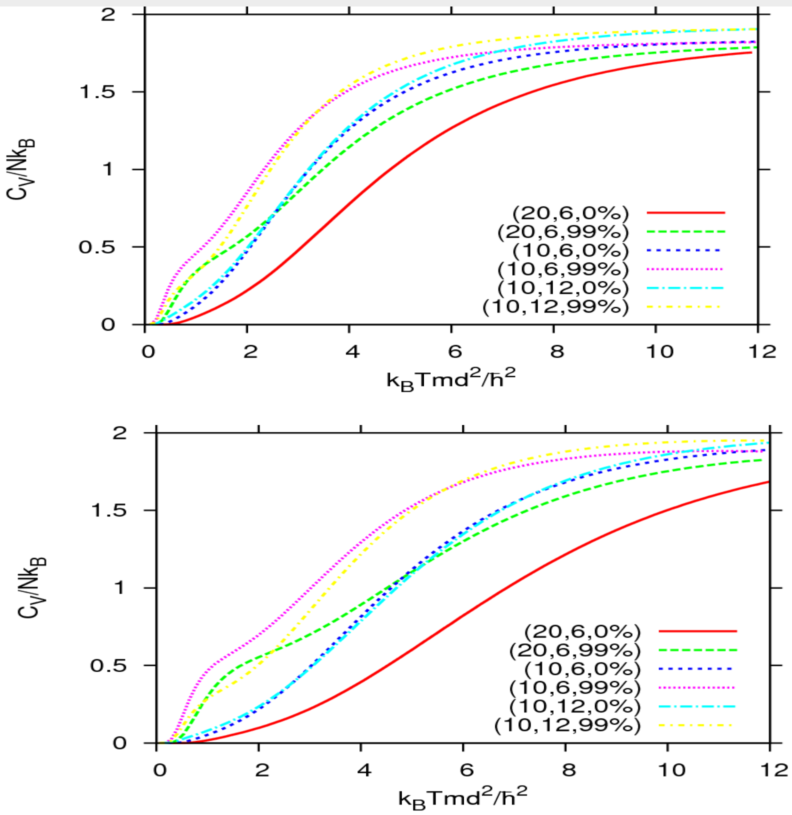
fermions



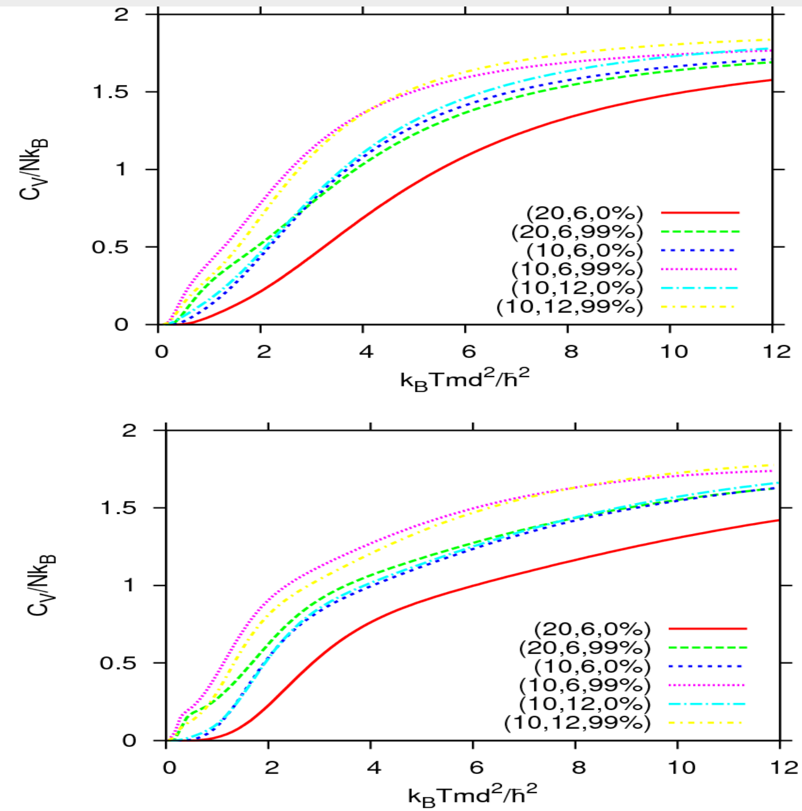


Heat Capacity

bosons



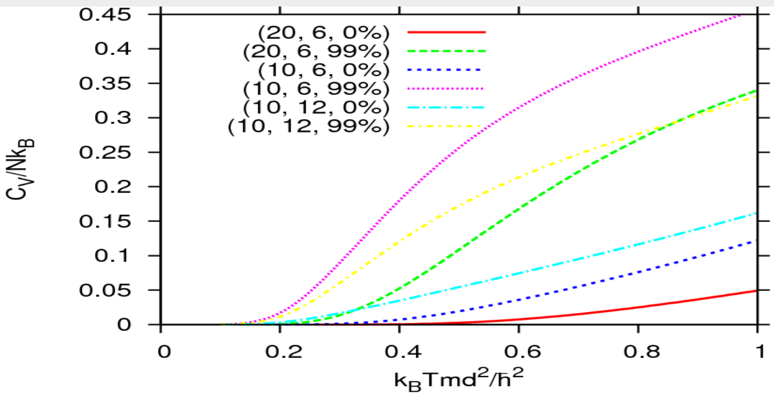
fermions

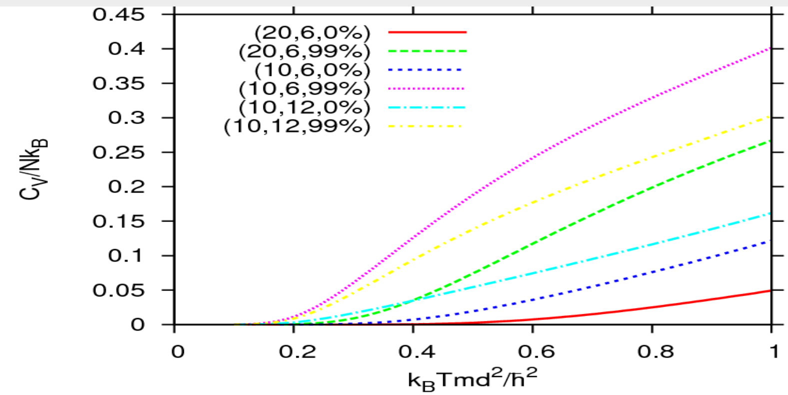


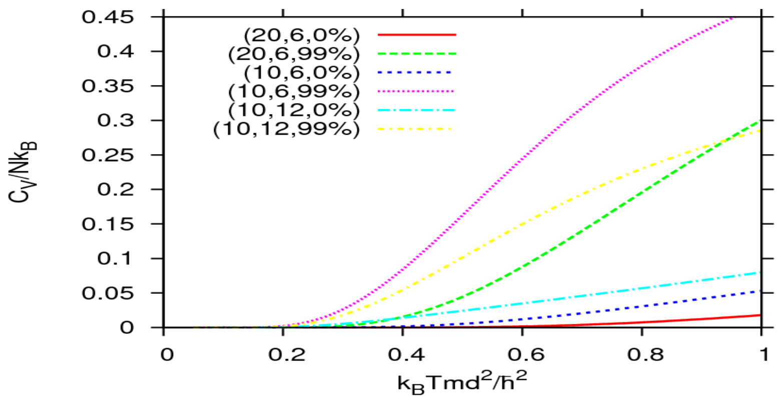
Heat Capacity, Low T

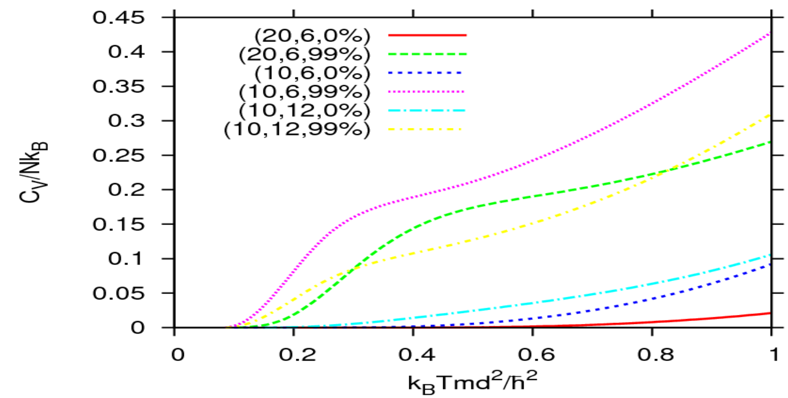
bosons

fermions









Conclusions (II)

- Availability of low-lying excitations strongly affects low T behavior
  - Sensitive to precise character of repulsive force
- High T behavior independent of statistics
- Low T competition between boson gap & number of boson states

Outlook

- More thermodynamic observables
- Thermodynamics of two component systems
- Virial coeffecients of quantum gases
- Different polarization angles