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Exchange and vibrational modes in bosonic quantum solids

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Vibrational Modes and Exchange in Bosonic Quantum Solids

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Obsessed with the Commensurate Solid

- Phonons are always there…
- As we lower the mass of the particles will we find…

  Other ground state?
  - Zero point vacancies…

  New excitations?
  - Exchange loops (probably not percolating… but present)

This is not necessary a search for an explanation of the experiments, but a search for what are we going to find if all the metallurgy is not present…

Phonons 001: A local description

$$H = \sum_{j=1}^{N}\left[\frac{p_j^2}{2m} + \frac{k}{2}\left(u_j - u_{j+1}\right)^2\right] = \sum_{j=1}^{N}\left[\frac{p_j^2}{2m} + ku_j^2 - ku_j u_{j+1}\right] \qquad \omega = \sqrt{\frac{2k}{m}}$$

$$u_j = \sqrt{\frac{\hbar}{2m\omega}}\left(a_j^\dagger + a_j\right)$$

$$p_j = i\sqrt{\frac{m\hbar\omega}{2}}\left(a_j^\dagger - a_j\right)$$

$$p_j^2 = \frac{\hbar m\omega}{2}\left(a_j^\dagger a_j + a_j a_j^\dagger - a_j^\dagger a_j^\dagger - a_j a_j\right)$$

$$u_j^2 = \frac{\hbar}{2m\omega}\left(a_j^\dagger a_j + a_j a_j^\dagger + a_j^\dagger a_j^\dagger + a_j a_j\right)$$

$$u_j u_{j+1} = \frac{\hbar}{2m\omega}\left(a_j^\dagger a_{j+1} + a_j a_{j+1}^\dagger + a_j^\dagger a_{j+1}^\dagger + a_j a_{j+1}\right)$$

$$H = \sum_{j=1}^{N}\left[\frac{\hbar\omega}{2}\left(a_j^\dagger a_j + a_j a_j^\dagger\right) - \frac{\hbar\omega}{4}\left(a_j^\dagger a_{j+1} + a_j a_{j+1}^\dagger + a_j^\dagger a_{j+1}^\dagger + a_j a_{j+1}\right)\right]$$

Phonons 001: A local description

$$H = \sum_{j=1}^{N} \left[\frac{\hbar\omega}{2} \left(a_j^\dagger a_j + a_j a_j^\dagger \right) - \frac{\hbar\omega}{4} \left(a_j^\dagger a_{j+1} + a_j a_{j+1}^\dagger + a_j^\dagger a_{j+1}^\dagger + a_j a_{j+1} \right) \right]$$

$$a_j = \frac{1}{\sqrt{N}} \sum_q a_q e^{iqaj}$$

$$H = \sum_q \left[\left(\frac{\hbar\omega}{2} - \frac{\hbar\omega}{4} \cos(qa) \right) \left(a_q^\dagger a_q + a_{-q} a_{-q}^\dagger \right) - \frac{\hbar\omega}{4} \cos(qa) \left(a_q^\dagger a_{-q}^\dagger + a_{-q} a_q \right) \right]$$

Phonons 001: A local description

$$H=\sum_q\left[\left(\frac{\hbar\omega}{2}-\frac{\hbar\omega}{4}\cos(qa)\right)\left(a_q^\dagger a_q+a_{-q}a_{-q}^\dagger\right)-\frac{\hbar\omega}{4}\cos(qa)\left(a_q^\dagger a_{-q}^\dagger+a_{-q}a_q\right)\right]$$

$$a_q^\dagger=u_q b_q^\dagger+v_q b_{-q}$$

$$a_q=v_q b_{-q}^\dagger+u_q b_q$$

$$u_q=\frac{1}{2}\left(\sqrt{\frac{\omega}{\Omega(q)}}+\sqrt{\frac{\Omega(q)}{\omega}}\right)$$

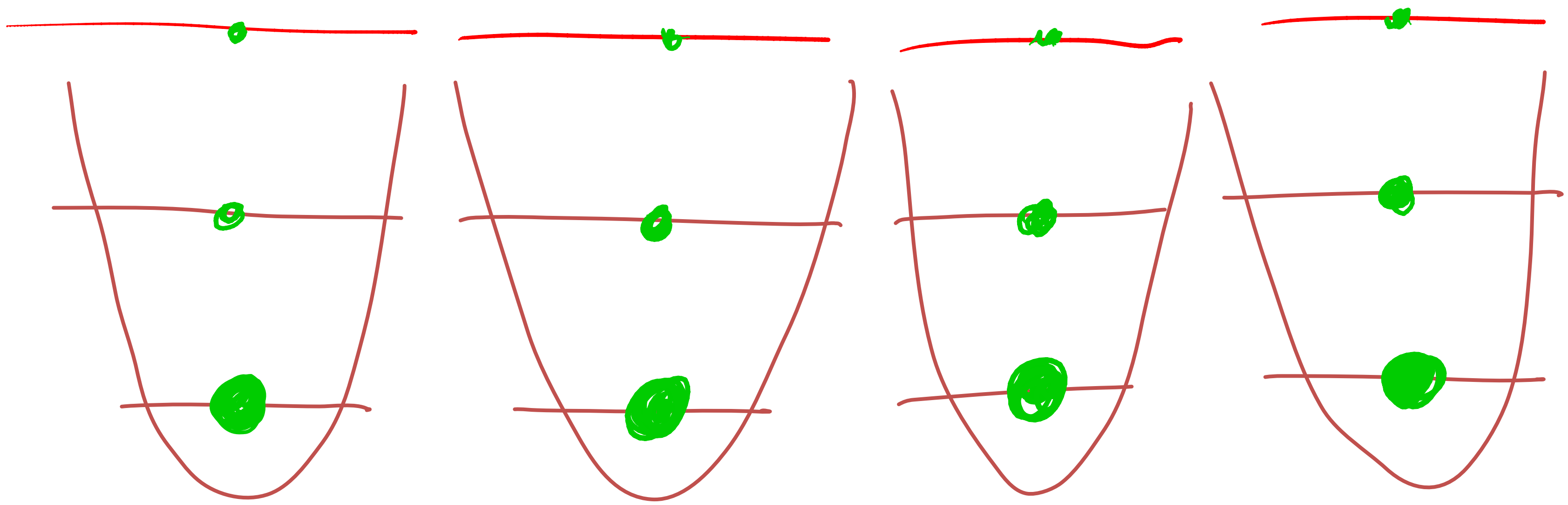
$$v_q=\frac{1}{2}\left(\sqrt{\frac{\omega}{\Omega(q)}}-\sqrt{\frac{\Omega(q)}{\omega}}\right)$$

$$H=\sum_q\left[\hbar\Omega(q)\left(b_q^\dagger b_q+\frac{1}{2}\right)\right]$$

$$\left|GS\right\rangle=\left|\varnothing_b\right\rangle=\exp\left\{\sum_q\lambda_q a_q^\dagger a_{-q}^\dagger\right\}\left|\varnothing_a\right\rangle$$

Phonons 001: A local description

$$\left|GS\right\rangle = \left|\varnothing_b\right\rangle = \exp\left\{\sum_q \lambda_q a_q^\dagger a_{-q}^\dagger\right\}\left|\varnothing_a\right\rangle = C\left(1 + \lambda_q a_q^\dagger a_{-q}^\dagger + \ldots\right)\left|\varnothing_a\right\rangle$$



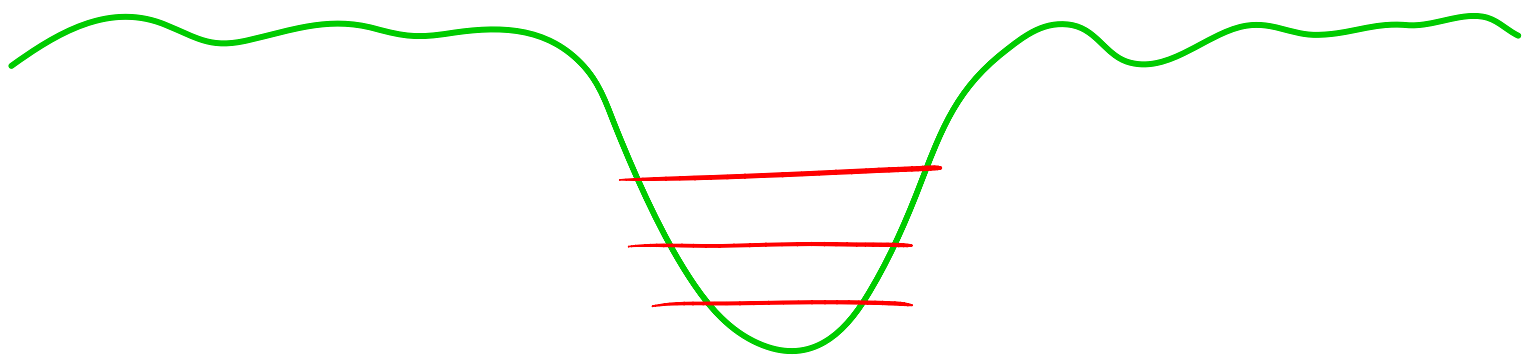
The Hamiltonian

$$H = \sum_{I=1}^{N} \frac{P_I^2}{2M} + \frac{1}{2}\sum_{I,J} V(\vec{r}_I - \vec{r}_J)$$

The “classical” solid wave function

$$\Psi = \prod_{J=1}^{N} \varphi(\vec{r}_J - \vec{R}_J)$$

A Hartree like calculation gives:
See for example P. W. Anderson, “Basic Notions of Condensed Matter Physics”
or the work by Varma and Werthamer



A localized basis set

Define a basis set of oscillators at every site:

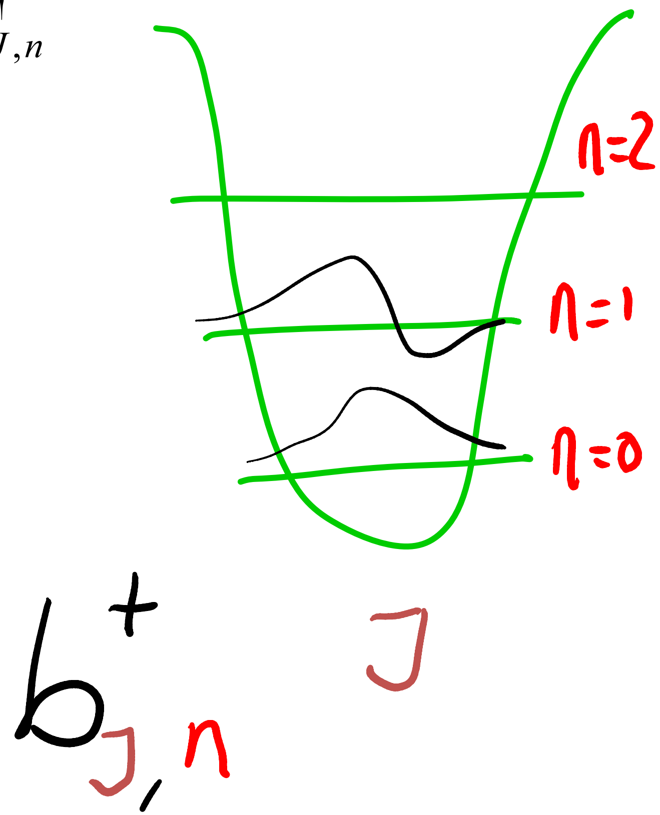
$$\psi^{\dagger}(\vec{r}) = \sum_{J,n} \varphi_n\left(\vec{r} - \vec{R}_J\right) b_{J,n}^{\dagger}$$

We will assume that the particles are hard core bosons:

$$\left[b_{I,n}, b_{J,n}^{\dagger}\right] = \delta_{I,J}\left(1 - 2n_{J,n}\right)$$

$$\left[b_{I,m}^{\dagger}, b_{J,n}^{\dagger}\right] = 0$$

$$\left[b_{I,m}, b_{J,n}\right] = 0$$



The Hamiltonian in its new clothes

$$H = -\frac{\hbar^2}{2M}\int d\vec{r}\,\psi^\dagger\left(\vec{r}\right)\nabla^2\psi\left(\vec{r}\right) + \iint d\vec{r}\,d\vec{r}\,'\psi^\dagger\left(\vec{r}\right)\psi^\dagger\left(\vec{r}'\right)V(\vec{r},\vec{r}\,')\psi\left(\vec{r}\,'\right)\psi\left(\vec{r}\right)$$

$$H = -\frac{\hbar^2}{2M}\sum_{\substack{I,J\\ n,m}} b_{I,n}^\dagger b_{J,m}\int d\vec{r}\,\varphi_n\left(\vec{r}-\vec{R}_I\right)\nabla^2\varphi_m\left(\vec{r}-\vec{R}_J\right) +$$

$$+\frac{1}{2}\sum_{\substack{I,J,K,L\\ n,m,r,s}} b_{I,n}^\dagger b_{K,m} b_{J,r}^\dagger b_{L,s}\iint d\vec{r}\,d\vec{r}\,'\varphi_n\left(\vec{r}-\vec{R}_I\right)\varphi_m\left(\vec{r}-\vec{R}_K\right)V(\vec{r},\vec{r}\,')\varphi_r\left(\vec{r}\,'-\vec{R}_J\right)\varphi_s\left(\vec{r}\,'-\vec{R}_L\right)$$

To make contact with the linear chain, we will assume 1D and harmonic interaction…

$$V(x,y) = -V_0 + \frac{k}{2}\left(\left|x-y\right| - a\right)^2$$

The Hamiltonian dressed with its new clothes

Even assuming a harmonic interaction and neglectic exchange, it looks terrible…

$$H = -\frac{\hbar\omega}{4}\sum_{I,m}\left[\sqrt{(m+1)(m+2)}\left(b^{\dagger}_{I,m+2}b_{I,m} + b^{\dagger}_{I,m}b_{I,m+2}\right) - (2m+1)b^{\dagger}_{I,m}b_{I,m}\right] -$$

$$-V_0\sum_{I,m,s} b^{\dagger}_{I,m}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s} +$$

$$+\frac{\hbar\omega}{4}\sum_{I,m,s}\left[\sqrt{(m+1)(m+2)}\left(b^{\dagger}_{I,m+2}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s} + b^{\dagger}_{I,m}b_{I,m+2}b^{\dagger}_{I+1,s}b_{I+1,s}\right) + (2m+1)b^{\dagger}_{I,m}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s}\right] -$$

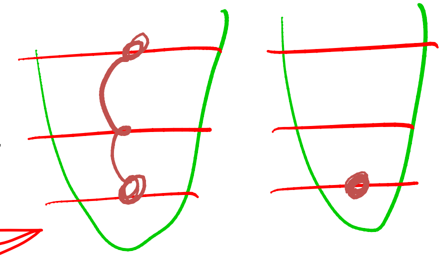
$$-\frac{\hbar\omega}{2}\sum_{I,m,s}\sqrt{m+1}\sqrt{s+1}\left(b^{\dagger}_{I,m+1}b_{I,m}b^{\dagger}_{I+1,s+1}b_{I+1,s} + b^{\dagger}_{I,m}b_{I,m+1}b^{\dagger}_{I+1,s}b_{I+1,s+1}\right) -$$

$$-\frac{\hbar\omega}{2}\sum_{I,m,s}\sqrt{m+1}\sqrt{s+1}\left(b^{\dagger}_{I,m+1}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s+1} + b^{\dagger}_{I,m}b_{I,m+1}b^{\dagger}_{I+1,s+1}b_{I+1,s}\right) +$$

$$+\frac{\hbar\omega}{4}\sum_{I,m,s}\left(\sqrt{(m+1)(m+2)}\left(b^{\dagger}_{I,s}b_{I,s}b^{\dagger}_{I+1,m+2}b_{I+1,m} + b^{\dagger}_{I,s}b_{I,s}b^{\dagger}_{I+1,m}b_{I+1,m+2}\right) + (2m+1)b^{\dagger}_{I,s}b_{I,s}b^{\dagger}_{I+1,m}b_{I+1,m}\right)$$

The Hamiltonian dressed with its new clothes

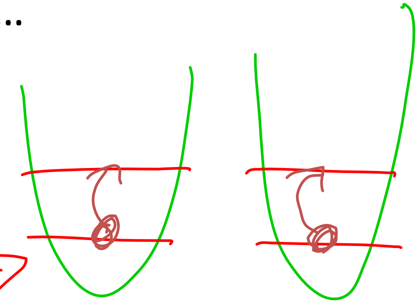
Even assuming a harmonic interaction, it looks terrible…



$$
\begin{aligned}
H = & -\frac{\hbar\omega}{4}\sum_{I,m}\left[\sqrt{(m+1)(m+2)}\left(b^{\dagger}_{I,m+2}b_{I,m}+b^{\dagger}_{I,m}b_{I,m+2}\right)-(2m+1)b^{\dagger}_{I,m}b_{I,m}\right]- \\
& -V_0\sum_{I,m,s} b^{\dagger}_{I,m}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s}+ \\
& +\frac{\hbar\omega}{4}\sum_{I,m,s}\left[\sqrt{(m+1)(m+2)}\left(b^{\dagger}_{I,m+2}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s}+b^{\dagger}_{I,m}b_{I,m+2}b^{\dagger}_{I+1,s}b_{I+1,s}\right)+(2m+1)b^{\dagger}_{I,m}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s}\right]- \\
& -\frac{\hbar\omega}{2}\sum_{I,m,s}\sqrt{m+1}\sqrt{s+1}\left(b^{\dagger}_{I,m+1}b_{I,m}b^{\dagger}_{I+1,s+1}b_{I+1,s}+b^{\dagger}_{I,m}b_{I,m+1}b^{\dagger}_{I+1,s}b_{I+1,s+1}\right)- \\
& -\frac{\hbar\omega}{2}\sum_{I,m,s}\sqrt{m+1}\sqrt{s+1}\left(b^{\dagger}_{I,m+1}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s+1}+b^{\dagger}_{I,m}b_{I,m+1}b^{\dagger}_{I+1,s+1}b_{I+1,s}\right)+ \\
& +\frac{\hbar\omega}{4}\sum_{I,m,s}\left(\sqrt{(m+1)(m+2)}\left(b^{\dagger}_{I,s}b_{I,s}b^{\dagger}_{I+1,m+2}b_{I+1,m}+b^{\dagger}_{I,s}b_{I,s}b^{\dagger}_{I+1,m}b_{I+1,m+2}\right)+(2m+1)b^{\dagger}_{I,s}b_{I,s}b^{\dagger}_{I+1,m}b_{I+1,m}\right)
\end{aligned}
$$

The Hamiltonian dressed with its new clothes

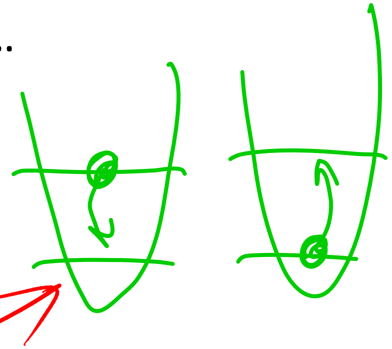
Even assuming a harmonic interaction, it looks terrible…



$$
\begin{aligned}
H = &-\frac{\hbar\omega}{4}\sum_{I,m}\left[\sqrt{(m+1)(m+2)}\left(b^{\dagger}_{I,m+2}b_{I,m}+b^{\dagger}_{I,m}b_{I,m+2}\right)-(2m+1)b^{\dagger}_{I,m}b_{I,m}\right]- \\
&-V_0\sum_{I,m,s} b^{\dagger}_{I,m}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s}+ \\
&+\frac{\hbar\omega}{4}\sum_{I,m,s}\left[\sqrt{(m+1)(m+2)}\left(b^{\dagger}_{I,m+2}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s}+b^{\dagger}_{I,m}b_{I,m+2}b^{\dagger}_{I+1,s}b_{I+1,s}\right)+(2m+1)b^{\dagger}_{I,m}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s}\right]- \\
&-\frac{\hbar\omega}{2}\sum_{I,m,s}\sqrt{m+1}\sqrt{s+1}\left(b^{\dagger}_{I,m+1}b_{I,m}b^{\dagger}_{I+1,s+1}b_{I+1,s}+b^{\dagger}_{I,m}b_{I,m+1}b^{\dagger}_{I+1,s}b_{I+1,s+1}\right)- \\
&-\frac{\hbar\omega}{2}\sum_{I,m,s}\sqrt{m+1}\sqrt{s+1}\left(b^{\dagger}_{I,m+1}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s+1}+b^{\dagger}_{I,m}b_{I,m+1}b^{\dagger}_{I+1,s+1}b_{I+1,s}\right)+ \\
&+\frac{\hbar\omega}{4}\sum_{I,m,s}\left(\sqrt{(m+1)(m+2)}\left(b^{\dagger}_{I,s}b_{I,s}b^{\dagger}_{I+1,m+2}b_{I+1,m}+b^{\dagger}_{I,s}b_{I,s}b^{\dagger}_{I+1,m}b_{I+1,m+2}\right)+(2m+1)b^{\dagger}_{I,s}b_{I,s}b^{\dagger}_{I+1,m}b_{I+1,m}\right)
\end{aligned}
$$

The Hamiltonian dressed with its new clothes

Even assuming a harmonic interaction, it looks terrible…



$$H=-\frac{\hbar\omega}{4}\sum_{I,m}\left[\sqrt{(m+1)(m+2)}\left(b^{\dagger}_{I,m+2}b_{I,m}+b^{\dagger}_{I,m}b_{I,m+2}\right)-(2m+1)b^{\dagger}_{I,m}b_{I,m}\right]-$$

$$-V_0\sum_{I,m,s}b^{\dagger}_{I,m}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s}+$$

$$+\frac{\hbar\omega}{4}\sum_{I,m,s}\left[\sqrt{(m+1)(m+2)}\left(b^{\dagger}_{I,m+2}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s}+b^{\dagger}_{I,m}b_{I,m+2}b^{\dagger}_{I+1,s}b_{I+1,s}\right)+(2m+1)b^{\dagger}_{I,m}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s}\right]-$$

$$-\frac{\hbar\omega}{2}\sum_{I,m,s}\sqrt{m+1}\sqrt{s+1}\left(b^{\dagger}_{I,m+1}b_{I,m}b^{\dagger}_{I+1,s+1}b_{I+1,s}+b^{\dagger}_{I,m}b_{I,m+1}b^{\dagger}_{I+1,s}b_{I+1,s+1}\right)-$$

$$-\frac{\hbar\omega}{2}\sum_{I,m,s}\sqrt{m+1}\sqrt{s+1}\left(b^{\dagger}_{I,m+1}b_{I,m}b^{\dagger}_{I+1,s}b_{I+1,s+1}+b^{\dagger}_{I,m}b_{I,m+1}b^{\dagger}_{I+1,s+1}b_{I+1,s}\right)+$$

$$+\frac{\hbar\omega}{4}\sum_{I,m,s}\left(\sqrt{(m+1)(m+2)}\left(b^{\dagger}_{I,s}b_{I,s}b^{\dagger}_{I+1,m+2}b_{I+1,m}+b^{\dagger}_{I,s}b_{I,s}b^{\dagger}_{I+1,m}b_{I+1,m+2}\right)+(2m+1)b^{\dagger}_{I,s}b_{I,s}b^{\dagger}_{I+1,m}b_{I+1,m}\right)$$

Analog of the ladder operators

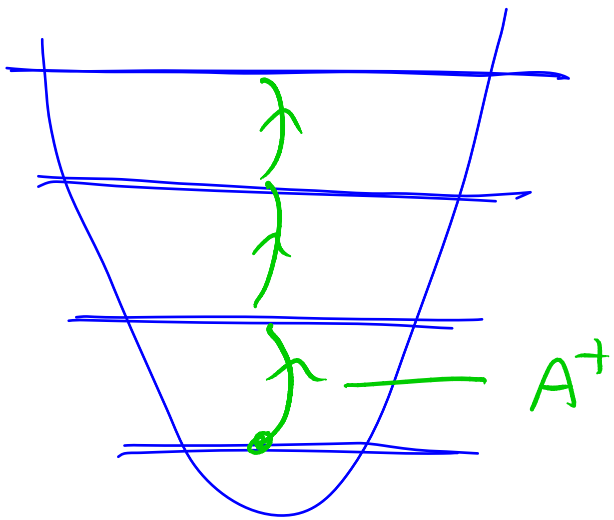
$$A_I^+ = \sum_{m=0} \sqrt{m+1}\, b^\dagger_{I,m+1} b_{I,m}$$

$$A_I^- = \sum_{m=0} \sqrt{m+1}\, b^\dagger_{I,m} b_{I,m+1}$$

$$n_I = \sum_{m=0} b^\dagger_{I,m} b_{I,m}$$

$$\left[A_I^-, A_K^+\right] = \delta_{I,K}\, n_K$$

$$\left[n_I, A_K^+\right] = 0\,.$$



The Hamiltonian again

$$H = \frac{\hbar\omega}{4}\sum_I \left(A_I^+ A_I^- + A_I^- A_I^+ - A_I^+ A_I^+ - A_I^- A_I^- \right) +$$

$$+\frac{\hbar k}{4M\omega}\sum_I \left(n_{I-1}n_I + n_I n_{I+1}\right)\left(A_I^+ A_I^- + A_I^- A_I^+ + A_I^+ A_I^+ + A_I^- A_I^- \right) -$$

$$-\frac{\hbar k}{2M\omega}\sum_I n_I n_{I+1}\left(A_I^+ A_{I+1}^- + A_I^- A_{I+1}^+ + A_I^+ A_{I+1}^+ + A_I^- A_{I+1}^- \right) -$$

$$-V_0 \sum_I n_I n_{I+1}$$

Same as the phonons of Solid State 101, but… with the occupation numbers

The simplest approximation

$$H = \frac{\hbar\omega}{4}\sum_I \left(A_I^+ A_I^- + A_I^- A_I^+ - A_I^+ A_I^+ - A_I^- A_I^- \right) +$$

$$+\frac{\hbar k}{4M\omega}\sum_I \left(n_{I-1} n_I + n_I n_{I+1} \right)\left(A_I^+ A_I^- + A_I^- A_I^+ + A_I^+ A_I^+ + A_I^- A_I^- \right) -$$

$$-\frac{\hbar k}{2M\omega}\sum_I n_I n_{I+1}\left(A_I^+ A_{I+1}^- + A_I^- A_{I+1}^+ + A_I^+ A_{I+1}^+ + A_I^- A_{I+1}^- \right) -$$

$$-V_0 \sum_I n_I n_{I+1}$$

$$\left\langle n_I n_{I+1} \right\rangle \equiv \chi \sim n^2 \qquad \omega = \sqrt{\frac{2k\chi}{M}}$$

The simplest approximation

$$H = \frac{\hbar\omega}{2}\sum_I \left(A_I^+ A_I^- + A_I^- A_I^+ \right) +$$

$$-\frac{\hbar\omega}{4}\sum_I \left(A_I^+ A_{I+1}^- + A_I^- A_{I+1}^+ + A_I^+ A_{I+1}^+ + A_I^- A_{I+1}^- \right) -$$

$$-V_0 N \chi$$

$$\left\langle n_I n_{I+1} \right\rangle \equiv \chi \sim n^2 \qquad \omega = \sqrt{\frac{2k\chi}{M}}$$

The local frequency selected to eliminate anomalous terms in the local vibrations

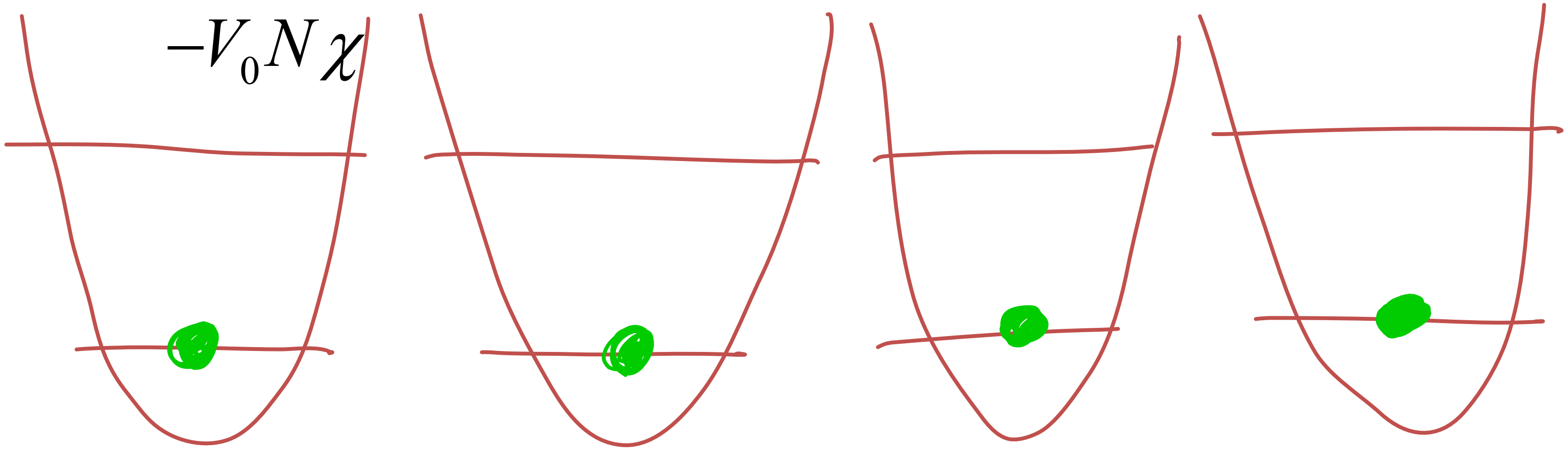
The simplest approximation

$$H = \frac{\hbar\omega}{2}\sum_I \left(A_I^+ A_I^- + A_I^- A_I^+ \right) +$$

$$\omega = \sqrt{\frac{2k\chi}{M}}$$

$$-\frac{\hbar\omega}{4}\sum_I \left(A_I^+ A_{I+1}^- + A_I^- A_{I+1}^+ + A_I^+ A_{I+1}^+ + A_I^- A_{I+1}^- \right) -$$

$$-V_0 N\chi$$



The local frequency selected to eliminate anomalous terms in the local vibrations

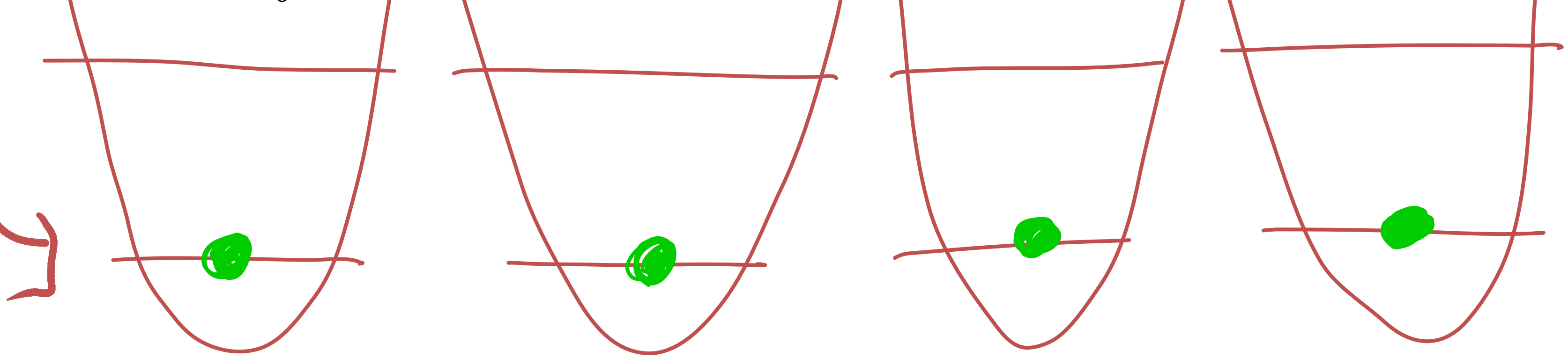
The simplest approximation

$$H = \frac{\hbar\omega}{2}\sum_I \left(A_I^+ A_I^- + A_I^- A_I^+\right) +$$

$$-\frac{\hbar\omega}{4}\sum_I \left(A_I^+ A_{I+1}^- + A_I^- A_{I+1}^+ + A_I^+ A_{I+1}^+ + A_I^- A_{I+1}^-\right) -$$

$$-V_0 N \chi$$

$$\omega = \sqrt{\frac{2k\chi}{M}}$$



The local frequency selected to eliminate anomalous terms in the local vibrations

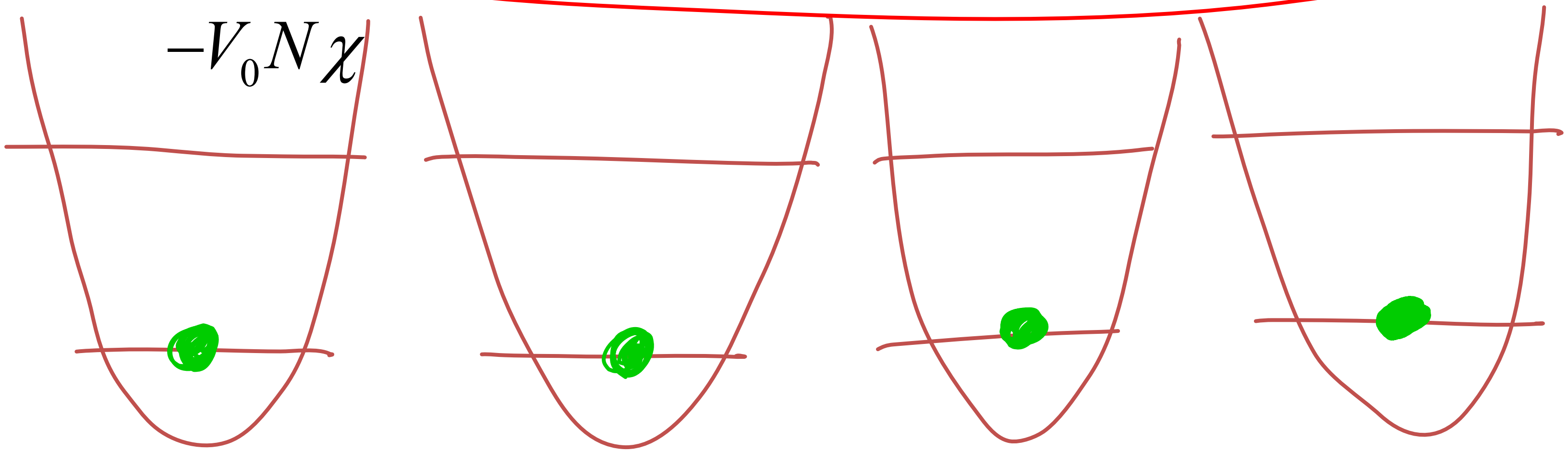
The simplest approximation

$$H = \frac{\hbar\omega}{2}\sum_I \left(A_I^+ A_I^- + A_I^- A_I^+ \right) +$$

$$-\frac{\hbar\omega}{4}\sum_I \left(A_I^+ A_{I+1}^- + A_I^- A_{I+1}^+ + A_I^+ A_{I+1}^+ + A_I^- A_{I+1}^- \right) -$$

$$-V_0 N \chi$$

$$\omega = \sqrt{\frac{2k\chi}{M}}$$



The local frequency selected to eliminate anomalous terms in the local vibrations

Fourier and diagonalize

$$H = \sum_q \left[\left(\frac{\hbar\omega}{2} - \frac{\hbar\omega}{4}\cos(qa) \right) \left(A_q^+ A_q^- + A_{-q}^- A_{-q}^+ \right) - \frac{\hbar\omega}{4}\cos(qa) \left(A_q^+ A_{-q}^+ + A_{-q}^- A_q^- \right) \right]$$
$$-V_0 N \chi$$

$$A_q^+ = u_q B_q^\dagger + v_q B_{-q}$$
$$A_q^- = v_q B_{-q}^\dagger + u_q B_q$$

$$H = \sum_q \hbar\Omega(q) \left(B_q^\dagger B_q + 1/2 \right) - V_0 N \chi$$

$$\Omega(q) = \sqrt{\frac{2k\chi}{m}\left(1 - \cos(qa)\right)} = \omega\sqrt{\left(1 - \cos(qa)\right)}$$

Ground state

$$E_{GS} = \sum_q \frac{\hbar\Omega(q)}{2} - V_0 N\chi$$

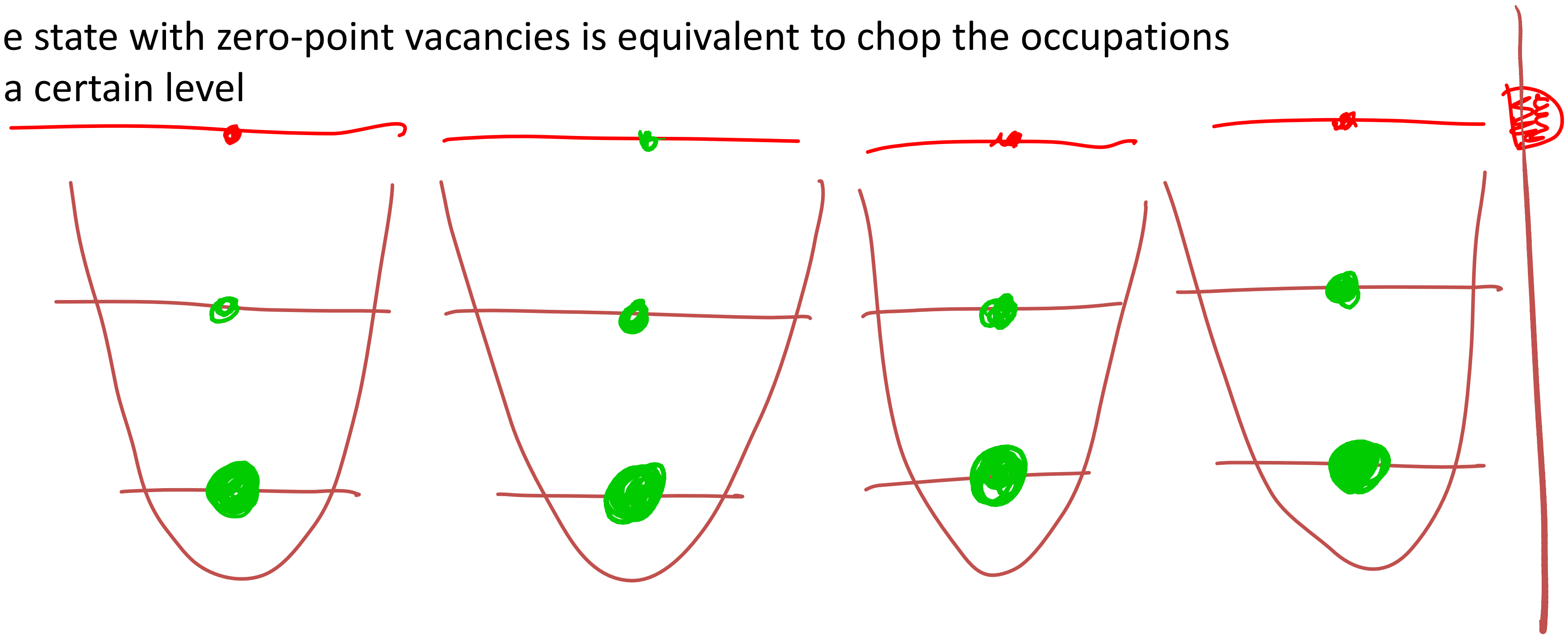
$$\Omega(q) = \sqrt{\frac{2k\chi}{m}\left(1-\cos(qa)\right)} = \omega\sqrt{\left(1-\cos(qa)\right)}$$

$$\left|GS\right\rangle = \left|\varnothing_b\right\rangle = C\exp\left\{\sum_q \frac{v_q}{u_q} A_q^\dagger A_{-q}^\dagger\right\}\left|\varnothing_a\right\rangle = C\left(1+\lambda_q A_q^\dagger A_{-q}^\dagger + \ldots\right)\left|\varnothing_a\right\rangle$$

The ground state has non zero population of higher energy states in the local description

$$\left|GS\right\rangle = \left|\varnothing_b\right\rangle = C\exp\left\{\sum_q \frac{v_q}{u_q} A_q^\dagger A_{-q}^\dagger\right\}\left|\varnothing_a\right\rangle = C\left(1+\lambda_q A_q^\dagger A_{-q}^\dagger + \ldots\right)\left|\varnothing_a\right\rangle$$

The state with zero-point vacancies is equivalent to chop the occupations at a certain level



Three Quantum Effects

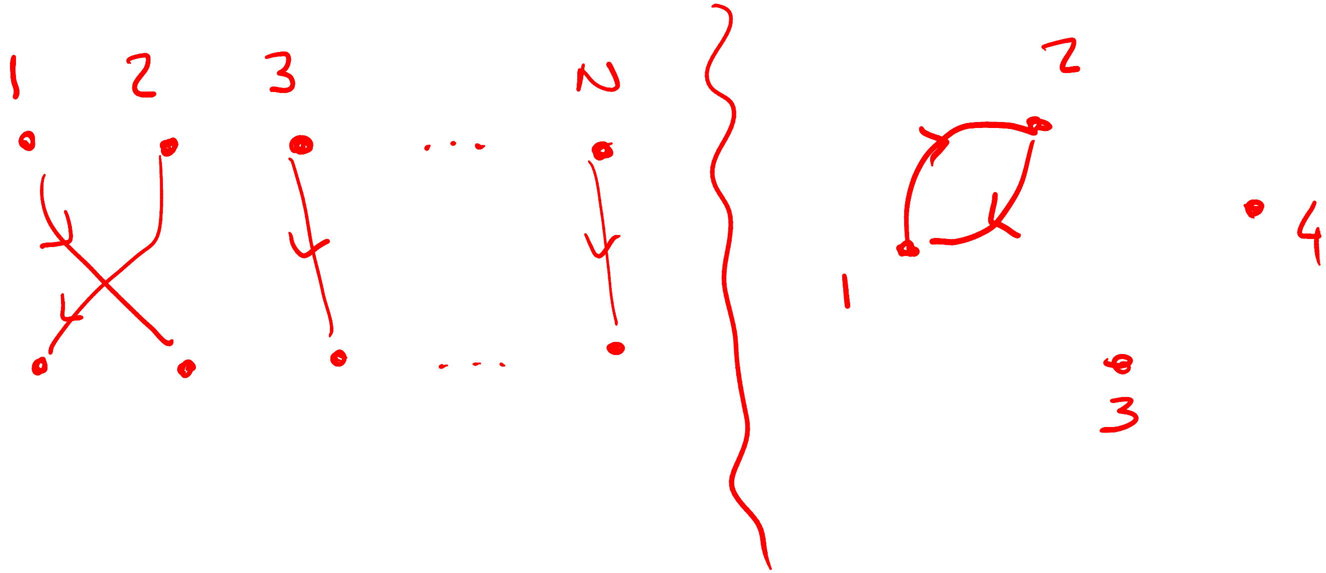
- Quantization of the dynamical variables
- Mixed particle number states
- Exchange (intrinsically many body…)

Exchange

$$\left|\psi_1,\cdots,\psi_N\right\rangle \in \mathbf{H}^{\otimes N}$$

However, in QM we cannot distinguish identical particles and the only allowable states for bosons are those fully symmetric against permutation of particles.

$$g \in S_N$$



Exchange

$$P_+ \left|\psi_1, \cdots, \psi_N\right\rangle = \frac{1}{N!} \sum_{g \in S_N} U(g) \left|\psi_1, \cdots, \psi_N\right\rangle$$

$$U(g) \left|\psi_1, \cdots, \psi_N\right\rangle = \left|\psi_{g^{-1}(1)}, \cdots, \psi_{g^{-1}(N)}\right\rangle$$

$$Z_{N,V}(\beta) = Tr\left(P_+ e^{-\beta H}\right) = \frac{1}{N!} \sum_{g \in S_N} Tr\left(U(g) e^{-\beta H}\right)$$

$$P_{N,V}(g) = \frac{Tr\left(U(g) e^{-\beta H}\right)}{Z_{N,V}(\beta)\, N!}$$

Exchange

$$Z_{N,V}(\beta) = Tr\left(P_+ e^{-\beta H}\right) = \frac{1}{N!}\sum_{g\in S_N} Tr\left(U(g)e^{-\beta H}\right)$$

$$H\left|n\right\rangle = E_n\left|n\right\rangle$$

$$Z_{N,V}(\beta) = \frac{1}{N!}\sum_{g\in S_N}\sum_{n}\left\langle n\right|U(g)\left|n\right\rangle e^{-\beta E_n}$$

$$P_{N,V}(g) = \frac{\sum_{n}\left\langle n\right|U(g)\left|n\right\rangle e^{-\beta E_n}}{Z_{N,V}(\beta)\,N!}$$

Exchange

$$Z_{N,V}\left(\beta\right)=Tr\left(P_{+}e^{-\beta H}\right)=\frac{1}{N!}\sum_{g\in S_N}Tr\left(U\left(g\right)e^{-\beta H}\right)$$

$$H\left|n\right\rangle = E_n\left|n\right\rangle$$

$$Z_{N,V}\left(\beta\right)=\frac{1}{N!}\sum_{g\in S_N}\sum_{n}\left\langle n\right|U\left(g\right)\left|n\right\rangle e^{-\beta E_n}$$

$$\langle \varphi_1 \varphi_2 | U(g) | \varphi_1 \varphi_2 \rangle = \int d\bar{r}_1 d\bar{r}_2\, \varphi_1^*(\bar{r}_1)\varphi_2^*(\bar{r}_2)\varphi_1(\bar{r}_2)\varphi_2(\bar{r}_1)$$

$$= \left| \int d\bar{r}\, \varphi_1^*(\bar{r})\, \varphi_2(\bar{r}) \right|^2$$

Feynman and the Bose gas

$$Z_{N,V}(\beta) = \frac{1}{N!}\sum_{g\in S_N} Tr\left(U(g)e^{-\beta H_0}\right)$$

$$= \frac{1}{N!}\sum_{g\in S_N} \int d\vec{r}_1 \cdots d\vec{r}_N \left\langle \vec{r}_1,\cdots,\vec{r}_N \right| U(g)e^{-\beta H_0} \left| \vec{r}_1,\cdots,\vec{r}_N \right\rangle$$

$$= \frac{1}{N!}\sum_{g\in S_N} \int d\vec{r}_1 \cdots d\vec{r}_N \left\langle \vec{r}_{g(1)},\cdots,\vec{r}_{g(N)} \right| e^{-\beta H_0} \left| \vec{r}_1,\cdots,\vec{r}_N \right\rangle$$

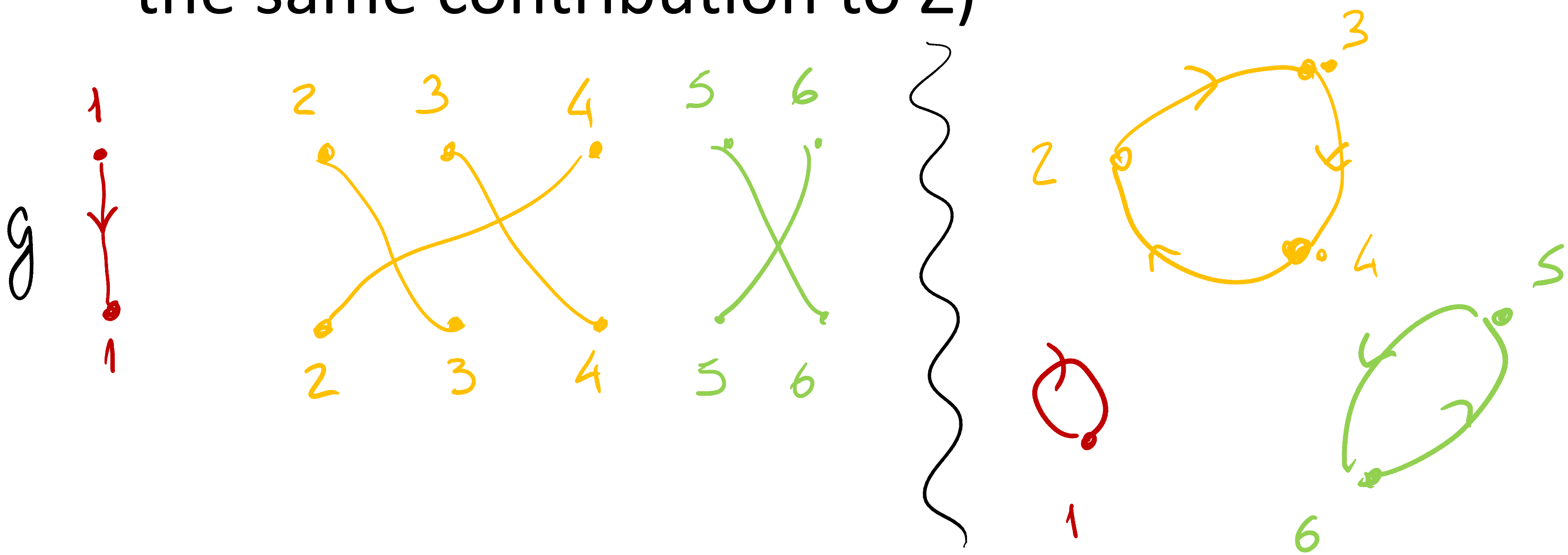
$$Z_{N,V}(\beta) = \frac{1}{\lambda^{3N} N!}\sum_{g\in S_N} \int d\vec{r}_1 \cdots d\vec{r}_N \exp\left\{ -\frac{\pi}{\lambda^2}\sum_{i=1}^{N}\left(\vec{r}_{g(i)} - \vec{r}_i\right)^2 \right\}$$

$$\lambda = \sqrt{\frac{2\pi\hbar^2\beta}{M}}$$

Following: H. Kleinert, Path Integral's book, based on Feynman's Stat. Mech.

Feynman and the Bose gas

- A permutation can be always factored into cycles (permutations with the same cycle structure belong to the same class and give the same contribution to Z)



Feynman and the Bose gas

$$Z_{N,V}(\beta) = \frac{1}{N!}\sum_{g}\prod_{w=1}^{N}\frac{N!}{C_w!\,w^{C_w}}\left[Z_{1,V}(w\beta)\right]^{C_w}$$

$$Z_{1,V}(w\beta) = \frac{V}{\lambda^3 w^{3/2}}$$

Order parameters in the Bose liquid

- Feynman
  - Feynman, R.P., 1953. Atomic Theory of the lambda Transition in Helium. *Physical Review*, 91(6), 1291.
- Penrose and Onsager
  - Penrose, O. & Onsager, L., 1956. Bose-Einstein Condensation and Liquid Helium. *Physical Review*, 104(3), 576.
- Sütõ
  - Sütõ, A., 1993. Percolation transition in the Bose gas. *Journal of Physics A: Mathematical and General*, 26(18), 4689-4710.
  - Sütõ, A., 2002. Percolation transition in the Bose gas: II. *Journal of Physics A: Mathematical and General*, 35(33), 6995-7002.
- Ueltschi
  - Ueltschi, D., 2006a. Feynman cycles in the Bose gas. *Journal of Mathematical Physics*, 47(12), 123303-15.
  - Ueltschi, D., 2006b. Relation between Feynman Cycles and Off-Diagonal Long-Range Order. *Physical Review Letters*, 97(17), 170601-4.

Order parameters in the Bose liquid

- Richard Feynman (1953):

  Density of particles in the infinite exchange cycle as order parameter.

$$\rho_p(\infty)$$

$$Z_{N,V}(\beta) = \frac{1}{\lambda^{*3N} N!} \sum_{g \in S_N} \int d\vec{r}_1 \cdots d\vec{r}_N \exp\left\{ -\frac{\pi}{\lambda^{*2}} \sum_{i=1}^{N} \left(\vec{r}_{g(i)} - \vec{r}_i \right)^2 \right\} \times \rho\left(\vec{r}_1, \cdots, \vec{r}_N \right)$$

Order parameters in the Bose liquid

- Penrose and Onsager (1956):

Off Diagonal Long Range Order

$$\sigma\left(x,y\right)=\left\langle c^{\dagger}(x)c(y)\right\rangle$$

$$\lim_{|x-y|\to\infty}\sigma\left(x,y\right)\neq 0$$

Absence of long range order necessary for the existence of ODLRO

Order parameters in the Bose liquid

- András Sütõ gave the first mathematical proof that:
  - Infinite cycles occur in the presence of condensation (1993)
  - No infinite cycle occurs in the absence of condensation (2002)

$$\sigma(x,0)=\sum_{n\geq 1} e^{-x^2/4n\beta}\rho_p(n)+\rho_p(\infty)$$

Claims that the uniqueness of the ground state replaces the absence of long range order as necesary condition for ODLRO

- Daniel Ueltschi in 2006 expored this relation in the presence of interactions

Exchange in solids

- Thouless, D., 1965. Exchange in Solid ^{3}He and Heisenberg Hamiltonian. *Proceedings of the Physical Society of London*, 86(553P), 893.
- Leggett, A.J., 1970. Can a Solid Be "Superfluid"? *Physical Review Letters*, 25(22), 1543.

School of M

lows: The effect is
same order of magn
id helium, namely t
interaction of He^3 nu
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change constant and
would give the order
$\lesssim J(\hbar^2/ma^2)^{-1} \sim 3\times 1$
emphasized that this
tive.

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Tunneling and Exchange in Quantum Solids*

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(Received 17 October 1968; revised manuscript received 14 May 1969)

Pairs of ^{3}He atoms in solid bcc ^{3}He have spatially symmetric or antisymmetric wave functions which correspond to energies ϵ^+ and ϵ^-, $\epsilon^{\pm}=\epsilon\pm\frac{1}{2}\Delta\epsilon$. The energy difference $\epsilon^+-\epsilon^-=\Delta\epsilon$ is due to a tunneling process and an interaction process. The effect of these two processes can be simulated by adding to the Hamiltonian of the solid an exchange Hamiltonian,

$$\mathcal{H}_x=-2\Delta\epsilon\sum_{ij}{}'\vec{\sigma}_i\cdot\vec{\sigma}_j=-2(\Delta\epsilon_T+\Delta\epsilon_x)\sum_{ij}{}'\vec{\sigma}_i\cdot\vec{\sigma}_j,$$

where $\Delta\epsilon$ is a sum of $\Delta\epsilon_T$ (due to the tunneling process) and $\Delta\epsilon_x$ (due to the interaction process). A theory of the magnitude and sign of $\Delta\epsilon_x$ and $\Delta\epsilon_T$ is given. We find $\Delta\epsilon_T<0$ and $\epsilon_x>0$. Using quite general arguments, we show that $|\Delta\epsilon_T|\gtrsim 2|\Delta\epsilon_x|$. The exchange in bcc solid ^{3}He is antiferromagnetic. Evaluation of the formulas for $\Delta\epsilon_T$ and $\Delta\epsilon_x$ using the ground-state wave function of Guyer and Sarkissian leads to $\Delta\epsilon=J$, in good agreement with experiment.

Exchange in solids

- Bernu, B. & Ceperley, D., 2005. Path integral calculations of exchange in solid ^{4}He. *Journal of Physics and Chemistry of Solids*, 66(8-9), 1462-1466.
  - Pointed that the Feynman-Kikuchi model was more for a solid than a liquid. However, the exchange constants are different.

$$J_p = J_o \exp\left[-\alpha L_p - \alpha' \sum_{i=1}^{n_p} \cos^4(\theta_i/2)\right].$$

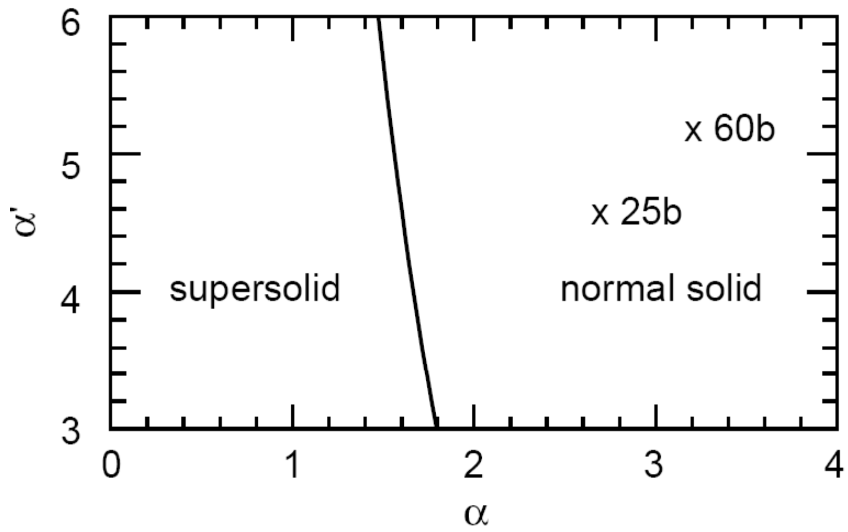
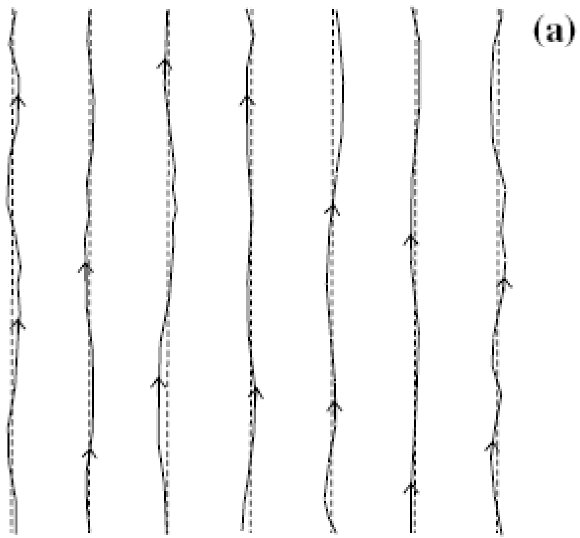


Fig. 2. Phase diagram of the generalized Feynman–Kikuchi model. The two points are near melting and at high pressure.

Exchange in solids

Nikolai Prokof'ev & Boris Svistunov. “Supersolid State of Matter.”
Physical Review Letters, **94**(15), 155302-4 (2005)



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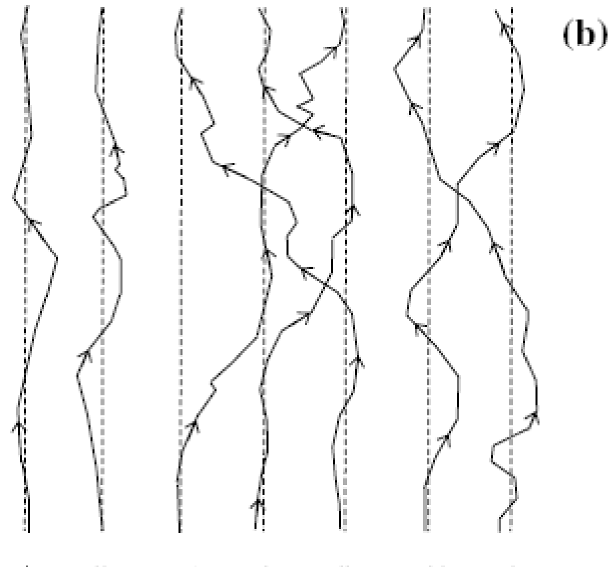

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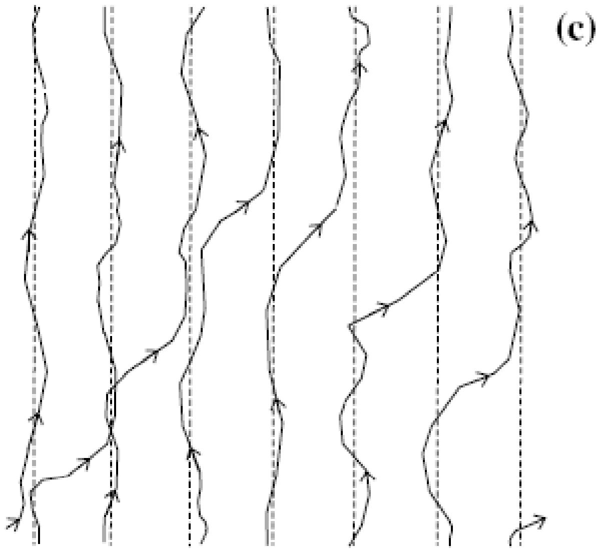


Exchange and Specific Heat

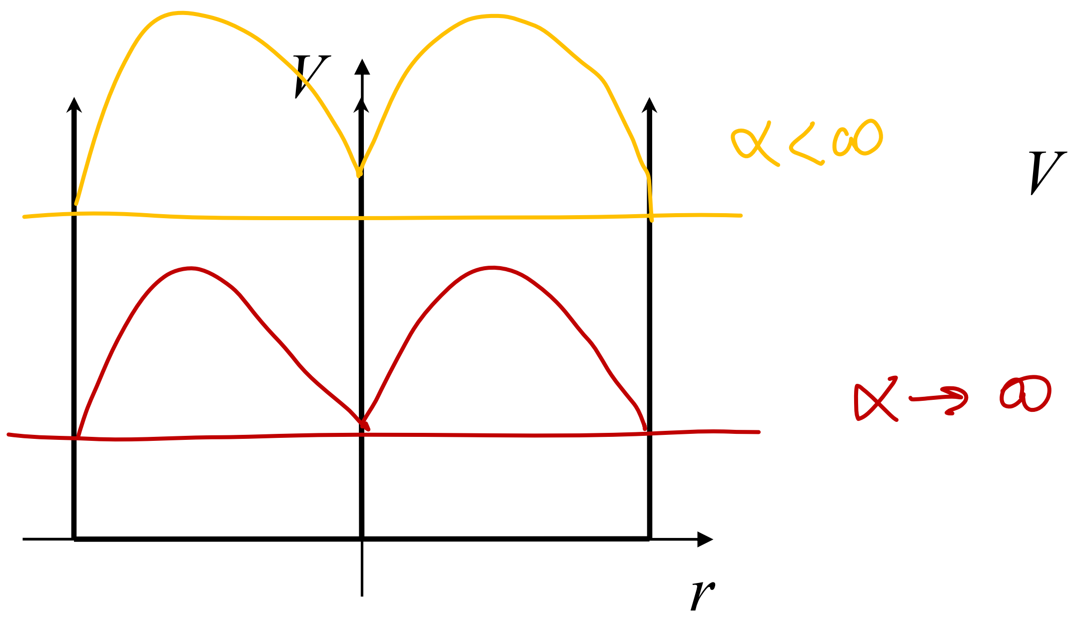
- Specific heat is a measure of the forms or degrees of freedom with which a system can absorb energy, e.g., the simple two-level system.
- The increment in the specific heat above Tc is observed in the non-interacting bose gas and in liquid helium.
- In both cases, can be traced back to the appearance of exchange as the “new” or “extra” excitation in the system.

A simple example of the effect of exchange on the specific heat

- Two particles with a delta interaction and the square well.

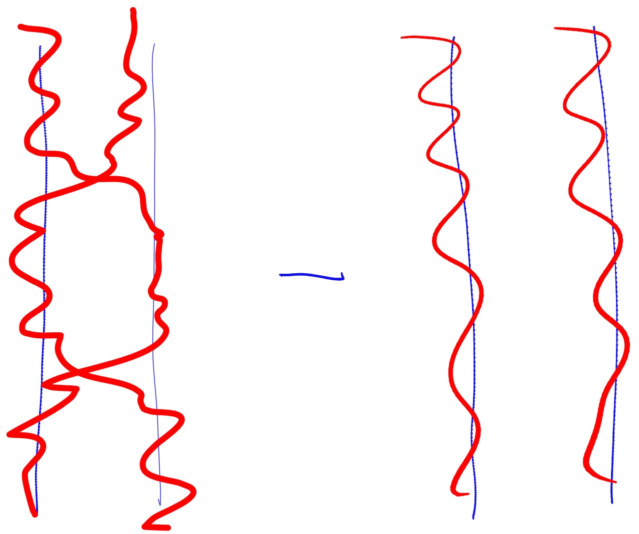
$$H = \frac{P^2}{2M} + \frac{p^2}{2\mu} + V\left(|r|\right)$$

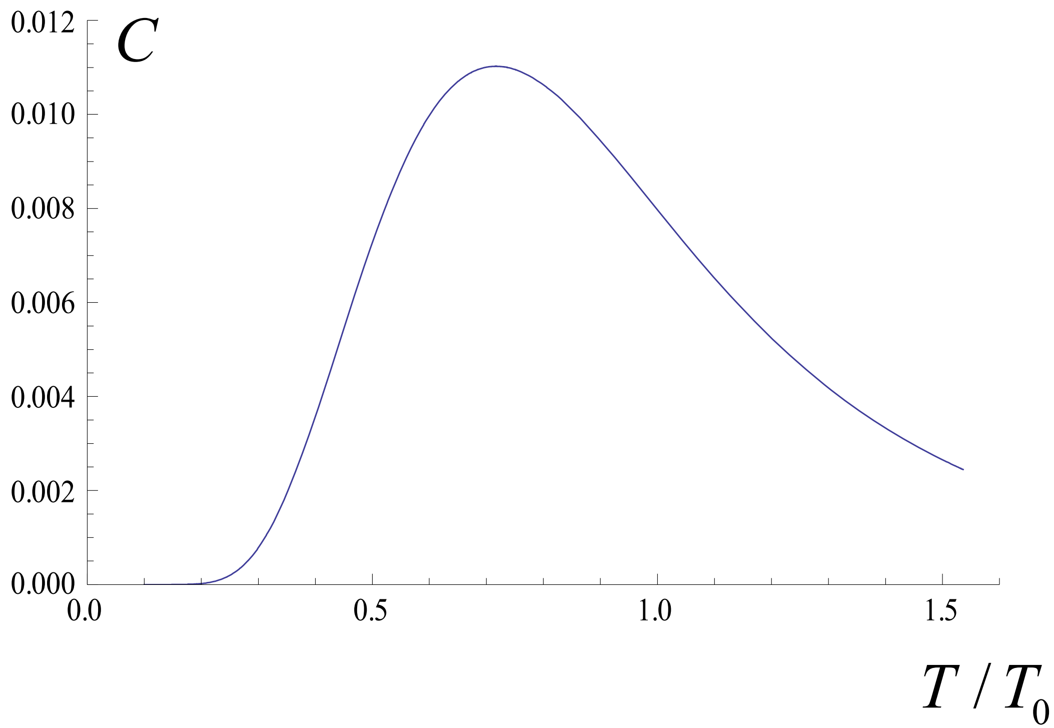
$$V\left(|r|\right) = \alpha\delta\left(r\right) + U\left(|r|\right)$$



A simple example of the effect of exchange on the specific heat

- Two particles with a delta interaction and the square well.





Fluctuations above Tc

- Koh, S., 2007. Moment of Inertia Just Above λ Point. *Journal of Low Temperature Physics*, 148(3), 121-126.
- Koh, S., 2006. Nonclassical rotational behavior at the vicinity of the lambda point. *Physical Review B (Condensed Matter and Materials Physics)*, 74(5), 054501-11.
- Anderson, P.W., 2008. Bose Fluids Above T_c: Incompressible Vortex Fluids and ``Supersolidity''. *Physical Review Letters*, 100(21), 215301-3.

Is there a Tc? Maybe the system never reaches the percolated state.

Still, experiments in a perfect solid would show superfluid/supersolid fluctuations

In the kitchen…

- Include exchange in the phonon description
- Dependence with the frequency of oscillation of the pendulum
- Pressure independence
- Realistic PIMC calculations
  - How far are we from the percolation limit
  - May be the defects push the system over the fence…

Do not forget the perfect solid… even if there are only fluctuations
it will be the manifestation of quantum effects… and that is always fun…