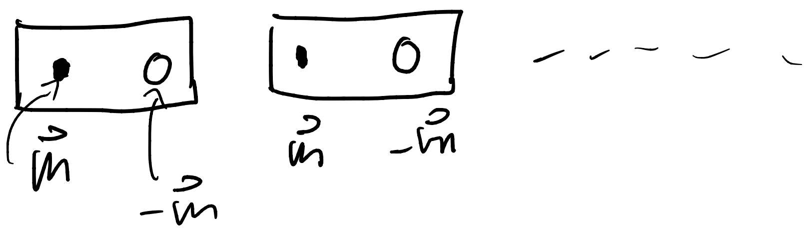
b) 1D anti-ferromagnet, $z=2$, $\vec{m}_j = (-1)^j \vec{m}$, $J<0$.

$\rightsquigarrow$ Group sites into unit cell with two sites



$$H \approx -J \sum_{i \in 2\mathbb{Z}} \left(2\vec{m}\left(\vec{S}_{i+1} - \vec{S}_i\right) + 2\vec{m}^2\right) = \sum_{i \in 2\mathbb{Z}} H^i_{MF}(\vec{m})$$

$$F_i(\vec{m}) = -\frac{1}{\beta}\log\left(\mathrm{Tr}\left(e^{-\beta H^i_{MF}(\vec{m})}\right)\right) = -\frac{1}{\beta}\log\left[\mathrm{Tr}\begin{array}{c}\begin{pmatrix} e^{2\beta J(m+m^2)} & & & \\ & e^{2\beta J m^2} & & \\ & & e^{2\beta J m^2} & \\ & & & e^{2\beta J(m^2-m)} \end{pmatrix} \\ \uparrow\uparrow \quad \uparrow\downarrow \quad \downarrow\uparrow \quad \downarrow\downarrow \end{array}\right]$$

$$= -\frac{1}{\beta}\left(2\beta J m^2 + \log\left(2 + 2\cosh(2\beta J m)\right)\right) =: F(m).$$

$$\partial_m F(m) = 0 \Leftrightarrow -4Jm = \frac{1}{\beta} \frac{4\beta J \sinh(2\beta J m)}{2 + 2\cosh(2\beta J m)} .$$

For small m: $m \approx -\frac{\beta J m}{2} \Rightarrow T_c = \frac{-J}{k_B 2} \overset{z=2}{\overset{\downarrow}{=}} \frac{-Jz}{k_B 4}$.

Comments:

↳ Mermin-Wagner theorem tells us that AFM order transition at finite T cannot happen in 1D.

↳ General rule of thumb: Mean-field theory is good in high spatial dimension (high coordination number z) and for small to moderate interactions.

[above critical dimension]

- Generic structure of mean-field decoupling:

$$H = \underbrace{H_0}_{\text{solution known}} + \sum_{i,j} \lambda_{i,j} O_i O_j$$

- Define $\delta O_j = O_j - \langle O_j \rangle$ and decompose $O_j = \langle O_j \rangle + \delta O_j$
- Approximate $\boxed{O_i O_j \underset{+\mathcal{O}(\delta^2)}{\approx} O_i \langle O_j \rangle + \langle O_i \rangle O_j - \langle O_i \rangle \langle O_j \rangle}$
- Replace $\{\langle O_i \rangle\}_i$ by free parameters $\{w_i\}_i$

$$\rightsquigarrow H \approx H_{MF}(\{w_i\}) = H_0 + \sum_{i,j} \lambda_{i,j} \left(O_i w_j + O_j w_i - w_i w_j \right)$$

With $Z = \mathrm{Tr}\left(e^{-\beta H_{MF}}\right)$ and $F = -\frac{1}{\beta}\log Z$, we get

$$\partial_{w_j} F = 0 \quad \forall_j \quad \Leftrightarrow \quad \boxed{\langle O_j \rangle_{MF} = w_j \quad \forall_j}$$

(self-consistency)

- Complementary approach to mean field theory: Variational optimization within the space of uncorrelated states (see part C).

- Bose-Hubbard model in Gutzwiller approximation (cf. sheet 2)

$$H = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i (n_i - 1).$$

– Basic idea: Perform mean-field decoupling of the kinetic term $b_i^\dagger b_j + \text{h.c.}$ to describe superfluid to Mott transition

- Gutzwiller ansatz: $|\Psi\rangle = \prod_i |\phi_i\rangle$ with $|\phi_i\rangle = \sum_{n=0}^{\infty} f_n^{(i)} |n\rangle^{(i)}$.

site

occupation number of site i

- Define $\langle\Psi| b_i |\Psi\rangle = \sum_{n=0}^{\infty} \sqrt{n+1}\, f_n^{(i)*} f_{n+1}^{(i)} =: \Psi_i$ (superfluid order parameter)

$\left[b_i f_{n+1}^{(i)} |n+1\rangle^{(i)} = \sqrt{n+1}\, f_{n+1}^{(i)} |n\rangle^{(i)} \right]$

$\left[{}^{(i)}\langle n|m\rangle^{(i)} =: \delta_{n,m} \right]$

- Perform mean field decoupling assuming $\Psi_i \equiv \Psi$.

$$H \approx \sum_i H_{MF}^{(i)}(\{\Psi, \Psi^*\}) = -\sum_i J \underbrace{z}_{\#NN} \big(b_i^\dagger \Psi + b_i \Psi^* - \underbrace{|\Psi|^2}_{\text{constant, often dropped}} \big) + \frac{U}{2} n_i (n_i - 1).$$

– Represent MF-Hamiltonian in local basis $|n\rangle^{(i)}$: drop (i) for brevity

occupation number

$$\langle n | H_{MF} - \mu \hat{n} | m \rangle = -zJ \left(\sqrt{m+1}\, \delta_{n,m+1}\, \psi + \sqrt{m}\, \delta_{n,m-1}\, \psi^* \right)$$

$$+ \frac{U}{2} n(n-1)\, \delta_{n,m} - \mu n\, \delta_{n,m} .$$

chemical potential

MF-energy

– Practical eigenvalue problem:

$$\begin{pmatrix} 0 & -zJ\psi^* & 0 & 0 & \cdots \\ -zJ\psi & -\mu & -\sqrt{2}\,zJ\psi^* & & \\ & -\sqrt{2}\,zJ\psi & U-2\mu & -\sqrt{3}\,zJ\psi^* & \\ 0 & & -\sqrt{3}\,zJ\psi & 3U-3\mu & \ddots \\ 0 & & & \ddots & \ddots \\ \vdots & & & & \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ \vdots \end{pmatrix} = \mathcal{E} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ \vdots \end{pmatrix}$$

– Practical MF iteration:

(i) Choose initial random value for Ψ.

(ii) Solve for the ground state of $H_{MF} - \mu \hat{n}$ and compute $\sum_{n=0}^{n_{max}} \sqrt{n+1}\, f_n^* f_{n+1} =: \tilde{\Psi}$.

(iii) Update $\Psi = \tilde{\Psi}$ in H_{MF}.

[repeat until Ψ self-consistent]

↳ Converge results upon increasing n_{max} (cutoff in boson number)

- Experimental observation of superfluid to Mott transition:

M. Greiner et al. Nature 415, 39 (2002).