中山大學
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# Bose-Hubbard Model


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# Cold Bosonic Atoms in Optical Lattices

## ·Hamiltonian

Hamilton operator for bosonic atoms

$$H = \int d^3x\, \psi^\dagger(\mathbf{x})\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{x}) + V_T(\mathbf{x})\right)\psi(\mathbf{x}) + \frac{1}{2}\frac{4\pi a_s\hbar^2}{m}\int d^3x\, \psi^\dagger(\mathbf{x})\psi^\dagger(\mathbf{x})\psi(\mathbf{x})\psi(\mathbf{x}),$$

$\psi(\boldsymbol{x})$ is a boson field operator for atoms in a given internal atomic state
$V_0(x)$ is the optical lattice potential
$V_T\,(x)$ describes an additional (slowly varying) external trapping potential

$$V_0(\mathbf{x}) = \sum_{j=1}^{3} V_{j0}\sin^2(kx_j)$$

$$k = 2\pi/\lambda \qquad a = \lambda/2$$

Expanding the field operators in the Wannier basis and keeping only the lowest vibrational states

$$\psi(\mathbf{x}) = \sum_i b_i w(\mathbf{x} - \mathbf{x}_i)$$

$$\hat{\Psi}(\mathbf{r}) = \sum_j \hat{b}_j\phi_j(\mathbf{r})$$

$$\Psi_\ell(r_\ell) = (k_0^2\tilde{\omega}_\ell/\pi)^{1/4}e^{-\tilde{\omega}_\ell k_0^2 r_\ell^2/2}$$

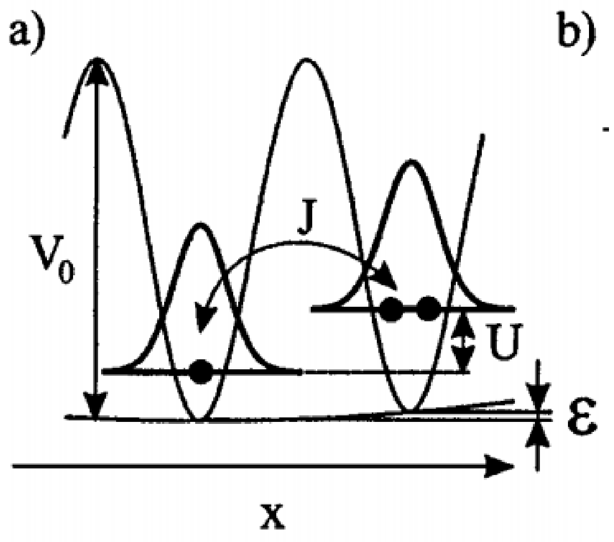
$$H = -J\sum_{\langle i,j\rangle} b_i^\dagger b_j + \sum_i \epsilon_i\hat{n}_i + \frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1),$$

近邻交叠积分最大

# Cold Bosonic Atoms in Optical Lattices

## ·Tight-Binding Model

仅用基态，假设基态能量为0




$$\psi(\mathbf{x}) = \sum_i b_i w(\mathbf{x} - \mathbf{x}_i)$$

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

where the operators $\hat{n}_i = b_i^\dagger b_i$ count the number of bosonic atoms at lattice site $i$;

the annihilation and creation operators $b_i$ and $b_i^\dagger$ obey the canonical commutation relations $\left[b_i, b_j^\dagger\right] = \delta_{ij}$.

The parameters $U = 4\pi a_s \hbar^2 \int d^3x|w(\mathbf{x})|^4/m$ correspond to the strength of the on site repulsion of two atoms on the lattice site $i$.

$J = -\int d^3x w^*(\mathbf{x} - \mathbf{x}_i)\left[-\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{x})\right]w(\mathbf{x} - \mathbf{x}_j)$ is the hopping matrix element between adjacent sites $i, j$.

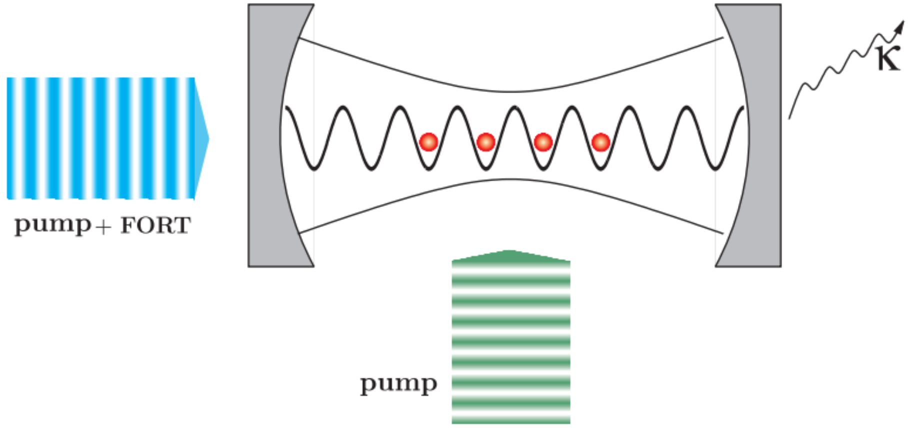
$\epsilon_i = \int d^3x V_T(\mathbf{x})|w(\mathbf{x} - \mathbf{x}_i)|^2 \approx V_T(\mathbf{x}_i)$ describes an energy offset of each lattice site.


Part.02

# Ultracold atoms in optical lattices generated by quantized light fields

## ·Single Atom Hamiltonian

N个质量为m，跃迁频率为$\omega_{eg}$的原子，与频率$\omega_c$的驻波单模腔场相互作用，还有一个$\omega_p$频率、与原子最大耦合强度为$h_0$的振幅为$\eta$的相干驱动光，弱耦合采用RWA，得到JC Model。




$$H^{(1)} = H_A^{(1)} + H_R^{(1)} + H_{Int}^{(1)}.$$

$$H_A^{(1)} = \frac{\hat{\mathbf{p}}^2}{2m} + V_e(\mathbf{x})\sigma^+\sigma^- + V_g(\mathbf{x})\sigma^-\sigma^+ + \hbar\omega_{eg}\sigma^+\sigma^- - i\hbar h(\mathbf{x})\left(\sigma^+ e^{-i\omega_p t} - \sigma^- e^{i\omega_p t}\right)$$

$$H_R^{(1)} = \hbar\omega_c a^\dagger a - i\hbar\eta\left(a e^{i\omega_p t} - a^\dagger e^{-i\omega_p t}\right),$$

$$H_{Int}^{(1)} = -i\hbar g(\mathbf{x})\left(\sigma^+ a - \sigma^- a^\dagger\right).$$

$$U(t) = \exp[i\omega_p t\left(\sigma^+\sigma^- + a^\dagger a\right)]$$

detuning

$$\Delta_c = \omega_p - \omega_c,\ \Delta_a = \omega_p - \omega_{eg}$$

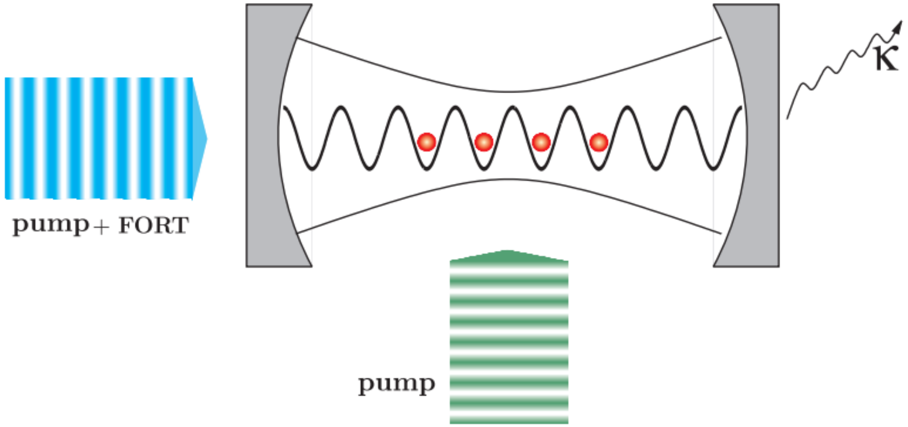
$$H_A^{(1)} = \frac{\hat{\mathbf{p}}^2}{2m} + V_e(\mathbf{x})\sigma^+\sigma^- + V_g(\mathbf{x})\sigma^-\sigma^+ - \hbar\Delta_a\sigma^+\sigma^- - i\hbar h(\mathbf{x})\left(\sigma^+ - \sigma^-\right)$$

$$H_R^{(1)} = -\hbar\Delta_c a^\dagger a - i\hbar\eta\left(a - a^\dagger\right),$$

$$H_{Int}^{(1)} = -i\hbar g(\mathbf{x})\left(\sigma^+ a - \sigma^- a^\dagger\right),$$

## ·Second Quantization

$$H_A^{(1)} = \frac{\hat{\mathbf{p}}^2}{2m} + V_e(\mathbf{x})\sigma^+\sigma^- + V_g(\mathbf{x})\sigma^-\sigma^+ - \hbar\Delta_a\sigma^+\sigma^- - i\hbar h(\mathbf{x})\left(\sigma^+ - \sigma^-\right)$$
$$H_R^{(1)} = -\hbar\Delta_c a^\dagger a - i\hbar\eta\left(a - a^\dagger\right),$$
$$H_{Int}^{(1)} = -i\hbar g(\mathbf{x})\left(\sigma^+ a - \sigma^- a^\dagger\right),$$




$$H = H_A + H_R + H_{A-R} + H_{A-P} + H_{A-A}.$$

$$H_A = \int \mathrm{d}^3\mathbf{x}\left[\Psi_g^\dagger(\mathbf{x})\left(-\frac{\hbar^2}{2m}\nabla^2 + V_g(\mathbf{x})\right)\Psi_g(\mathbf{x}) + \Psi_e^\dagger(\mathbf{x})\left(-\frac{\hbar^2}{2m}\nabla^2 - \hbar\Delta_a + V_e(\mathbf{x})\right)\Psi_e(\mathbf{x})\right]$$

$$H_{A-A} = \frac{U}{2}\int \mathrm{d}^3\mathbf{x}\Psi_g^\dagger(\mathbf{x})\Psi_g^\dagger(\mathbf{x})\Psi_g(\mathbf{x})\Psi_g(\mathbf{x}),\ U = 4\pi a_s\hbar^2/m.$$

$$H_{A-R} = -i\hbar\int \mathrm{d}^3\mathbf{x}\Psi_g^\dagger(\mathbf{x})g(\mathbf{x})a^\dagger\Psi_e(\mathbf{x}) + \mathrm{h.c.},$$

$$H_{A-P} = -i\hbar\int \mathrm{d}^3\mathbf{x}\Psi_g^\dagger(\mathbf{x})h(\mathbf{x})\Psi_e(\mathbf{x}) + \mathrm{h.c.}.$$

$$\hat{\Psi}_e^\dagger(\mathbf{r})\hat{\Psi}_g(\mathbf{r}) = \hat{\sigma}_+(\mathbf{r})$$
$$\hat{\Psi}_g^\dagger(\mathbf{r})\hat{\Psi}_e(\mathbf{r}) = \hat{\sigma}_-(\mathbf{r})$$

$$\left[\Psi_f(\mathbf{x}), \Psi_{f'}^\dagger(\mathbf{x}')\right] = \delta^3\left(\mathbf{x} - \mathbf{x}'\right)\delta_{f,f'}$$
$$\left[\Psi_f(\mathbf{x}), \Psi_{f'}(\mathbf{x}')\right] = \left[\Psi_f^\dagger(\mathbf{x}), \Psi_{f'}^\dagger(\mathbf{x}')\right] = 0,$$

## ·Heisenberg Equations

$$\frac{\partial \Psi_e(\mathbf{x})}{\partial t} = i\left[\frac{\hbar}{2m}\nabla^2 - \frac{V_e(\mathbf{x})}{\hbar} + \Delta_a\right]\Psi_e(\mathbf{x})$$ free evolution

$$- \left[g(\mathbf{x})a + h(\mathbf{x})\right]\Psi_g(\mathbf{x}).$$ 光子吸收及基态湮灭

$$\frac{\partial \Psi_g(\mathbf{x})}{\partial t} = i\left[\frac{\hbar}{2m}\nabla^2 - \frac{V_g(\mathbf{x})}{\hbar} - \frac{U}{\hbar}\Psi_g^\dagger(\mathbf{x})\Psi_g(\mathbf{x})\right]\Psi_g(\mathbf{x})$$

$$+ \left[g(\mathbf{x})a^\dagger + h(\mathbf{x})\right]\Psi_e(\mathbf{x}).$$ 光子发射及激发态产生

$$\frac{\partial a}{\partial t} = i\Delta_c a + \eta + \int d^3\mathbf{x}\, g(\mathbf{x})\Psi_g^\dagger(\mathbf{x})\Psi_e(\mathbf{x}).$$

$$\hat{\Psi}_e^\dagger(\mathbf{r})\hat{\Psi}_g(\mathbf{r}) = \hat{\sigma}_+(\mathbf{r})$$

$$\hat{\Psi}_g^\dagger(\mathbf{r})\hat{\Psi}_e(\mathbf{r}) = \hat{\sigma}_-(\mathbf{r})$$

$$\left[\Psi_f(\mathbf{x}), \Psi_{f'}^\dagger(\mathbf{x}')\right] = \delta^3(\mathbf{x}-\mathbf{x}')\,\delta_{f,f'}$$

$$\left[\Psi_f(\mathbf{x}), \Psi_{f'}(\mathbf{x}')\right] = \left[\Psi_f^\dagger(\mathbf{x}), \Psi_{f'}^\dagger(\mathbf{x}')\right] = 0,$$

T=0，弱激发态

large atom-pump detuning $\Delta_a$

$$\Psi_e(\mathbf{x},t) = -\frac{i}{\Delta_a}\left[h(\mathbf{x}) + g(\mathbf{x})a(t)\right]\Psi_g(\mathbf{x},t).$$

$g(\mathbf{x})$

$$\frac{\partial a}{\partial t} = i\left[\Delta_c - \frac{1}{\Delta_a}\int d^3\mathbf{x}\, g^2(\mathbf{x})\Psi_g^\dagger(\mathbf{x})\Psi_g(\mathbf{x})\right]a - \frac{i}{\Delta_a}\int d^3\mathbf{x}\, h(\mathbf{x})\Psi_g^\dagger(\mathbf{x})\Psi_g(\mathbf{x}) + \eta.$$

$$\frac{\partial \Psi_g(\mathbf{x})}{\partial t} = i\left[\frac{\hbar}{2m}\nabla^2 - \frac{V_g(\mathbf{x})}{\hbar} - \frac{h^2(\mathbf{x})}{\Delta_a} - \frac{g^2(\mathbf{x})}{\Delta_a}a^\dagger a - \frac{h(\mathbf{x})g(\mathbf{x})}{\Delta_a}(a + a^\dagger) - \frac{U}{\hbar}\Psi_g^\dagger(\mathbf{x})\Psi_g(\mathbf{x})\right]\Psi_g(\mathbf{x})$$

## ·Effective Hamiltonian

$$\frac{\partial a}{\partial t} = i\left[\Delta_c - \frac{1}{\Delta_a}\int d^3\mathbf{x} g^2(\mathbf{x})\Psi_g^\dagger(\mathbf{x})\Psi_g(\mathbf{x})\right]a - \frac{i}{\Delta_a}\int d^3\mathbf{x} h(\mathbf{x})\underset{g(\mathbf{x})}{\uparrow}\Psi_g^\dagger(\mathbf{x})\Psi_g(\mathbf{x}) + \eta.$$

$$\frac{\partial \Psi_g(\mathbf{x})}{\partial t} = i\left[\frac{\hbar}{2m}\nabla^2 - \frac{V_g(\mathbf{x})}{\hbar} - \frac{h^2(\mathbf{x})}{\Delta_a} - \frac{g^2(\mathbf{x})}{\Delta_a}a^\dagger a - \frac{h(\mathbf{x})g(\mathbf{x})}{\Delta_a}(a + a^\dagger) - \frac{U}{\hbar}\Psi_g^\dagger(\mathbf{x})\Psi_g(\mathbf{x})\right]\Psi_g(\mathbf{x})$$

$$\Downarrow$$

$$H_{\text{eff}} = \int d^3\mathbf{x}\Psi_g^\dagger(\mathbf{x})\left\{-\frac{\hbar^2}{2m}\nabla^2 + V_g(\mathbf{x}) + \frac{\hbar}{\Delta_a}\left[h^2(\mathbf{x}) + g^2(\mathbf{x})a^\dagger a + h(\mathbf{x})g(\mathbf{x})(a + a^\dagger)\right]\right\}\Psi_g(\mathbf{x})$$
$$+ \frac{U}{2}\int d^3\mathbf{x}\Psi_g^\dagger(\mathbf{x})\Psi_g^\dagger(\mathbf{x})\Psi_g(\mathbf{x})\Psi_g(\mathbf{x}) - i\hbar\eta(a - a^\dagger) - \hbar\Delta_c a^\dagger a.$$

$$\Downarrow$$ Single particle Hamiltonian

$$H_{\text{eff}}^{(1)} = \frac{\mathbf{p}^2}{2m} + V_g(\mathbf{x}) + \frac{\hbar}{\Delta_a}\left[h^2(\mathbf{x}) + g^2(\mathbf{x})a^\dagger a + h(\mathbf{x})g(\mathbf{x})(a + a^\dagger)\right] - i\hbar\eta(a - a^\dagger) - \hbar\Delta_c a^\dagger a.$$

## ·1D Open System

$$h(\mathbf{x}) = h_0 \cos(k_p y)$$
$$V_g(\mathbf{x}) = V_g(x)$$
$$g(x) = g_0 \cos(kx)$$

$$\dot{\varrho} = \frac{1}{i\hbar}[H_{\text{eff}}, \varrho] + \mathcal{L}\varrho.$$

$$\mathcal{L}\varrho = \kappa\left(2a\varrho a^\dagger - a^\dagger a \varrho - \varrho a^\dagger a\right)$$

Cavity loss κ

$$\frac{\partial a}{\partial t} = i\left[\Delta_c - \frac{1}{\Delta_a}\int \mathrm{d}^3\mathbf{x} g^2(\mathbf{x})\Psi_g^\dagger(\mathbf{x})\Psi_g(\mathbf{x})\right] a - \frac{i}{\Delta_a}\int \mathrm{d}^3\mathbf{x} h(\mathbf{x})\Psi_g^\dagger(\mathbf{x})\Psi_g(\mathbf{x}) + \eta.$$

$g(\mathbf{x})$

Langevin equation

$$\dot{a} = \left\{ i\left[\Delta_c - \frac{g_0^2}{\Delta_a}\int \mathrm{d}x \Psi_g^\dagger(x)\cos^2(kx)\Psi_g(x)\right] - \kappa \right\} a - i\frac{g_0 h_0}{\Delta_a}\int \mathrm{d}x \Psi_g^\dagger(x)\cos(kx)\Psi_g(x) + \eta + \Gamma_{in}$$

Cavity loss κ

Noise operator

外部真空T=0，噪声算符的平均值为0，不进入动力学

## ·Bose-Hubbard Hamiltonian

$$\Psi_g(x) = \sum_k b_k w(x-x_k) \qquad w(x) = w_0(x)$$

$$H_{\text{eff}} = \int d^3\mathbf{x}\Psi_g^\dagger(\mathbf{x})\left\{-\frac{\hbar^2}{2m}\nabla^2 + V_g(\mathbf{x}) + \frac{\hbar}{\Delta_a}\left[h^2(\mathbf{x}) + g^2(\mathbf{x})a^\dagger a + h(\mathbf{x})g(\mathbf{x})\left(a+a^\dagger\right)\right]\right\}\Psi_g(\mathbf{x})$$
$$+\frac{U}{2}\int d^3\mathbf{x}\Psi_g^\dagger(\mathbf{x})\Psi_g^\dagger(\mathbf{x})\Psi_g(\mathbf{x})\Psi_g(\mathbf{x}) - i\hbar\eta\left(a-a^\dagger\right) - \hbar\Delta_c a^\dagger a.$$

$$V_g(x) = V_{\text{cl}}\cos^2(k_F x)$$

低激发腔场势阱太小，故增加外部捕获势

$$H = \sum_{k,l} E_{kl} b_k^\dagger b_l + \left(\hbar U_0 a^\dagger a + V_{\text{cl}}\right)\sum_{k,l} J_{kl} b_k^\dagger b_l$$
$$+ \hbar\eta_{\text{eff}}\left(a+a^\dagger\right)\sum_{k,l}\tilde{J}_{kl} b_k^\dagger b_l - i\hbar\eta\left(a-a^\dagger\right)$$
$$+ \frac{1}{2}\sum_{i,j,k,l} U_{ijkl} b_i^\dagger b_j^\dagger b_k b_l - \hbar\Delta_c a^\dagger a,$$

$$E_{kl} = \int dx\, w(x-x_k)\left(-\frac{\hbar^2}{2m}\nabla^2\right)w(x-x_l),$$
$$J_{kl} = \int dx\, w(x-x_k)\cos^2(kx)w(x-x_l),$$
$$\tilde{J}_{kl} = \int dx\, w(x-x_k)\cos(kx)w(x-x_l).$$
$$U_{ijkl} = g_{1D}\int dx w(x-x_i)w(x-x_j)w(x-x_k)w(x-x_l)$$

cos(k)在两个井之间一正一负

$$\tilde{J}_{k,k+1} = 0$$


Part.03

# Quantum phases in an optical lattice

## ·Bogoliubov Approximation

$$H=-t\sum_{\langle i,j\rangle} c_i^\dagger c_j+\frac{1}{2}U\sum_i c_i^\dagger c_i^\dagger c_i c_i-\mu\sum_i c_i^\dagger c_i,$$

momentum space

$$c_i=\frac{1}{\sqrt{N_s}}\sum_{\mathbf{k}} a_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_i},\quad c_i^\dagger=\frac{1}{\sqrt{N_s}}\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger e^{i\mathbf{k}\cdot\mathbf{r}_i},$$

$$\Sigma_i e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i}=N_s\delta_{\mathbf{k},\mathbf{k}'}$$

$$H=\sum_{\mathbf{k}}(-\overline{\epsilon}_{\mathbf{k}}-\mu)a_{\mathbf{k}}^\dagger a_{\mathbf{k}}+\frac{1}{2}\frac{U}{N_s}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{k}''}\sum_{\mathbf{k}'''} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}^\dagger a_{\mathbf{k}''}a_{\mathbf{k}'''}\delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''},$$

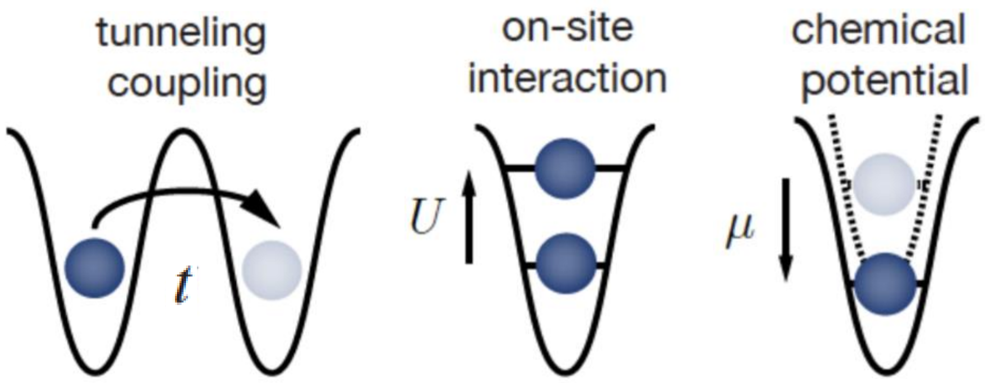
$$\overline{\epsilon}_{\mathbf{k}}=2t\Sigma_{j=1}^{d}\cos(k_j a)$$

For a Bose condensed gas $N_0 \gg 1$: $N_0=\langle a_0^\dagger a_0\rangle\approx\langle a_0 a_0^\dagger\rangle$ $N_0=\langle a_0^\dagger\rangle\langle a_0\rangle$ $\langle a_0^\dagger\rangle=\langle a_0\rangle=\sqrt{N_0}$

Bogoliubov approach:

$$a_0^\dagger\to\sqrt{N_0}+a_0^\dagger,\quad a_0\to\sqrt{N_0}+a_0,$$

minimizing the energy of the gas with respect to the number of condensate atoms $N_0$



**·Bogoliubov Approximation**

$$H=\sum_{\mathbf{k}}(-\overline{\epsilon}_{\mathbf{k}}-\mu)a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\frac{1}{2}\frac{U}{N_s}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{k}''}\sum_{\mathbf{k}'''}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}'}^{\dagger}a_{\mathbf{k}''}a_{\mathbf{k}'''}\delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''},$$

$$a_0^{\dagger}\to\sqrt{N_0}+a_0^{\dagger},\quad a_0\to\sqrt{N_0}+a_0,$$ minimizing the energy

波动线性项=0 $H^{(1)}=\left(-\overline{\epsilon}_0-\mu+\frac{U}{N_s}N_0\right)\sqrt{N_0}(a_0^{\dagger}+a_0),$

$\mu=Un_0-zt$ condensate density $n_0=N_0/N_s$ the number of nearest neighbors $z=2d$

化学势能是增加一个粒子所需的能量：包含在自身格点的相互作用能增加和可能hopping的能量减小

Effective Hamiltonian

$$H^{\text{eff}}=\left(-zt-\mu+\frac{1}{2}Un_0\right)N_0+\sum_{\mathbf{k}}(-\overline{\epsilon}_{\mathbf{k}}-\mu)a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\frac{1}{2}Un_0\sum_{\mathbf{k}}(a_{\mathbf{k}}a_{-\mathbf{k}}+4a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+a_{-\mathbf{k}}^{\dagger}a_{\mathbf{k}}^{\dagger}).$$

Matrix form 令 $\epsilon_{\mathbf{k}}=zt-\overline{\epsilon}_{\mathbf{k}}$

$$H^{\text{eff}}=-\frac{1}{2}Un_0N_0-\frac{1}{2}\sum_{\mathbf{k}}(\epsilon_{\mathbf{k}}+Un_0)+\frac{1}{2}\sum_{\mathbf{k}}(a_{\mathbf{k}}^{\dagger},a_{-\mathbf{k}})\times\begin{bmatrix}\epsilon_{\mathbf{k}}+Un_0 & Un_0\\ Un_0 & \epsilon_{\mathbf{k}}+Un_0\end{bmatrix}\begin{pmatrix}a_{\mathbf{k}}\\ a_{-\mathbf{k}}^{\dagger}\end{pmatrix}$$

**·Bogoliubov Approximation**

$$H^{\mathrm{eff}} = -\frac{1}{2}Un_0N_0 - \frac{1}{2}\sum_{\mathbf{k}}(\epsilon_{\mathbf{k}} + Un_0) + \frac{1}{2}\sum_{\mathbf{k}}(a_{\mathbf{k}}^{\dagger}, a_{-\mathbf{k}}) \times \begin{bmatrix} \epsilon_{\mathbf{k}} + Un_0 & Un_0 \\ Un_0 & \epsilon_{\mathbf{k}} + Un_0 \end{bmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^{\dagger} \end{pmatrix}$$

diagonalized

$$\begin{pmatrix} b_{\mathbf{k}} \\ b_{-\mathbf{k}}^{\dagger} \end{pmatrix} = \begin{bmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ v_{\mathbf{k}}^{*} & u_{\mathbf{k}}^{*} \end{bmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^{\dagger} \end{pmatrix} \equiv \mathbf{B} \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^{\dagger} \end{pmatrix}$$

$$|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1$$

$$n = \frac{1}{N_s}\sum_{\mathbf{k}} \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle_{H^{\mathrm{eff}}},$$

$$\hbar\omega_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + 2Un_0\epsilon_{\mathbf{k}}},$$

$$|v_{\mathbf{k}}|^2 = |u_{\mathbf{k}}|^2 - 1 = \frac{1}{2}\left(\frac{\epsilon_{\mathbf{k}} + Un_0}{\hbar\omega_{\mathbf{k}}} - 1\right).$$

$$H^{\mathrm{eff}} = -\frac{1}{2}Un_0N_0 + \frac{1}{2}\sum_{\mathbf{k}}[\hbar\omega_{\mathbf{k}} - (\epsilon_{\mathbf{k}} + Un_0)] + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}$$

$$n = n_0 + \frac{1}{N_s}\sum_{\mathbf{k}\neq 0}[(|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2)\langle b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} \rangle_{H^{\mathrm{eff}}} + |v_{\mathbf{k}}|^2].$$

Bose distribution

$$n = n_0 + \frac{1}{N_s}\sum_{\mathbf{k}\neq 0}\left(\frac{\epsilon_{\mathbf{k}} + Un_0}{\hbar\omega_{\mathbf{k}}}\frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}} - 1} + \frac{\epsilon_{\mathbf{k}} + Un_0 - \hbar\omega_{\mathbf{k}}}{2\hbar\omega_{\mathbf{k}}}\right)$$

T=0, $\beta \to \infty$

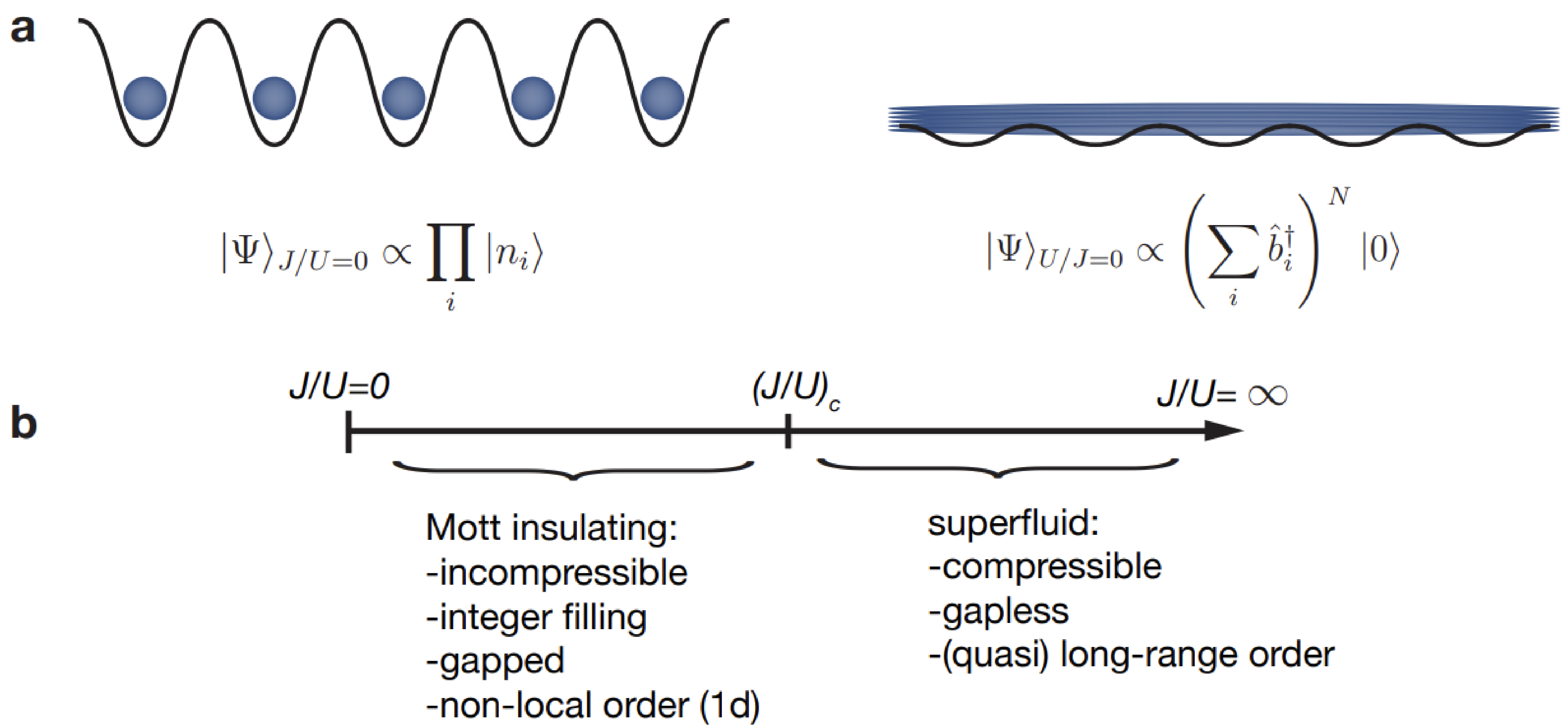
$\boldsymbol{k} = 2\pi\boldsymbol{q}/a$

$$n = n_0 + \frac{1}{2}\int_{-1/2}^{1/2} d\mathbf{q}\left(\frac{\epsilon_{\mathbf{q}} + Un_0}{\hbar\omega_{\mathbf{q}}} - 1\right)$$

$$\epsilon_{\mathbf{q}} = 2t\Sigma_{i=1}^{d}[1 - \cos(2\pi q_i)]$$

$$\hbar\omega_{\mathbf{q}} = (\epsilon_{\mathbf{q}}^2 + 2Un_0\epsilon_{\mathbf{q}})^{1/2}$$

# Quantum phases in an optical lattice



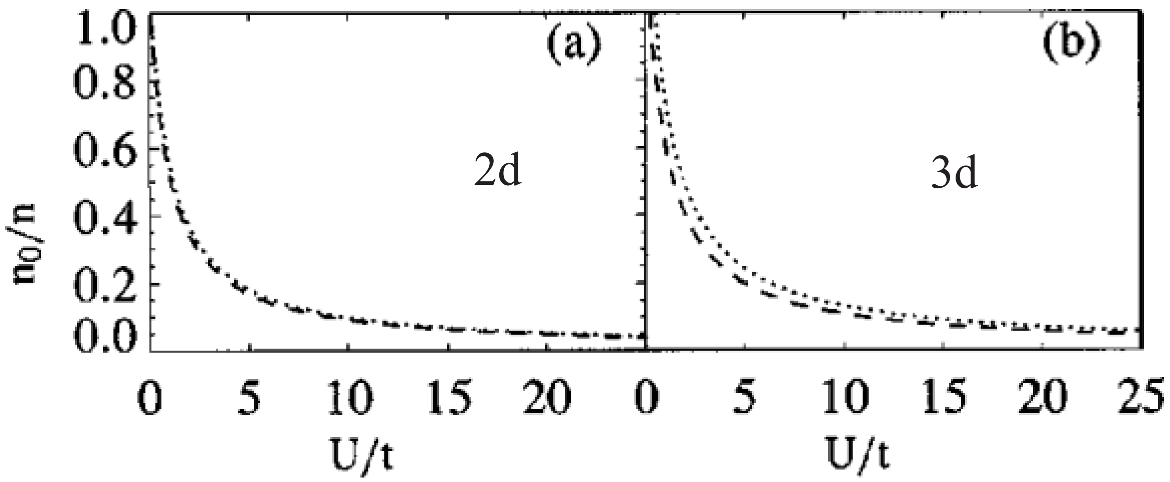

Probing correlated quantum many-body systems at the single-particle level
-Manuel Endres

# Quantum phases in an optical lattice

·**Bogoliubov Approximation**

$$n=n_0+\frac{1}{2}\int_{-1/2}^{1/2}d\mathbf{q}\left(\frac{\epsilon_\mathbf{q}+Un_0}{\hbar\omega_\mathbf{q}}-1\right)$$

对于n=Z，应当没有超流解




n=0.5(dashed line), 1(dotted line)

**Asymptotic behavior** $U/t\rightarrow\infty$ $\epsilon_\mathbf{q}\leqslant 4\pi^2|\mathbf{q}|^2t.$

$$\int_{-1/2}^{1/2}d\mathbf{q}\frac{\epsilon_\mathbf{q}+Un_0}{\sqrt{\epsilon_\mathbf{q}^2+2U\epsilon_\mathbf{q}n_0}}\geqslant\frac{1}{2\pi}\sqrt{\frac{Un_0}{2t}}\int_{-1/2}^{1/2}\frac{d\mathbf{q}}{|\mathbf{q}|}=\mathrm{I_d}$$

$$n\approx n_0+\frac{1}{4\pi}\sqrt{\frac{Un_0}{2t}}I_d-\frac{1}{2}$$

$$n_0=\left(\frac{1}{2}\sqrt{\frac{I_d^2}{16\pi^2}\frac{U}{2t}+4n+2}-\frac{I_d}{8\pi}\sqrt{\frac{U}{2t}}\right)^2$$

一直存在正的解，没有超流-绝缘体转变，只有极限才有$n_0$=0

**·Mean-field Approach**

The superfluid order parameter $\psi = \sqrt{n_i} = \langle c_i^\dagger \rangle = \langle c_i \rangle$

$$H = -t\sum_{\langle i,j\rangle} c_i^\dagger c_j + \frac{1}{2}U\sum_i c_i^\dagger c_i^\dagger c_i c_i - \mu \sum_i c_i^\dagger c_i,$$

做代换

$$c_i^\dagger c_j = \langle c_i^\dagger \rangle c_j + c_i^\dagger \langle c_j \rangle - \langle c_i^\dagger \rangle \langle c_j \rangle = \psi(c_i^\dagger + c_j) - \psi^2$$

$$H^{\mathrm{eff}} = -zt\psi \sum_i (c_i^\dagger + c_i) + zt\psi^2 N_s + \frac{1}{2}U\sum_i c_i^\dagger c_i^\dagger c_i c_i - \mu \sum_i c_i^\dagger c_i,$$

$\bar{U} = U/zt,\ \bar{\mu} = \mu/zt$ 消除维度依赖

the number of nearest neighbors $z = 2d$

$$H_i^{\mathrm{eff}} = \frac{1}{2}\bar{U}\hat{n}_i(\hat{n}_i - 1) - \bar{\mu}\hat{n}_i - \psi(c_i^\dagger + c_i) + \psi^2$$ 转化为最小化单粒子基态能量

·**Mean-field Approach**

Second-order perturbation theory $H^{\text{eff}}=H^{(0)}+\psi V$

$$H^{(0)}=\frac{1}{2}\bar{U}\hat{n}(\hat{n}-1)-\bar{\mu}\hat{n}+\psi^2,\qquad V=-(c^\dagger+c),\qquad E_g^{(0)}=\{E_n^{(0)}|n=0,1,2,\dots\}_{\min}.$$

$$E_g^{(0)}=\begin{cases}0 & \text{if } \bar{\mu}<0,\\ \frac{1}{2}\bar{U}g(g-1)-\bar{\mu}g & \text{if } \bar{U}(g-1)<\bar{\mu}<\bar{U}g.\end{cases}$$

比较$g$粒子与$g\pm 1$粒子能量

只有两个不为0

$$E_g^{(2)}=\psi^2\sum_{n\neq g}\frac{|\langle g|V|n\rangle|^2}{E_g^{(0)}-E_n^{(0)}},\quad\Longrightarrow\quad E_g^{(2)}=\frac{g}{\bar{U}(g-1)-\bar{\mu}}+\frac{g+1}{\bar{\mu}-\bar{U}g}.$$

$$E_g(\psi)=a_0(g,\bar{U},\bar{\mu})+a_2(g,\bar{U},\bar{\mu})\psi^2+\mathcal{O}(\psi^4),\qquad a_2(g,\bar{U},\bar{\mu})=\frac{g}{\bar{U}(g-1)-\bar{\mu}}+\frac{g+1}{\bar{\mu}-\bar{U}g}+1=0,$$

# Quantum phases in an optical lattice

·**Mean-field Approach**

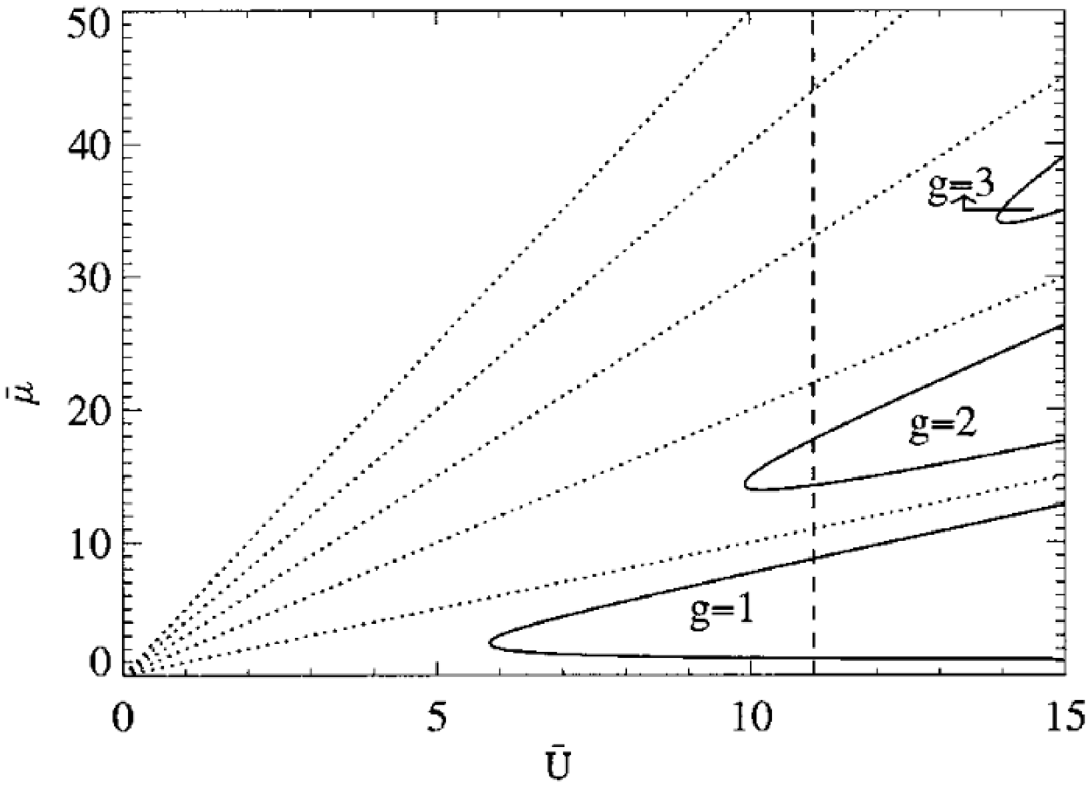
$$E_g(\psi)=a_0(g,\bar{U},\bar{\mu})+a_2(g,\bar{U},\bar{\mu})\psi^2+\mathcal{O}(\psi^4),\qquad a_2(g,\bar{U},\bar{\mu})=\frac{g}{\bar{U}(g-1)-\bar{\mu}}+\frac{g+1}{\bar{\mu}-\bar{U}g}+1=0,$$

$a_2>0$则$\psi=0$，$a_2<0$则$\psi>0$，则$a_2=0$为相变点

$$\bar{\mu}_{\pm}=\frac{1}{2}[\bar{U}(2g-1)-1]\pm\frac{1}{2}\sqrt{\bar{U}^2-2\bar{U}(2g+1)+1},$$

令两者相等可以得到临界$\bar{U}_c$

$$\bar{U}_c=2g+1+\sqrt{(2g+1)^2-1},$$



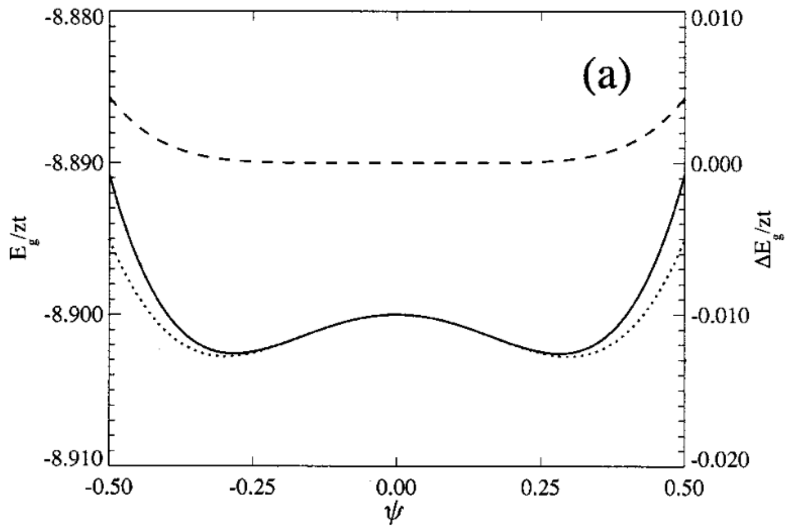
# Quantum phases in an optical lattice

## ·Mean-field Approach

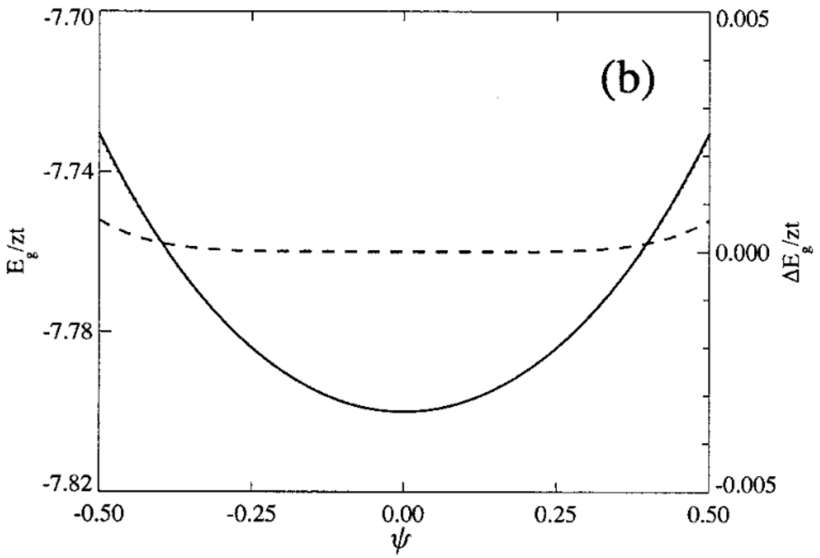
Fourth-order perturbation theory

$$E_g(\psi)=a_0(g,\overline{U},\overline{\mu})+a_2(g,\overline{U},\overline{\mu})\psi^2+a_4(g,\overline{U},\overline{\mu})\psi^4,$$

$$a_4(g,\overline{U},\overline{\mu})=\frac{g(g-1)}{[\overline{U}(g-1)-\overline{\mu}]^2[\overline{U}(2g-3)-2\overline{\mu}]}+\frac{(g+1)(g+2)}{(\overline{\mu}-\overline{U}g)^2[2\overline{\mu}-\overline{U}(2g+1)]}-\left(\frac{g}{\overline{U}(g-1)-\overline{\mu}}+\frac{g+1}{\overline{\mu}-\overline{U}g}\right)\times\left(\frac{g}{[\overline{U}(g-1)-\overline{\mu}]^2}+\frac{g+1}{(\overline{\mu}-\overline{U}g)^2}\right)$$




$\overline{U}=11$ and $\overline{\mu}=8.9$




$\overline{U}=11$ and $\overline{\mu}=7.8$

# Quantum phases in an optical lattice

**·Mean-field Approach**

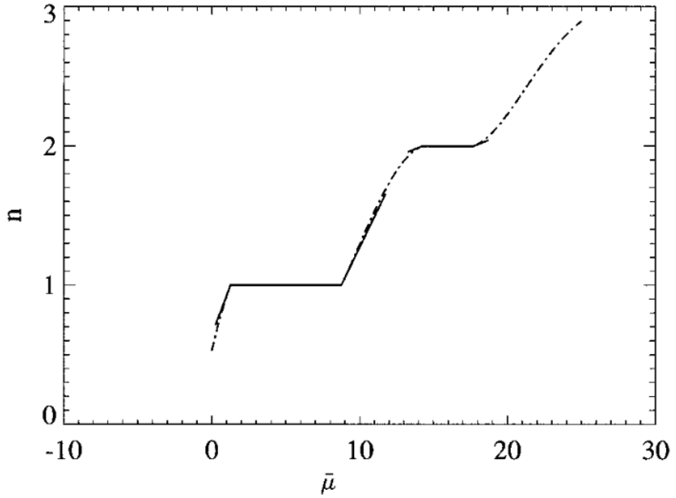
$\bar{\mu}=n\bar{U}$ 此时n+1和n粒子能量相同，利用二重简并微扰(文章写的n与n-1)

$$E_g(\psi)|_{\bar{\mu}=n\bar{U}}=-\frac{1}{2}\bar{U}n(n+1)+\psi^2-|\psi|\sqrt{n+1},$$

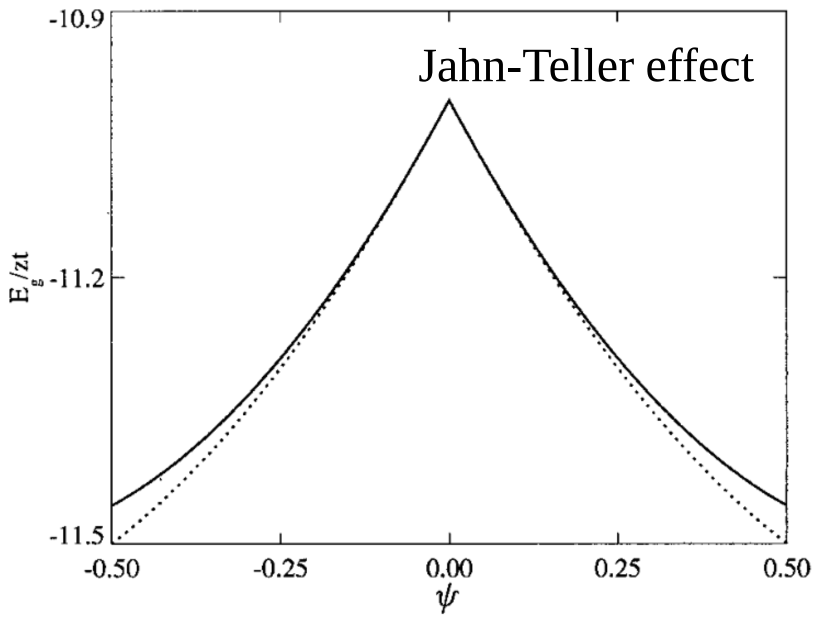
grand-canonical ensemble $\psi_{\min}=[-a_2(g,\bar{U},\bar{\mu})/2a_4(g,\bar{U},\bar{\mu})]^{1/2}$

$$n=-\frac{\partial\langle H^{\mathrm{eff}}\rangle}{\partial\mu}=-\frac{\partial E_g(\psi=\psi_{\min})}{\partial\bar{\mu}}=g-\frac{\partial}{\partial\bar{\mu}}\left(\frac{a_2(g,\bar{U},\bar{\mu})^2}{4a_4(g,\bar{U},\bar{\mu})}\right)$$

在$\mu_\pm$之间，n为常数！
对应mott绝缘体




$\bar{U}=U/zt=11$




$\bar{U}=\bar{\mu}=11$

·**Dispersion Relations** 将涨落视为准粒子和准空穴激发，计算二者色散关系

定义复变函数 $a_i^*(\tau)$ and $a_i(\tau)$ $Z=\mathrm{Tr}\, e^{-\beta\hat{H}}=\int \mathcal{D}a^*\mathcal{D}a \exp\{-S[a^*,a]/\hbar\}$,

作用量

$$S[a^*,a]=\int_0^{\hbar\beta} d\tau\left[\sum_i a_i^*\left(\hbar\frac{\partial}{\partial\tau}-\mu\right)a_i-\sum_{ij} t_{ij}a_i^*a_j+\frac{1}{2}U\sum_i a_i^*a_i^*a_ia_i\right],$$

Hubbard-Stratonovich transformation

$$S[a^*,a,\psi^*,\psi]=S[a^*,a]+\int_0^{\hbar\beta} d\tau\sum_{ij}(\psi_i^*-a_i^*)t_{ij}\times(\psi_j-a_j)$$

$\psi^*$ and $\psi$ 是序参量场

$$S[a^*,a,\psi^*,\psi]=\int_0^{\hbar\beta} d\tau\left[\sum_i a_i^*\left(\hbar\frac{\partial}{\partial\tau}-\mu\right)a_i+\frac{1}{2}U\sum_i a_i^*a_i^*a_ia_i-\sum_{ij} t_{ij}(a_i^*\psi_j+\psi_i^*a_j)+\sum_{ij} t_{ij}\psi_i^*\psi_j\right]$$

$S^{(0)}[a^*,a]$ 为$t_{ij}=0$的项

$$\exp(-S^{\mathrm{eff}}[\psi^*,\psi]/\hbar)\equiv\exp\left(-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\sum_{ij} t_{ij}\psi_i^*\psi_j\right)\int \mathcal{D}a^*\mathcal{D}a\times\exp\{-S^{(0)}[a^*,a]/\hbar\}\times\exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\left(-\sum_{ij} t_{ij}(a_i^*\psi_j+\psi_i^*a_j)\right)\right]$$

## ·Dispersion Relations

利用Taylor展开到二阶(这里很迷)

$$\langle a_i^* a_j^* \rangle_{S^{(0)}} = \langle a_i a_j \rangle_{S^{(0)}} = 0,$$

$$\langle a_i^* a_j \rangle_{S^{(0)}} = \langle a_i a_j^* \rangle_{S^{(0)}} = \langle a_i a_i^* \rangle_{S^{(0)}} \delta_{i,j},$$

$$S^{(2)}[\psi^*,\psi] = -\frac{1}{2\hbar}\left\langle \left( \int_0^{\hbar\beta} d\tau \sum_{ij} t_{ij}(a_i^*\psi_j + \psi_i^* a_j) \right)^2 \right\rangle_{S^{(0)}} + \int_0^{\hbar\beta} d\tau \sum_{ij} t_{ij}\psi_i^*\psi_j$$

$$= -\frac{1}{2\hbar}\left\langle \int_0^{\hbar\beta}\int_0^{\hbar\beta} d\tau d\tau' \sum_{iji'j'} t_{ij}t_{i'j'}(a_i^*\psi_j + \psi_i^* a_j)(a_{i'}^*\psi_{j'} + \psi_{i'}^* a_{j'}) \right\rangle_{S^{(0)}} + \int_0^{\hbar\beta} d\tau \sum_{ij} t_{ij}\psi_i^*\psi_j .$$

First term

$$S^{(2)}[\psi^*,\psi] = \int_0^{\hbar\beta} d\tau \left\{ \sum_{ij} t_{ij}\psi_i^*(\tau)\psi_j(\tau) - \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau' \sum_{iji'j'} t_{ij}t_{i'j'}\psi_j^*(\tau) \times \langle a_i(\tau) a_{i'}^*(\tau')\rangle_{S^{(0)}}\psi_{j'}(\tau') \right\}$$

$$t_{ij} = t_{ji} = \begin{cases} t & \text{for nearest neighbors} \\ 0 & \text{otherwise.} \end{cases}$$

$\Downarrow$

直接带入跳跃1次的 $\sum_{ij} t_{ij}\psi_i^*(\tau)\psi_j(\tau) = \sum_i t\psi_i^*(\tau)\psi_{i\pm\{1\}}(\tau)$

Momentum space $\sum_{ij} t_{ij}\psi_i^*(\tau)\psi_j(\tau) = \sum_{\mathbf{k}} 2t\psi_{\mathbf{k}}(\tau)\psi_{\mathbf{k}}^*(\tau)\sum_{j=1}^{d} \cos(k_j a).$

## ·Dispersion Relations

$$\langle a_i^* a_j^* \rangle_{S^{(0)}} = \langle a_i a_j \rangle_{S^{(0)}} = 0,$$

$$\langle a_i^* a_j \rangle_{S^{(0)}} = \langle a_i a_j^* \rangle_{S^{(0)}} = \langle a_i a_i^* \rangle_{S^{(0)}} \delta_{i,j},$$

跳跃2次的 $\sum_{ji'j'} t_{ij} t_{i'j'} \psi_j^*(\tau) \langle a_i(\tau) a_{i'}^*(\tau') \rangle_{S^{(0)}} \psi_{j'}(\tau')$

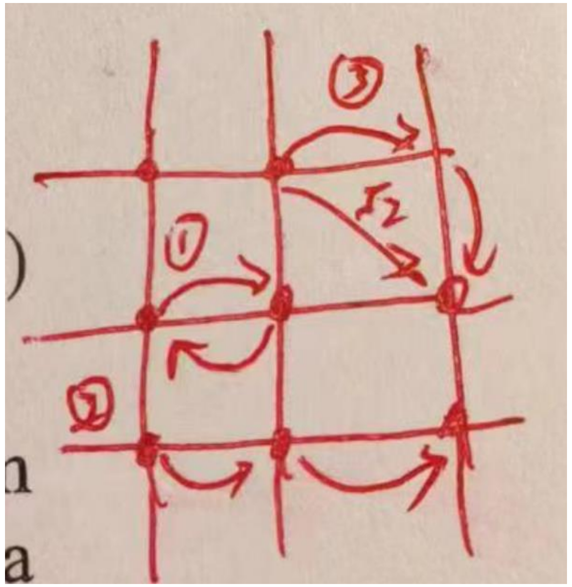
$$= \langle a_i(\tau) a_i^*(\tau') \rangle_{S^{(0)}} \sum_{jj'} t_{ij} t_{ij'} \psi_j^*(\tau) \psi_{j'}(\tau')$$

$$4 \sum_{i}^{d} \sum_{j \neq i}^{d} \cos(k_i a) \cos(k_j a)$$

$$= t^2 \langle a_i(\tau) a_i^*(\tau') \rangle_{S^{(0)}} \sum_j \{ z \psi_j^*(\tau) \psi_j(\tau') + \psi_j^*(\tau) \psi_{j \pm \{2\}}(\tau') + \psi_j^*(\tau) \psi_{j \pm \{\sqrt{2}\}}(\tau') \}$$

① ② ③

$$z = 2d \qquad 2 \sum_{i}^{d} \cos(2 k_j a)$$



$$= \langle a_i(\tau) a_i^*(\tau') \rangle_{S^{(0)}} \sum_{\mathbf{k}} \psi_{\mathbf{k}}^*(\tau) \psi_{\mathbf{k}}(\tau') \bar{\epsilon}_{\mathbf{k}}^2, \qquad \bar{\epsilon}_{\mathbf{k}} = 2t \Sigma_{j=1}^{d} \cos(k_j a).$$

## ·Dispersion Relations

处理时间依赖，引入Matsubara frequency $\hbar\omega_n=\pi(2n)/\hbar\beta$

$$\psi_{\mathbf{k}}(\tau)=\sum_n \frac{1}{\sqrt{\hbar\beta}}\psi_{\mathbf{k}n}e^{-i\omega_n\tau},\quad \psi_{\mathbf{k}}^*(\tau)=\sum_n \frac{1}{\sqrt{\hbar\beta}}\psi_{\mathbf{k}n}^*e^{+i\omega_n\tau}.$$

引入虚的时间排序算符，将场期望转换为对算符的期望

$$\langle a_i(\tau)a_{i'}^*(\tau')\rangle_{S^{(0)}}=\langle \mathrm{T}[a_i(\tau)a_{i'}^\dagger(\tau')]\rangle_{S^{(0)}}.$$

利用阶跃函数可以表示为

$$\langle \mathrm{T}[a_i(\tau)a_{i'}^\dagger(\tau')]\rangle_{S^{(0)}}=\theta(\tau-\tau')\langle a_i(\tau)a_{i'}^\dagger(\tau')\rangle_{S^{(0)}}+\theta(\tau'-\tau)\langle a_{i'}^\dagger(\tau')a_i(\tau)\rangle_{S^{(0)}}.$$

$$E_{g+1}^{(0)}-E_g^{(0)}=-\mu+gU>0,$$
$$E_g^{(0)}-E_{g-1}^{(0)}=-\mu+(g-1)U<0.$$

$$E_g^{(0)}=\begin{cases}0 & \text{if } \bar{\mu}<0,\\ \frac{1}{2}\bar{U}g(g-1)-\bar{\mu}g & \text{if } \bar{U}(g-1)<\bar{\mu}<\bar{U}g.\end{cases}$$

$$\begin{aligned}\langle a_i(\tau)a_{i'}^*(\tau')\rangle_{S^{(0)}}=\theta(\tau-\tau')(1+g)\\ \times\exp\{-(E_{g+1}^{(0)}-E_g^{(0)})(\tau-\tau')/\hbar\}\\ +\theta(\tau'-\tau)g\exp\{(E_{g-1}^{(0)}-E_g^{(0)})\\ \times(\tau-\tau')/\hbar\}.\end{aligned}$$

e指数是考虑Heisenberg绘景导致的吗？
为什么没有i

# Quantum phases in an optical lattice

## ·Dispersion Relations

代入并利用阶跃函数的性质可得

$$S^{(2)}[\psi^*,\psi]=\sum_n\sum_{\mathbf{k}}|\psi_{\mathbf{k}n}|^2\bar{\epsilon}_{\mathbf{k}}\times\left(1-\frac{\bar{\epsilon}_{\mathbf{k}}}{\hbar}\int_{-\infty}^{0}d\tau'(1+g)\times\exp\{(-i\hbar\omega_n-\mu+gU)\tau'/\hbar\}-\frac{\bar{\epsilon}_{\mathbf{k}}}{\hbar}\int_{0}^{\infty}d\tau' g\exp\{-(i\hbar\omega_n+\mu-(g-1)U)\tau'/\hbar\}\right)$$

即

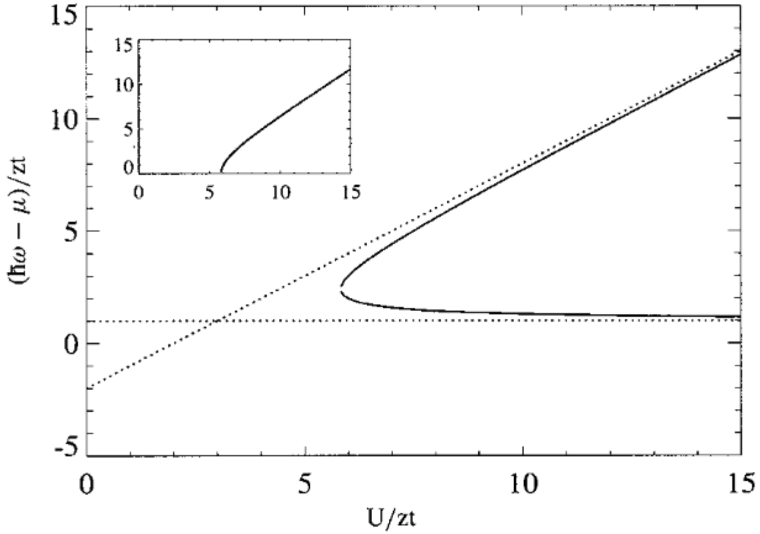
$$S^{(2)}[\psi^*,\psi]=\sum_n\sum_{\mathbf{k}}|\psi_{\mathbf{k}n}|^2\bar{\epsilon}_{\mathbf{k}}\times\left[1-\bar{\epsilon}_{\mathbf{k}}\left(\frac{g+1}{-i\hbar\omega_n-\mu+gU}+\frac{g}{i\hbar\omega_n+\mu-(g-1)U}\right)\right].$$

带入实能量$\hbar\omega$，$i\omega_n\to\omega$，并令其等于0，得到等式

$$0=\left[1-\bar{\epsilon}_{\mathbf{k}}\left(\frac{g+1}{-\hbar\omega-\mu+gU}+\frac{g}{\hbar\omega+\mu-(g-1)U}\right)\right]$$

即为准粒子和准空穴色散关系

$$\hbar\omega_{qp,qh}=-\mu+\frac{U}{2}(2g-1)-\frac{\bar{\epsilon}_{\mathbf{k}}}{2}\pm\frac{1}{2}\sqrt{\bar{\epsilon}_{\mathbf{k}}^2-(4g+2)U\bar{\epsilon}_{\mathbf{k}}+U^2}.$$




$\mathbf{k}=0$ in the $g=1$

$$\lim_{U\to\infty}\hbar\omega_{qp}=-\mu+gU-(g+1)\bar{\epsilon}_0 \qquad \lim_{U\to\infty}\hbar\omega_{qh}=-\mu+(g-1)U+g\bar{\epsilon}_0$$

$$=E^{(0)}_{g+1}-E^{(0)}_{g}-(g+1)zt, \qquad =E^{(0)}_{g}-E^{(0)}_{g-1}+gzt,$$

一阶修正来自于hopping，i节点准粒子激发则有$\langle c_j^\dagger c_i\rangle$=(g+1)t，而空穴激发则$\langle c_i^\dagger c_j\rangle$=gt