Bose-Fermi Mixtures in Optical Lattices

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1. Bose-Hubbard-Modell

Second-quantized Hamiltonian for bosons [1]:

$$\hat{H} = \int d^3x\, \hat{\psi}^\dagger(\mathbf{x}) \left[-\frac{\hbar^2}{2m_\mathrm{B}}\nabla^2 + \sum_{j=1}^{3} V_0 \sin(k_L x_j) \right] \hat{\psi}(\mathbf{x}) + \frac{2\pi a_\mathrm{BB}\hbar^2}{m_\mathrm{B}} \int d^3x\, \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{x})$$

Decomposition in Wannier-states:

$$\hat{\psi}(\mathbf{x}) = \sum_i \hat{a}_i w_B(\mathbf{x}-\mathbf{x}_i)$$

Derivation of the Bose-Hubbard-Hamiltonian [1–5]:

$$\hat{H}_\mathrm{BHM} = -J_\mathrm{B} \sum_{<i,j>} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2}\sum_i \hat{a}_i^\dagger\hat{a}_i^\dagger\hat{a}_i\hat{a}_i - \mu_\mathrm{B}\sum_i \hat{a}_i^\dagger\hat{a}_i$$

Coefficients [6–8]:

$$J_\mathrm{B} = -\int d^3x\, w_B^*(\mathbf{x}-\mathbf{x}_i)\left[-\frac{\hbar^2}{2m_\mathrm{B}}\nabla^2 + \sum_{j=1}^{3} V_0\sin(k_L x_j)\right] w_B(\mathbf{x}-\mathbf{x}_j)$$

$$U = \frac{4\pi a_\mathrm{BB}\hbar^2}{m_\mathrm{B}}\int d^3x\, |w_B(\mathbf{x}-\mathbf{x}_i)|^4$$

Harmonic approximation:

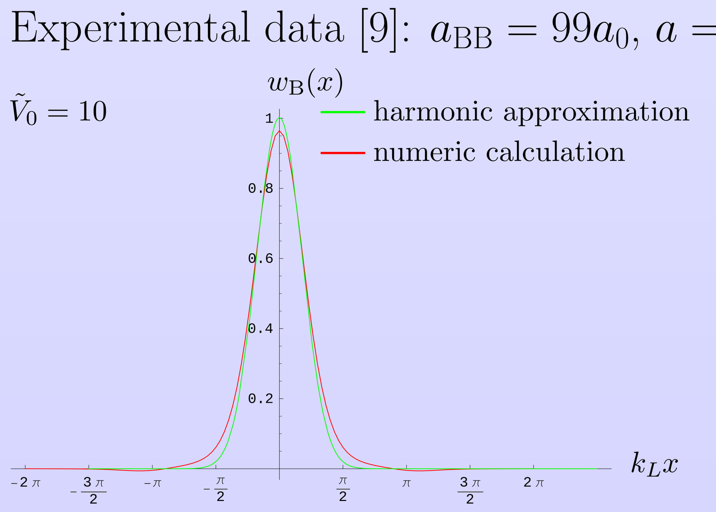
$$w_\mathrm{B}(x) = \sqrt[4]{\frac{\pi}{a^2}}\sqrt[8]{\frac{V_0}{E_R}} \exp\left[-\frac{\pi^2}{2}\sqrt{\frac{V_0}{E_R}}\left(\frac{x}{a}\right)^2\right]$$

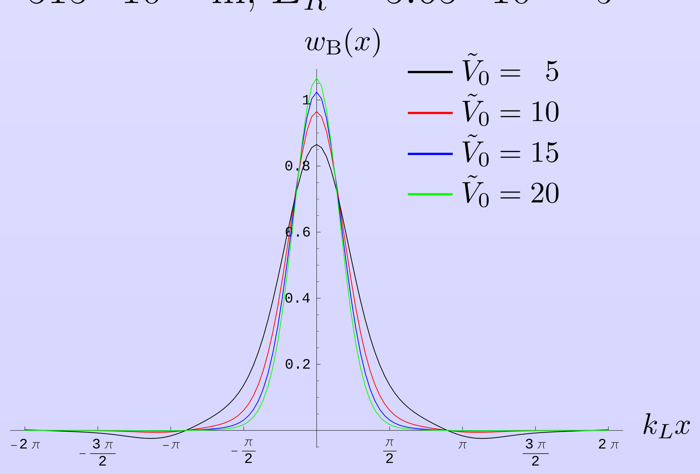
$$U = \sqrt{8\pi}E_R \frac{a_\mathrm{BB}}{a}\left(\frac{V_0}{E_R}\right)^{3/4}$$

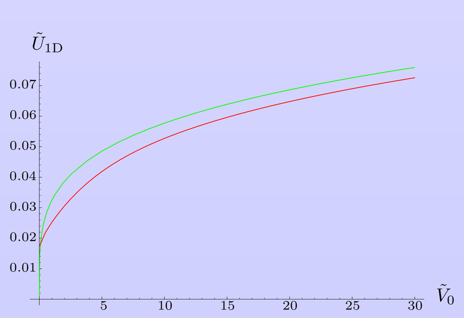
$$J_\mathrm{B} = \left(\frac{\pi^2}{4}-1\right) V_0 \exp\left[-\frac{\pi^2}{4}\sqrt{\frac{V_0}{E_R}}\right]$$

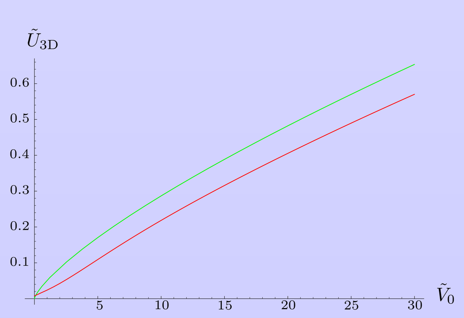
Recoil energy: $\tilde{X} = \frac{X}{E_R}$, $E_R = \frac{\hbar^2 k_L^2}{2m_\mathrm{B}}$, $k_L = \frac{\pi}{a}$

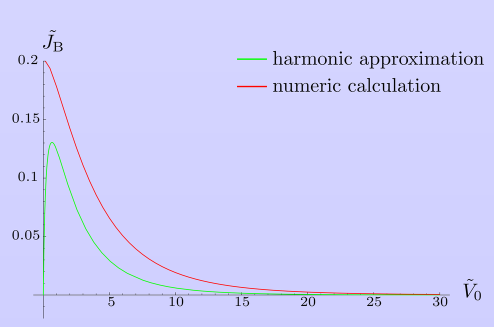
Experimental data [9]: $a_\mathrm{BB} = 99a_0$, $a = 515\cdot 10^{-9}$ m, $E_R = 5.65\cdot 10^{-29}$ J











2. Mean-Field Theory

Mean-field ansatz [4,10]:

$$\hat{a}_i^\dagger \hat{a}_j \approx \langle\hat{a}_i^\dagger\rangle\hat{a}_j + \langle\hat{a}_j\rangle\hat{a}_i^\dagger - \langle\hat{a}_i^\dagger\rangle\langle\hat{a}_j\rangle \quad \text{with} \quad \psi = \langle\hat{a}_i^\dagger\rangle = \langle\hat{a}_j\rangle$$

Mean-field Hamiltonian:

$$\hat{H}_\mathrm{MF} = \sum_i -J_\mathrm{B} z[\psi(\hat{a}_i + \hat{a}_i^\dagger) - \psi^2] + \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) - \mu_\mathrm{B}\hat{n}_i$$

Solution [4,5,10,11]:

$$\mathcal{F}(\psi^*,\psi) = -k_B T \ln \mathrm{Tr}\left\{ e^{-\hat{H}_\mathrm{MF}/k_B T}\right\} = a_0 + a_2|\psi|^2 + a_4|\psi|^4 + \dots$$

$T = 0$: $a_0 = E_n$

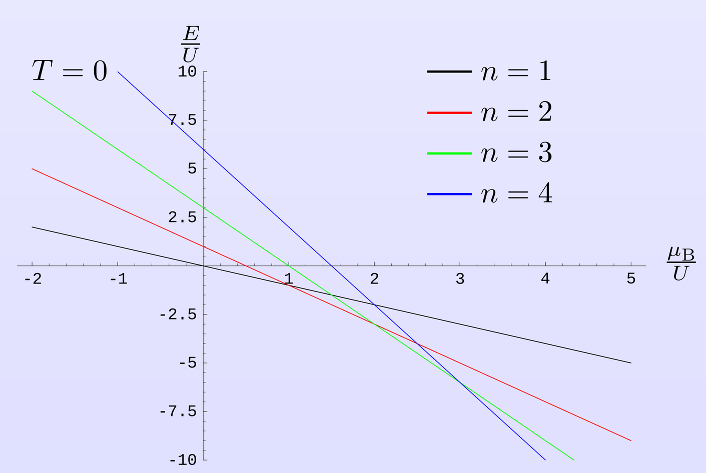
$$a_2 = J_\mathrm{B} z + J_\mathrm{B}^2 z^2 \frac{U + \mu_\mathrm{B}}{(\mu_\mathrm{B} - Un)[U(n-1) - \mu_\mathrm{B}]}$$

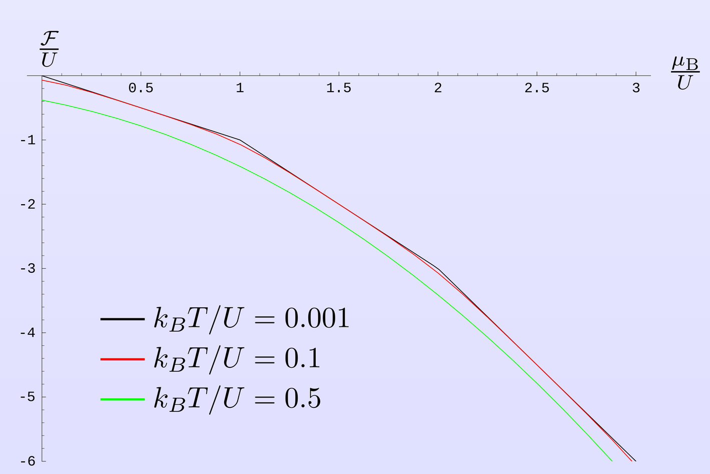
$T > 0$: $a_0 = -k_B T \ln \sum_{n=0}^{\infty} e^{-E_n/k_B T}$

$$a_2 = J_\mathrm{B} z + \frac{J_\mathrm{B}^2 z^2}{\mathcal{Z}} \sum_{n=0}^{\infty} \frac{U+\mu_\mathrm{B}}{(\mu_\mathrm{B} - Un)[U(n-1)-\mu_\mathrm{B}]} e^{-E_n/k_B T}$$

$$\mathcal{Z} = \sum_{n=0}^{\infty} e^{-E_n/k_B T}$$

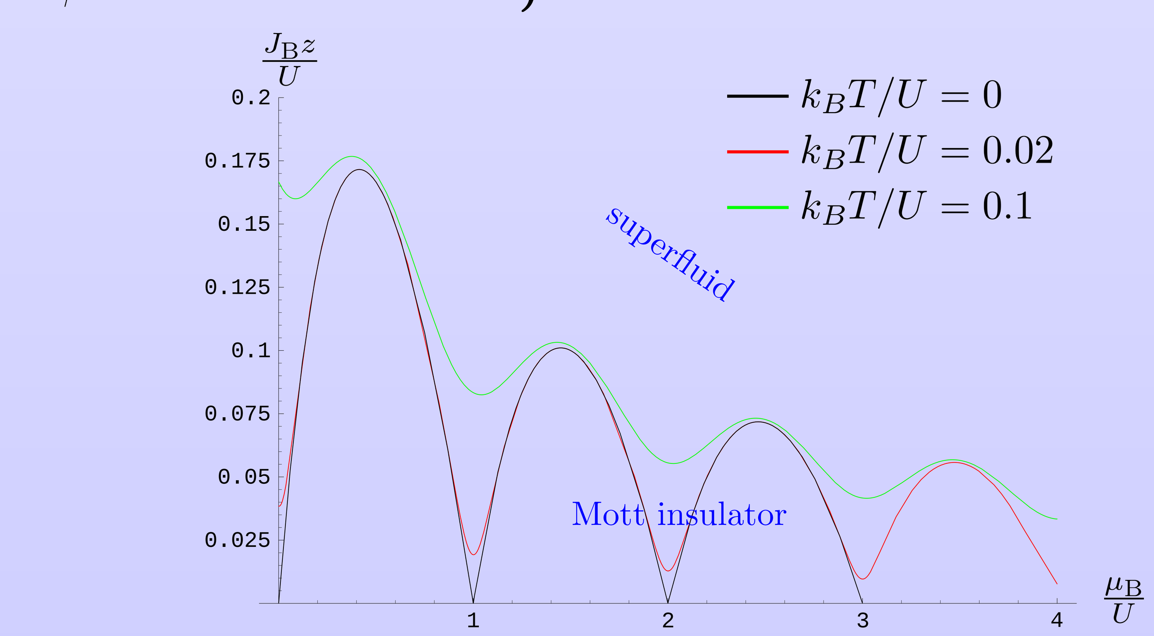
$$E_n = \frac{U}{2}n(n-1) - \mu_\mathrm{B} n$$





Phase transition [4,6]:

$$\left.\begin{array}{l} \frac{\partial \mathcal{F}}{\partial\psi} = \psi(2a_2 + 4a_4\psi^2) = 0 \\ \frac{\partial^2\mathcal{F}}{\partial\psi^2} = 2a_2 + 12a_4\psi^2 > 0 \end{array}\right\} \Rightarrow \left\{\begin{array}{ll} \psi = 0 & \text{if } a_2 > 0 \text{ Mott insulator} \\ \psi = \sqrt{-\frac{a_2}{2a_4}} & \text{if } a_2 < 0 \text{ superfluid}\end{array}\right.$$



3. Bose-Fermi-Hubbard

Add fermions [7,12]:

$$\hat{H}_F = \int d^3x\, \hat{\phi}^\dagger(\mathbf{x})\left[-\frac{\hbar^2}{2m_F}\nabla^2 + \sum_{j=1}^{3} V_0 \sin(kx_j)\right]\hat{\phi}(\mathbf{x}) + \frac{2\pi a_\mathrm{BF}\hbar^2(m_F + m_B)}{m_F m_B}\int d^3x\, \hat{\psi}^\dagger(\mathbf{x})\hat{\phi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\phi}(\mathbf{x})$$

Bose-Fermi-Hubbard Hamiltonian:

$$\hat{H}_\mathrm{BFH} = -\sum_{<i,j>}(J_\mathrm{B}\hat{a}_i^\dagger\hat{a}_j + J_\mathrm{F}\hat{b}_i^\dagger\hat{b}_j) + \frac{U}{2}\sum_i \hat{a}_i^\dagger\hat{a}_i^\dagger\hat{a}_i\hat{a}_i + U_\mathrm{BF}\sum_i \hat{a}_i^\dagger\hat{a}_i\hat{b}_i^\dagger\hat{b}_i - \mu_\mathrm{B}\sum_i \hat{a}_i^\dagger\hat{a}_i - \mu_\mathrm{F}\sum_i \hat{b}_i^\dagger\hat{b}_i$$

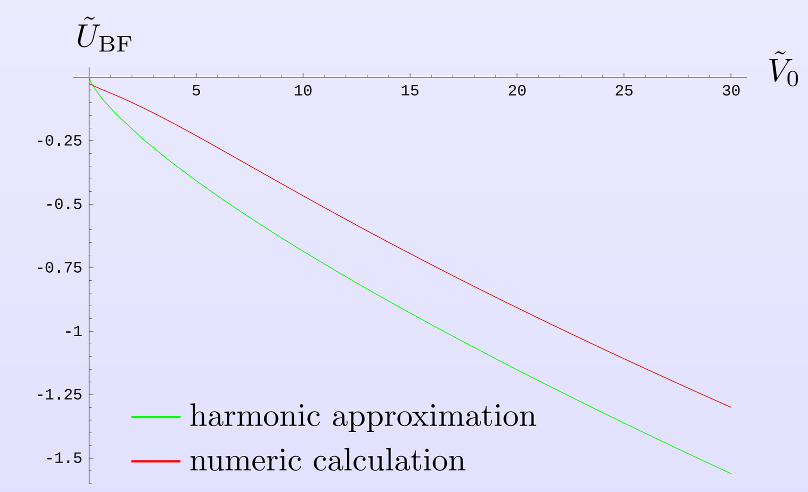
$$U_\mathrm{BF} = \frac{2\pi a_\mathrm{BF}\hbar^2(m_F + m_B)}{m_F m_B}\int d^3x\, |w_B(\mathbf{x}-\mathbf{x}_i)|^2 |w_F(\mathbf{x}-\mathbf{x}_i)|^2$$

Harmonic approximation [13]:

$$\tilde{U}_\mathrm{BF} = 4\sqrt{\pi}\,\frac{a_\mathrm{BF}}{a}\left(1 + \frac{m_B}{m_F}\right)\left(1 + \sqrt{\frac{m_B}{m_F}}\right)^{-3/2}\tilde{V}_0^{3/4}$$

Experimental data [9]:

$a_\mathrm{BF} = -205a_0$
$m_B/m_F = 87/40$



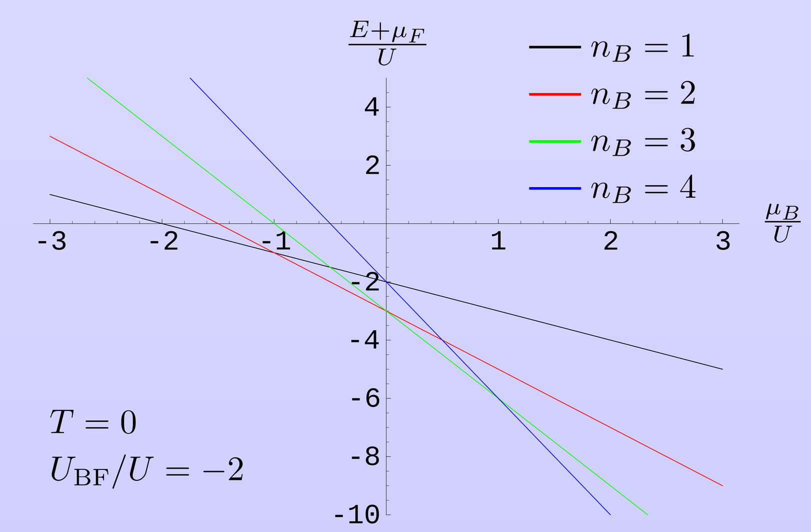
Solution of Bose-Fermi-Hubbard for $T = 0$:

$$E(\psi^*,\psi) = a_0 + a_2|\psi|^2 + a_4|\psi|^4 + \dots$$

$$a_0 = \frac{U}{2}n_B(n_B - 1) - \mu_B n_B - \mu_F n_F + U_\mathrm{BF} n_B n_F + O(J_\mathrm{F})$$

$$a_2 = J_\mathrm{B} z + J_\mathrm{B}^2 z^2 \frac{U + \mu_\mathrm{B} - U_\mathrm{BF} n_F}{(\mu_\mathrm{B} - U_\mathrm{BF} n_F - U n_B)[U(n_B - 1) - \mu_\mathrm{B} + U_\mathrm{BF} n_F]}$$

For $J_\mathrm{F} = J_\mathrm{B} = 0$ and $n_\mathrm{F} = 1$:



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