



Visibility of Atomic Cloud Released from Optical Lattices

Alexander Hoffmann¹, Francisco Ednilson Alves dos Santos¹, and Axel Pelster²

¹Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

²Fachbereich Physik, Universität Duisburg-Essen, Lotharstrasse 1, 47048 Duisburg, Germany

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1. Bose-Hubbard Model

Second-quantized Hamiltonian for bosons [1]:

$$\hat{H} = \int d^3x \hat{\psi}^\dagger(\mathbf{x}) \left[-\frac{\hbar^2}{2m} \nabla^2 + \sum_{j=1}^3 V_0 \sin^2\left(\frac{\pi}{a} x_j\right) \right] \hat{\psi}(\mathbf{x}) + \frac{2\pi a_s \hbar^2}{m} \int d^3x \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) \hat{\psi}(\mathbf{x})$$

Decomposition in Wannier states:

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

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

$$\hat{H}_{\text{BH}} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \sum_i \left\{ \frac{U}{2} \hat{a}_i^\dagger \hat{a}_i \hat{a}_i - \mu \hat{a}_i^\dagger \hat{a}_i \right\}$$

Bose-Hubbard coefficients [6-8]:

$$J = - \int d^3x w^*(\mathbf{x} - \mathbf{x}_i) \left[-\frac{\hbar^2}{2m} \nabla^2 + \sum_{j=1}^3 V_0 \sin^2\left(\frac{\pi}{a} x_j\right) \right] w(\mathbf{x} - \mathbf{x}_j)$$

$$U = \frac{4\pi a_s \hbar^2}{m} \int d^3x |w(\mathbf{x} - \mathbf{x}_i)|^4$$

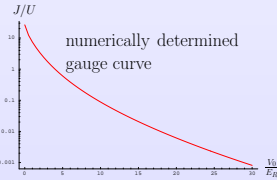
Recoil energy $E_R = \hbar^2 \pi^2 / 2ma^2$

Data of Bloch group [9,10]:

Lattice spacing $a = 425$ nm

Bosons used in experiment: ⁸⁷Rb

s-wave scattering length $a_s = 100a_0$



2. Mean-Field Theory

Mean-field ansatz [3,11]:

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

Mean-field Hamiltonian:

$$\hat{H}_{\text{MF}} = \sum_i \left\{ -Jz[\psi(\hat{a}_i + \hat{a}_i^\dagger) - \psi^2] + \frac{U}{2} \hat{n}_i(\hat{n}_i - 1) - \mu \hat{n}_i \right\}$$

Landau expansion [2,3,11,12]:

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

$$T = 0: \quad a_0 = E_n = \frac{U}{2} n(n-1) - \mu n$$

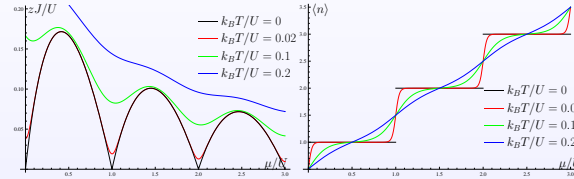
$$a_2 = Jz - J^2 z^2 \frac{U + \mu}{(\mu - Un)[U(n-1) - \mu]}$$

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

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

Second-order phase transition [3,6] due to $a_4 > 0$ [12]:

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



3. Quantum Corrections

Hamiltonian motivated by variational perturbation theory [13,14]

$$\hat{H} = \hat{H}_{\text{MF}} + \eta(\hat{H}_{\text{BH}} - \hat{H}_{\text{MF}})$$

\Rightarrow Order parameter ψ is variational parameter

Dirac interaction picture $\hat{H} = \hat{H}_0 + \hat{V}$:

$$\hat{H}_0 = \sum_i \left\{ \frac{U}{2} \hat{a}_i^\dagger \hat{a}_i \hat{a}_i - \mu \hat{a}_i^\dagger \hat{a}_i \right\}$$

$$\hat{V} = -\eta J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j - (1-\eta) J z \sum_i (\psi \hat{a}_i + \psi \hat{a}_i^\dagger - \psi^2)$$

Result in zeroth order of η :

$$a_2^{(0)} = Jz - J^2 z^2 \frac{\sum_{n=0}^{\infty} \frac{U+\mu}{(\mu-Un)[U(n-1)-\mu]} e^{-\beta E_n}}{\sum_{n=0}^{\infty} e^{-\beta E_n}}$$

Result in first order of η :

$$a_2^{(1)} = \frac{J \sum_{n=0}^{\infty} \frac{U+\mu}{(\mu-Un)[U(n-1)-\mu]} e^{-\beta E_n}}{\sum_{n=0}^{\infty} e^{-\beta E_n}} a_2^{(0)}$$

\Rightarrow Same phase border for all temperatures.

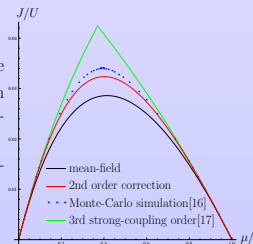
Result in second order of η for $T = 0$, $n = 1$, and $z = 6$:

$$a_2^{(2)} = J^3 \frac{36(3\mu^4 - 4\mu^3 U - 7\mu^2 U^2 - 5\mu U^3 - 3U^4)}{(U - \mu)^3 (3U - \mu)^3} - J^3 \frac{6(U + \mu)^2}{(U - \mu)^2 \mu^2}$$

- Monte-Carlo is believed to be very precise

- Analytical result for quantum correction numerically verified by exact diagonalization of mean-field Hamiltonian [15]

- Strong-coupling approach compares particle and hole states



4. Time-of-Flight

Density in momentum space [18]:

$$n(\mathbf{k}) = \langle \hat{\psi}^\dagger(\mathbf{k}) \hat{\psi}(\mathbf{k}) \rangle = |w(\mathbf{k})|^2 S(\mathbf{k}), \quad S(\mathbf{k}) = \sum_{i,j} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} \langle \hat{a}_i^\dagger \hat{a}_j \rangle$$

Time-of-flight: $\hat{n}(x, y, t) = \int_{-\infty}^{\infty} dz n(\mathbf{k} = \frac{m\mathbf{r}}{\hbar t})$

Second-order strong-coupling expansion:

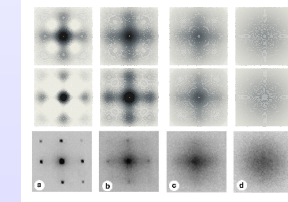
$$S(\mathbf{k}, T) = S_0(T) + 2 \frac{J}{U} S_1(T) \sum_{i=1}^3 \cos(k_i a) + 4 \frac{J^2}{U^2} S_2(T) \left[-3 + \sum_{i,j=1}^3 \cos(k_i a) \cos(k_j a) \right]$$

with the coefficients

$$S_0(T) = N_S \frac{\sum_{n=0}^{\infty} n e^{-\beta E_n}}{\sum_{n=0}^{\infty} e^{-\beta E_n}} - N_S \frac{\beta J^2}{U} \left[\frac{\sum_{n,m=0}^{\infty} n \frac{n(m+1)}{m-n+1} e^{-\beta(E_n+E_m)}}{\sum_{n,m=0}^{\infty} e^{-\beta(E_n+E_m)}} - \frac{\sum_{n=0}^{\infty} n e^{-\beta E_n}}{\sum_{n=0}^{\infty} e^{-\beta E_n}} \frac{\sum_{m=0}^{\infty} \frac{n(m+1)}{m-n+1} e^{-\beta(E_n+E_m)}}{\sum_{m=0}^{\infty} e^{-\beta(E_n+E_m)}} \right]$$

$$S_1(T) = N_S \frac{2 \sum_{n,m=0}^{\infty} \frac{(n+1)n}{(m-n+1)(m-n+1)} e^{-\beta(E_n+E_m)}}{\sum_{n,m=0}^{\infty} e^{-\beta(E_n+E_m)}}$$

$$S_2(T) = N_S \frac{3 \sum_{n,m,l=0}^{\infty} \left[\frac{n(m+1)(l+1)}{(m-n+1)(l-n+1)} + \frac{ml(l+1)}{(l-n+1)(l-m+1)} \right] e^{-\beta(E_n+E_m+E_l)}}{\sum_{n,m,l=0}^{\infty} e^{-\beta(E_n+E_m+E_l)}}$$



first-order calculation ($T = 0$)

second-order calculation ($T = 0$)

experimental absorption pictures [10]

(a) $V_0 = 8E_R$, (b) $V_0 = 14E_R$, (c) $V_0 = 18E_R$, and (d) $V_0 = 30E_R$.

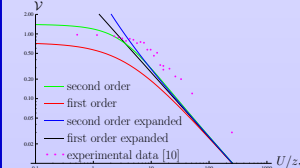
5. Visibility

Definition of visibility [9,10]: $\mathcal{V} = \frac{\tilde{n}_{\text{max}} - \tilde{n}_{\text{min}}}{\tilde{n}_{\text{max}} + \tilde{n}_{\text{min}}}$

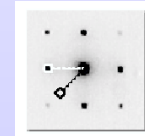
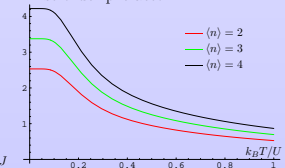
First order expanded:

$$\mathcal{V} = \frac{zJ}{U} \frac{S_1(T) (1 - \cos(\sqrt{2}\pi))}{3 S_0(T)} \quad \text{prefactor}$$

$T = 0$ and $n = 2$:



First order prefactor:





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