Ginzburg-Landau Theory for Bosons in Optical Lattices

Axel Pelster

Hanse-Wissenschaftskolleg
Institute for Advanced Study

1. Introduction

2. Landau Theory

3. Green Functions

4. Equilibrium Results

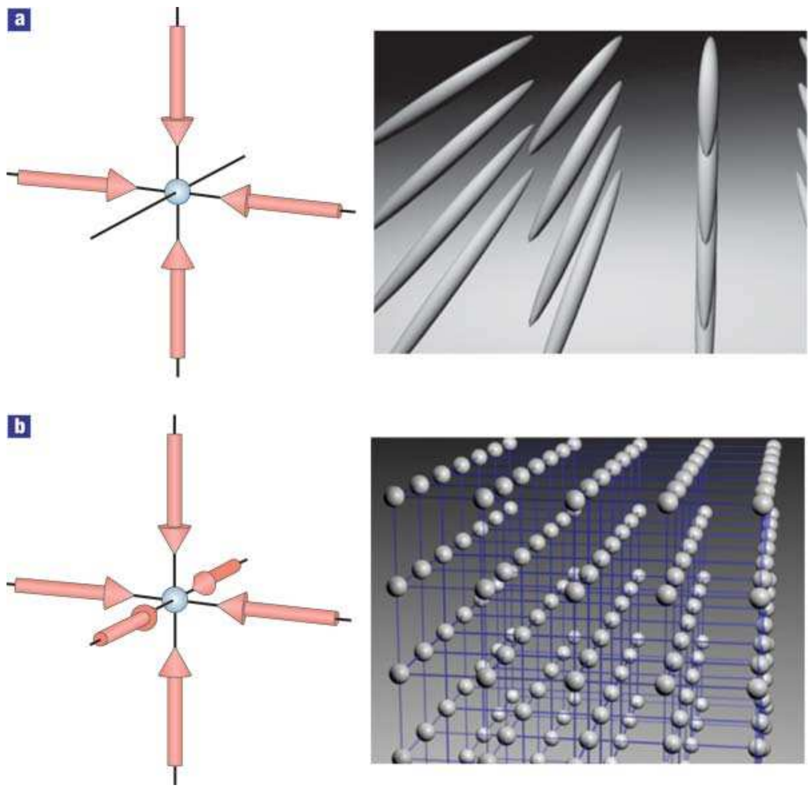
5. Ginzburg-Landau Theory

6. Nonequilibrium Results

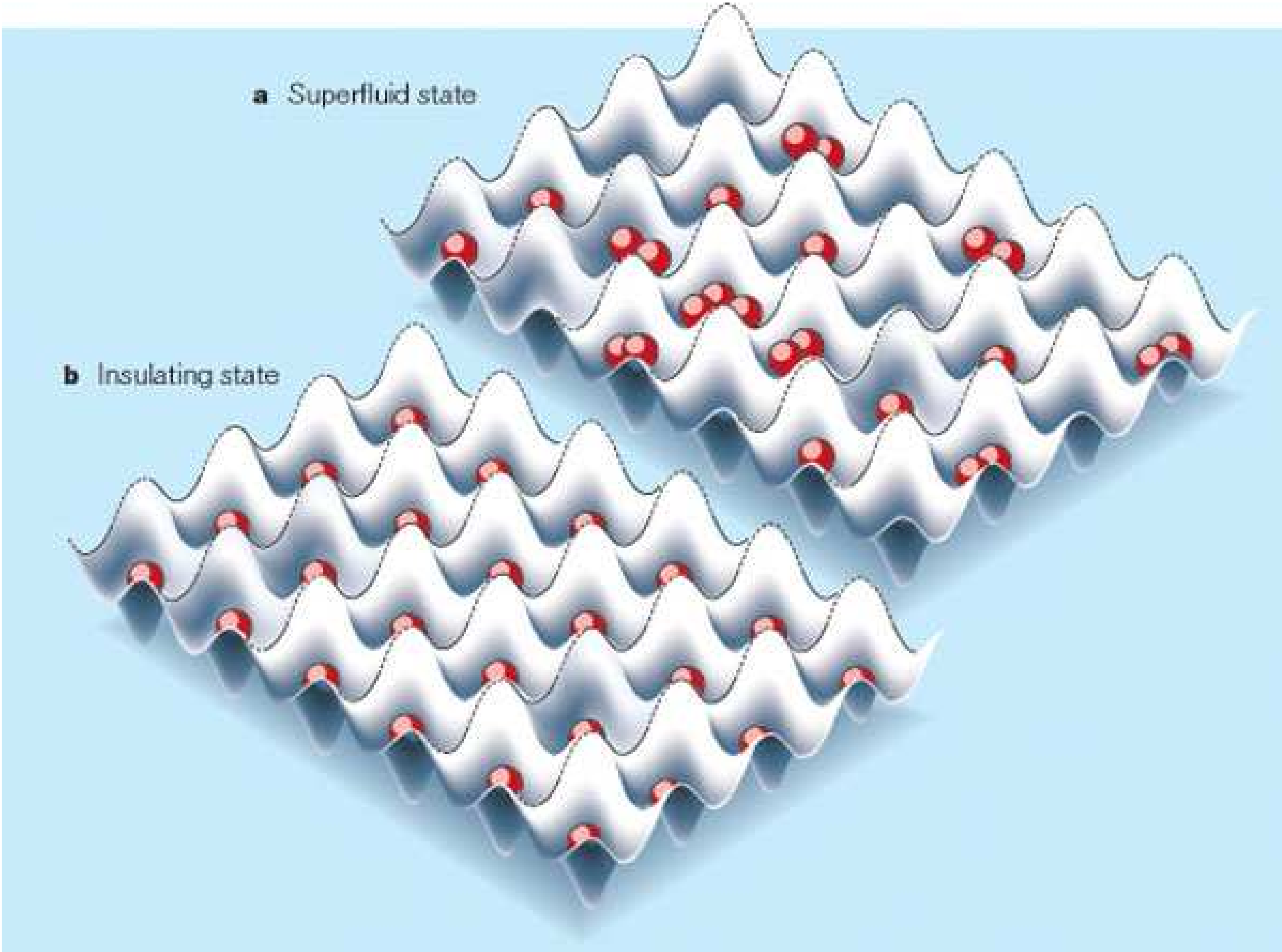
7. Summary and Outlook

1.1 Optical Lattice

- **Counter-propagating laser beams create periodic potential**
- **Different possible topologies at 1D, 2D, and 3D**
- **Hopping and interactions are highly controllable**



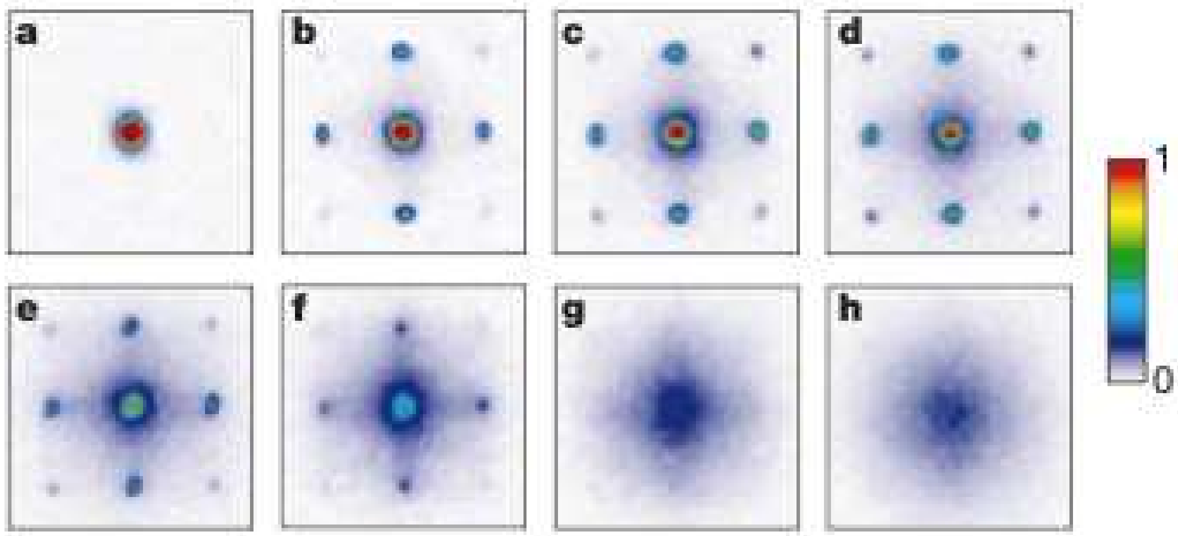
1.2 Quantum Phase Transition



1.3 Time-of-Flight Absorption Pictures

- **Superfluid phase:**
  delocalization in space, localization in Fourier space

- **Mott phase:**
  localization in space, delocalization in Fourier space

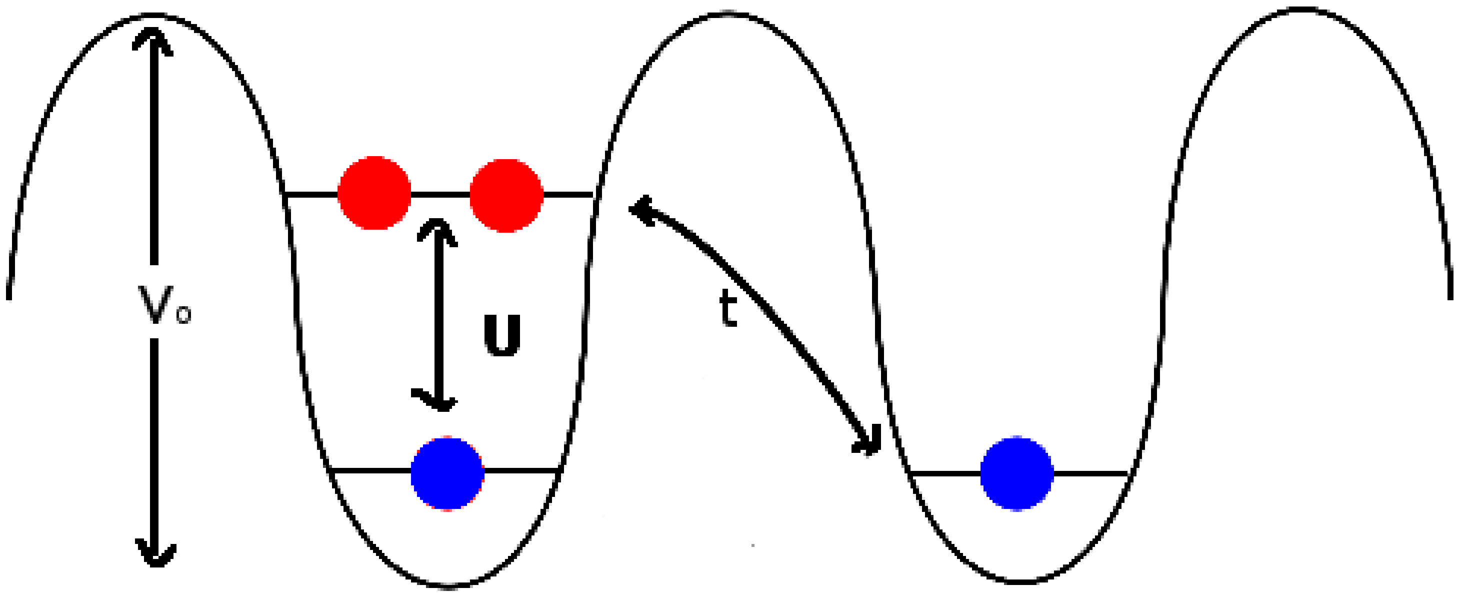


Greiner, Mandel, Esslinger, Hänsch, and Bloch, Nature **415**, 39 (2002)

1.4 Theoretical Description

Bose-Hubbard Hamiltonian:

$$\hat{H}_{\mathrm{BH}} = -t \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \sum_i \left[\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i \right], \qquad \hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$$



1.5 Mean-Field Theory

Bose-Hubbard Hamiltonian:

$$\hat{H}_{\mathrm{BH}} = -t \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \sum_i \left[\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i \right], \qquad \hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$$

Ansatz: $\sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j \rightarrow 2d \sum_i (\psi^* \hat{a}_i + \psi \hat{a}_i^\dagger - |\psi|^2)$

Partition function: $Z = \mathrm{Tr}\left[e^{-\beta \hat{H}_{\mathrm{MF}}(\psi^*, \psi)} \right] = e^{-\beta F_{\mathrm{MF}}(\psi^*, \psi)}$

Self-consistency relations:

$$\begin{cases} \dfrac{\partial F_{\mathrm{MF}}}{\partial \psi} = 0 \\ \dfrac{\partial F_{\mathrm{MF}}}{\partial \psi^*} = 0 \end{cases} \Longrightarrow \begin{cases} \langle \hat{a}_i^\dagger \rangle = \psi^* \\ \langle \hat{a}_i \rangle = \psi \end{cases}$$

Landau expansion: $F_{\mathrm{MF}}(\psi^*, \psi) = a_0 + a_2 |\psi|^2 + a_4 |\psi|^4 + \cdots$

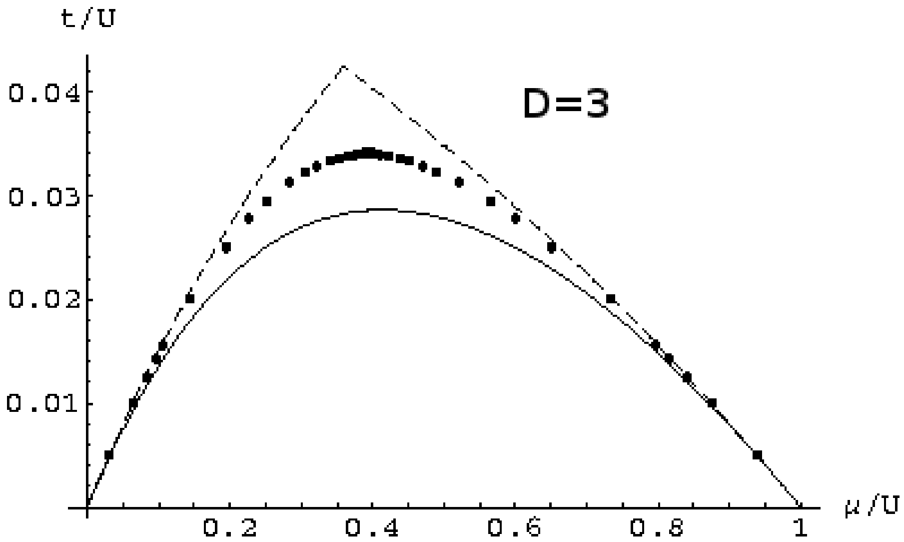
If $a_4 > 0$, then $a_2 = 0$ defines SF-MI phase boundary

1.6 State of the Art

Mean-field result:

$$t_c = U/\left[2d\left(\frac{n+1}{n-b}+\frac{n}{1-n+b}\right)\right] \quad , \qquad b = \frac{\mu}{U}$$

Quantum Phase Diagram:



Dashed: **3rd order strong-coupling**
PRB **53**, 2691, 1996

Line: **Mean-field result**
PRB **40**, 546, 1989

Dots: **Monte-Carlo data**
PRA **75**, 013619, 2007

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2.1 Landau Theory

Bose-Hubbard Hamiltonian with Current:

$$\hat{H}_{\rm BH}(J^*,J) = \hat{H}_{\rm BH} + \sum_i \left(J^* \hat{a}_i + J \hat{a}_i^\dagger \right)$$

Grand-Canonical Free Energy: $F = -\frac{1}{\beta} \ln {\rm Tr} \left[e^{-\beta \hat{H}_{\rm BF}(J^*,J)} \right]$

$$\psi = \langle \hat{a}_i \rangle = \frac{1}{N_{\rm s}} \frac{\partial F(J^*,J)}{\partial J^*} \quad ; \quad \psi^* = \langle \hat{a}_i^\dagger \rangle = \frac{1}{N_{\rm s}} \frac{\partial F(J^*,J)}{\partial J}$$

Legendre Transformation: $\Gamma(\psi^*,\psi) = \psi^* J + \psi J^* - F/N_{\rm s}$

$$\frac{\partial \Gamma}{\partial \psi^*} = J \quad ; \quad \frac{\partial \Gamma}{\partial \psi} = J^*$$

$\Longrightarrow$ **Physical limit of vanishing current**

Landau expansion: $\Gamma = a_0 + a_2 |\psi|^2 + a_4 |\psi|^4 + \cdots$

$\Longrightarrow$ **Landau coefficients in tunneling expansion**

2.2 Technical Details

Hopping Expansion:

$$F(J^*, J) = F_0(t) + \sum_{p=1}^{\infty} c_{2p}(t)|J|^{2p}$$

$$c_p(t) = \sum_{n=0}^{\infty} (-t)^n \alpha_p^{(n)}$$

Legendre Transformation:

$$\Gamma(\psi^*, \psi) = -F_0(t) + \frac{1}{c_2(t)}|\psi|^2 - \frac{c_4(t)}{c_2(t)^4}|\psi|^4 + \cdots$$

Phase boundary:

$$\frac{1}{c_2(t_c)} = \frac{1}{\alpha_2^{(0)}} \left\{ 1 + \frac{\alpha_2^{(1)}}{\alpha_2^{(0)}} t_c + \left[\left(\frac{\alpha_2^{(1)}}{\alpha_2^{(0)}} \right)^2 - \frac{\alpha_2^{(2)}}{\alpha_2^{(0)}} \right] t_c^2 + \cdots \right\} = 0$$

Note: Choose smallest critical t_c.

2.3 Explicit Results

$$
\begin{aligned}
\alpha_2^{(0)} &= \frac{b+1}{U(b-n)(b+1-n)} \\
\alpha_2^{(1)} &= \frac{2d(b+1)^2}{U^2(b-n)^2(b+1-n)^2}
\end{aligned}
$$

$$
\begin{aligned}
\alpha_2^{(2)} = \; & 2\left\{2d(b+1)^3(b-2-n)(b+3-n) + n(b-n)(b+1-n)\right. \\
& \left. \times(1+n)(4+3b+2n)\left[-3-2n+2(b^2+b-2bn+n^2)\right]\right\} \\
& / \left[U^3(b-n-2)(b-n)^3(b+1-n)^3(b+3-n)\right]
\end{aligned}
$$

Here n is number of particles at each site and $b = \mu/U$.

Santos and Pelster, PRA **79**, 013614 (2009)

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3.1 Green Function Method

Imaginary-Time Green's Function:

$$
\begin{aligned}
G_1(\tau', j'|\tau, j) &= \frac{1}{Z_{\rm BH}} \mathrm{Tr}\left\{ e^{-\beta \hat{H}_{\rm BH}} \hat{T} \left[\hat{a}_{j,\rm H}(\tau) \hat{a}^\dagger_{j',\rm H}(\tau') \right] \right\} \\
\hat{a}_{j,\rm H}(\tau) &= e^{\hat{H}_{\rm BH}\tau/\hbar}\, \hat{a}_j\, e^{-\hat{H}_{\rm BH}\tau/\hbar} \\
Z_{\rm BH} &= \mathrm{Tr}\left[e^{-\beta \hat{H}_{\rm BH}} \right]
\end{aligned}
$$

Motivation:

- Quantum phase diagram
- Excitation spectra
- Absorption measurements

3.2 Cumulant Expansion

Hopping Expansion:

$$\hat{H}_{\mathrm{BH}} = \underbrace{-\sum_{i,j} t_{i,j}\hat{a}_i^\dagger \hat{a}_j}_{\text{perturbation}} + \underbrace{\sum_i \left[\frac{U}{2}\hat{n}_i(\hat{n}_i - 1) - \mu\hat{n}_i\right]}_{=\hat{H}^{(0)}}, \qquad \hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$$

Motivated by Fermi-Hubbard model: Metzner, PRB **43**, 8549 (1993)

Expansion in hopping matrix element:

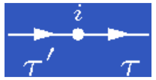
$$G_1^{(n)}(\tau', i'|\tau, i) = \frac{Z^{(0)}}{Z}\frac{1}{n!}\sum_{i_1,j_1,\ldots,i_n,j_n} t_{i_1 j_1}\ldots t_{i_n j_n}\int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n$$
$$\times G_{n+1}^{(0)}(\tau_1, j_1;\ldots;\tau_n, j_n;\tau', i'|\tau_1, i_1;\ldots;\tau_n, i_n;\tau, i)$$

Decomposition into *local* cumulants:

$$G_2^{(0)}(\tau_1', i_1';\tau_2', i_2'|\tau_1, i_1;\tau_2, i_2) = \delta_{i_1,i_2}\delta_{i_1',i_2'}\delta_{i_1,i_1'}C_2^{(0)}(\tau_1',\tau_2'|\tau_1,\tau_2)$$
$$+\delta_{i_1,i_1'}\delta_{i_2,i_2'}C_1^{(0)}(\tau_1'|\tau_1)C_1^{(0)}(\tau_2'|\tau_2) + \delta_{i_1,i_2'}\delta_{i_2,i_1'}C_1^{(0)}(\tau_2'|\tau_1)C_1^{(0)}(\tau_1'|\tau_2)$$

3.3 Diagrammatic Representation

Diagrammatica:



$= C_1^{(0)}(\tau'|\tau)\,,$ 

$= C_2^{(0)}(\tau_1', \tau_2'|\tau_1, \tau_2)\,,$  $= t_{ij}$

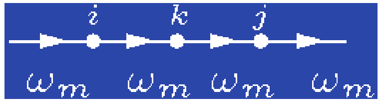
In Matsubara space with $E_n = \frac{U}{2}n(n-1) - \mu n$

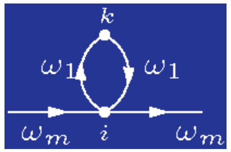
$$C_1^{(0)}(\omega_m) = \frac{1}{\mathcal{Z}^{(0)}} \sum_{n=0}^{\infty} \left[\frac{(n+1)}{E_{n+1} - E_n - i\omega_m} - \frac{n}{E_n - E_{n-1} - i\omega_m} \right] e^{-\beta E_n}$$

First two orders of perturbation series:

$G_1^{(1)}(\omega_m; i, j) \;=$ 

$= t\delta_{d(i,j),1} C_1^{(0)}(\omega_m)^2$

$G_1^{(2)}(\omega_m; i, j) \;=$ 

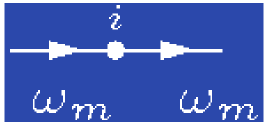
$+$ 

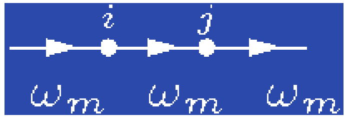
$$= t^2 \left[\delta_{d(i,j),2} + 2\delta_{d(i,j),\sqrt{2}} + 2d\delta_{i,j} \right] C_1^{(0)}(\omega_m)^3$$

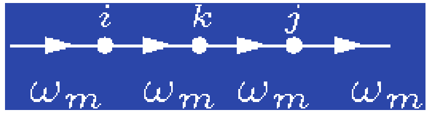
$$+ t^2 2d\delta_{i,j} \sum_{\omega_1} C_1^{(0)}(\omega_m) C_2^{(0)}(\omega_m, \omega_1|\omega_m, \omega_1)$$

3.4 Resummation

First-order:

$\tilde{G}_1^{(1)}(\omega_m; i, j) =$ 

$+$ 

$+$ 

$+ \dots$

Easily summed in Fourier space:

$$\tilde{G}_1^{(1)}(\omega_m, \mathbf{k}) = \frac{C_1^{(0)}(\omega_m)}{1 - t(\mathbf{k})\, C_1^{(0)}(\omega_m)} \quad , \qquad t(\mathbf{k}) = 2t \sum_{l=1}^{d} \cos(k_l a)$$

- **Phase boundary given by divergency of** $G_1(\omega_m = 0; \mathbf{k} = \mathbf{0})$.
- **First-order result reproduces mean-field result.**
- **Improved by taking one-loop diagram into account.**
- **Reproduces in zero-temperature limit result of Landau theory.**

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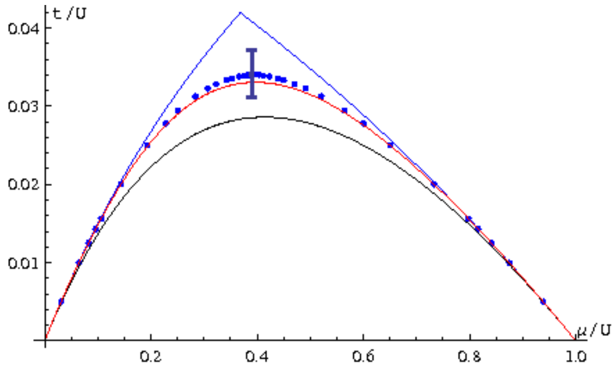
4.1 Quantum Phase Diagram

Zero temperature:



Error bar: **Extrapolated strong-coupling series**

Black line: **Mean-field**

Blue line: **3rd strong-coupling order**

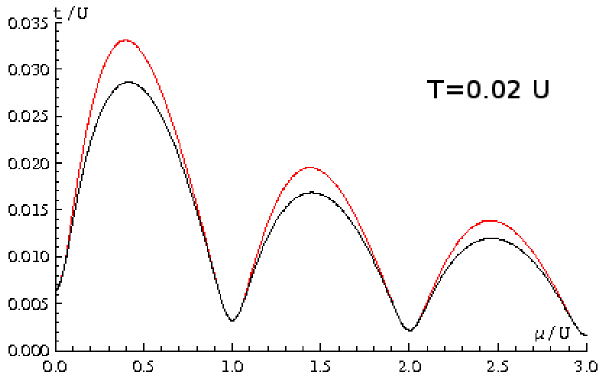
Red line: **Landau theory**

Blue dots: **Monte-Carlo data**

Santos and Pelster, PRA **79**, 013614 (2009)

Extension to higher orders: Teichmann *et al.*, PRB **79**, 100503(R) (2009)

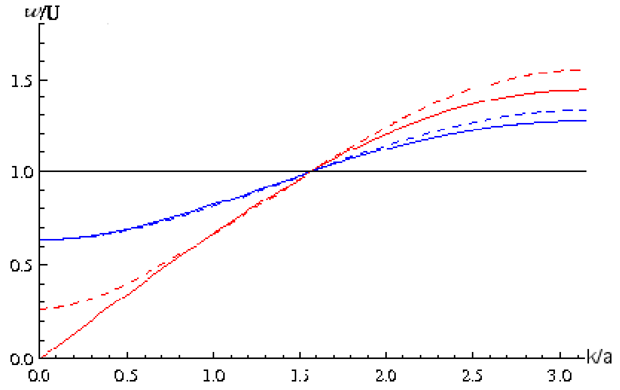
Finite Temperature:



Black: **First order (Mean field)**

Red: **Second order (One-loop corrected)**

4.2 Excitation Spectrum

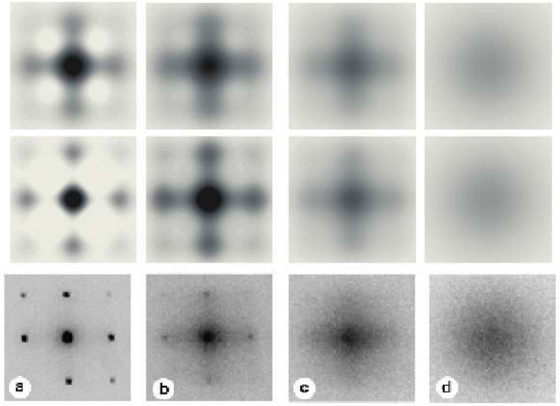


- **Solid black:** $t = 0$
- **Solid blue:** $t = 0.017\,U$ **(first order)**
- **Dotted blue:** $t = 0.017\,U$ **(second order)**
- **Solid red:** $t = 0.029\,U$ **(first order)**
- **Dotted red:** $t = 0.029\,U$ **(second order)**

- **Excitation spectrum given by poles of real-time Green's function**
- **Spectrum gapped in Mott phase**
- **Spectrum becomes gapless at phase boundary**
- **Only quantitative effects from finite temperature**

4.3 Absorption Measurements

Time-of-Flight Pictures:

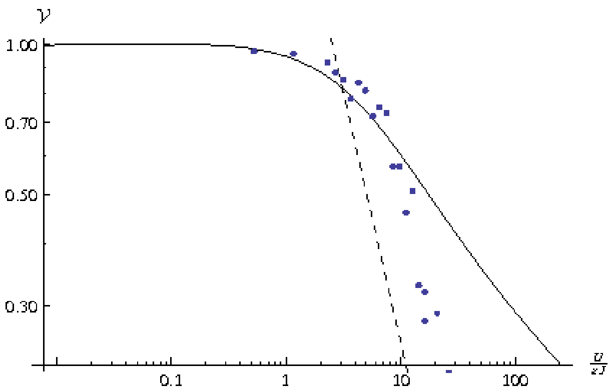


Top to bottom: First-order perturbation theory,

Second-order perturbation theory, experiment.

Left to right: $V_0 = 8, 14, 18, 30 E_\mathrm{R}$

Visibility:



Contrast Measure: $\nu = \dfrac{n_\mathrm{max} - n_\mathrm{min}}{n_\mathrm{max} + n_\mathrm{min}}$

Solid: First-order (Wannier functions)

Dashed: First-order (harmonic approximation)

Dots: Experimental data (Bloch's group)

Hoffmann and Pelster, PRA **79**, 053623 (2009)

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5.1 Ginzburg-Landau Theory

Effective Action:

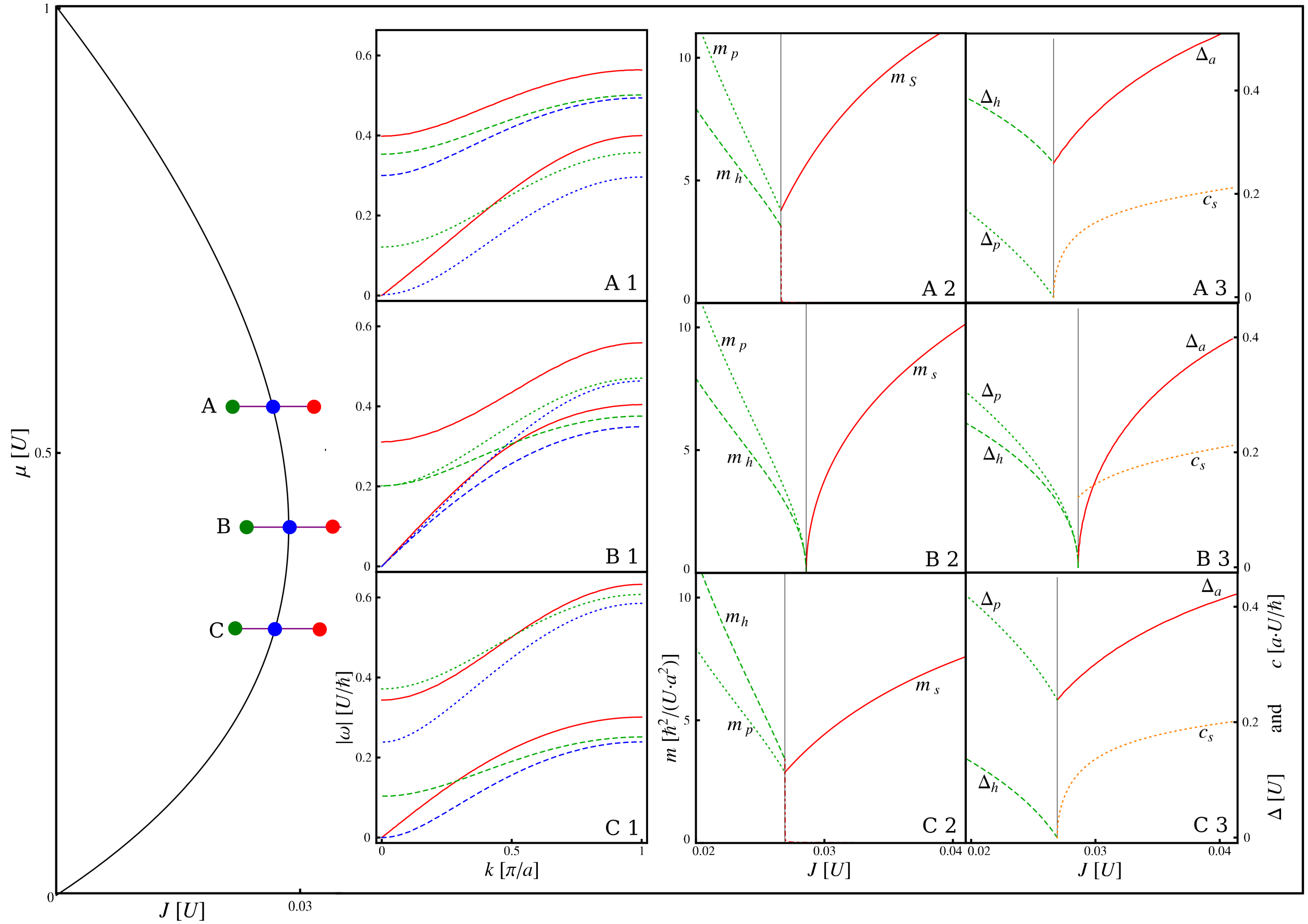
$$\Gamma = \Gamma_0 + \sum_{i,j} \sum_m \Big[b_2(i;\omega_m)\delta_{ij} - J_{ij} \Big] \psi_i(\omega_m)\psi_j^*(\omega_m)$$
$$+ \sum_i \sum_{m_1,m_2,m_3,m_4} b_4(i;\omega_{m_1},\omega_{m_2},\omega_{m_3},\omega_{m_4})\psi_i(\omega_{m_1})\psi_i(\omega_{m_2})\psi_i^*(\omega_{m_3})\psi_i^*(\omega_{m_4}) + \dots$$

Equations of Motion:

$$\sum_{i',m'} \left[\begin{array}{cc} \left.\dfrac{\partial^2\Gamma}{\partial\psi_i^*(\omega_m)\partial\psi_{i'}(\omega_{m'})}\right|_{\mathrm{eq}} & \left.\dfrac{\partial^2\Gamma}{\partial\psi_i^*(\omega_m)\partial\psi_{i'}^*(\omega_{m'})}\right|_{\mathrm{eq}} \\ \left.\dfrac{\partial^2\Gamma}{\partial\psi_i(\omega_m)\partial\psi_{i'}(\omega_{m'})}\right|_{\mathrm{eq}} & \left.\dfrac{\partial^2\Gamma}{\partial\psi_i(\omega_m)\partial\psi_{i'}^*(\omega_{m'})}\right|_{\mathrm{eq}} \end{array} \right] \left[\begin{array}{c} \delta\psi_{i'}(\omega_{m'}) \\ \delta\psi_{i'}^*(\omega_{m'}) \end{array} \right] = \left[\begin{array}{c} 0 \\ 0 \end{array} \right]$$

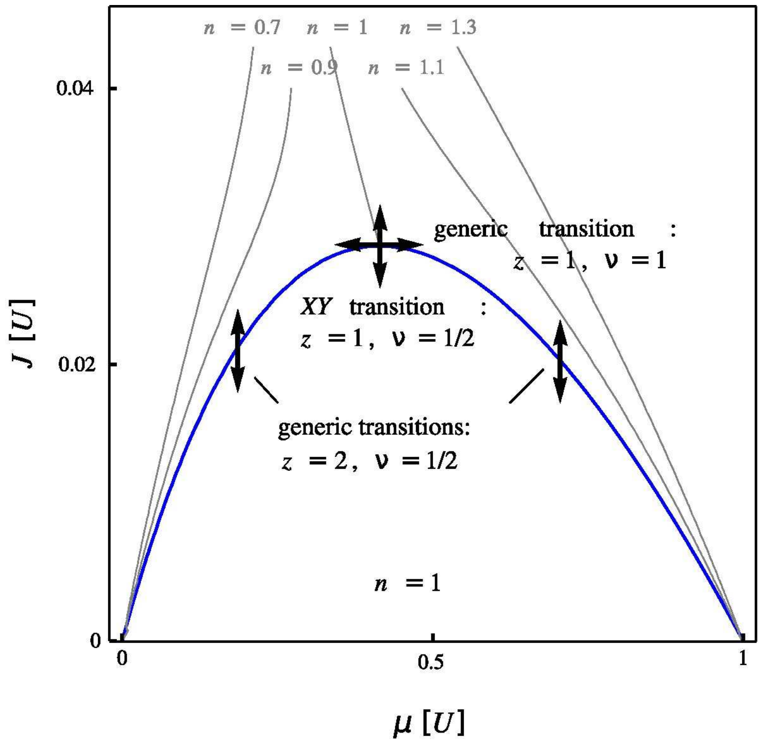
Bradlyn, Santos, and Pelster, PRA **79**, 013615 (2009)

5.2 Excitation Spectra



Graß, Santos, and Pelster, PRA **84**, 013613 (2011)

5.3 Critical Exponents



- **Scaling behavior:** $\Delta \sim (J - J_{\rm PB})^{z\nu}$
- **Two universality classes:**
  - Generic transition: driven by density variation $z\nu = 1$ (=mean field)
  - XY-like transition: driven by hopping variation $z\nu = 1/2$ (only at lobe tip)

Fisher *et al.*, PRB **40**, 546 (1989)

5.4 Discussion:

- **Modes in Superfluid Phase**
  - **Two modes** $\longrightarrow$ Phase/amplitude excitations
    Huber *et al.*, PRB **75**, 085106 (2007)
  - **Sound mode** $\longrightarrow$ Goldstone theorem, Bogoliubov theory, Bragg spectroscopy
    Ernst *et al.*, Nat. Phys. **6**, 56 (2009)
  - **Gapped mode** $\longrightarrow$ Condensate filling at constant density, lattice modulation
    Stöferle *et al.*, PRL **92**, 130403 (2004)

- **Deep in Superfluid Phase:**
  - Hopping expansion not supposed to be good far away from phase boundary
  - Nevertheless: Consider $U \ll J, \mu$ and expand in U
    $\Rightarrow$ **Gross-Pitaevski equation**: $i\hbar\frac{\partial \Psi_i}{\partial t} = -\sum_j J_{ij}\Psi_j - \mu\Psi_i - U\Psi_i|\Psi_i|^2$
  - Yields **Bogoliubov sound mode:**

$$\hbar\omega(\boldsymbol{k}) = \sqrt{\left(4J\sum \sin^2(k_i a/2)\right)^2 + 2nU\left(4J\sum \sin^2(k_i a/2)\right)}$$

  - Gapped mode: Solve equation of motion first, and apply the limit $U \longrightarrow 0$ then
    $\Rightarrow \omega = 2|\mu|$

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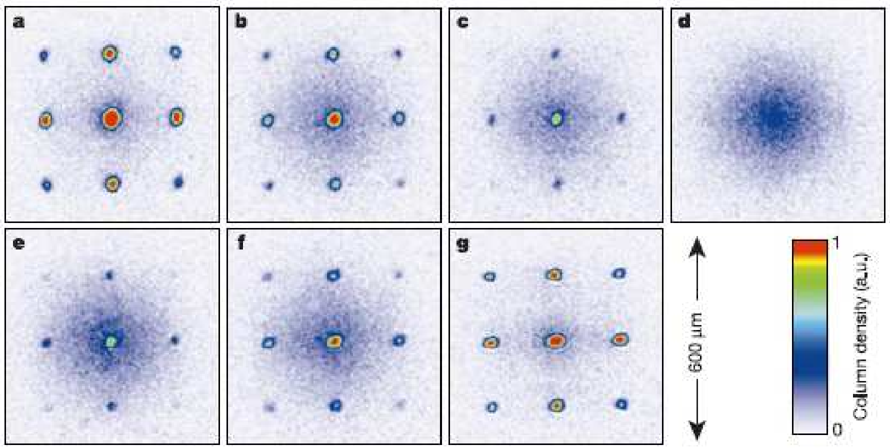
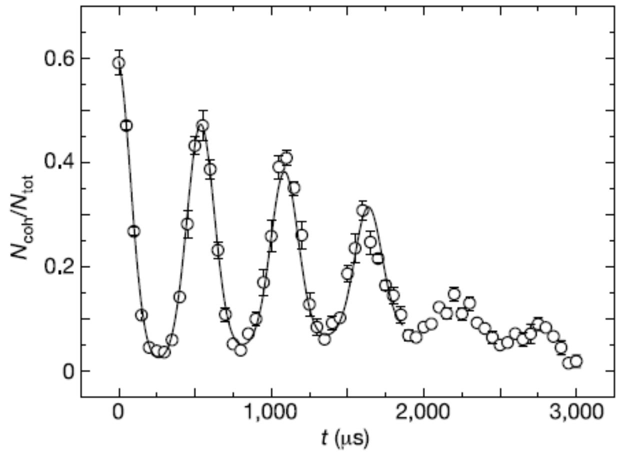
6.1 Collapse and Revival of Matter Waves

- **Inhomogeneous Bose-Hubbard Hamiltonian:**

$$\hat{H}_{\rm BH} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \sum_i \left[\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu_i \hat{n}_i \right], \qquad \mu_i = \mu - \frac{m}{2} \omega^2 \mathbf{x}_i^2$$

- **Experiment:**





– Time-of-flight absorption pictures:

Greiner *et al.*, Nature **419**, 51 (2002)

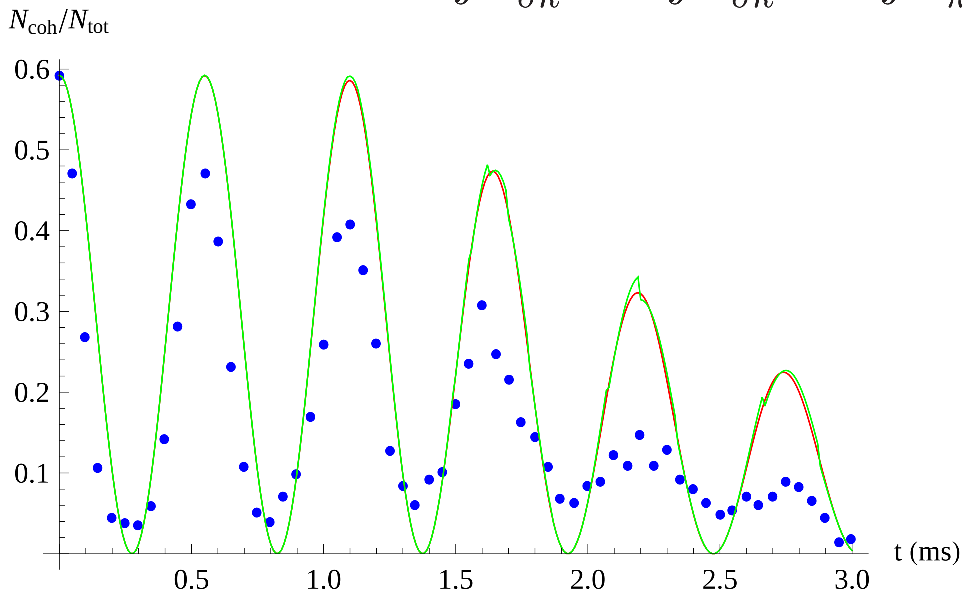
– Periodic potential depth suddenly changed from $8\ E_R$ to $22\ E_R$

6.2 Preliminary Results from Ginzburg-Landau Theory

- Condensed fraction extracted from $130\ \mu m \times 130\ \mu m$ squares around interference peaks

- **Measured coherent fraction:**

$$N_{\rm coh} = \int_{-\delta k}^{\delta k} dk_x \int_{-\delta k}^{\delta k} dk_y \int_{-\pi/a}^{\pi/a} dk_z |\phi(\mathbf{k}, t)|^2$$



- **blue dots**: experimetal data
- **solid green**: numerical solution
- **solid red**: Large-time approximation

- **Physical origin of damping:**
phase decoherence due to trap

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7.1 Selected Research Topics

- **Thermometer:**
  - visibility and excitation spectrum are candidates
  - experimental procedure: adiabatic heating

- **Hopping Expansion in Schwinger-Keldysh Formalism:**
  - temperature and time
  - theoretical inconsistency:

    Bradlyn, Santos, and Pelster, PRA **79**, 013615 (2009)

    Graß, Santos, and Pelster, PRA **84**, 013613 (2011)

- **Jaynes-Cummings-Hubbard Model:**

  Nietner and Pelster, PRA **85**, 043831 (2012)

- **Disordered Bosons in Lattice:**

  Krutitsky, Pelster, and Graham, NJP **8**, 187 (2006)

7.2 Posters

- **D. Hinrichs**, A. Pelster, and M. Holthaus:
  Critical properties of the Bose-Hubbard model

- N. Gheeraert, S. Chester, S. Eggert, and **A. Pelster**:
  Mean-field theory for the extended Bose-Hubbard model

- **T. Wang**, X.-F. Zhang, A. Pelster, and S. Eggert:
  Anisotropic superfluidity of bosons in optical Kagome superlattice

- W. Cairncross and **A. Pelster**:
  Stability analysis for Bose-Einstein condensates under parametric resonance

- **B. Nikolic**, A. Balaz, and A. Pelster:
  Bose-Einstein condensation in weak disorder potential