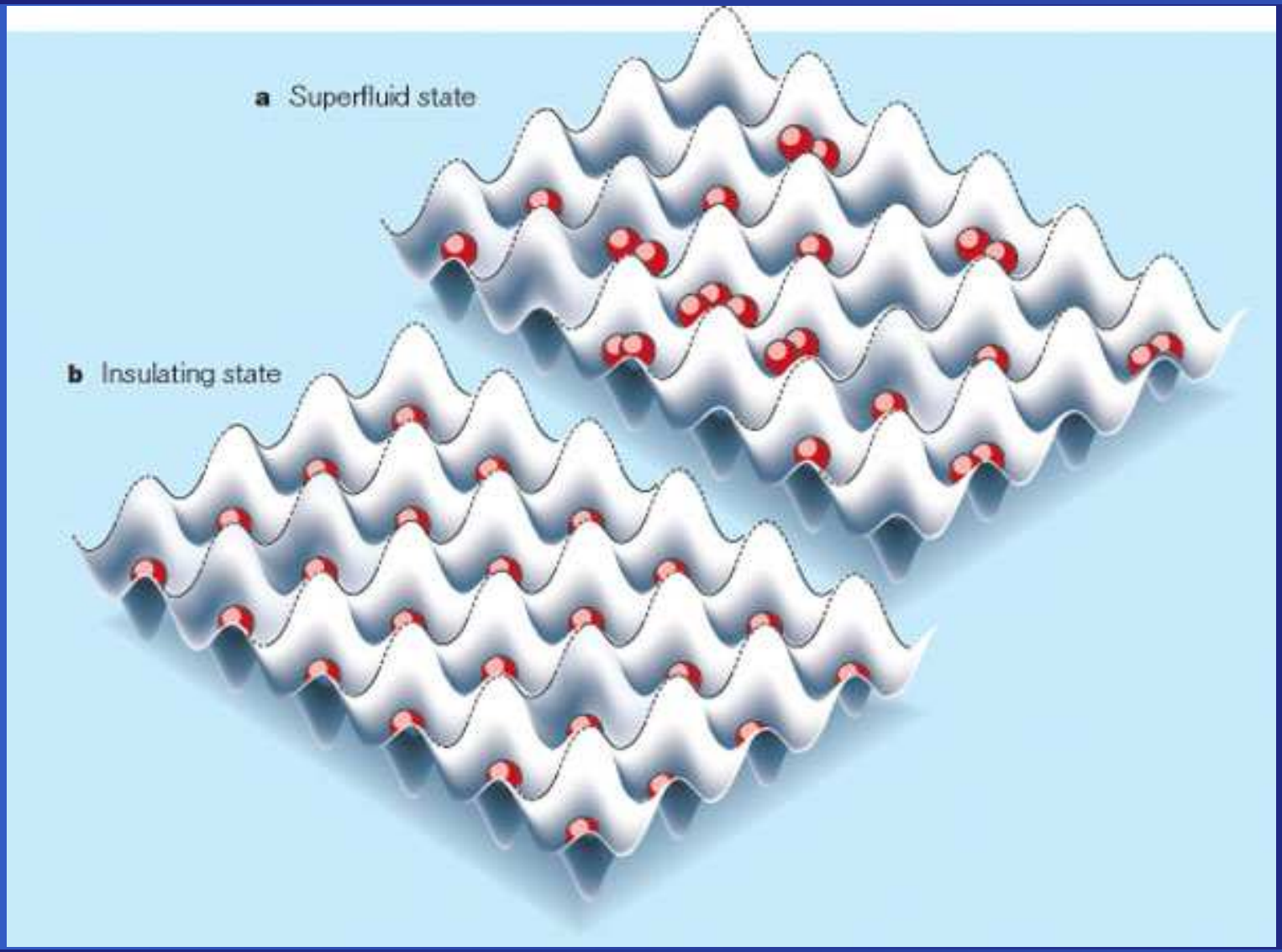
Quantum Phase Diagram of Bosons in Optical Lattices

Ednilson Santos, Matthias Ohliger, Alexander Hoffmann, and Axel Pelster

Outline of the talk

1. Experimental facts
2. Theoretical description
3. Mean-field theory
4. State of the art
5. Effective potential method
6. Green's function method
7. Results
8. Conclusion

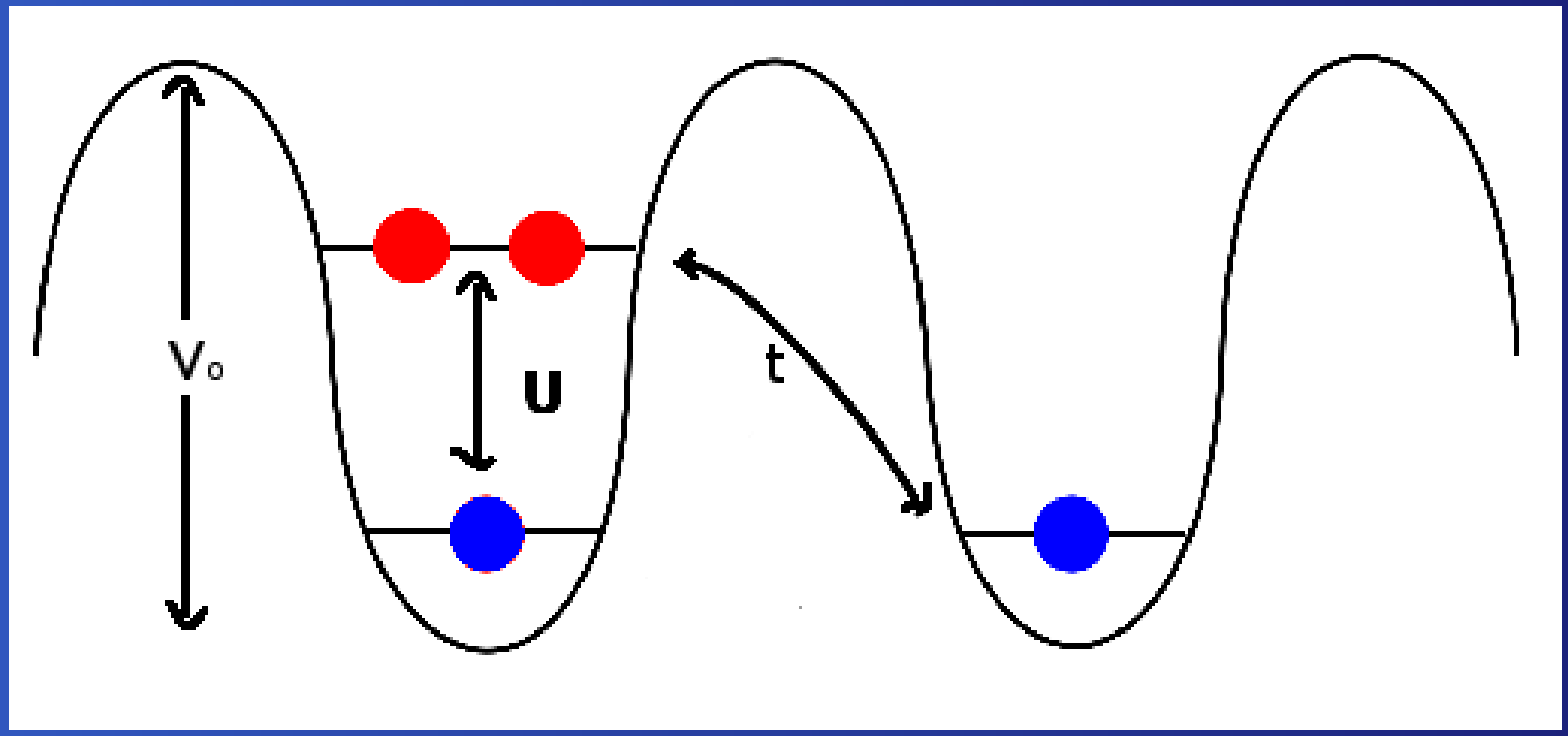
1 - Experimental facts



2 - Theoretical description

Bose-Hubbard Hamiltonian:

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



3 - Mean-field theory

Bose-Hubbard Hamiltonian:

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

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

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

Self-consistency relations: $\begin{cases} \frac{\partial F_{\rm MF}}{\partial \psi} = 0 \\ \frac{\partial F_{\rm MF}}{\partial \psi^*} = 0 \end{cases} \Longrightarrow \begin{cases} \langle \hat{a}_i^\dagger \rangle = \psi^* \\ \langle \hat{a}_i \rangle = \psi \end{cases}$

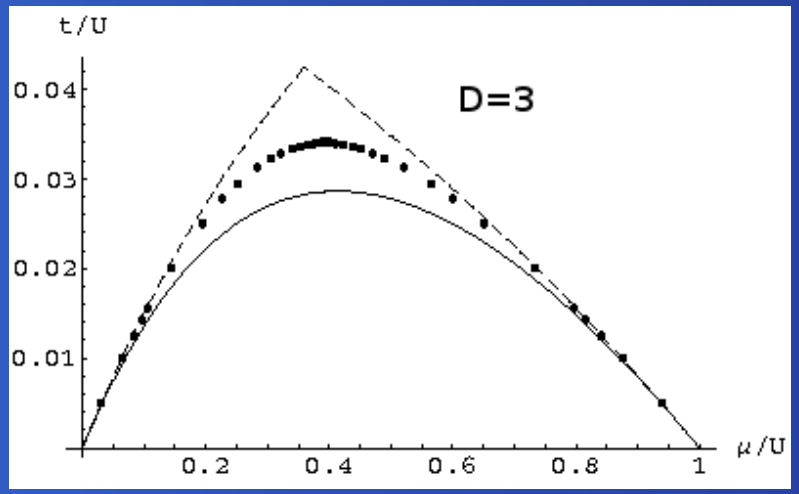
Landau expansion: $F_{\rm MF}(\psi^*, \psi) = a_0 + a_2 |\psi|^2 + a_4 |\psi|^4 + \cdots$

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

4 - State of the art

Mean-field result:

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



Dashed: 3rd order strong-coupling

Phys. Rev. B, 53:2691, 1996

Line: Mean-field result

Phys. Rev. B, 40:546, 1989

Dots: Monte-Carlo data

Phys. Rev. A, 75:013619, 2007

5 - Effective potential method

Bose-Hubbard Hamiltonian with current:

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

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

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

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

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

Physical limit of vanishing current:

$$\frac{\partial \Gamma}{\partial \psi^*} = 0 \quad ; \quad \frac{\partial \Gamma}{\partial \psi} = 0$$

5.1 - Details

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

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

with: $c_{2n}(t) = \sum_{p=0}^{\infty}(-t)^p \alpha_{2n}^{(p)}$

Phase boundary:

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

5.2 - Phase boundary

First order: $t_c^{(1)} = -\frac{\alpha_2^{(0)}}{\alpha_2^{(1)}}$

Remark: Identical to mean-field phase boundary.

Second order:

$$t_c^{(2)} = \frac{\overline{\alpha}_1}{2\left(\overline{\alpha}_2 - \overline{\alpha}_1^2\right)} + \frac{1}{2\left(\overline{\alpha}_2 - \overline{\alpha}_1^2\right)}\sqrt{\overline{\alpha}_1^2 - 4\left(\overline{\alpha}_1^2 - \overline{\alpha}_2\right)}$$

with: $\overline{\alpha}_1 = \frac{\alpha_2^{(1)}}{\alpha_2^{(0)}} \quad ; \quad \overline{\alpha}_2 = \frac{\alpha_2^{(2)}}{\alpha_2^{(0)}}$

Note: Choose the smallest critical $t_c^{(2)}$.

5.3 - Explicit results

$$\alpha_2^{(0)} = \frac{b+1}{U(b-n)(b+1-n)}$$

$$\alpha_2^{(1)} = \frac{2d(b+1)^2}{U^2(b-n)^2(b+1-n)^2}$$

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

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

6 - Green's function method

- Green's function contains many important information about the system:
  - Quantum phase diagram
  - Time-of-flight pictures
  - Excitation spectra
  - Thermodynamic properties

Imaginary-time Green's function:

$$G_1(\tau', j'|\tau, j) = \frac{1}{Z}\mathrm{Tr}\left\{e^{-\beta\hat{H}_{\mathrm{BH}}}\hat{T}\left[\hat{a}_{j,\mathrm{H}}(\tau)\hat{a}^{\dagger}_{j',\mathrm{H}}(\tau')\right]\right\}$$

with $\hat{a}_{j,\mathrm{H}}(\tau) = e^{\hat{H}_{\mathrm{BH}}\tau/\hbar}\hat{a}_j e^{-\hat{H}_{\mathrm{BH}}\tau/\hbar}$

and $Z = \mathrm{Tr}\left[e^{-\beta\hat{H}_{\mathrm{BH}}}\right] = e^{-\beta F}$.

6.1 - Decomposition

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

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:

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

6.2 - Diagrammatic representation

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

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

$= t_{ij}$

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

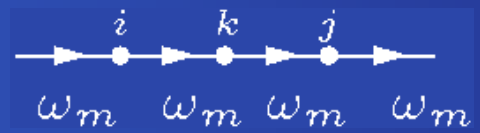
$$C_1^{(0)}(\omega_m) = \frac{1}{\mathcal{Z}^{(0)}} \sum_{n=0}^{\infty} \left[\frac{(n+1)}{E_{n+1} - E_n - i\omega_m} - \frac{n}{E_n - E_{n-1} - i\omega_m} \right] e^{-\beta E_n}$$

First two orders of perturbation series:

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

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

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



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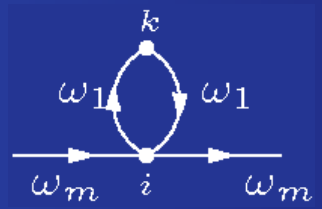


$$= t^2(\delta_{d(i,j),2} + 2\delta_{d(i,j),\sqrt{2}} + 2d\delta_{i,j}) C_1^{(0)}(\omega_m)^3$$

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

6.3 - Resumation

First-order:

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

$+ \ldots$

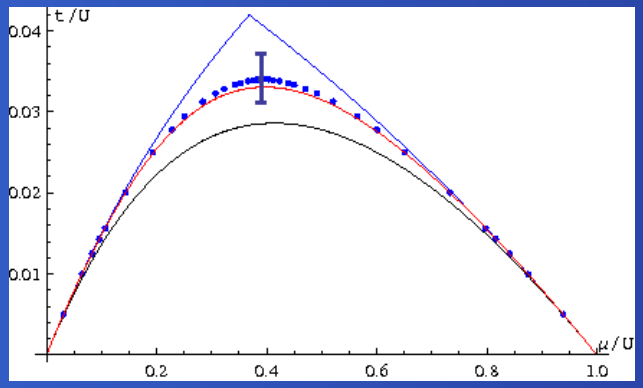
Easily summed in Fourier space:

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

- 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 effective potential approach.

7 - Results

Phase diagram for zero temperature:



Error bar: Extrapolated strong-coupling series.

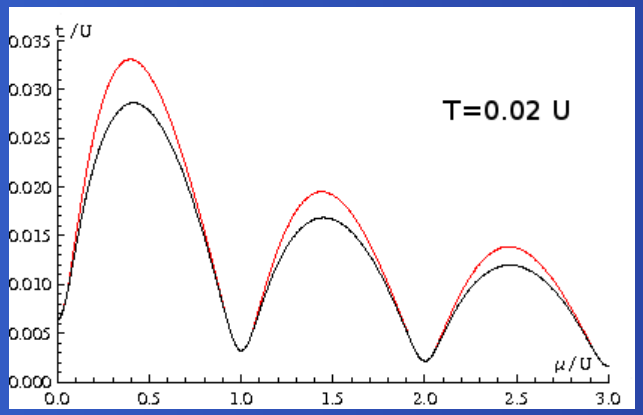
Black line: Mean-field.

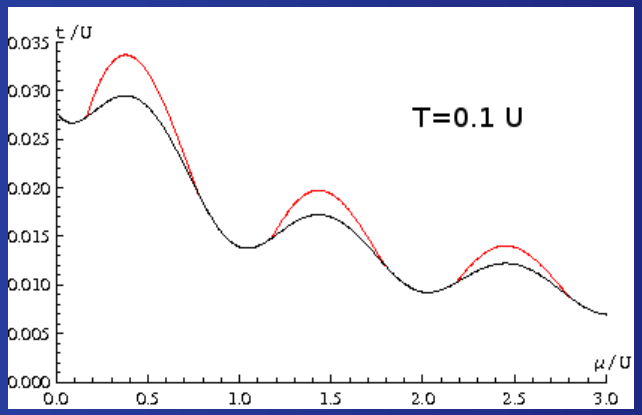
Blue line: 3rd strong-coupling order.

Red line: Effective potential (arXiv:0806.2812).

Blue dots: Monte-Carlo data.

Phase diagram for finite temperature:

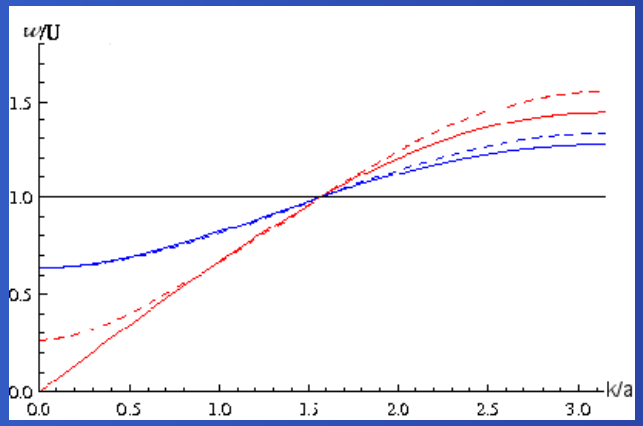




Black: First order (Mean field). Red: Second order (One-loop corrected)

7.1 - More Results

Excitation spectrum:



Solid black: $t = 0$.

Solid blue: $t = 0.017\,U$ (first order).

Dotted blue: $t = 0.017\,U$ (second order).

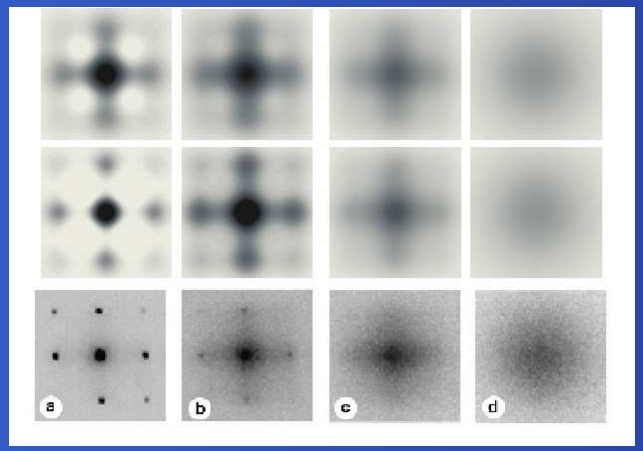
Solid red: $t = 0.029\,U$ (first order).

Dotted red: $t = 0.029\,U$ (second order).

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

7.2 - More Results

Time-of-flight pictures:

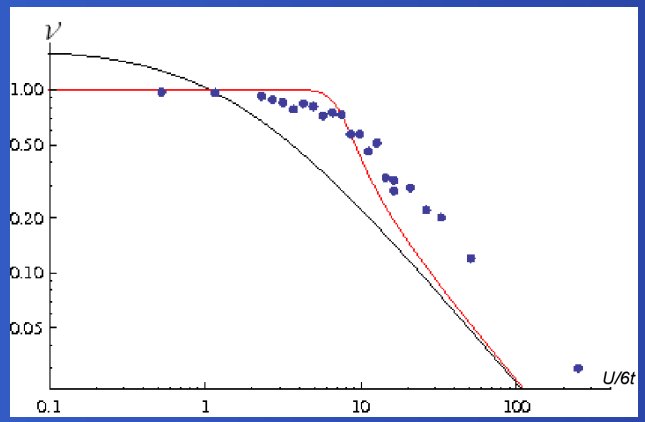


Top to bottom: First-order perturbation theory, Second-order perturbation theory, experiment.

Left to right: $V_0 = 8, 14, 18, 30 E_R$.

Time-of-flight pictures represent momentum distribution.

Visibility:



Measure for interference patterns in TOF pictures

$$\nu = \frac{n_{\max} - n_{\min}}{n_{\max} + n_{\min}}$$

Black: First-order perturbation theory

Red: Second-order perturbation theory

Dots: Experimental data (Bloch's group)

8 - Conclusions

- Monte-Carlo data are believed to be very precise
- Effective potential method gives a difference of 3% from the Monte-Carlo data at the lobe tip.
- Green's function approach allows the calculation of visibility and excitation spectrum. They are candidates for thermometer as they are measurable quantities.
- Four-point correlations – Hanbury-Brown-Twiss effect
- Dynamic quantum phase transition – Collapse and Revival