CARL VON OSSIETZKY universität OLDENBURG

Critical properties of the Bose-Hubbard model

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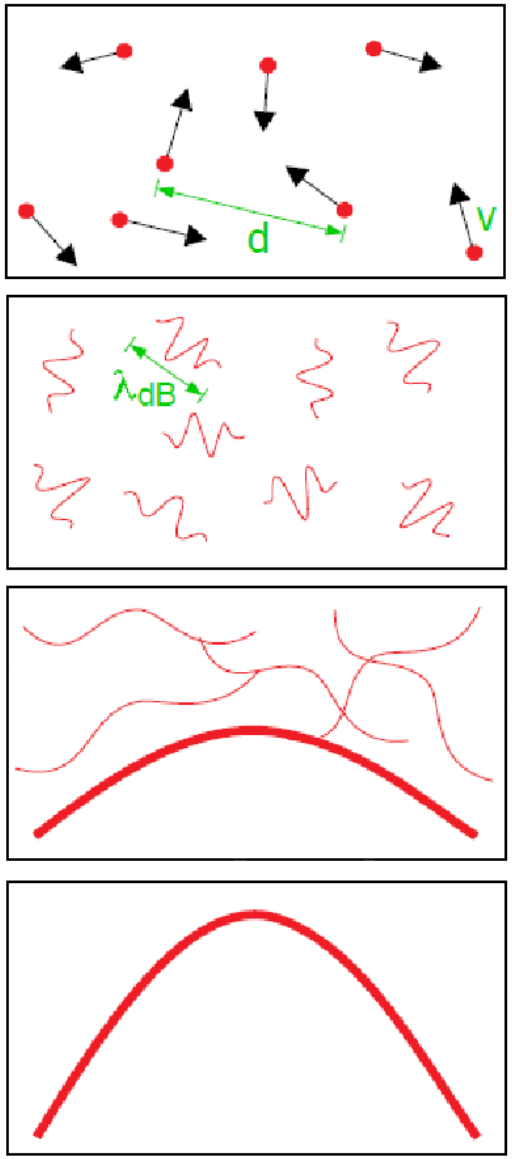
28.11.2012

Outline

Cold atoms

A. E. Leanhardt et al., Science **301**, 1513 (2003):
450 pK $= 450 \cdot 10^{-12}$ K $= 0.00000000045$ K

Cold atoms



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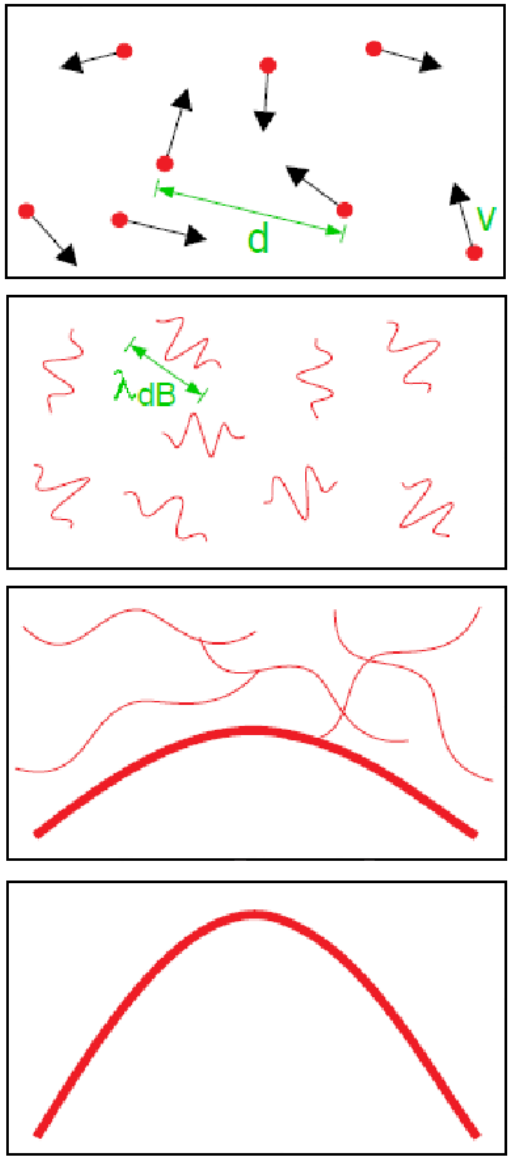

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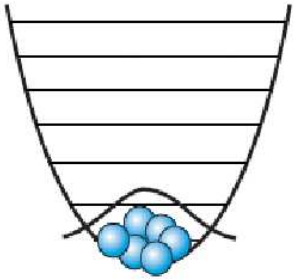
macroscopic occupation of the ground state for $T \to 0$



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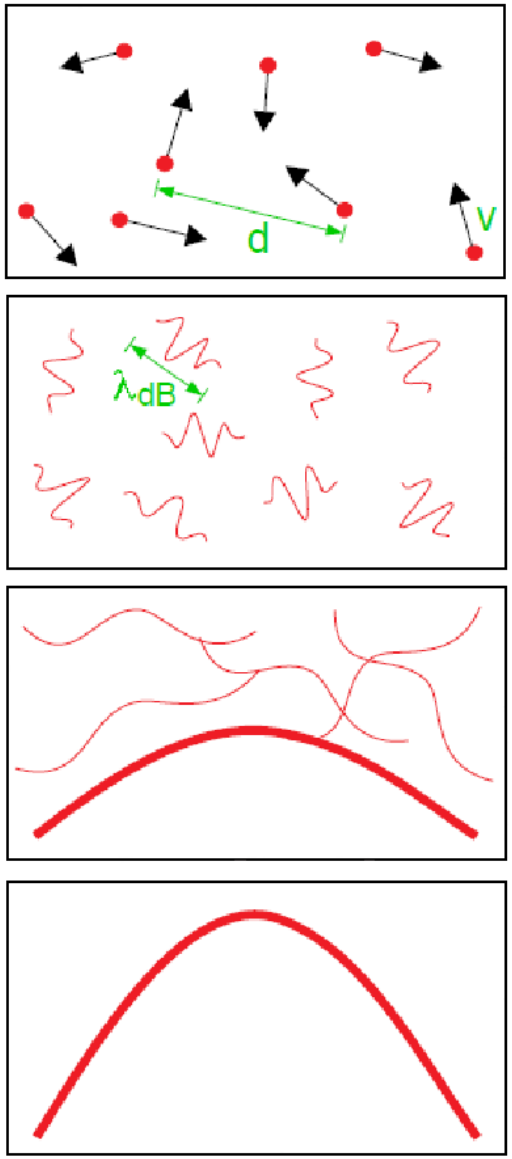

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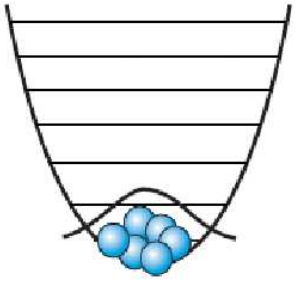
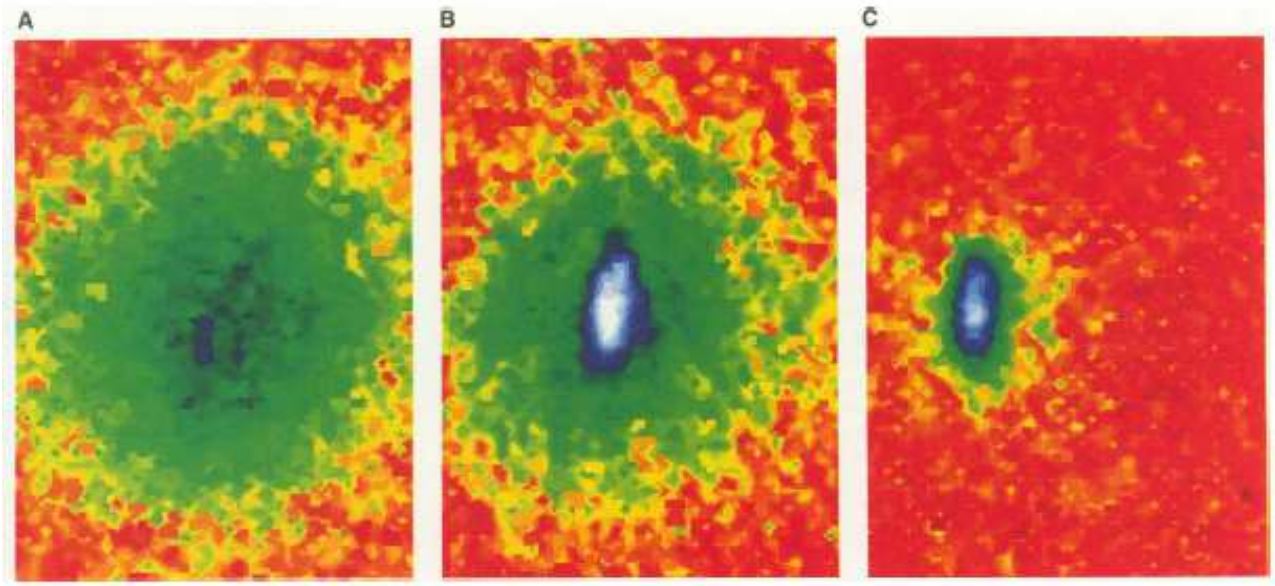


Phase space density: $n\lambda_{\text{dB}}^3 \approx 2.6$

Bose-Einstein condensation

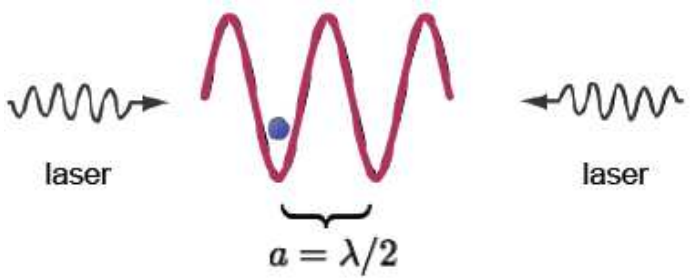


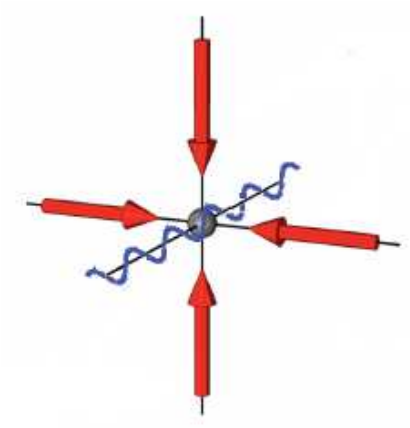
A: $1.7\ \mu$K, B: 170 nK, C: 20 nK

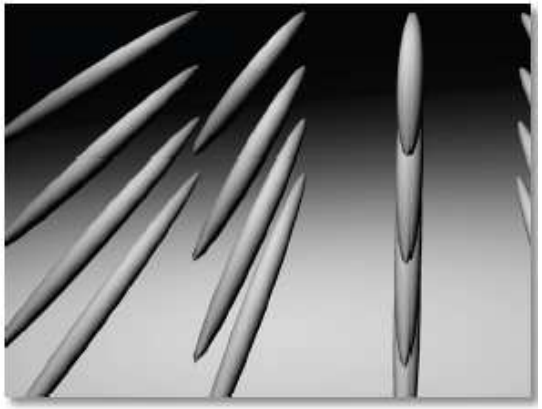
$$T < T_c \approx 180 \text{ nK}: \ n\lambda_{dB}^3 \approx 10^2 \gg 2.6$$

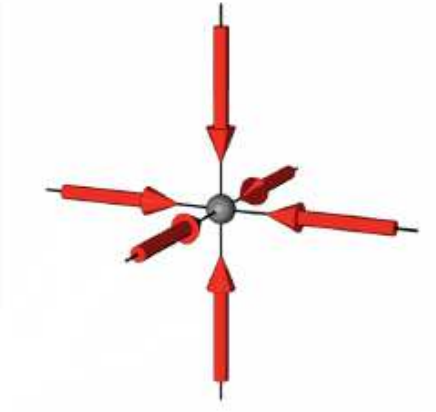
M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Science **269**, 198 (1995)

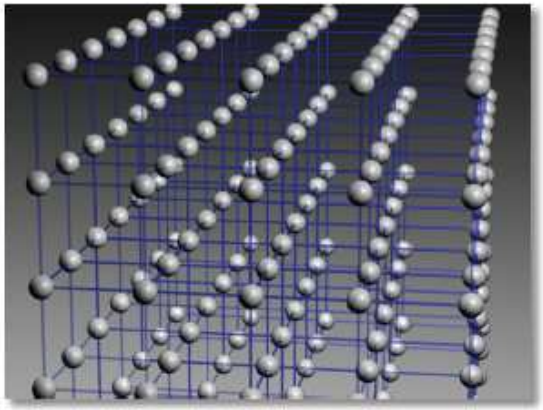
Optical lattices







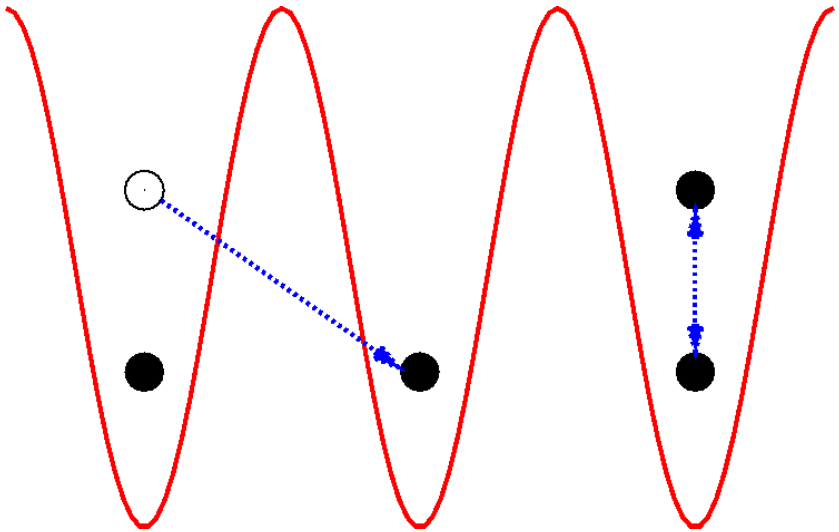




Outline

Bose-Hubbard model

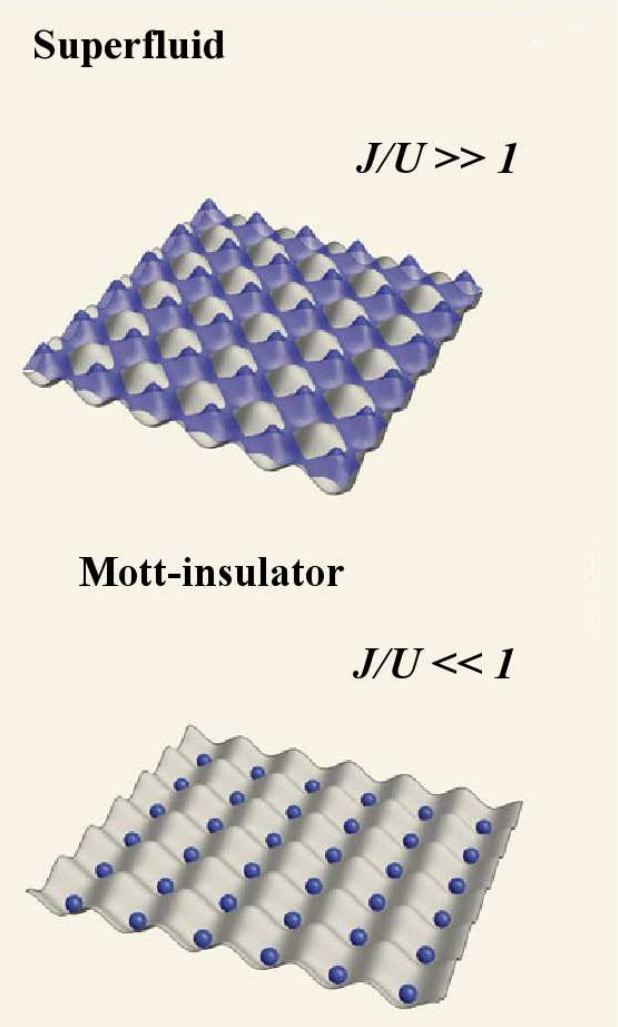
$$\hat{H}_{\mathrm{BH}} = \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) - J\sum_{\langle i,j\rangle} \hat{b}_i^\dagger \hat{b}_j - \mu \sum_i \hat{n}_i$$



$\hat{n}_i$	number of particles on lattice site i
$\hat{b}_i^\dagger / \hat{b}_i$	creation/annihilation of a particle on lattice site i
$\hat{b}_i^\dagger \hat{b}_j$	tunneling of a particle from site j to site i
$\langle i,j\rangle$	restriction of tunneling processes to nearest-neighbor tunneling

Quantum phase transition: Superfluid → Mott-insulator

$$\hat{H}_{\mathrm{BH}} = \frac{1}{2}\sum_{i=1}^{M}\hat{n}_i(\hat{n}_i - 1) - J/U\sum_{\langle i,j\rangle}\hat{b}_i^\dagger\hat{b}_j - \mu/U\sum_{i=1}^{M}\hat{n}_i$$



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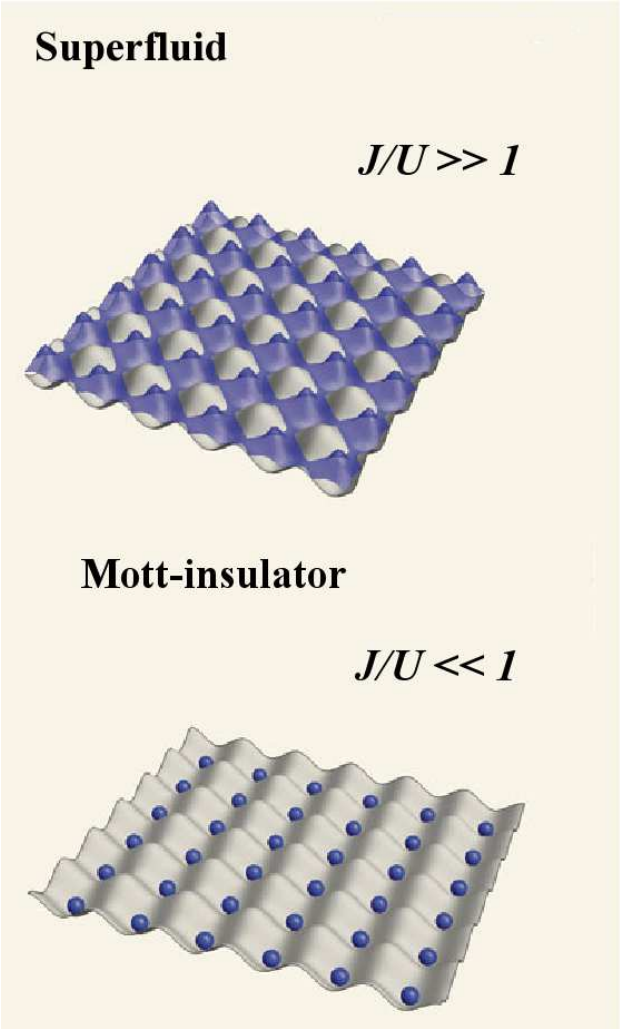
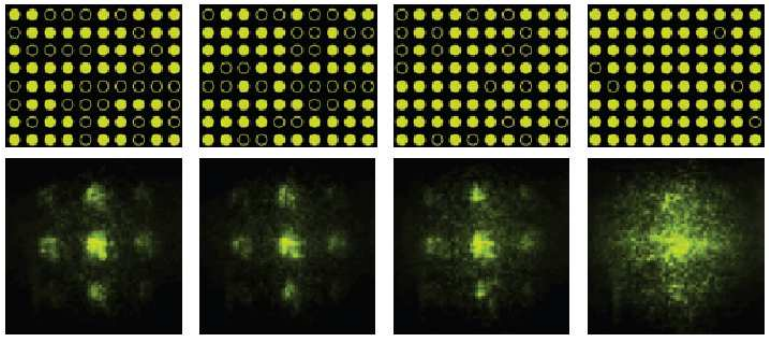


$J/U >> 1$ $J/U << 1$



W. S. Bakr et al., Science **329**, 547 (2010)

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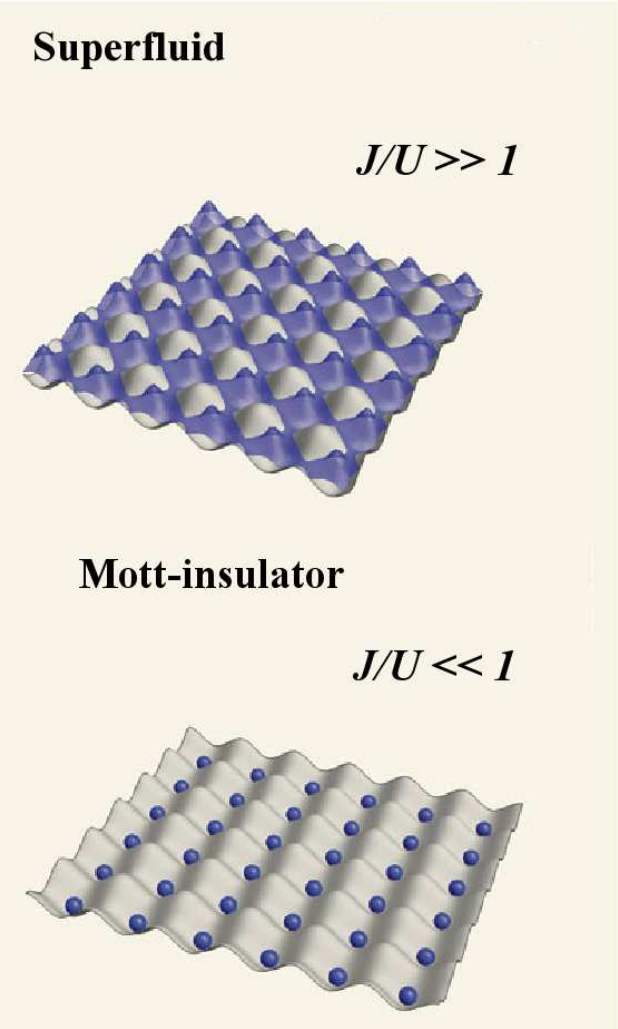

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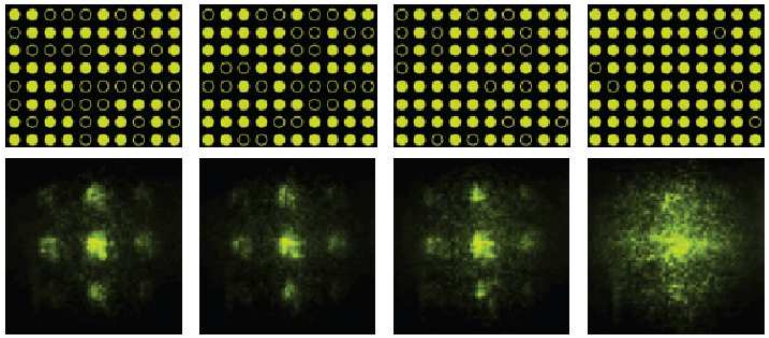

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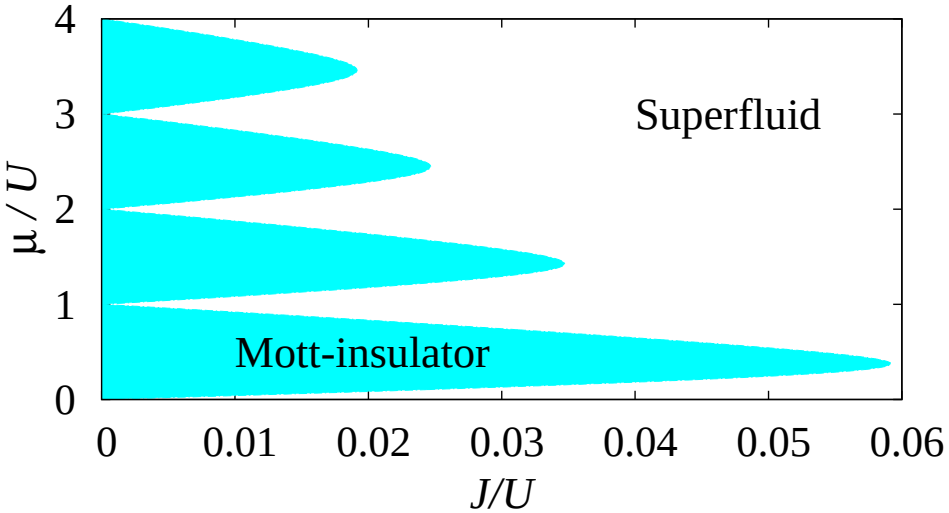

Method of the effective potential

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F. E. A. dos Santos and A. Pelster, Phys. Rev. A **79**, 013614 (2009).

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- Breaking of the $U(1)$-symmetry of the Bose-Hubbard model:

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- Expansion of the free energy in powers of J/U and $|\eta|^2$:

$$\mathcal{F}(J/U,\mu/U,|\eta|^2) = \langle \hat{H} \rangle = M \left(f_0(J/U,\mu/U) + \sum_{k=1}^{\infty} c_{2k}(J/U,\mu/U)|\eta|^{2k} \right)$$

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- Definition of the order parameter:

$$\psi = \frac{1}{M}\frac{\partial \mathcal{F}}{\partial \eta^*} = \langle \hat{b}_i \rangle \,, \quad \psi^* = \frac{1}{M}\frac{\partial \mathcal{F}}{\partial \eta} = \langle \hat{b}_i^\dagger \rangle$$

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Method of the effective potential

- Legendre-transformation of the free energy $\mathcal{F}$ to the effective potential Γ:

$$\Gamma = \mathcal{F} - M\left(\eta\,\psi^* + \eta^*\psi\right)$$

$$\frac{1}{M}\Gamma(J/U,\mu/U) = f_0 - \frac{1}{c_2}|\psi|^2 + \frac{c_4}{c_2^4}|\psi|^4 + \left(\frac{c_6}{c_2^6} - \frac{4c_4^2}{c_2^7}\right)|\psi|^6 + \mathcal{O}(|\psi|^8)$$
$$:= f_0 + a_2|\psi|^2 + a_4|\psi|^4 + a_6|\psi|^6 + \mathcal{O}(|\psi|^8)$$

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- Self-consistent determination of the order parameter ψ_0, ψ_0^*:

$$\frac{1}{M}\frac{\partial\Gamma}{\partial\psi^*} = -\eta\,, \quad \frac{1}{M}\frac{\partial\Gamma}{\partial\psi} = -\eta^* \quad \text{and} \quad \hat{H}_{|\eta=\eta^*=0} = \hat{H}_{\text{BH}}$$

$|\psi|^4$-approach: $\rho_{c,4} = |\psi_{0,4}|^2 = -\dfrac{a_2}{2a_4}$

$|\psi|^6$-approach: $\rho_{c,6} = |\psi_{0,6}|^2 = \dfrac{1}{3}\dfrac{-a_4 + \sqrt{a_4^2 - 3a_2a_6}}{a_6}$

Superfluid density

The superfluid part is defined by a vanishing viscosity.

Wave function of the condensate: $\Psi_0(\mathbf{x}) = \mathrm{e}^{\mathrm{i}\varphi(\mathbf{x})}|\psi_0|$ with $\varphi(\mathbf{x}) = \boldsymbol{\theta}\mathbf{x}/L$

$$\text{superfluid velocity: } \mathbf{v}_s = \langle \mathbf{p}/m \rangle = \frac{\hbar}{m}\,\nabla\varphi(\mathbf{x}) = (\hbar/m)\boldsymbol{\theta}/L$$

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The kinetic energy of the superfluid part is then given by

$$\mathcal{F}(\theta/L) - \mathcal{F}(0) = \frac{1}{2} m \rho_{\mathsf{sf}} M v_s^2 = \frac{1}{2} m \rho_{\mathsf{sf}} M \left(\frac{\hbar}{m}\right)^2 \left(\frac{\theta}{L}\right)^2 .$$

$$\rho_{\mathsf{sf}} = \lim_{\theta/L \to 0} \frac{1}{J/U} \left(\frac{L}{\theta}\right)^2 \frac{1}{M} \left[\Gamma(\theta/L) - \Gamma(0)\right] \quad \text{with} \quad \frac{\hbar^2}{2m} = J/U$$

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$$\text{twisted boundary conditions: } \hat{b}_i \to \mathrm{e}^{\mathrm{i}\mathbf{x}\frac{\boldsymbol{\theta}}{L}}\,\hat{b}_i \quad \text{and} \quad \hat{b}_i^\dagger \to \mathrm{e}^{-\mathrm{i}\mathbf{x}\frac{\boldsymbol{\theta}}{L}}\,\hat{b}_i^\dagger$$

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Kato's perturbation theory

$$\mathcal{F} = M\left(f_0 + \sum_{k=1}^{\infty} c_{2k}|\eta|^{2k}\right) = E_m + \sum_{n=1}^{\infty} \text{tr}\left[\sum_{\{\alpha_n\}} \hat{S}^{\alpha_1}\hat{V}\hat{S}^{\alpha_2}\ldots\hat{S}^{\alpha_n}\hat{V}\hat{S}^{\alpha_{n+1}}\right]$$

$$\hat{S}^{\alpha} = \begin{cases} -|m\rangle\langle m| & , \alpha = 0 \\ \sum_{\ell\neq m} \frac{|\ell\rangle\langle\ell|}{(E_m - E_\ell)^{\alpha}} & , \alpha > 0 \end{cases} \quad \text{and} \quad \sum_{k=1}^{n+1} \alpha_k = n - 1\ .$$

Ground state of the Mott-insulator: $|m\rangle = |g\rangle\ldots|g\rangle$, $g = N/M$ integer

T. Kato, Prog. Theor. Phys. **4**, 514 (1949).

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$\mathbf{n = 2}$: $\alpha_1 + \alpha_2 + \alpha_3 = 1 \rightarrow$ (1,0,0), (0,1,0), (0,0,1)

$$\text{tr}\left[S^1\hat{V}S^0\hat{V}S^0 + S^0\hat{V}S^0\hat{V}S^1 + S^0\hat{V}S^1\hat{V}S^0\right]$$

$$= \sum_j \left[\underbrace{\langle j|i\rangle\ldots\langle m|j\rangle + \langle j|m\rangle\ldots\langle i|j\rangle}_{=0}\right] + \sum_{\ell\neq m} \frac{\langle m|\hat{V}|\ell\rangle\langle\ell|\hat{V}|m\rangle}{E_m - E_\ell}$$

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Diagrammatic calculation of the ground state energy

$$E_m^{(2)} = \sum_{\ell \neq m} \frac{\langle m|\hat{V}|\ell\rangle\langle\ell|\hat{V}|m\rangle}{E_m - E_\ell}\,, \quad \hat{H}_{\mathsf{BH}} = \underbrace{\sum_i \left(\frac{1}{2}\hat{n}_i(\hat{n}_i - 1) - \mu/U\hat{n}_i\right)}_{\hat{H}_0} \underbrace{-J/U \sum_{\langle i,j\rangle} \hat{b}_i^\dagger \hat{b}_j}_{\hat{V}}$$

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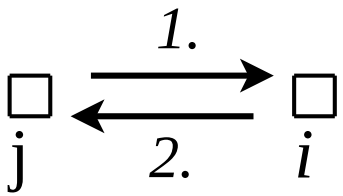

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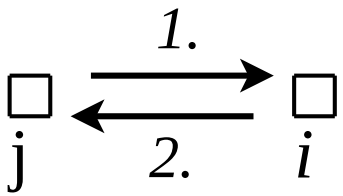

1. $\hat{V}|m\rangle = \hat{V}\left(|g\rangle_i|g\rangle_j\right) = -J/U\sqrt{g(g+1)}\left(|g+1\rangle_i|g-1\rangle_j\right) \ , \quad |\ell\rangle = |g{+}1\rangle_i|g{-}1\rangle_j$

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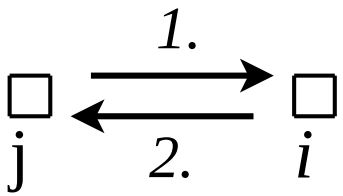

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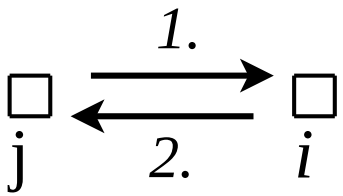
Diagrammatic calculation of the ground state energy

$$E_m^{(2)} = \sum_{\ell \neq m} \frac{\langle m|\hat{V}|\ell\rangle\langle\ell|\hat{V}|m\rangle}{E_m - E_\ell} \ , \quad \hat{H}_{\mathsf{BH}} = \underbrace{\sum_i \left(\frac{1}{2}\hat{n}_i(\hat{n}_i - 1) - \mu/U\hat{n}_i\right)}_{\hat{H}_0} \underbrace{-J/U \sum_{\langle i,j\rangle} \hat{b}_i^\dagger \hat{b}_j}_{\hat{V}}$$



1. $\hat{V}|m\rangle = \hat{V}\left(|g\rangle_i|g\rangle_j\right) = -J/U\sqrt{g(g+1)}\left(|g+1\rangle_i|g-1\rangle_j\right) \ , \quad |\ell\rangle = |g{+}1\rangle_i|g{-}1\rangle_j$

2. $\hat{V}|\ell\rangle = -J/U\sqrt{g(g+1)}\left(|g\rangle_i|g\rangle_j\right) = -J/U\sqrt{g(g+1)}|m\rangle$

$$E_\ell = E_m + 1$$

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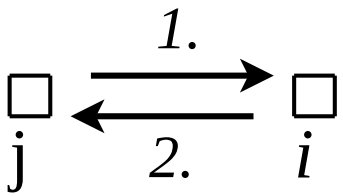

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$$E_\ell = E_m + 1$$

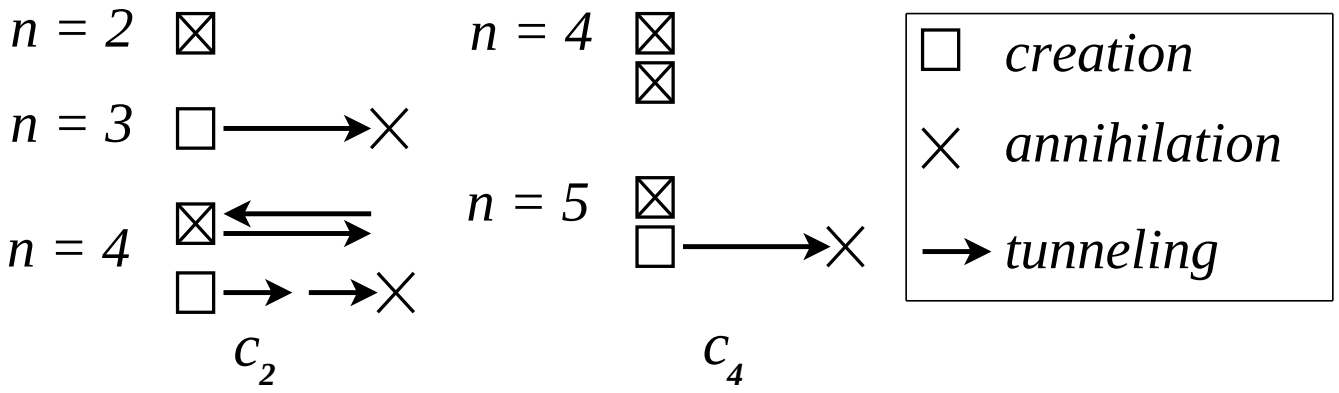
$$E_m^{(2)} = -wg(g+1)(J/U)^2$$

For example, $w = 2D$ for a D-dimensional square lattice

Diagrammatic calculation of c_{2k}

$$\hat{H}_0 = \sum_i \left(\frac{1}{2} \hat{n}_i (\hat{n}_i - 1) - \mu/U \hat{n}_i \right)$$

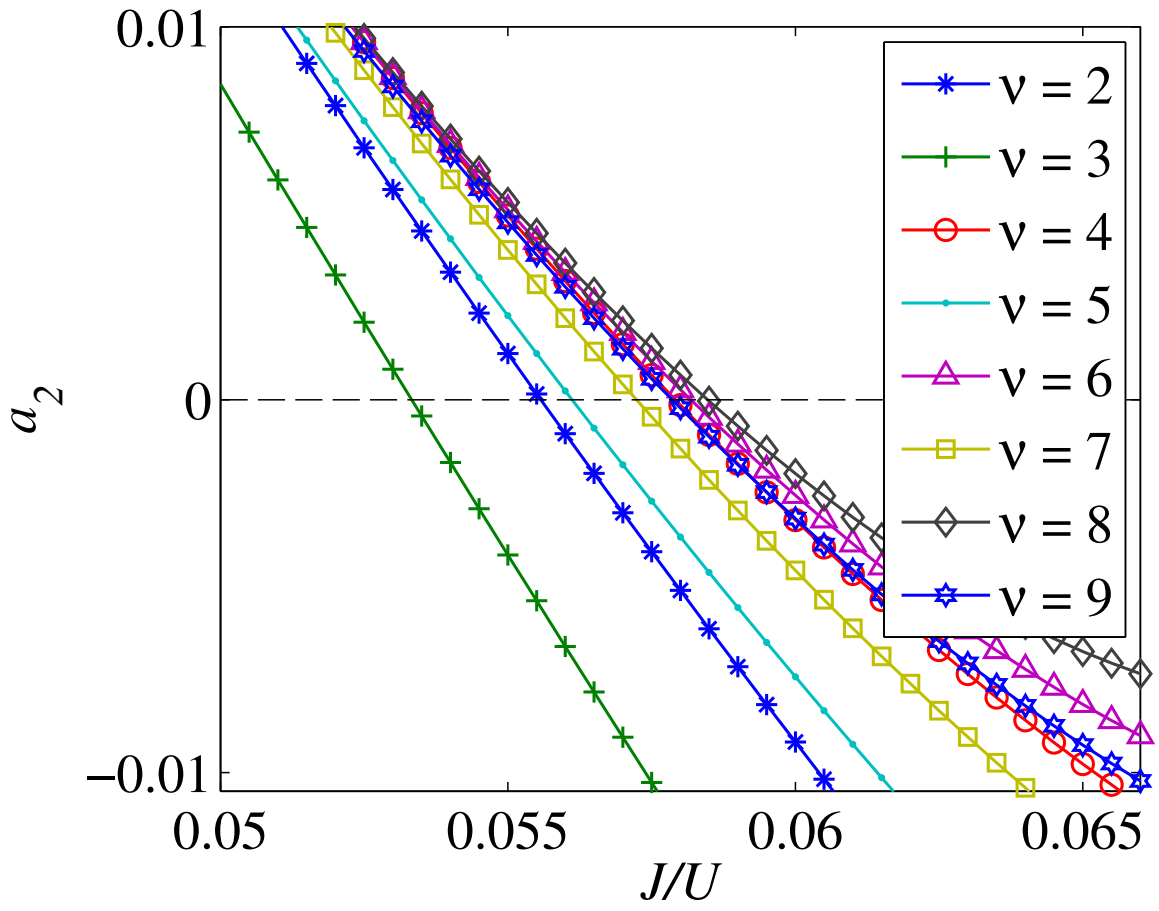
$$\hat{V} = -J/U \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \sum_i \left(\eta \, \hat{b}_i^\dagger + \eta^* \hat{b}_i \right)$$



A. Eckardt, Phys. Rev. B **79**, 195131 (2009).

Outline

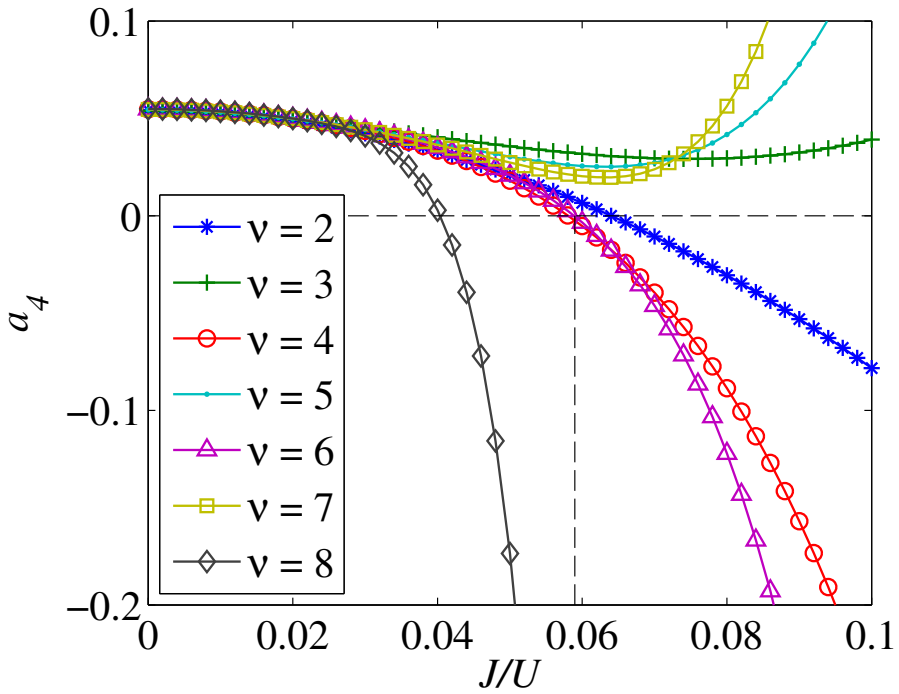
Coefficient a_2 of the effective potential for $D = 2$

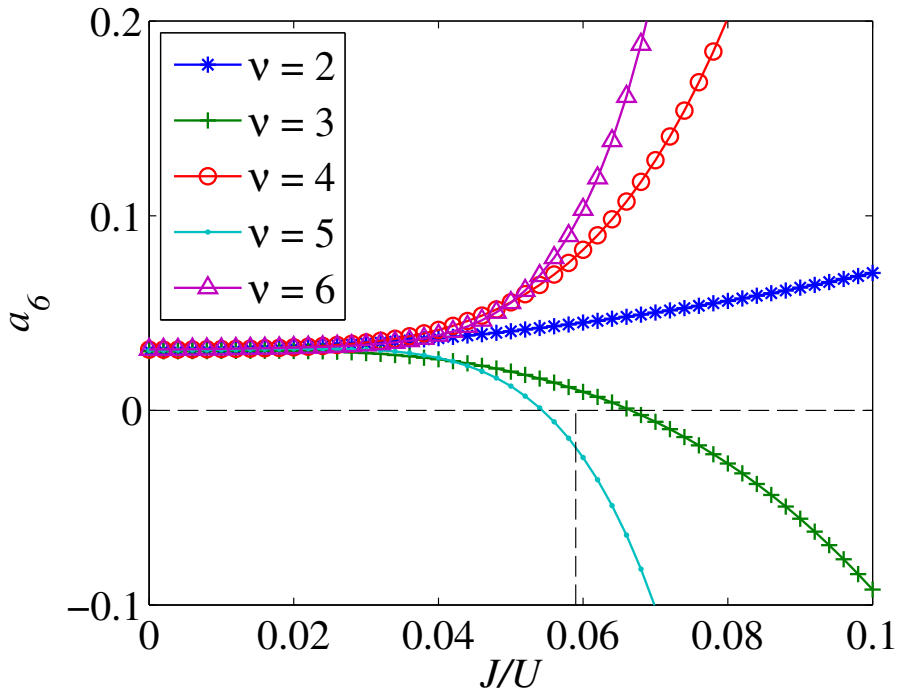


- Zeros where a_2 changes its sign

Coefficients a_4 & a_6 of the effective potential

$D = 2$:

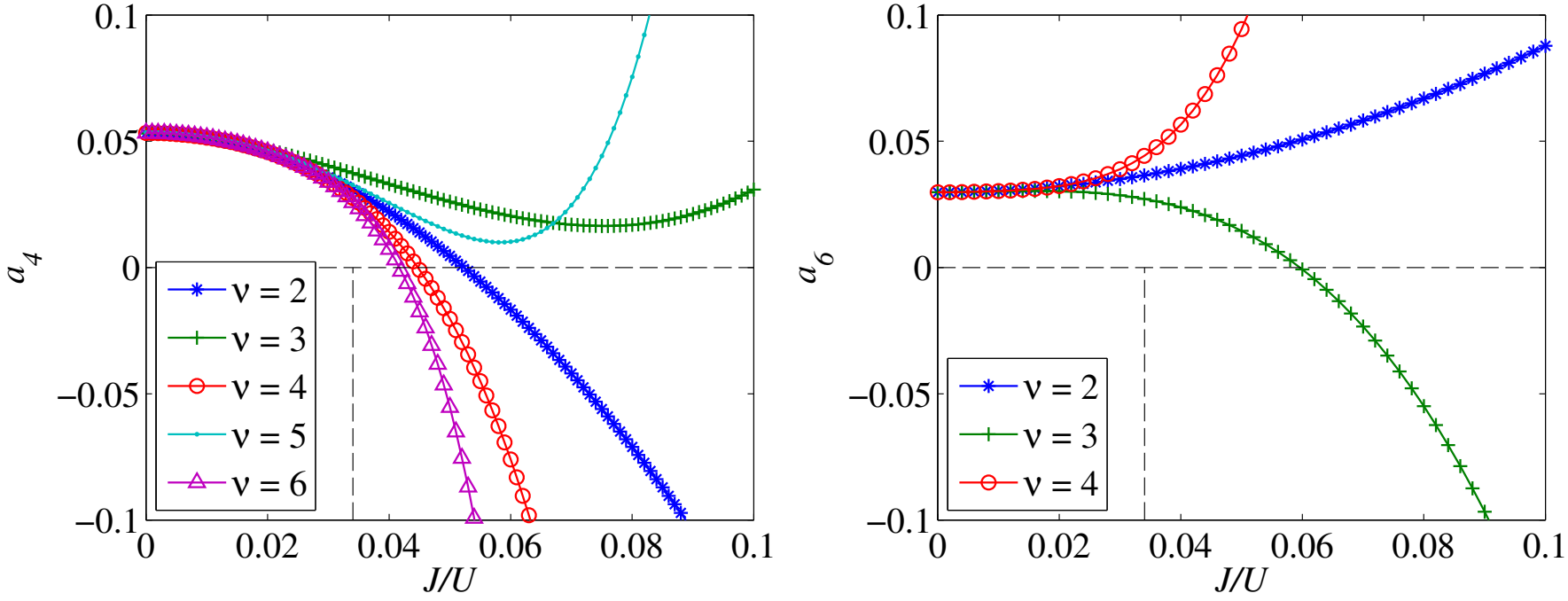




- Alternating behavior of even and odd orders
- Zeros in the direct vicinity of $(J/U)_c$

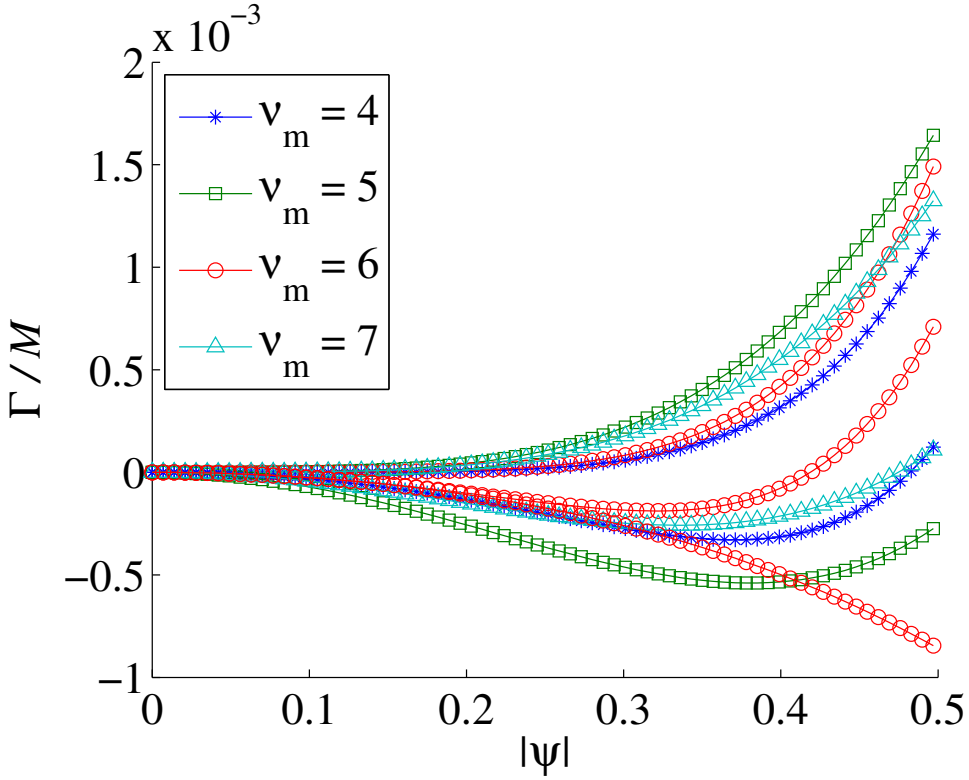
Coefficients a_4 & a_6 of the effective potential

$\underline{D = 3}$:



- Alternating behavior of even and odd orders
- Small range with $J/U > (J/U)_c$ where $a_4 > 0$ and $a_6 > 0$ for all orders

Effective potential for $D = 2$



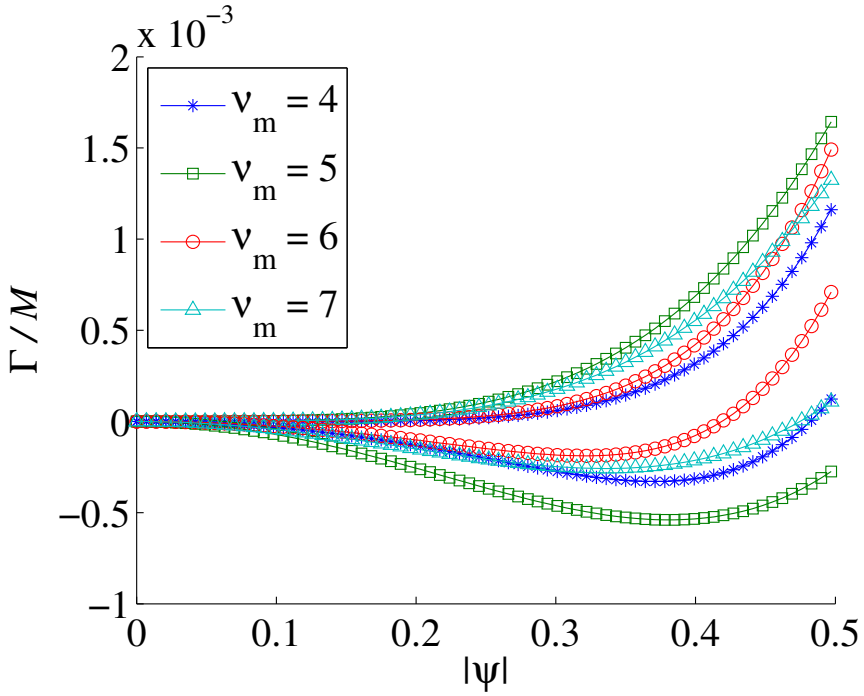
upper curves: $J/U = (J/U)_c \approx 0.059$
lower curves: $J/U = 0.06$

odd orders ($|\psi|^4$-approach): $\frac{1}{M}\Gamma = f_0 + a_2|\psi|^2 + a_4|\psi|^4$

even orders ($|\psi|^6$-approach): $\frac{1}{M}\Gamma = f_0 + a_2|\psi|^2 + a_4|\psi|^4 + a_6|\psi|^6$

Determination of the phase boundary

$$\frac{1}{M}\Gamma = f_0 + a_2|\psi|^2 + a_4|\psi|^4 + a_6|\psi|^6$$



Landau's argument
Phase transition happens if $a_2 = -1/c_2$ changes its sign.
alternatively: $a_2 = 0$

N. Teichmann, D.H., and M. Holthaus, PRB **79**, 100503(R) (2009).
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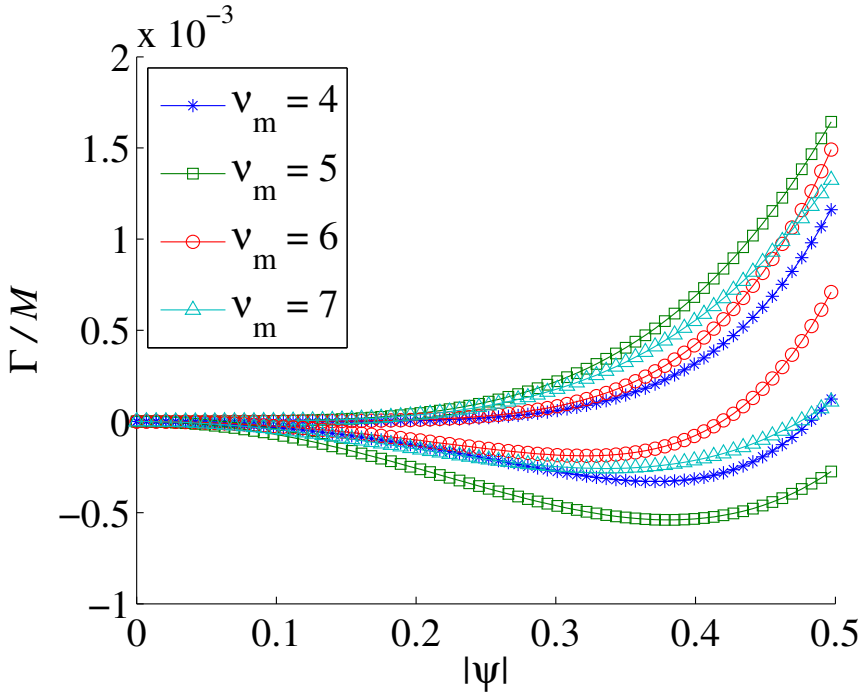

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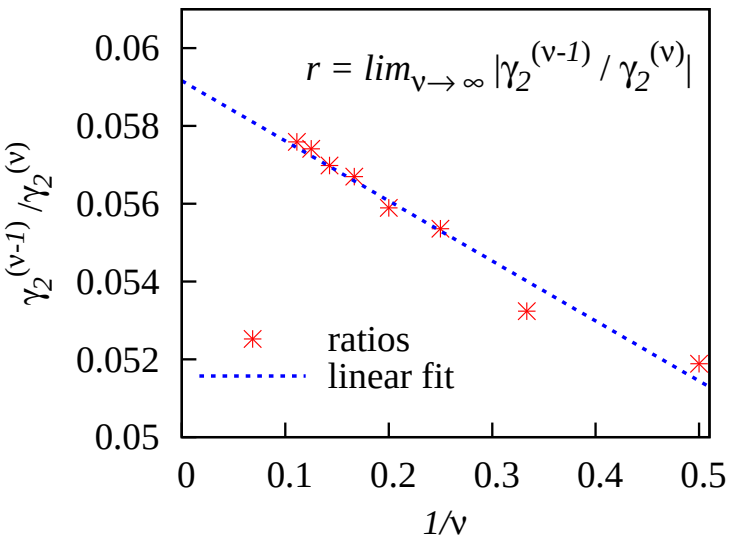
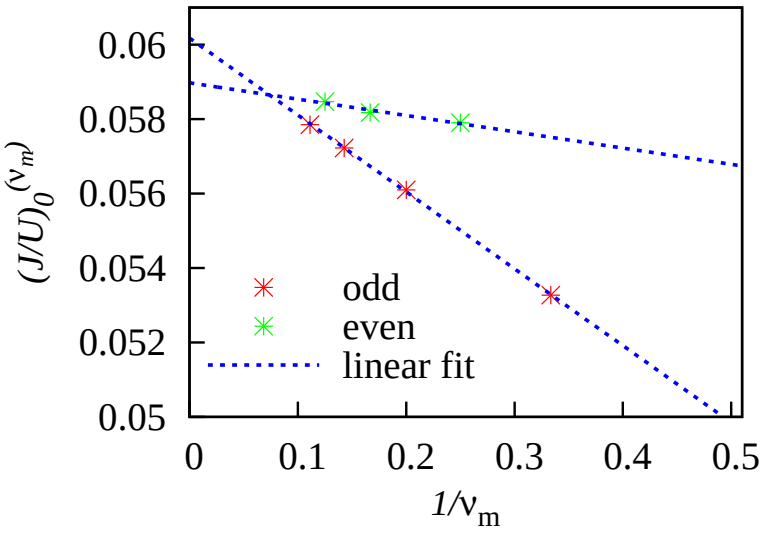
1. Radius of convergence r of $c_2 = \sum_\nu \gamma_2^{(\nu)} (J/U)^\nu$, $r = \lim_{\nu\to\infty} |\gamma_2^{(\nu-1)}/\gamma_2^{(\nu)}|$

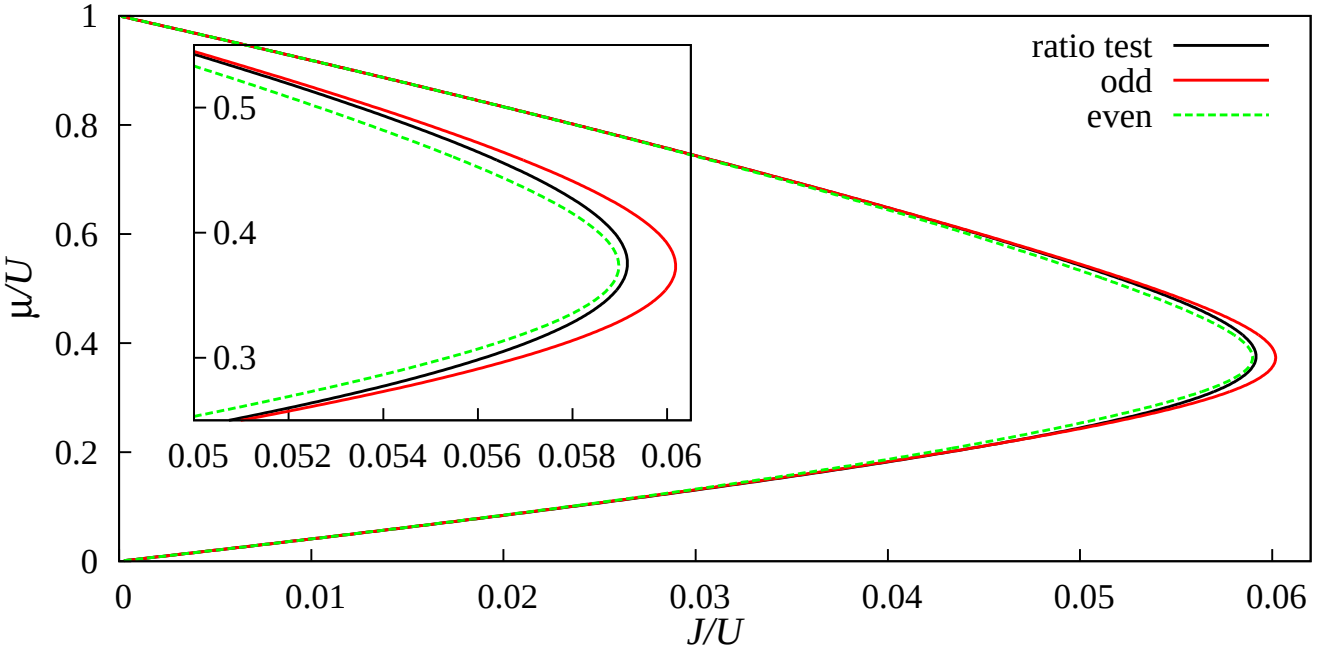
2. Zeros $(J/U)_0^{(\nu_m)}$ of the Taylor expansion of $-1/c_2$

N. Teichmann, D.H., and M. Holthaus, PRB **79**, 100503(R) (2009).
N. Teichmann, D.H., and M. Holthaus, EPL **91**, 10004 (2010).

Comparison of the phase boundaries







Particle density

Alternative determination of the phase boundary by setting

$$\langle \hat{n} \rangle = -\frac{1}{M} \left(\frac{\partial \Gamma}{\partial (\mu/U)} \right)_{\psi=\psi_0} \stackrel{!}{=} 1 \, .$$

Depends on a_2, a_4, a_6, whereas the condition via the zeros depends only on a_2.

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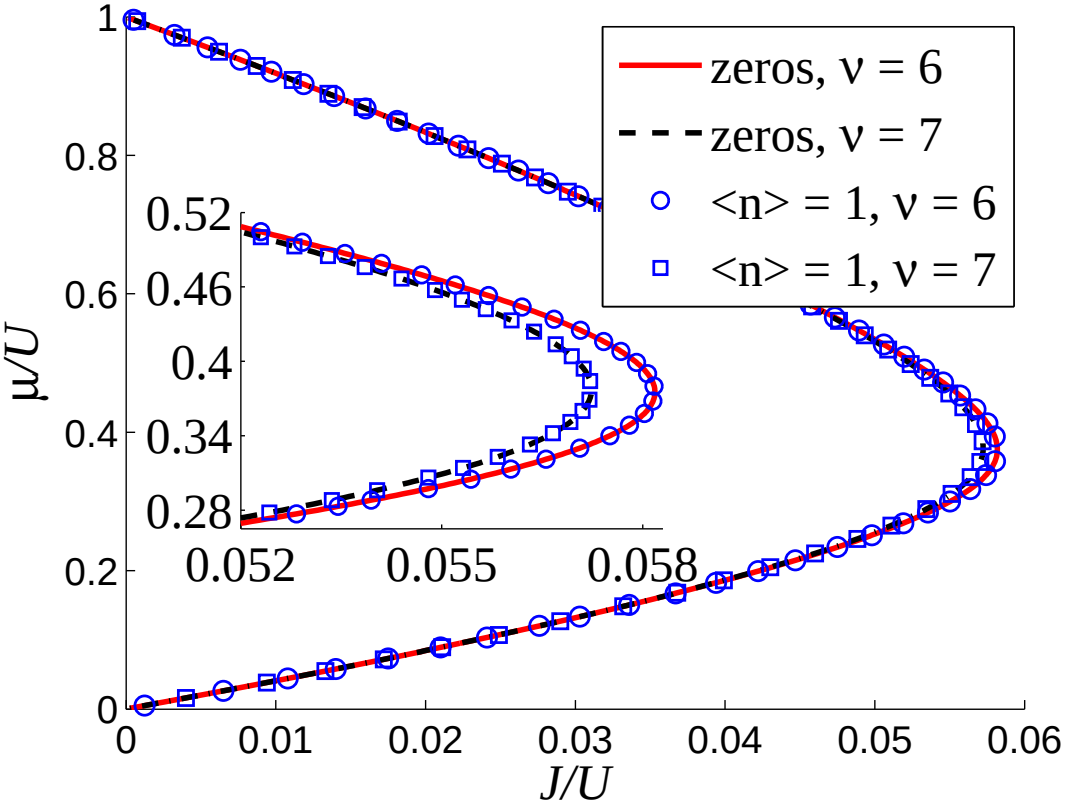
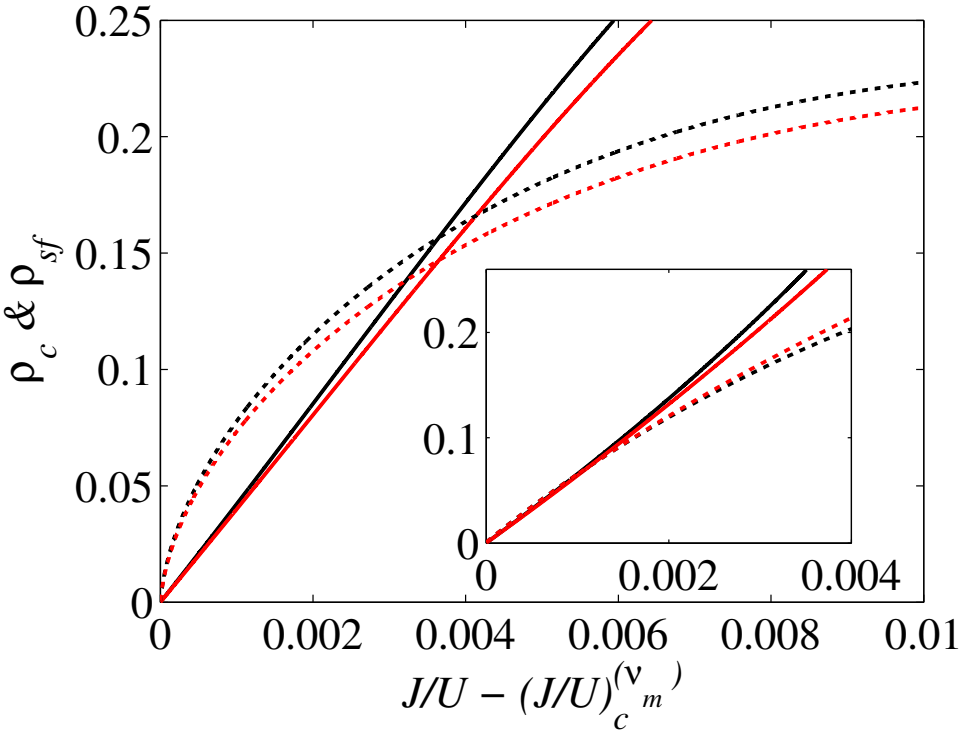


Outline

Comparison of the densities



black curves: ρ_{sf}
red curves: ρ_{c}
solid lines (odd orders): $|\psi|^4$-approach
dotted lines (even orders): $|\psi|^6$-approach

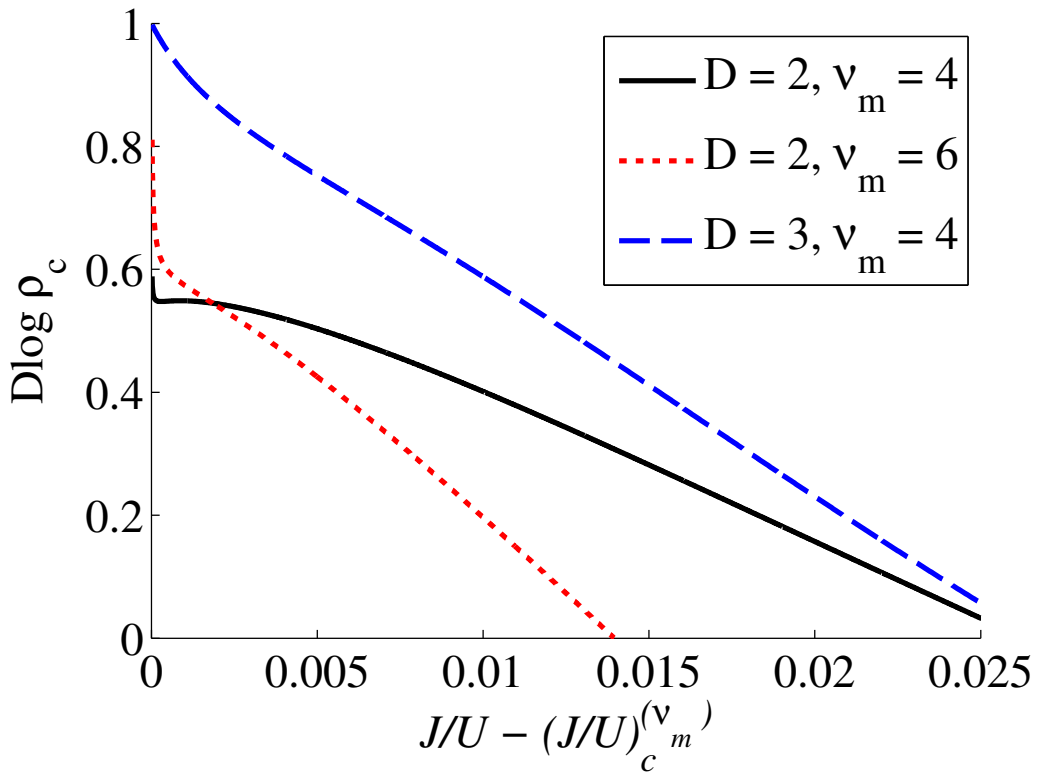
densities: $\rho \propto x^\sigma$, $x = J/U - (J/U)_c^{(\nu_m)}$

$D = 2 : \sigma \approx 2/3$ ($(D+1)$-dimensional XY-model)
$D = 3 : \sigma = 1$ (upper critical dimension, mean-field)

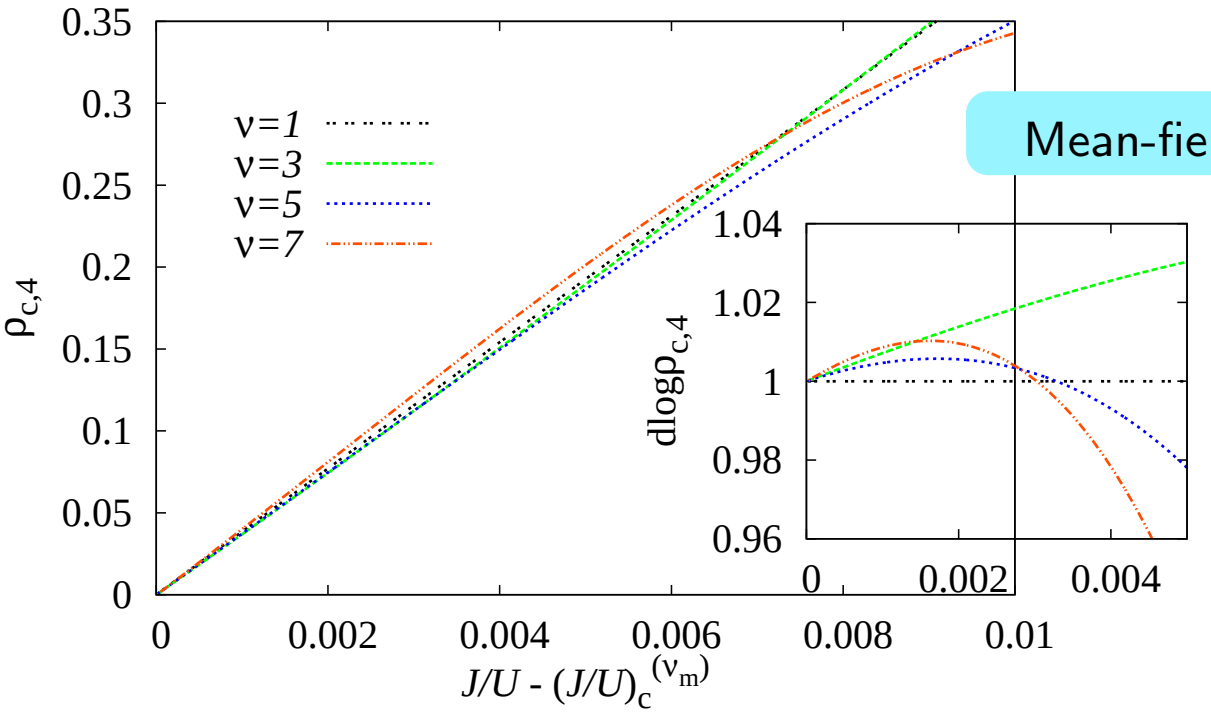
Critical exponents of the even orders via the $|\psi|^6$-approach

densities: $\rho \propto x^\sigma \rightarrow \mathrm{d}\log\rho := \lim_{x\to 0} \frac{\mathrm{d}\log\rho}{\mathrm{d}\log x} = \sigma$

$$D = 2 : \sigma \approx 2/3$$
$$D = 3 : \sigma = 1$$



Critical exponents of the odd orders via the $|\psi|^4$-approach



Mean-field results for odd orders

H. Kleinert, Phys. Rev. D **57**, 2264 (1998).

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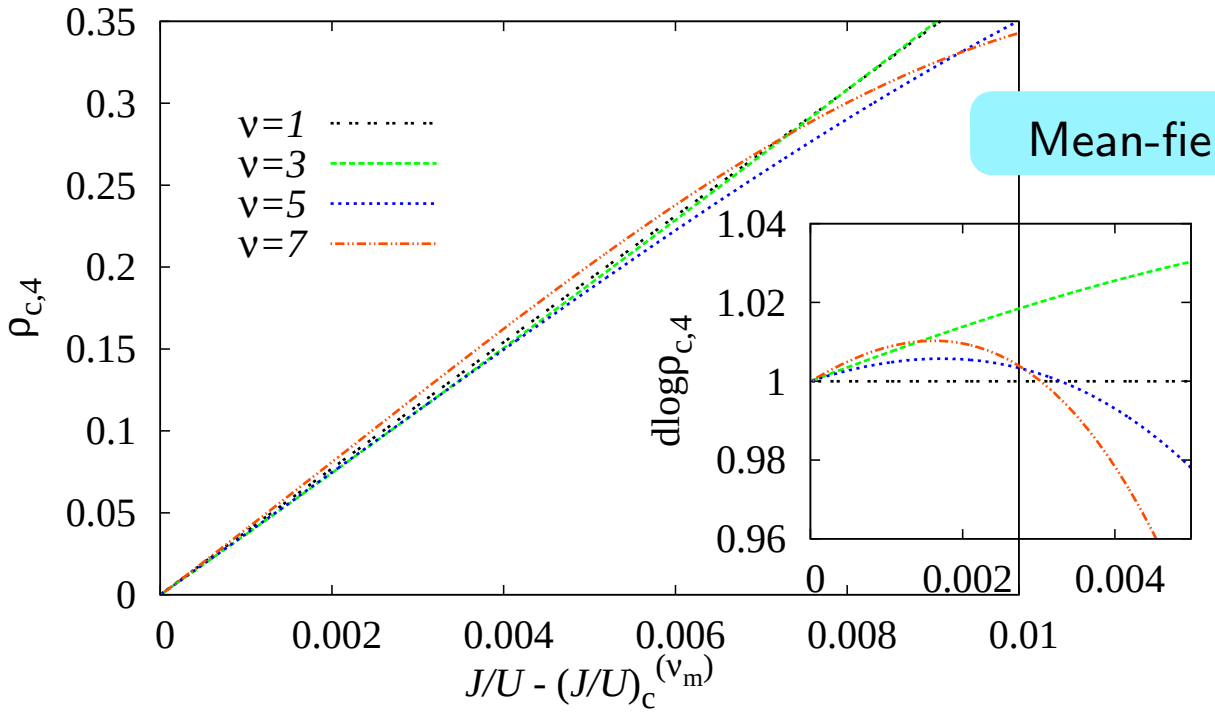

Mean-field results for odd orders

Variational perturbation theory

$$f(g) = \sum_{i=0}^{\infty} a_i g^i \underset{g\to\infty}{\overset{VPT}{\longmapsto}} f^{\infty}(g) = g^{p/q} \sum_{i=0}^{\infty} b_i (g^{-2/q})^i$$

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Variational perturbation theory

$$\rho(g) = \sum_{i=0}^{\infty} a_i g^i \qquad \rho^{\infty}(g) = g^{p/q} \sum_{i=0}^{\infty} b_i (g^{-2/q})^i$$

$$h(g) = \mathrm{d} \log \rho(g) \ , \quad h^{\infty}(g',p',q') = p/q$$

$$p' = 0 \quad \text{because} \quad p/q = g^{p'/q'} b_0 + g^{p'/q'} b_1 g^{-2/q'}$$

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$$\mathrm{d}\log h(g) = F_1(g)\ , \quad F_1^{\infty}(g'',q') = 0$$

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Condensate density	Superfluid density	H. Kleinert
$q' = 2.4615$	$\theta/L \to 0 \quad : q' = 2.7818$	$q' \approx 2.52$

Critical exponents for $D = 2$

$|\psi|^4$-approach

ν_m	$\beta_c^{(\nu_m)}$	$\upsilon^{(\nu_m)}$
3	1.3774	1.4291
5	1.0206	1.0836
7	1.0334	1.0221

$|\psi|^6$-approach

ν_m	$\beta_c^{(\nu_m)}$	$\upsilon^{(\nu_m)}$ (θ/L)	
		0.001	0.01
4	0.5715	0.6446	0.6463
6	0.6153	0.6525	0.6541

	β_c	υ
$|\psi|^4$-approach	0.7028	0.6784
$|\psi|^6$-approach	0.7029	0.6681
M. Campostrini et al. ($3D$ XY-model)	0.6970(2)	0.67155(27)

M. Campostrini et al., Phys. Rev. B **63**, 214503 (2001)

Conclusion

- Precise determination of the phase boundary
- Qualitatively correct densities
- Remarkably precise determination of critical exponents

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Thank you for your attention.