Bose-Hubbard Model (BHM) at Finite Temperature

- a Layman's (Sebastian Schmidt) proposal -

pick up Diploma work at FU-Berlin with

PD Dr. Axel Pelster (Uni Duisburg-Essen)

~ Diagrammatic techniques, high-order, resummation theory

Prof. Hagen Kleinert (FU-Berlin)

~*Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, World Scientific, 4th edition

Ultracold Atoms – What's Hot?

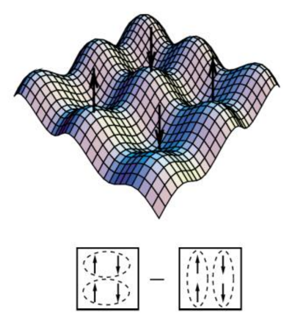
<u>Quantum Information (QI)</u>

Atom Chip

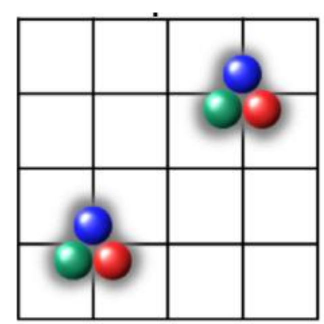
Schmiedmayer (TU Vienna)

<u>Quantum Simulation (QS)</u>

High Tc



QCD



W. Hofstetter (Frankfurt U)

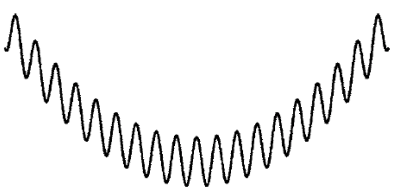
Experiment+Theory

Need to know what I simulate

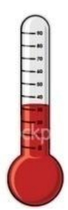
↓

Quantitative agreement between Theory and Experiment

Challenges:



Trapping homogeneous —LDA→ inhomogeneous



Thermometer?

Finite T Superfluid density, Mott phase ???

Numerical vs Analytical

DMRG, DMFT, NRG,...

Monte-Carlo (1D, 2D, 3D)

BUT:
- Large-scale/flexibility?
- Fermions: Monte-Carlo sign
- "Cassandra" Problem

Mean-Field Theory
+ Quantum Corrections

Perturbation Theory
+ Resummation

BHM=Benchmark

Disorder, Geometries
Flavour, Spinor,....
Fermi-Hubbard

Outline

- **Formulation of the Problem**

  Bose Hubbard Model

  Finite-T Phase Diagram

- **Status Quo**

  Bogoliubov

  Strong Coupling

  Decoupling

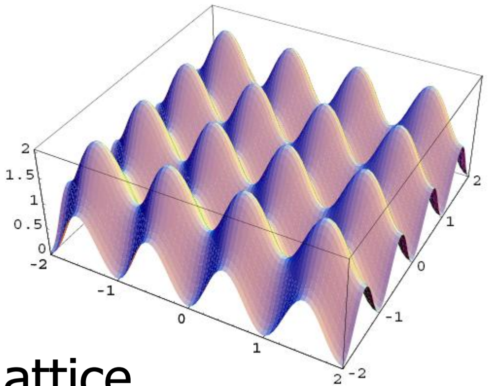
  Monte-Carlo as a Benchmark

- **Proposal:**

  “From Above”

  “From Below”

Bose-Hubbard Model



Lattice

$$V_{\text{ext}} = V_0 \sum_{i=1}^{3} \sin^2(\frac{\pi}{a} x_i)$$

$$\hat{H} = \int d^3x \left\{ \hat{\psi}^\dagger(\mathbf{x}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}} - \mu \right] \hat{\psi}(\mathbf{x}) + \frac{2\pi a_{\text{BB}}\hbar^2}{m} \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{x}) \right\}$$

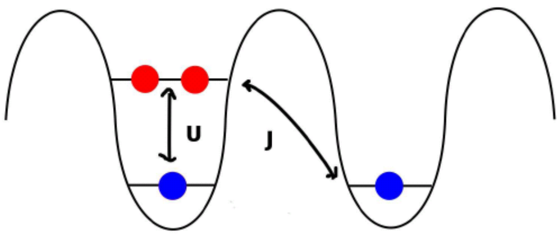
Pseudopotential

Wannier Representation

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

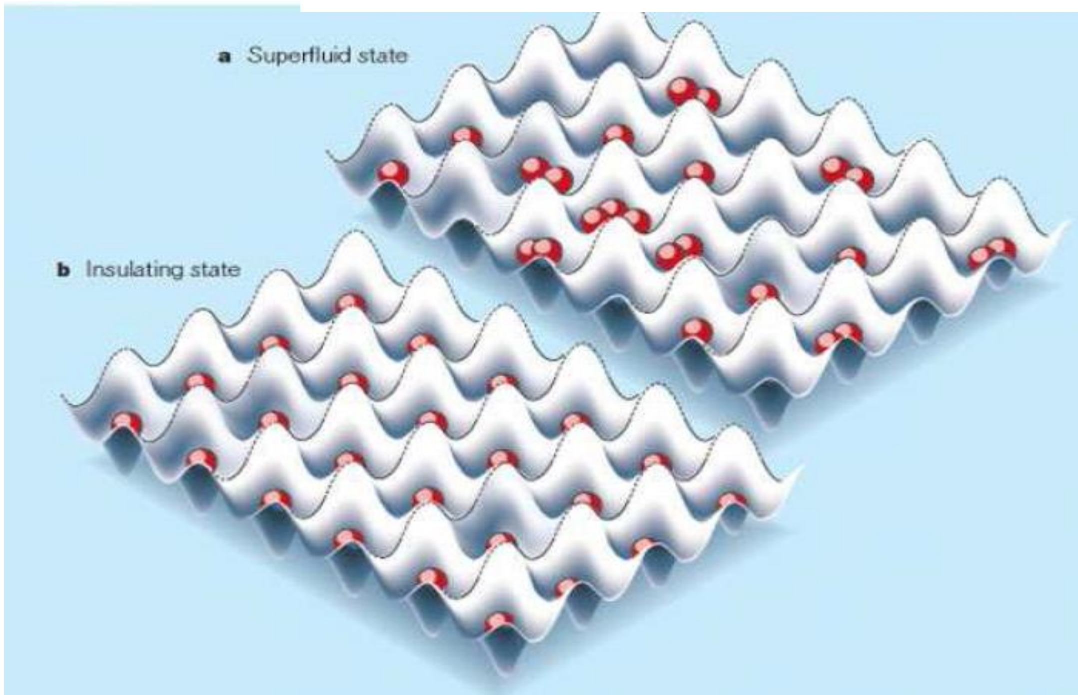
- Lowest band
- N.N. hopping

$$\hat{H}_{\text{BHM}} = -J \sum_{<i,j>} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i - \mu \sum_i \hat{a}_i^\dagger \hat{a}_i$$



Superfluid-Mott Insulator

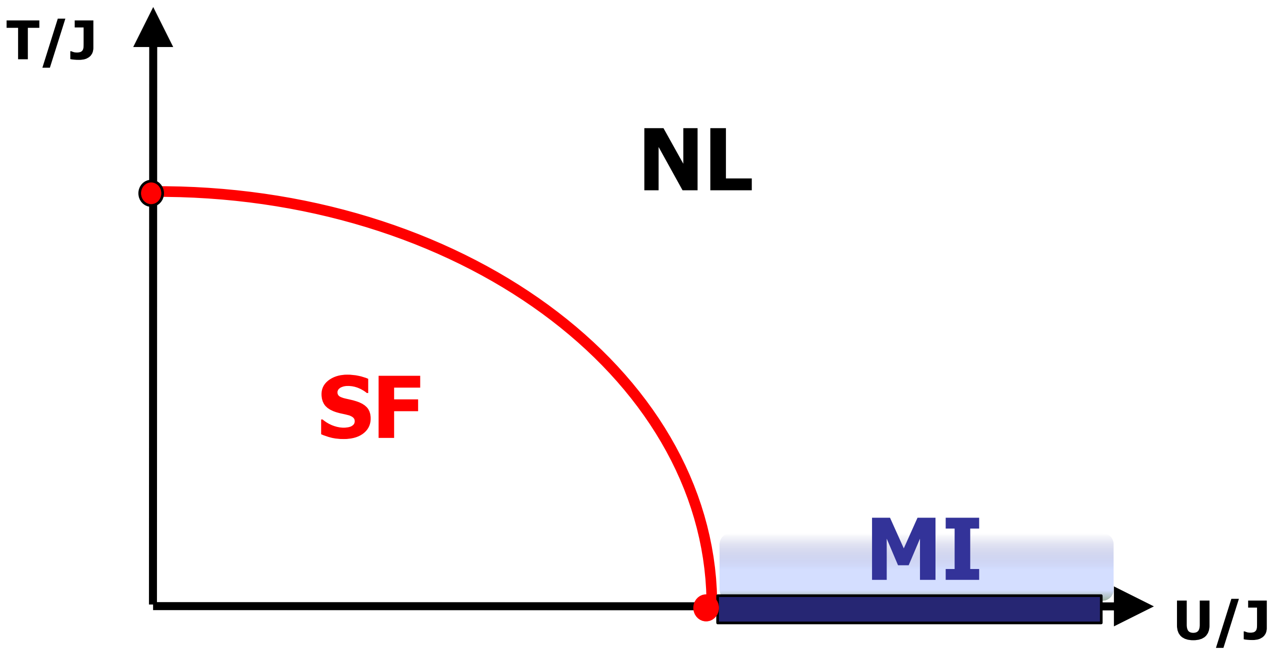
Superfluid $|\Psi_N\rangle(U=0) = \frac{1}{\sqrt{N!}}\left(\frac{1}{\sqrt{N_L}}\sum_{\mathbf{R}} \hat{a}^\dagger_{\mathbf{R}}\right)^N |0\rangle$



Mott Insulator $|\Psi_{N=N_L}\rangle(J=0) = \left(\prod_{\mathbf{R}} \hat{a}^\dagger_{\mathbf{R}}\right)|0\rangle$

Finite-T Phase Diagram

Formulation of the Problem



What is T_c (U_c) in 3D ?

Bogoliubov

<u>Momentum Representation</u>

$$c_i = \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}} a_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_i}$$

Cubic lattice

$$H = \sum_{\mathbf{k}} (-\overline{\epsilon_{\mathbf{k}}} - \mu) a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}$$

$$\overline{\epsilon_{\mathbf{k}}} = 2t\Sigma_{j=1}^{d} \cos(k_j a)$$

$$+ \frac{1}{2} \frac{U}{N_s} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \sum_{\mathbf{k}''} \sum_{\mathbf{k}'''} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}'}^{\dagger} a_{\mathbf{k}''} a_{\mathbf{k}'''} \delta_{\mathbf{k}+\mathbf{k}',\mathbf{k}''+\mathbf{k}'''}$$

<u>Ansatz:</u>

$$a_{\mathbf{0}} \to \sqrt{N_0} + a_{\mathbf{0}}$$

$$n_0 = N_0 / N_s$$

Expand up to quadratic fluctuations & Minimize wrt. condensate density

Linear order: $\mu = U n_0 - z t$

Quadratic order:

$$H^{\text{eff}} = -\frac{1}{2} U n_0 N_0 - \frac{1}{2} \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} + U n_0) + \frac{1}{2} \sum_{\mathbf{k}} (a_{\mathbf{k}}^{\dagger}, a_{-\mathbf{k}}) \times \begin{bmatrix} \epsilon_{\mathbf{k}} + U n_0 & U n_0 \\ U n_0 & \epsilon_{\mathbf{k}} + U n_0 \end{bmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^{\dagger} \end{pmatrix},$$

Bogoliubov

Quadratic fluctuations

$$H^{\text{eff}} = -\frac{1}{2}Un_0N_0 - \frac{1}{2}\sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} + Un_0) + \frac{1}{2}\sum_{\mathbf{k}} (a_{\mathbf{k}}^{\dagger}, a_{-\mathbf{k}}) \times \begin{bmatrix} \epsilon_{\mathbf{k}} + Un_0 & Un_0 \\ Un_0 & \epsilon_{\mathbf{k}} + Un_0 \end{bmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^{\dagger} \end{pmatrix},$$

⇩

Bogoliubov Transformation

$$\begin{pmatrix} b_{\mathbf{k}} \\ b_{-\mathbf{k}}^{\dagger} \end{pmatrix} = \begin{bmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ v_{\mathbf{k}}^{*} & u_{\mathbf{k}}^{*} \end{bmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^{\dagger} \end{pmatrix} \equiv \mathbf{B} \begin{pmatrix} a_{\mathbf{k}} \\ a_{-\mathbf{k}}^{\dagger} \end{pmatrix}$$

⇩

$$H^{\text{eff}} = -\frac{1}{2}Un_0N_0 + \frac{1}{2}\sum_{\mathbf{k}} [\hbar\omega_{\mathbf{k}} - (\epsilon_{\mathbf{k}} + Un_0)] + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}},$$

Quasiparticle Energies $\hbar\omega_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + 2Un_0\epsilon_{\mathbf{k}}}$

No Gap Sound Modes !

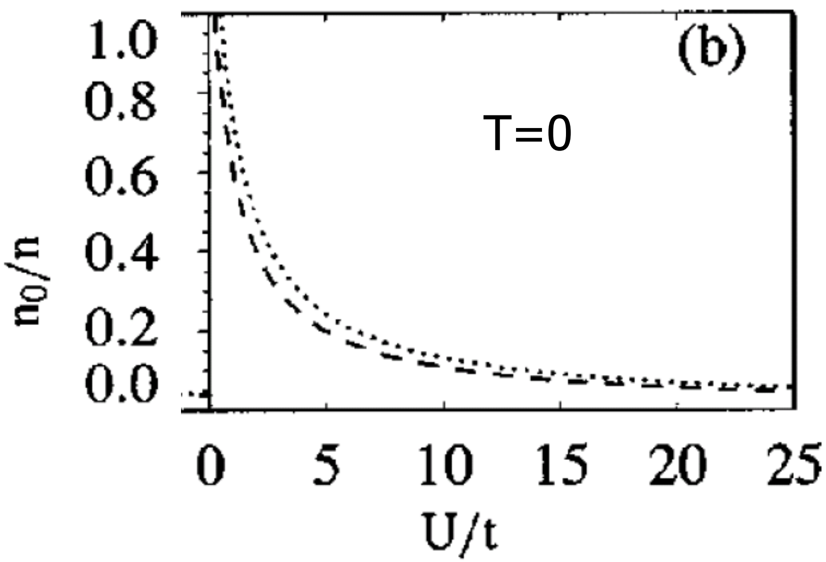
Bogoliubov

Phase transition via Condensate fraction

$$n = \frac{1}{N_s} \sum_{\mathbf{k}} \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle_{H^{\text{eff}}}$$

$$n = n_0 + \frac{1}{N_s} \sum_{\mathbf{k} \neq 0} \left(\frac{\epsilon_{\mathbf{k}} + U n_0}{\hbar \omega_{\mathbf{k}}} \frac{1}{e^{\beta \hbar \omega_{\mathbf{k}}} - 1} + \frac{\epsilon_{\mathbf{k}} + U n_0 - \hbar \omega_{\mathbf{k}}}{2 \hbar \omega_{\mathbf{k}}} \right)$$

van Oosten et al.,
PRA 63, 053601 (2001)



$n = 0.5$ (dashed line)

$n = 1.0$ (dotted line)

NO Phase transition at T=0 !

BUT Good description of the condensate at weak coupling

Decoupling

Ansatz in site-basis

$$\hat{a}_i = \langle \hat{a}_i \rangle + \delta \hat{a}_i$$

with $\psi = \langle \hat{a}_j \rangle$

consistent mean-field theory

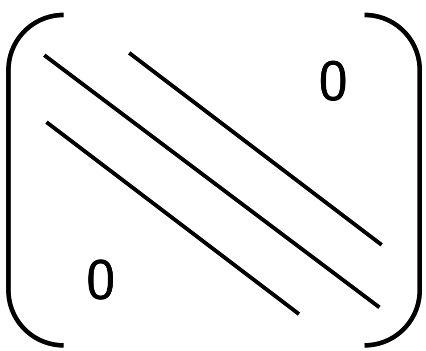
$$\hat{a}_i^\dagger \hat{a}_j \approx \langle \hat{a}_i^\dagger \rangle \hat{a}_j + \langle \hat{a}_j \rangle \hat{a}_i^\dagger - \langle \hat{a}_i^\dagger \rangle \langle \hat{a}_j \rangle$$

Mean field Hamiltonian

$$\hat{H}_{\mathrm{MF}} = \sum_i -Jz(\psi^* \hat{a}_i + \psi \hat{a}_i^\dagger - |\psi|^2) + \frac{U}{2}\hat{n}_i(\hat{n}_i - 1) - \mu \hat{n}_i$$

Diagonalization in site-basis

$$\hat{H}_{\mathrm{MF}} =$$



K. Sheshardi et al., EPL 22, 257 (1993)

Perturbation Theory

$$\hat{H}_0 = -Jz\psi^2 + \frac{U}{2}\hat{n}(\hat{n} - 1) - \mu \hat{n}$$

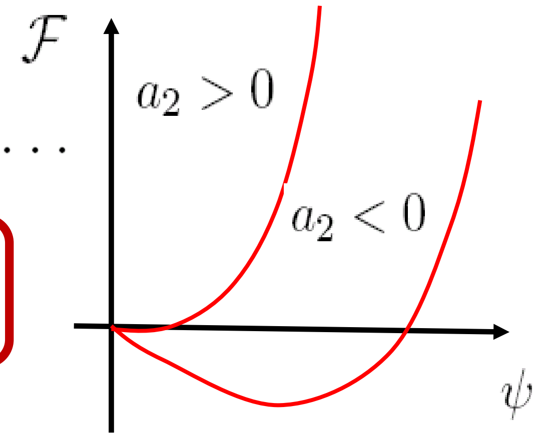
$$\hat{V} = -Jz\psi(\hat{a} + \hat{a}^\dagger)$$

van Oosten et al., PRA 63, 053601 (2001)

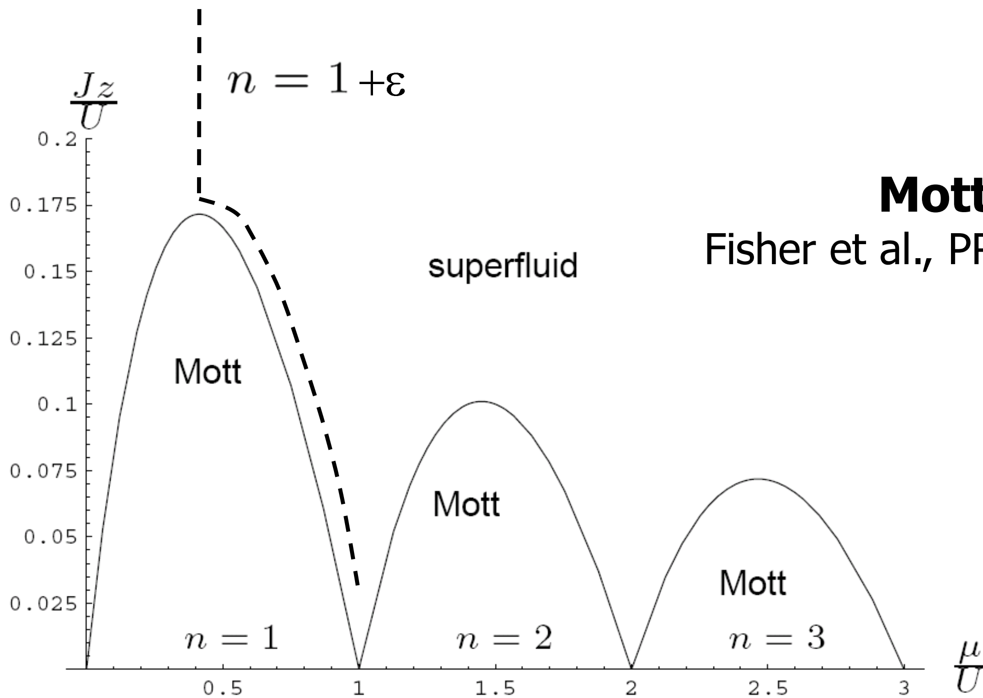
Decoupling

Phase transition ~Landau expansion

$$\mathcal{F}(\psi^*,\psi) = a_0 + a_2|\psi|^2 + a_4|\psi|^4 + \ldots$$



$$a_2 = Jz + J^2 z^2 \frac{U+\mu}{(\mu - Un)[U(n-1)-\mu]} \overset{!}{=} 0$$



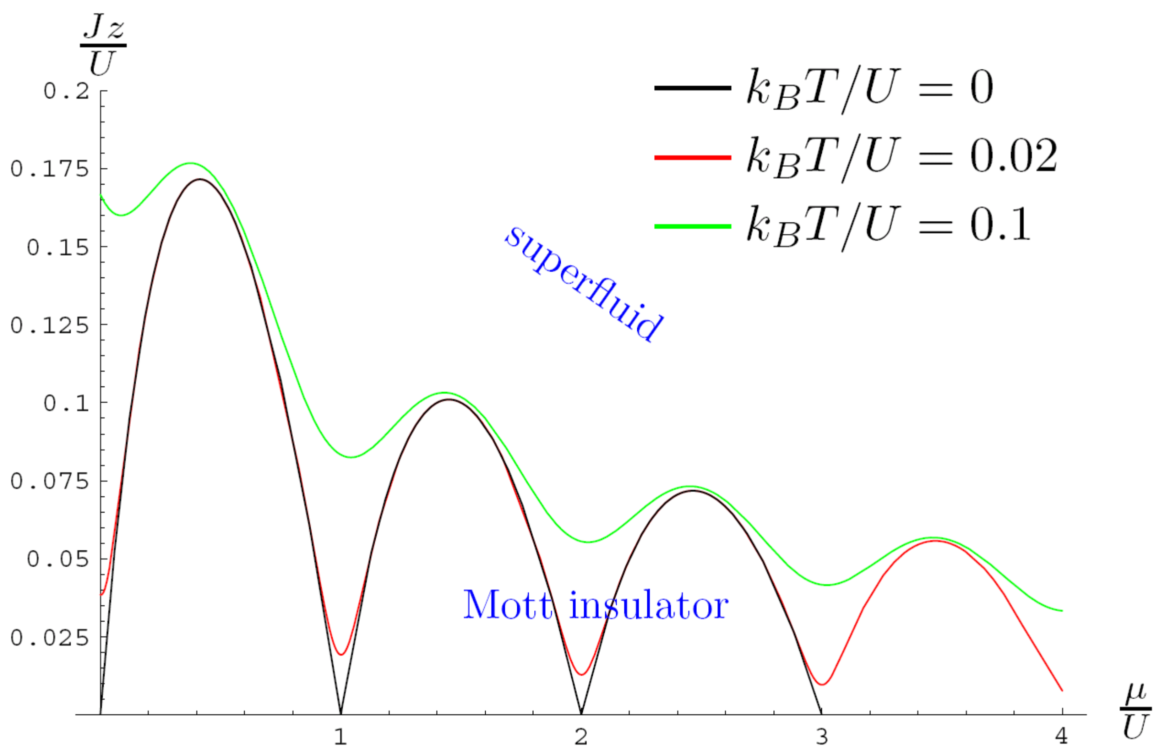
Mott Lobes

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

Alexander Hoffmann,
Diploma Thesis, FU-Berlin (2006)

Decoupling

Finite Temperature



Alexander Hoffmann,
Diploma Thesis, FU-Berlin (2007)

Strong Coupling

$$\hat{H}_{\mathrm{BHM}} = \underbrace{-J \sum_{<i,j>} \hat{a}_i^\dagger \hat{a}_j}_{V} + \underbrace{\frac{U}{2}\sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i - \mu \sum_i \hat{a}_i^\dagger \hat{a}_i}_{H_0}$$

Unperturbed system is site-diagonal!

$$E_G^{(0)}(N = N_s) = \frac{U}{2}\sum_i n_i\,(n_i - 1) - \mu_i \sum_i n_i$$

$$|\psi_G^{(0)}(N = N_s)\rangle = \left(\prod_i \hat{a}_i^\dagger\right)|0\rangle$$

→ Rayleigh-Schroedinger perturbation theory

Particle (hole) excitation gap

$$\Delta_\pm = E_G(N = N_s) - E_G(N = N_s \pm 1)$$

$\Delta_\pm^{(0)} = U$ Phase Transition: $\Delta_\pm = 0$

3rd order +linear extrapolation

Freericks & Monien, PRB 53, 2691 (1996)

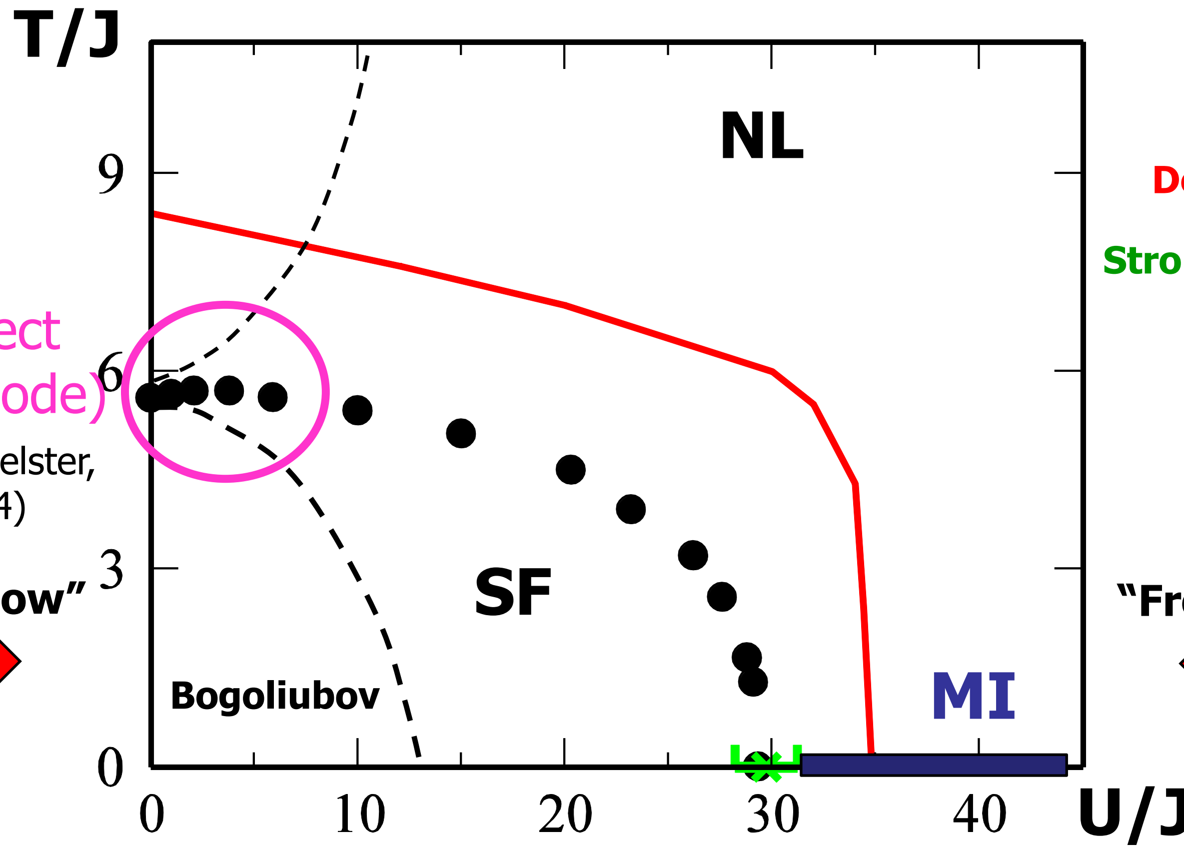
$$(U/J)_c = 29.7 \quad (3D, n = 1)$$

Status Quo

Reentrant
classical field effect
(zero Matsubara mode)

H.Kleinert, S.Schmidt, A.Pelster,
PRL 93, 160402 (2004)

"From Below"



Decoupling

Strong-Coupling

"From Above"

● Monte-Carlo Data

B. Capogrosso-Sansone, N. V. Prokofev, B. V. Svistunov, PRB 75, 134302 (2007)

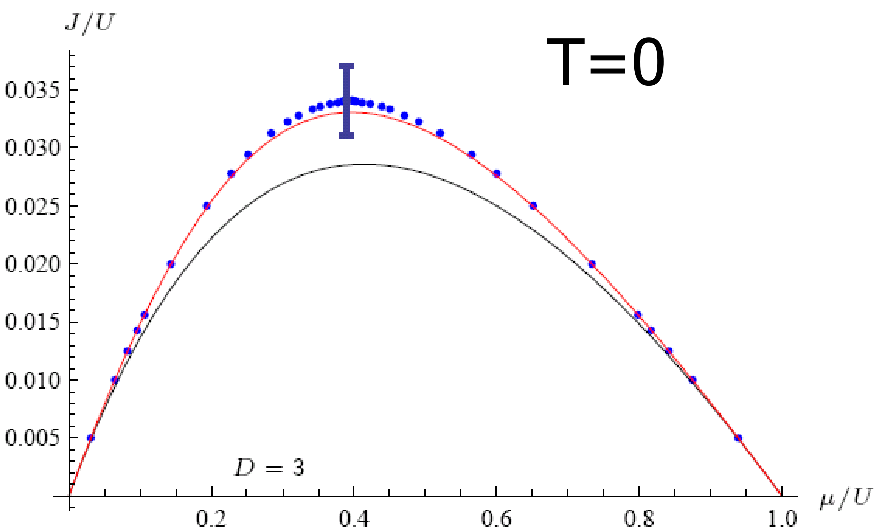
From Above

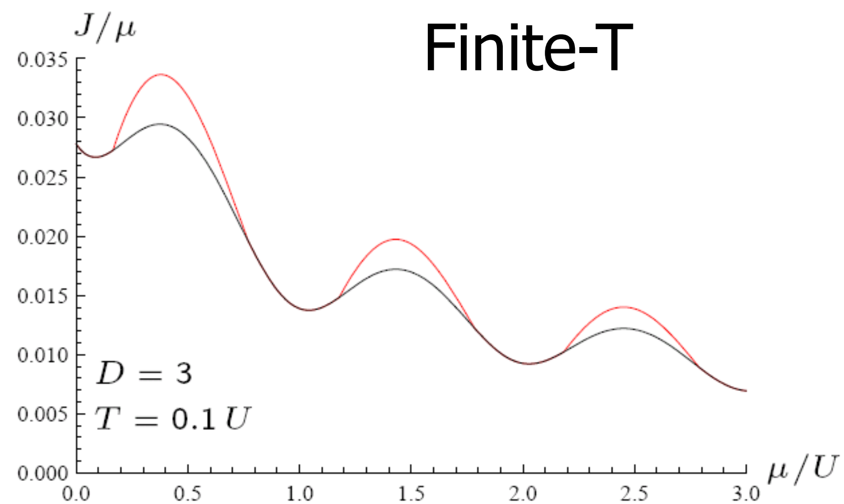
Diagrammatic Strong Coupling + Resummation @ T>0

Ohliger & Pelster, unpublished (2008)

•Decoupling MFT= Subset of strong-coupling diagrams $D \to \infty$
•Quantum Correction completely analytic !

Phase diagram, Time-of-flight pictures, Visibility, Spin-1 Bosons,…..





Ednilson Santos, FU-Berlin, PhD Thesis (in preparation)

From Below

Imaginary time path integral

$$\mathcal{Z} = \oint \mathcal{D}\psi^* \oint \mathcal{D}\psi \, e^{-\mathcal{A}[\psi^*,\psi]/\hbar}$$

Classical fields

Bosonic Action

$$\mathcal{A}[\psi^*,\psi] = \mathcal{A}^{(0)}[\psi^*,\psi] + \mathcal{A}^{(\mathrm{int})}[\psi^*,\psi]$$

$$\mathcal{A}^{(0)}[\psi^*,\psi] = \int_0^{\hbar\beta} d\tau \int d^D x \, \psi^*(\mathbf{x},\tau) \left\{ \hbar \frac{\partial}{\partial \tau} + \hat{H}(\mathbf{x}) - \mu \right\} \psi(\mathbf{x},\tau)$$

$$\mathcal{A}^{(\mathrm{int})}[\psi^*,\psi] = \frac{1}{2} \int_0^{\hbar\beta} d\tau \int d^D x \int d^D x' \, V^{(\mathrm{int})}(\mathbf{x},\mathbf{x}') \, \psi^*(\mathbf{x},\tau)\psi(\mathbf{x},\tau)\psi^*(\mathbf{x}',\tau)\psi(\mathbf{x}',\tau)$$

From Below

Motivation: Generic approach for superfluid phase?

Background field

$$\psi(\mathbf{x},\tau) = \Psi + \delta\psi(\mathbf{x},\tau)$$

$$\mathcal{Z} = \oint \mathcal{D}\delta\psi^* \oint \mathcal{D}\delta\psi \, e^{-\mathcal{A}[\Psi^*+\delta\psi^*,\Psi+\delta\psi]/\hbar}$$

$$\mathcal{A}[\Psi^* + \delta\psi^*, \Psi + \delta\psi] = \mathcal{A}^{(0)}[\delta\psi^*, \delta\psi] + \mathcal{A}^{(2)}[\delta\psi^*, \delta\psi] + \mathcal{A}^{(\mathrm{cor})}[\delta\psi^*, \delta\psi]$$

Tree Level — Quadratic Fluctuations — Perturbation

Free Energy $\Gamma[\Psi^*, \Psi] = -\frac{1}{\beta} \ln \mathcal{Z}$

From Below

One-Loop Approximation

Tree Level

$$\Gamma^{(0)}[\Psi^*, \Psi] = \quad V\left(-\mu|\Psi|^2 + \frac{\mathrm{U}}{2}|\Psi|^4\right)$$

Quadratic Fluctuations

$$e^{-\beta\Gamma^{(1)}[\Psi^*,\Psi]} = \oint \mathcal{D}\delta\psi^* \oint \mathcal{D}\delta\psi \, e^{-\mathcal{A}^{(2)}[\delta\psi^*,\delta\psi]/\hbar}$$

$$\mathcal{A}^{(2)}[\delta\psi^*, \delta\psi] = \frac{1}{2}\int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau' \int d^D x \int d^D x' \begin{pmatrix} \delta\psi(\mathbf{x},\tau) \\ \delta\psi^*(\mathbf{x},\tau) \end{pmatrix}^\dagger G^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') \begin{pmatrix} \delta\psi(\mathbf{x}',\tau') \\ \delta\psi^*(\mathbf{x}',\tau') \end{pmatrix}$$

with Kernel

$$G^{-1}(\mathbf{x},\tau;\mathbf{x}',\tau') = \delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau')\frac{1}{\hbar}$$

$$\times \begin{pmatrix} \hbar\partial_{\tau'} + \epsilon(-i\hbar\boldsymbol{\nabla}') - \mu + 2\mathrm{U}|\Psi|^2 & \mathrm{U}\Psi^2 \\ \mathrm{U}\Psi^{*2} & -\hbar\partial_{\tau'} + \epsilon(-i\hbar\boldsymbol{\nabla}') - \mu + 2\mathrm{U}|\Psi|^2 \end{pmatrix}$$

⇨ Fourier & Matsubara decomposition of Fluctuations and Kernel ⇨ $\Gamma^{(1)}[\Psi^*, \Psi] = \frac{1}{2\beta}\,\mathrm{Tr}\,\ln\, G^{-1}$

From Below

One-Loop Approximation

Loop counter

$$\Gamma[\Psi^*,\Psi] = V\left(-\mu|\Psi|^2 + \frac{U}{2}|\Psi|^4\right) + \frac{\eta}{2}\sum_{\mathbf{k}} E(\mathbf{k}) + \frac{\eta}{\beta}\sum_{\mathbf{k}} \ln\left[1 - e^{-\beta E(\mathbf{k})}\right] + \mathcal{O}(\eta^2)$$

Quasiparticle Energies $E(\mathbf{k}) = \sqrt{\left[\epsilon(\mathbf{k}) - \mu + 2U|\Psi|^2\right]^2 - U^2\,|\Psi|^4}$

Extremalization wrt. $n_0 = \Psi^*\Psi$ ⇨ **Bogoliubov**

very general approach: long-range, multi-component, disorder etc

allows for systematic diagrammatic analysis
Def: 1^{st} Bogoliubov Correction = 2-Loop Background

(has never been calculated?)

From Below

Two-Loop Approximation

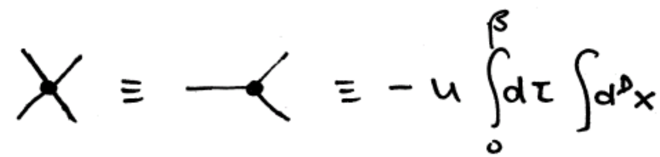
$$\mathcal{A}^{(\mathrm{cor})}[\delta\psi^*,\delta\psi] = \int_0^{\hbar\beta} d\tau \int d^D x \int d^D x' \, V^{(\mathrm{int})}(\mathbf{x},\mathbf{x}') \left\{ \left[\Psi^*(\mathbf{x},\tau)\delta\psi(\mathbf{x},\tau) + \delta\psi^*(\mathbf{x},\tau)\Psi(\mathbf{x},\tau) \right] \right.$$
$$\left. \times \delta\psi^*(\mathbf{x}',\tau)\delta\psi(\mathbf{x}',\tau) + \frac{1}{2}\,\delta\psi^*(\mathbf{x},\tau)\delta\psi(\mathbf{x},\tau)\delta\psi^*(\mathbf{x}',\tau)\delta\psi(\mathbf{x}',\tau) \right\} . \qquad (6.55$$

Taylor Expansion

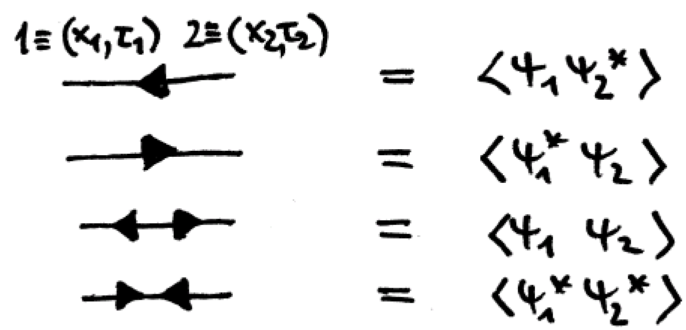
Ensemble Average $\langle \bullet \rangle = e^{\beta\Gamma^{(1)}[\Psi^*,\Psi]} \oint \mathcal{D}\delta\psi^* \oint \mathcal{D}\delta\psi \, \bullet \, e^{-\mathcal{A}^{(2)}[\delta\psi^*,\delta\psi]/\hbar}$ ⇨ Wick Theorem

Feynman Rules

Pseudopotential



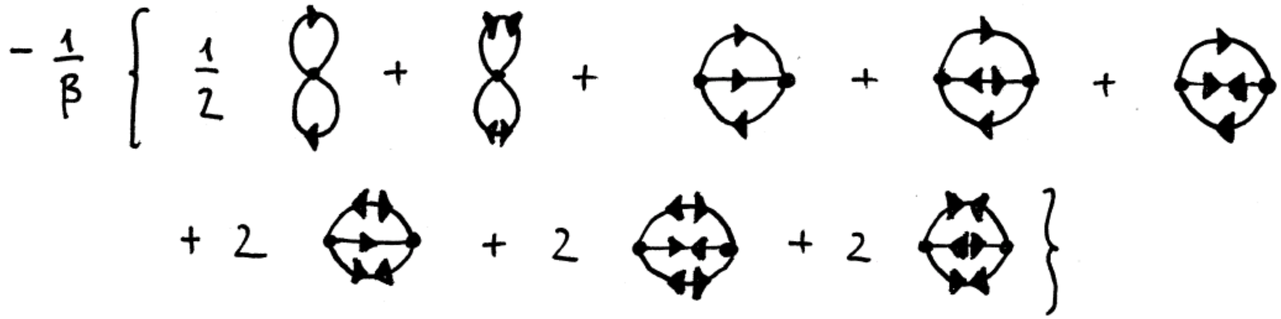
$$G(\mathbf{x},\tau;\mathbf{x}',\tau') = \begin{pmatrix} G_{\psi\psi^*}(\mathbf{x},\tau;\mathbf{x}',\tau') & G_{\psi\psi}(\mathbf{x},\tau;\mathbf{x}',\tau') \\ G_{\psi^*\psi^*}(\mathbf{x},\tau\;\;\mathbf{x}',\tau') & G_{\psi^*\psi}(\mathbf{x},\tau\;\;\mathbf{x}',\tau') \end{pmatrix}$$



From Below

Two-Loop Approximation

$$\Gamma^{(2)}[\Psi^*, \Psi] =$$



NO Divergencies on the lattice!

- Diagrams are finite!!!!
- Automating higher orders (Resummation via VPT)