Effective Action Approach to Bosons in Optical Lattices

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1. Effective Potential (Landau Theory)

Bose-Hubbard Hamiltonian [1–3]:

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

Coupling to global source [4–6]:

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

Grand-canonical free energy in hopping expansion:

$$F(J^*,J)=N_{\rm s}\left(F_0+\sum_{p=1}^{\infty}c_{2p}(t)|J|^{2p}\right), \qquad c_{2p}(t)=\sum_{n=0}^{\infty}(-t)^n\alpha_{2p}^{(n)}$$

Order parameter:

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

Legendre transformation yields effective potential:

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

Legendre identities:

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

Physical limit of vanishing currents:

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

Effective potential in hopping expansion:

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

Location of second-order phase transition:

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

First hopping order for $T=0$ yields mean-field result [1]:

$$t_c^{(1)}=-\frac{\alpha_2^{(0)}}{\alpha_2^{(1)}}=U/\left[2d\left(\frac{n+1}{n-b}+\frac{n}{1-n+b}\right)\right] \quad , \qquad b=\frac{\mu}{U}$$

Second hopping order for $T=0$ [7]:

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

with coefficients for $n=1$:

$$\overline{\alpha}_1=\frac{2(b+1)d}{(b-1)b}$$

$$\overline{\alpha}_2=\frac{4d\left[-12b^3+b(9-8d)-3d+b^4(6+d)-3b^2(1+2d)\right]}{(-1+b)^2b^2\left(-3-2b+b^2\right)}$$

2. Effective Action (Ginzburg-Landau Theory)

Coupling to local sources [5,6]:

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

Grand-canonical free energy functional ($\hbar=1$):

$$\mathcal{F}\left[J_i^*(\tau),J_i(\tau)\right]=F_0-\frac{1}{\beta}\left\{\sum_{i_1,i_2}\int_0^\beta d\tau_1\int_0^\beta d\tau_2\,G^{(2)}(i_1,\tau_1|i_2,\tau_2)J_{i_1}(\tau_1)J_{i_2}^*(\tau_2)\right.$$
$$\left.+\sum_{\substack{i_1,i_2\\i_3,i_4}}\int_0^\beta d\tau_1\int_0^\beta d\tau_2\int_0^\beta d\tau_3\int_0^\beta d\tau_4\,G^{(4)}(i_1,\tau_1;i_2,\tau_2|i_3,\tau_3;i_4,\tau_4)J_{i_1}(\tau_1)J_{i_2}(\tau_2)J_{i_3}^*(\tau_3)J_{i_4}^*(\tau_4)+\cdots\right\}$$

In Matsubara space with $\omega_m=2\pi m/\beta$:

$$\mathcal{F}\left[J_i^*(\omega_m),J_i(\omega_m)\right]=F_0-\frac{1}{\beta}\left\{\sum_{i_1,i_2}\sum_{m_1,m_2}G^{(2)}(i_1,\omega_{m_1}|i_2,\omega_{m_2})J_{i_1}(\omega_{m_1})J_{i_2}^*(\omega_{m_2})\right.$$
$$\left.+\sum_{\substack{i_1,i_2\\i_3,i_4}}\sum_{\substack{m_1,m_2\\m_3,m_4}}G^{(4)}(i_1,\omega_{m_1};i_2,\omega_{m_2}|i_3,\omega_{m_3};i_4,\omega_{m_4})J_{i_1}(\omega_{m_1})J_{i_2}(\omega_{m_2})J_{i_3}^*(\omega_{m_3})J_{i_4}^*(\omega_{m_4})+\cdots\right\}$$

Order parameter field:

$$\psi_i(\omega_m)=\langle\hat{a}_i(\omega_m)\rangle=\beta\frac{\delta\mathcal{F}}{\delta J_i^*(\omega_m)} \quad , \quad \psi_i^*(\omega_m)=\left\langle\hat{a}_i^\dagger(\omega_m)\right\rangle=\beta\frac{\delta\mathcal{F}}{\delta J_i(\omega_m)}$$

Legendre transformation yields effective action:

$$\Gamma\left[\psi_i^*(\omega_m),\psi_i(\omega_m)\right]=\mathcal{F}-\frac{1}{\beta}\sum_i\sum_m\left[\psi_i^*(\omega_m)J_i(\omega_m)+\psi_i(\omega_m)J_i^*(\omega_m)\right]$$

Equations of motion:

$$\frac{\delta\Gamma}{\delta\psi_i^*(\omega_m)}=0 \quad , \quad \frac{\delta\Gamma}{\delta\psi_i(\omega_m)}=0$$

Static solutions yield average number of particles per site and compressibility:

$$\langle n\rangle=-\frac{1}{N_s}\frac{\partial\Gamma}{\partial\mu}\bigg|_{\psi=\psi_{\rm eq}} \quad , \quad \kappa=-\frac{1}{N_s}\frac{\partial^2\Gamma}{\partial\mu^2}\bigg|_{\psi=\psi_{\rm eq}}$$

Dynamical solutions yield dispersion relations for amplitude and phase excitations:

$$\frac{\delta\Gamma\left[\psi_{\rm eq}+\delta A_i(\tau)\right]}{\delta(\delta A_i(\tau))}=0\rightarrow\omega_A(\mathbf{k}) \quad , \quad \frac{\delta\Gamma\left[\psi_{\rm eq}e^{i\theta_i(\tau)}\right]}{\delta\theta_i(\tau)}=0\rightarrow\omega_\theta(\mathbf{k})$$

Second sound dispersion relation [8,9]:

$$\omega_s(\mathbf{k})=\sqrt{\omega_A(\mathbf{k})\omega_\theta(\mathbf{k})}$$

Peierls phase factor: $\hat{a}_i\rightarrow\hat{a}_i e^{i\frac{\mathbf{x}_i}{L}\cdot\boldsymbol{\phi}}$

Calculate superfluid density from $\Gamma(\boldsymbol{\phi})$ [10,11]:

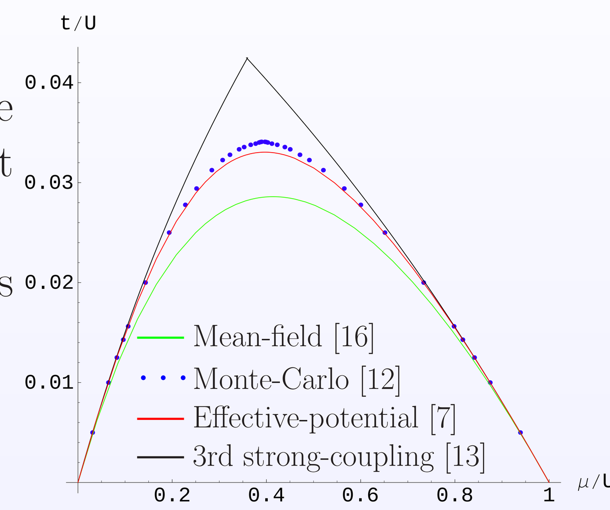
$$\rho=\lim_{|\boldsymbol{\phi}|\rightarrow0}\frac{2m^*L^2}{N_s|\boldsymbol{\phi}|^2}\left[\Gamma(\boldsymbol{\phi})|_{\psi=\psi_{\rm eq}(\boldsymbol{\phi})}-\Gamma(0)|_{\psi=\psi_{\rm eq}(0)}\right]$$

Result in first hopping order: $\rho=\psi_{\rm eq}^*\psi_{\rm eq}$

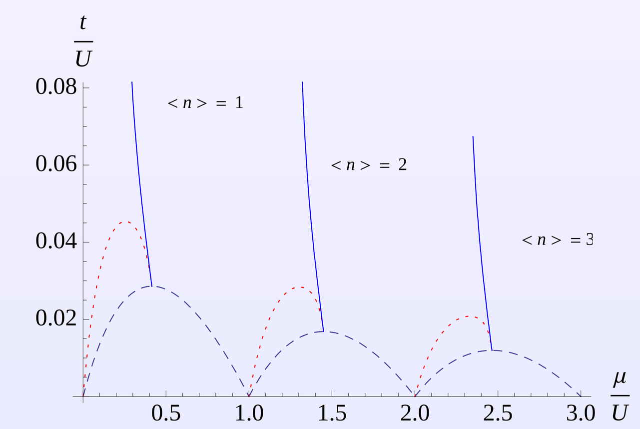
3. Results

Phase diagram for zero temperature:

- Recent Monte-Carlo simulations are believed to be very precise [12]
- Effective-potential method gives a difference less that 3% from the Monte-Carlo data at the lobe tip [7]
- Strong-coupling approach [13] compares particle and hole states
- Extension to higher hopping orders [14].
- Extension to $T>0$ [15].

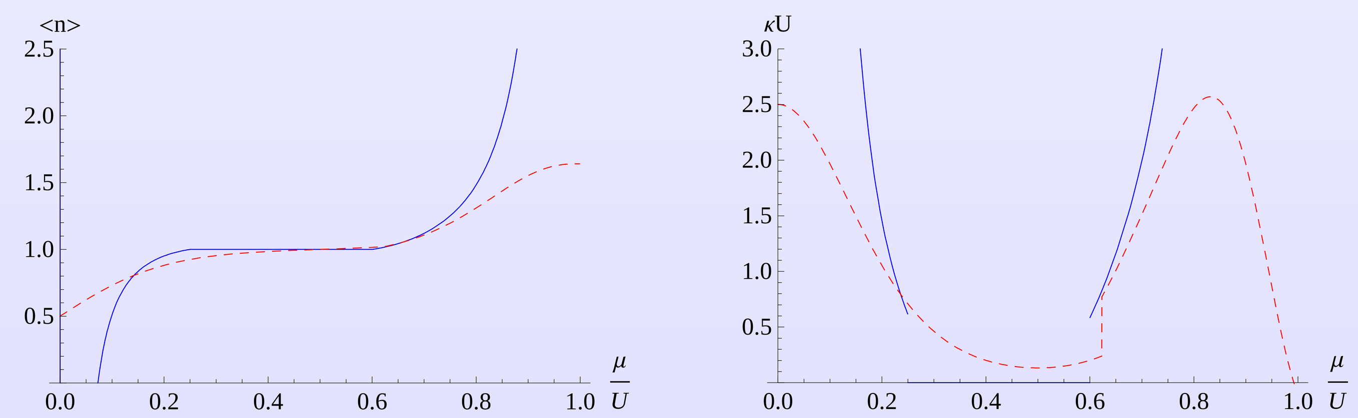


Contours of constant $\langle n\rangle$:



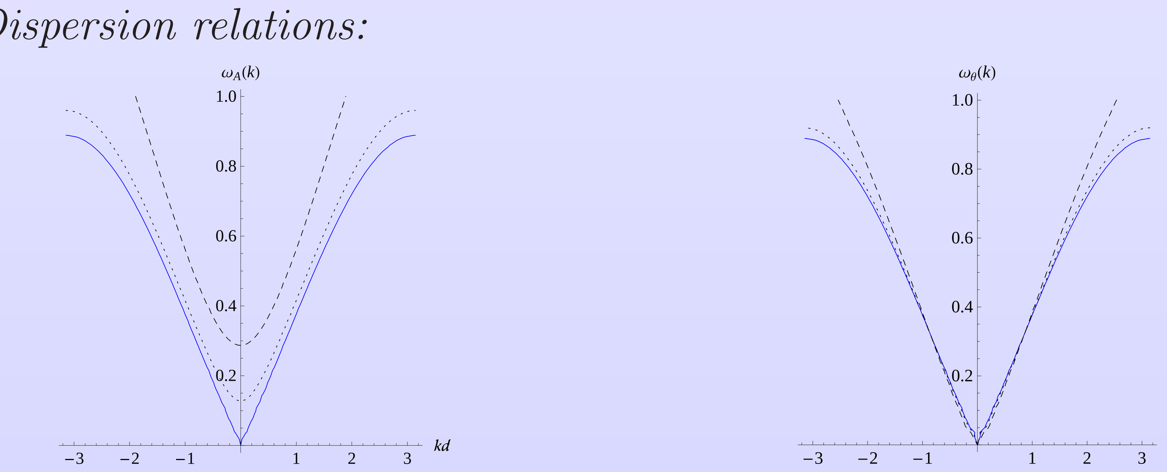
- Inside superfluid phase $\langle n\rangle$ should increase with μ
- Mean-field (dotted) theory violates this general property [17]
- Field-theoric (solid) method has a larger range of validity [17]

Average number of particles per lattice site and compressibility:



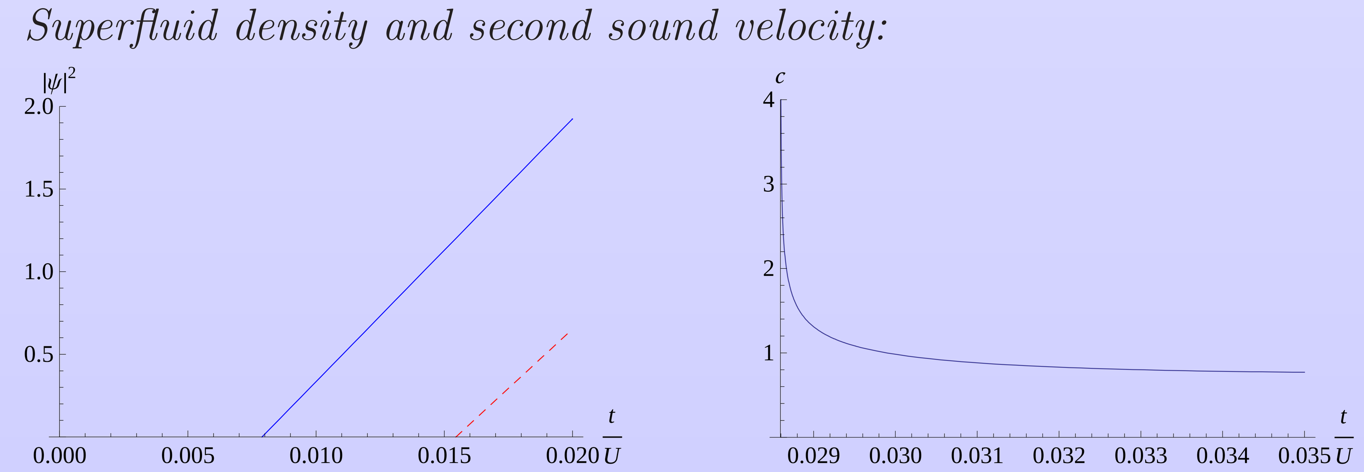
Solid blue: $T/U=0$. Dashed red: $T/U=0.1/k_B$ [17].

Dispersion relations:



Dotted: $t=0.3\,U$. Dashed: $t=0.35\,U$. Solid: $t=t_c\approx0.028\,U$. $\mu/U=\sqrt{2}-1$ [17].

Superfluid density and second sound velocity:



Superfluid velocity. $\mu/U=0.9U$.

Second sound velocity. $\mu/U=\sqrt{2}-1$ [17].

Solid blue: $T/U=0$. Dashed red: $T/U=0.1k_b$.

Outlook: Time-of-flight absorption pictures [18–20]

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References

[1] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher. Boson localization and the superfluid-insulator transition. *Phys. Rev. B*, **40**:546, 1989.

[2] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller. Cold bosonic atoms in optical lattices. *Phys. Rev. Lett.*, **81**:3108, 1998.

[3] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch. Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms. *Nature*, **415**:39, 2002.

[4] J. W. Negele and H. Orland. *Quantum Many-Particle Systems*. Perseus Books, 1998.

[5] H. Kleinert and V. Schulte-Frohlinde. *Critical Properties of* Φ^4 *Theories*. World Scientific, 2001.

[6] J. Zinn-Justin. *Quantum Field Theory and Critical Phenomena*. Oxford University Press, 2002.

[7] F. E. A. dos Santos and A. Pelster. On the quantum phase diagram of bosons in optical lattices. *Phys. Rev. A* `(in press)`. `arXive/0806.2812`.

[8] P. B. Weichman. Crossover scaling in a dilute bose superfluid near zero temperature. *Phys. Rev. B*, **38**:8739, 1988.

[9] H. Kleinert. *Multivalued Fields. In Condensed Matter, Electromagnetism, and Gravitation*. World Scientific, 2008.

[10] M. N. Fischer, M. N. Barber, and D. Jasnow. Helicity modulus, superfluidity, and scaling in isotropic systems. *Phys. Rev. A*, **8**:1111, 1973.

[11] R. Roth and K. Burnett. Superfluidity and interference pattern of ultracold bosons in optical lattices. *Phys. Rev. A*, **67**:031602(R), 2003.

[12] B. Capogrosso-Sansone, E. Kozik, N. Prokof'ev, and B. Svistunov. On-site number statistics of ultracold lattice bosons. *Phys. Rev. A*, **75**:013619, 2007.

[13] J. K. Freericks and H. Monien. Strong-coupling expansion for the pure and disorderd Bose-Hubbard model. *Phys. Rev. B*, **53**:2691, 1996.

[14] N. Teichmann, D. Hinrichs, M. Holthaus, and A. Eckardt. Bose-Hubbard phase diagram with arbitrary filling. `arXive/0810.0643`.

[15] M. Ohliger and A. Pelster. Green's function approach to the Bose-Hubard model. `arXive/0810.4399`.

[16] S. Sachdev. *Quantum Phase Transitions*. Cambridge University Press, 1999.

[17] B. Bradlyn, F. E. A. dos Santos, and A. Pelster. Effective action approach for quantum phase transitions in bosonic lattices. `arXive/0809.0706`.

[18] F. Gerbier, A. Widera, S. Fölling, O. Mandel, T. Gericke, and I Bloch. Interference pattern and visibility of a mott insulator. *Phys. Rev. A*, **72**:053606, 2005.

[19] F. Gerbier, S. Foelling, A. Widera, and I. Bloch. Visibility of a Bose-condensed gas released from an optical lattice at finite temperatures. `arXive/0701.420`.

[20] A. Hoffmann and A. Pelster. Visibility of cold atomic gases in optical lattices for finite temperatures. `arXive/0809.0771`.