Green's Function Approach to the Bose-Hubbard Model

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1. Green's Function Approach

Bose-Hubbard model

$$\hat H = \hat H_0 + \sum_{i,j} t_{i,j}\hat a_i^\dagger \hat a_j \quad t_{i,j} = t \text{ if } i,j \text{ nearest neighbors}; \quad t_{i,j}=0 \text{ otherwise}$$

Strong-coupling Hamiltonian:

$$\hat H_0 = \sum_i \left[\frac{U}{2}\hat n_i(\hat n_i - 1) - \mu \hat n_i\right], \quad \hat H_0|n\rangle = N_S E_n|n\rangle, \quad E_n = \frac{U}{2}n(n-1) - \mu n$$

Imaginary-time Green's function ($\hbar = k_B = 1$):

$$G_1(\tau', j'|\tau, j) = \frac{1}{\mathcal Z}\mathrm{Tr}\left\{e^{-\beta \hat H_{BH}}\hat T\left[\hat a_{j,H}(\tau)\hat a^\dagger_{j',H}(\tau')\right]\right\} \quad \text{with} \quad \mathcal Z = \mathrm{Tr}\{e^{-\beta \hat H_{BH}}\}$$

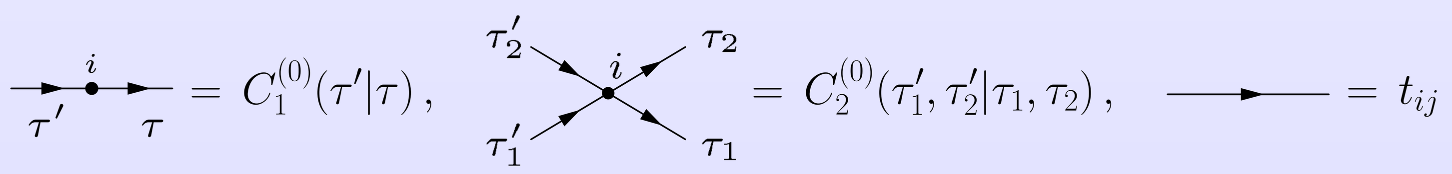
Expansion in hopping matrix element:

$$G_1^{(n)}(\tau', i'|\tau, i) = \frac{\mathcal Z^{(0)}}{\mathcal Z}\frac{1}{n!}\sum_{i_1,j_1,\dots,i_n,j_n} t_{i_1j_1}\dots t_{i_nj_n}\int_0^\beta d\tau_1\dots\int_0^\beta d\tau_n$$
$$\times\, G^{(0)}_{n+1}(\tau_1, j_1; \dots; \tau_n, j_n; \tau', i'|\tau_1, i_1; \dots; \tau_n, i_n, \tau, i)$$

Locality of $\hat H_0$ allows decomposition of $n+1$-particle unperturped Green's functions into *local* cumulants, e.g.

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

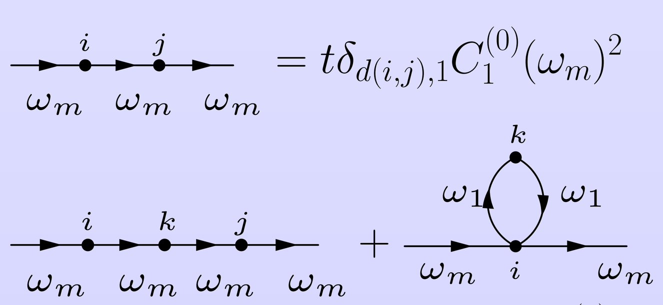
Diagrammatic representation [1]:



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

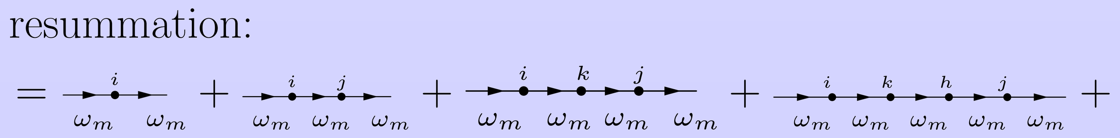
$$C_1^{(0)}(\omega_m) = \frac{1}{\mathcal Z^{(0)}}\sum_{n=0}^\infty\left[\frac{(n+1)}{E_{n+1}-E_n-i\omega_m} - \frac{n}{E_n - E_{n-1} - i\omega_m}\right]e^{-\beta E_n}$$

First two orders of perturbation series:



$$=t^2(\delta_{d(i,j),2} + 2\delta_{d(i,j),\sqrt2} + 2d\delta_{i,j})C_1^{(0)}(\omega_m)^3$$
$$+\, t^2 2d\delta_{i,j}\sum_{\omega_1}C_1^{(0)}(\omega_m)C_2^{(0)}(\omega_m,\omega_1|\omega_m,\omega_1)$$

First-order resummation:



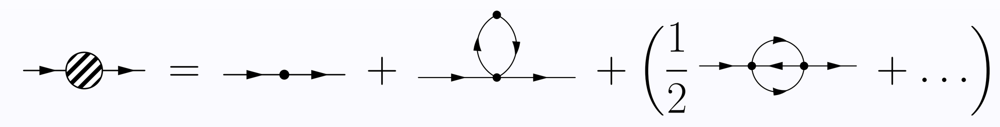
Easily summed in Fourier space:

$$\tilde G_1^{(1)}(\omega_m, \mathbf k) = \frac{C_1^{(0)}(\omega_m)}{1 - t(\mathbf k)\,C_1^{(0)}(\omega_m)}, \qquad t(\mathbf k) = 2t\sum_{l=1}^d \cos(k_l a)$$

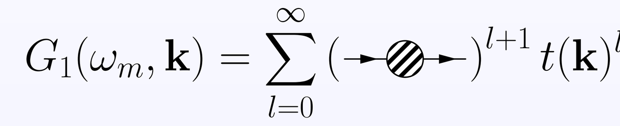
Phase boundary given by divergence of $G_1(\omega_m = 0; \mathbf k = \mathbf 0)$.
First-order result reproduces mean-field result [2,3].

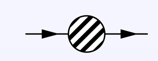
One-loop corrections:

Sum over all one-particle irreducable diagrams:



Full Green's function obtained by:

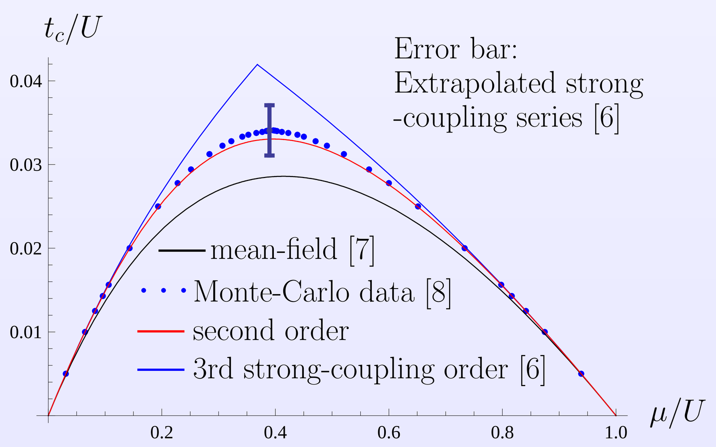


One-loop approximation by considering only the first two terms in 

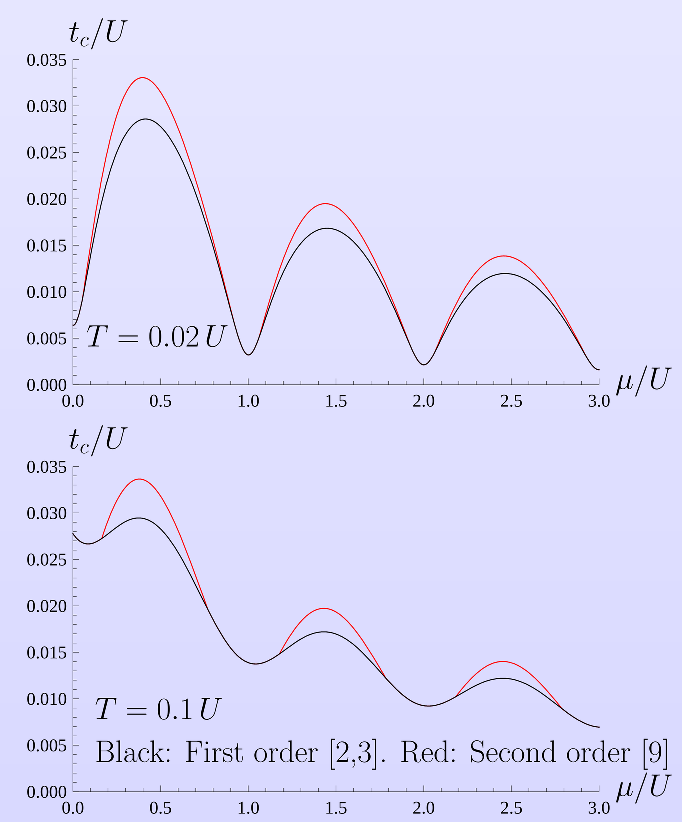
2. Results for $3d$ System

Phase diagram for zero temperature:

- Second order gives a difference of less than 3% from high-precision Monte-Carlo data at the lobe tip.
- Second order reproduces effective potential result [4], numerically extentable to higher orders [5]
- Strong-coupling approach compares particle and hole states



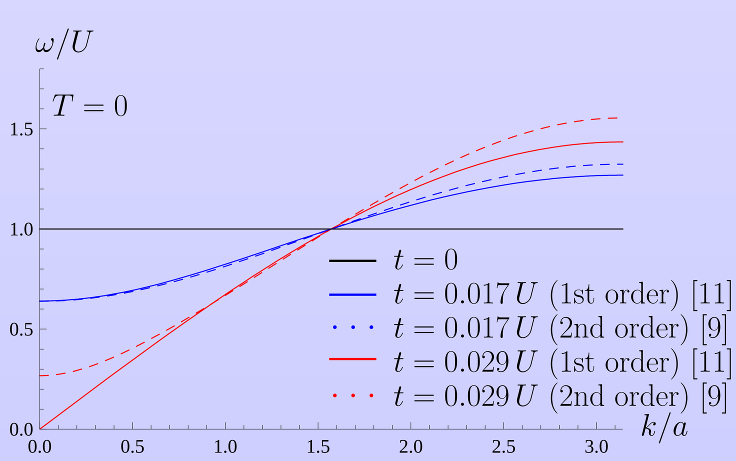
Phase diagram for finite temperature:



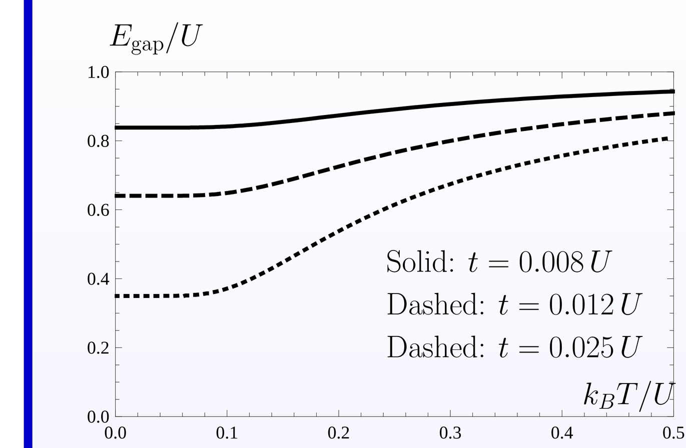
- Both thermal and quantum fluctuations shift phase boundary towards larger values of critical hopping
- One-loop corrections most important near quantum critical point (tip of lobes)
- Temperature effects most important between lobes due to larger thermal fluctuations
- One-loop corrections slightly larger for lower temperature

Excitation spectrum:

- 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
- Spectrum in superfluid phase by effective action method [10]



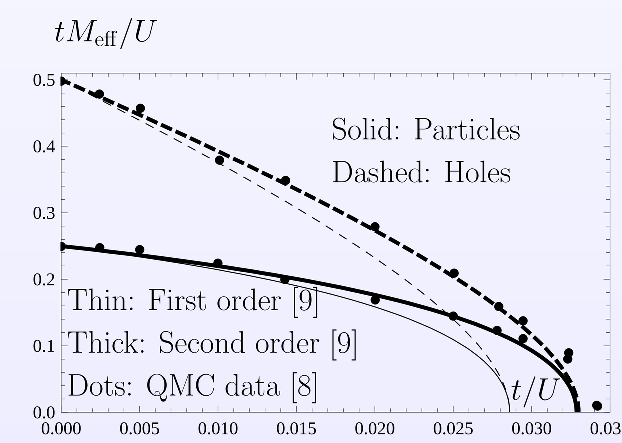
Excitation gap:



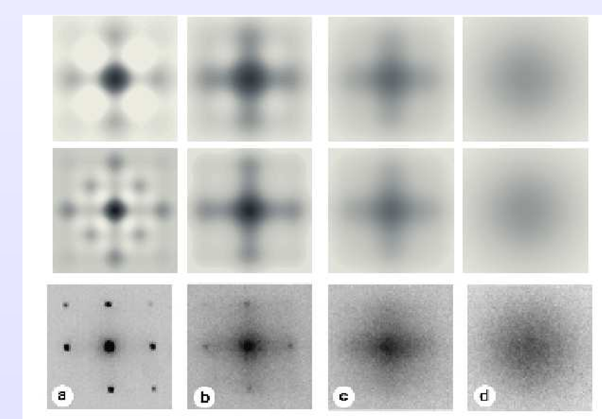
- Characteristic gap in Mott phase
- Gets larger with higher temperature due to thermal fluctuations
- Could serve as thermometer in experiments

Effective Masses:

- Quasi-particles and quasi-holes carry effective masses
- Effective mass vanishes at quantum critical point
- Good agreement with QMC data



Time-of-flight:



Top to bottom: First-order perturbation theory, Second-order perturbation theory [12], experiment [13]. Left to right: $V_0 = 8, 14, 18, 30\,E_R$

- Time-of-Flight pictures give momentum-space density
- Obtained from Green's function [14]:

$$n_{\mathbf k} = \langle\hat\psi^\dagger(\mathbf k)\hat\psi(\mathbf k)\rangle = |w(\mathbf k)|^2\sum_{i,j}e^{i\mathbf k(\mathbf r_i - \mathbf r_j)}\lim_{\tau'\searrow 0}G_1(\tau', i|0, j)$$

$w(\mathbf k)$: Wannier function

- 2d pictures by integration along z-axis

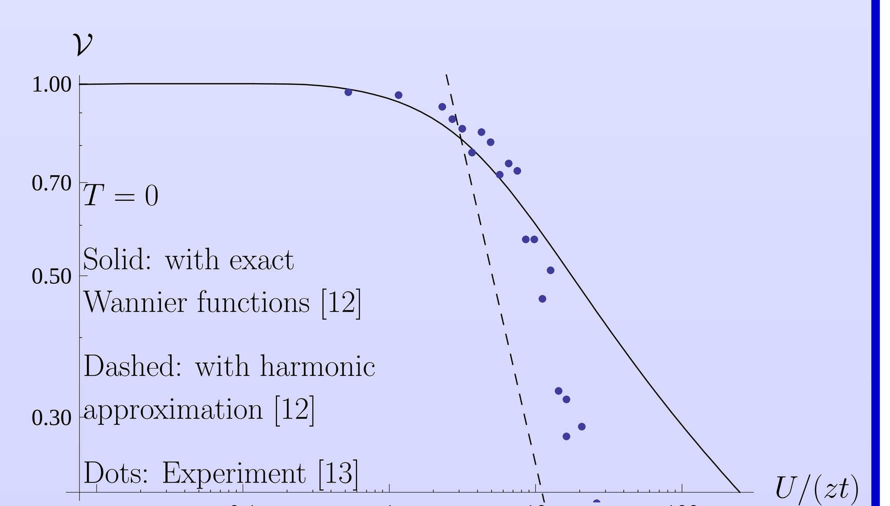
Visibility:

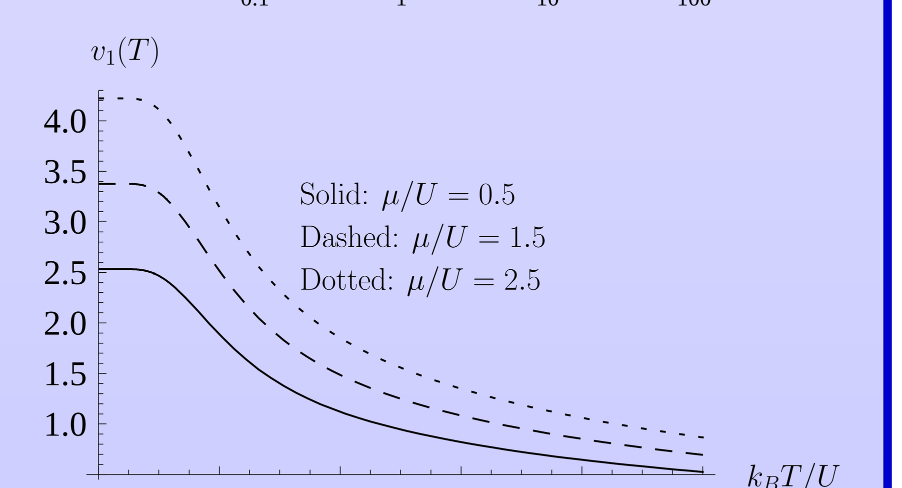
- Measure for interference patterns in TOF pictures

$$\mathcal V = \frac{n_{max} - n_{min}}{n_{max} + n_{min}}$$

- Harmonic (Gaussian) approximation of Wannier functions yields considerable errors compared to exact numerical treatment
- Behavior for small t [12]:

$$\mathcal V = v_1(T)\frac{zt}{U} + v_2(T)\left(\frac{zt}{U}\right) + \dots$$





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