Diagrammatic Green's Functions Approach to the Bose-Hubbard Model

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  - Experimental realization
  - Bose-Hubbard model
  - Motivation

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- Imaginary-time Green's functions
  - Hopping expansion
  - Cumulant decomposition
  - Diagrammatic rules

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- Time-of-flight

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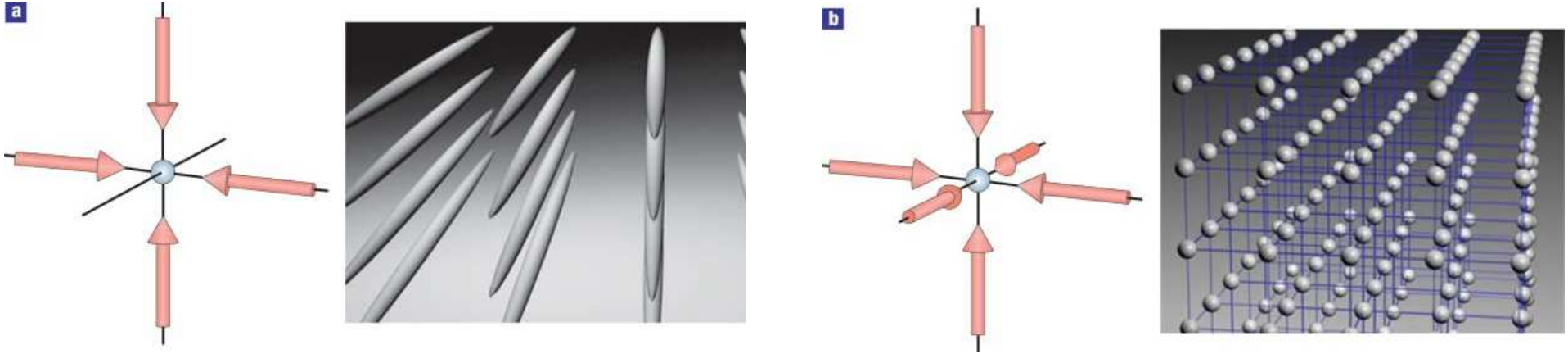
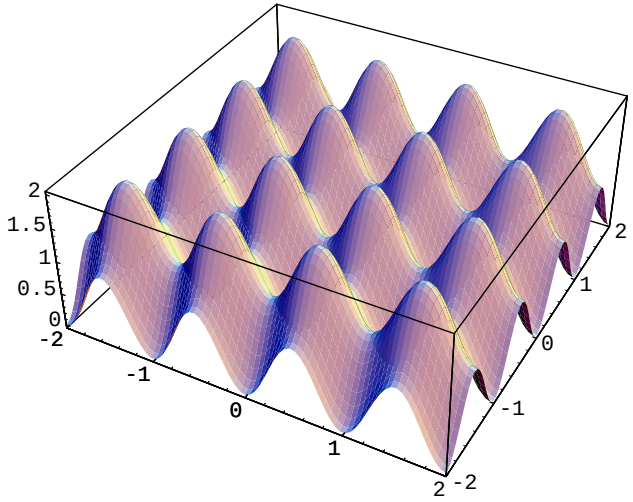
Experimental realization



- Optical lattice produced by counter-propagating lasers
- $V \propto \sin^2(2\pi x/\lambda)$
- Relative strength of hopping and interaction controllable
- (Quasi) one-, two-, and three-dimensional configurations possible



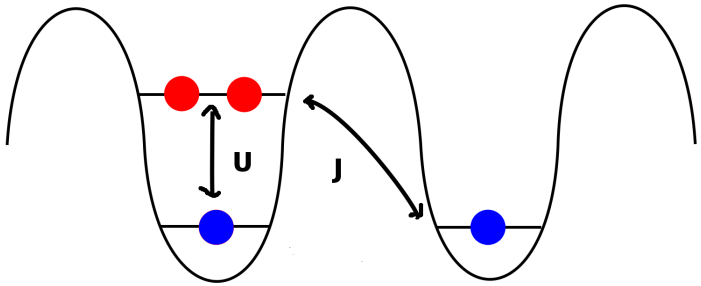
Bose-Hubbard model

- Bose-Hubbard Hamiltonian:

$$\hat{H}_{\text{BHM}} = \hat{H}_0 + \hat{H}_1$$

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

$$\hat{H}_1 = -J \sum_{<i,j>} \hat{a}_i^\dagger \hat{a}_j = -\sum_{i,j} J_{i,j} \hat{a}_i^\dagger \hat{a}_j$$



$$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$$

$$J_{ij} = \begin{cases} J & \text{if } i, j \text{ nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$

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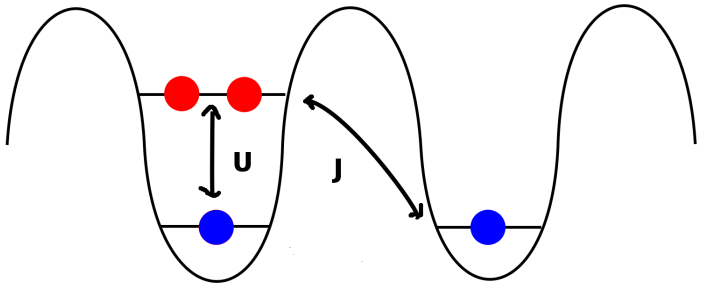

- $\hat{H}_0$ site-diagonal:

$$\hat{H}_0 |n\rangle = N_S E_n |n\rangle$$

$$E_n = \frac{U}{2} n(n-1) - \mu n$$

- Perturbative expansion in $\hat{H}_1$

Motivation

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

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  - Time-of-flight pictures
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- Motivated by:
  - F. Nogueira's "Primer to the Bose-Hubbard model"
  - Diagrammatic calculations for Fermions by W. Metzner, PRB **43**, 8549 (1993)

Imaginary-time Green's function

- Definition:

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

$$\text{with } \mathcal{Z} = \mathrm{Tr}\{e^{-\beta \hat{H}}\}$$

- Heisenberg operators in imaginary time ($\hbar = 1$):

$$\hat{O}_{\mathrm{H}}(\tau) = e^{\hat{H}\tau} \hat{O} e^{-\hat{H}\tau}$$

Dirac interaction picture

- Time evolution of operators determined only by $\hat{H}_0$:

$$\hat{O}_{\mathrm{D}}(\tau) = e^{\hat{H}_0 \tau} \hat{O} e^{-\hat{H}_0 \tau}$$

- Dirac time evolution operator calculated by Dyson series:

$$\begin{aligned}\hat{U}_{\mathrm{D}}(\tau, \tau_0) =& \sum_{n=0}^{\infty} (-1)^n \int_{\tau_0}^{\tau} d\tau_1 \ldots \int_{\tau_0}^{\tau_{n-1}} d\tau_n \hat{H}_{1\mathrm{D}}(\tau_1) \ldots \hat{H}_{1\mathrm{D}}(\tau_n) \\ =& \hat{T} \exp\left(- \int_{\tau_0}^{\tau} d\tau_1 \hat{H}_{1\mathrm{D}}(\tau_1) \right)\end{aligned}$$

Partition function

- Full partition function:

$$\mathcal{Z} = \mathrm{Tr}\left\{e^{-\beta \hat{H}_0} \hat{U}_{\mathrm{D}}(\beta, 0)\right\}$$

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- nth order contibution:

$$\mathcal{Z}^{(n)} = \frac{1}{n!}\mathcal{Z}^{(0)} \sum_{i_1, j_1, \ldots, i_n, j_n} J_{i_1 j_1} \ldots J_{i_n j_n} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \ldots \int_0^\beta d\tau_n$$
$$\times\, G_n^{(0)}(\tau_1, j_1; \ldots; \tau_n, j_n | \tau_1, i_1; \ldots; \tau_n, i_n)$$

- Unperturbed n-particle Green's function:

$$G_n^{(0)}(\tau_1', i_1'; \ldots; \tau_n', i_n' | \tau_1, i_1; \ldots; \tau_n, i_n) = \left\langle \hat{T} \hat{a}_{i_1'}^\dagger(\tau_1') \hat{a}_{i_1}(\tau_1) \ldots \hat{a}_{i_n'}^\dagger(\tau_n') \hat{a}_{i_n}(\tau_n) \right\rangle^{(0)}$$

Cumulant decomposition

- Decompose $G_n^{(0)}(\tau_1', i_1'; \ldots; \tau_n', i_n' | \tau_1, i_1; \ldots; \tau_n, i_n)$ into "simple" parts
- $\hat{H}_0$ not harmonic $\Rightarrow$ Wick's theorem not applicable

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- But: Decomposition into cumulants
- $\hat{H}_0$ site-diagonal $\Rightarrow$ cumulants local. Example:

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

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- Denote contributions diagrammatically:
  Points for cumulants, lines for hopping matrix elements
- Perturbation theory in number of *lines*

Calculation of cumulants

- Generating functional:

$$C_0^{(0)}[j,j^*] = \log \left\langle \hat{T}\exp\left(\int_0^\beta d\tau j^*(\tau)\hat{a}(\tau) + j(\tau)\hat{a}^\dagger(\tau)\right)\right\rangle^{(0)}$$

- Cumulants calculated by functional derivatives:

$$C_n^{(0)}(\tau_1',\ldots,\tau_n'|\tau_1,\ldots,\tau_n) = \frac{\delta^{2n}}{\delta j(\tau_1')\ldots\delta j(\tau_n')\delta j^*(\tau_1)\ldots\delta j^*(\tau_n)} C_0^{(0)}[j,j^*]\Big|_{j=j^*=0}$$

Calculation of cumulants

- One- and two-particle cumulants:

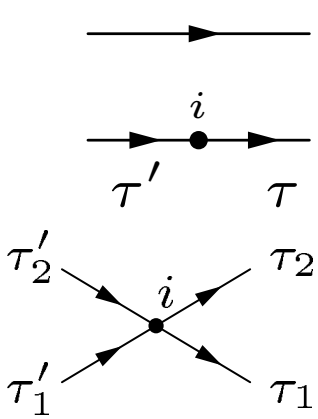
$$C_1^{(0)}(\tau', |\tau) = \langle \hat{T}\hat{a}^\dagger(\tau')\hat{a}(\tau)\rangle^{(0)} = \frac{1}{\mathcal{Z}^{(0)}} \sum_{n=0}^{\infty} \langle n|\hat{T}\hat{a}^\dagger(\tau')\hat{a}(\tau)|n\rangle\, e^{-\beta E_n}$$

$$= \frac{1}{\mathcal{Z}^{(0)}} \sum_{n=0}^{\infty} \Big[\Theta(\tau-\tau')(n+1)\, e^{(E_n - E_{n+1})(\tau-\tau')} + \Theta(\tau'-\tau)\, n\, e^{(E_n - E_{n-1})(\tau'-\tau)}\Big]\, e^{-\beta E_n}$$

$$C_2^{(0)}(\tau_1', \tau_2'|\tau_1, \tau_2) = \langle \hat{T}\hat{a}^\dagger(\tau_1')\hat{a}^\dagger(\tau_2')\hat{a}(\tau_1)\hat{a}(\tau_2)\rangle^{(0)} - C_1^{(0)}(\tau_1', \tau_1)C_1^{(0)}(\tau_2', \tau_2) - C_1^{(0)}(\tau_1', \tau_2)C_1^{(0)}(\tau_2', \tau_1)$$

Diagrammatic rules for $\mathcal{Z}^{(n)}$

1. Draw all possible combinations of vertices with total n entering and n leaving lines
2. Connect them in all possible ways and assign time variables and hopping matrix elements onto the lines
3. Sum over all site indices and integrate all time variables from 0 to β



$$= J_{ij}$$

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

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

Calculation of free energy

- Grand-canonical free energy:

$$\mathcal{F} = -\frac{1}{\beta}\log\mathcal{Z}\,, \quad \mathcal{F}^{(0)} = -\frac{N_S}{\beta}\log\mathcal{Z}^{(0)}\,, \quad \mathcal{Z}^{(0)} = \sum_n e^{-\beta E_n}$$

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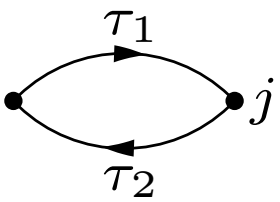
- First correction:

$\mathcal{F}^{(2)} = \frac{-1}{2\beta}$ 

$$= \frac{-1}{2\beta}\sum_{i,j} J_{i,j}J_{j,i}\int_0^\beta d\tau_1\int_0^\beta d\tau_2\, C_1^{(0)}(\tau_2|\tau_1)C_1^{(0)}(\tau_1|\tau_2)$$

$$= -\frac{N_S 2DJ^2}{U\mathcal{Z}^{(0)2}}\sum_{n,k}\left[\frac{(n+1)k}{k-n+1} + \frac{n(k+1)}{n-k+1}\right]e^{-\beta(E_n+E_k)}$$

Diagrammatic rules for Green's functions

$$G_1(\tau', i'|\tau, i) = \frac{1}{\mathcal{Z}} \mathsf{Tr}\left\{ e^{-\beta \hat{H}_0} \hat{T} \hat{a}^\dagger_{i'}(\tau') \hat{a}_i(\tau) \hat{U}_\mathsf{D}(\beta, 0) \right\}$$

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

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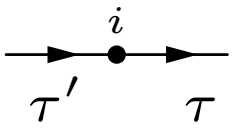
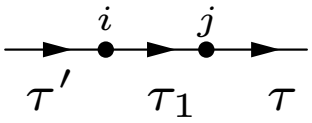
- Diagrams have external lines with *fixed* time and site variables
- Disconnected diagrams cancelled by $\mathcal{Z}^{(0)}/\mathcal{Z}$
- Zeroth and first order:

$G_1^{(0)}(\tau', i|\tau, j) =$ 

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

$G_1^{(1)}(\tau', i|\tau, j) =$ 

$= J \delta_{d(i,j),1} \int_0^\beta d\tau_1 \, C_1^{(0)}(\tau'|\tau_1) C_1^{(0)}(\tau_1|\tau)$

Calculations in Matsubara space

- Translational invariance in time suggests Matsubara transform:

$$C_1^{(0)}(\omega_m) = \frac{1}{\mathcal{Z}^{(0)}} \sum_n \left[\frac{(n+1)}{E_{n+1} - E_n - i\omega_m} - \frac{n}{E_n - E_{n-1} - i\omega_m} \right] e^{-\beta E_n}, \ \omega_m = \frac{2\pi}{\beta} m$$

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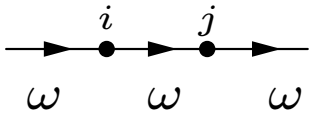
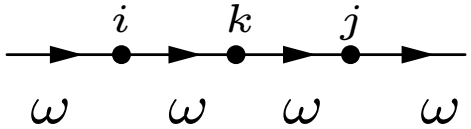
- In rule 3 integration over τ replaced by summation over ω_m under consideration of frequency conservation on vertices:

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



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

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



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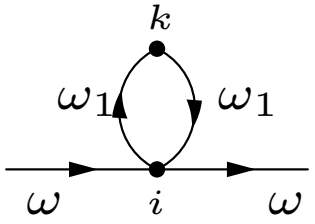

$$= J^2(\delta_{d(i,j),2} + 2\delta_{d(i,j),\sqrt{2}} + 2D\delta_{i,j}) C_1^{(0)}(\omega)^3$$
$$+ J^2 2D\delta_{i,j} \sum_{\omega_1} C_1^{(0)}(\omega_1) C_2^{(0)}(\omega, \omega_1 | \omega, \omega_1)$$

Equal-time correlations

- Momentum space density:

$$\hat{n}_{\mathbf{k}} = \langle \hat{\psi}^\dagger(\mathbf{k})\hat{\psi}(\mathbf{k})\rangle = |w(\mathbf{k})|^2 \underbrace{\sum_{i,j} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} \langle \hat{a}_i^\dagger \hat{a}_j \rangle}_{S(\mathbf{k})}, \quad \langle \hat{a}_i^\dagger \hat{a}_j \rangle = \lim_{\tau' \nearrow 0} G_1(\tau', i|0, j)$$

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- Quasi-momentum distribution:

$$S(\mathbf{k}) = K_0 + K_1 \frac{J(\mathbf{k})}{U} + K_2 \frac{J^2(\mathbf{k})}{U^2} + \dots, \qquad J(\mathbf{k}) = 2J \sum_{l=1}^{3} \cos(k_l a)$$

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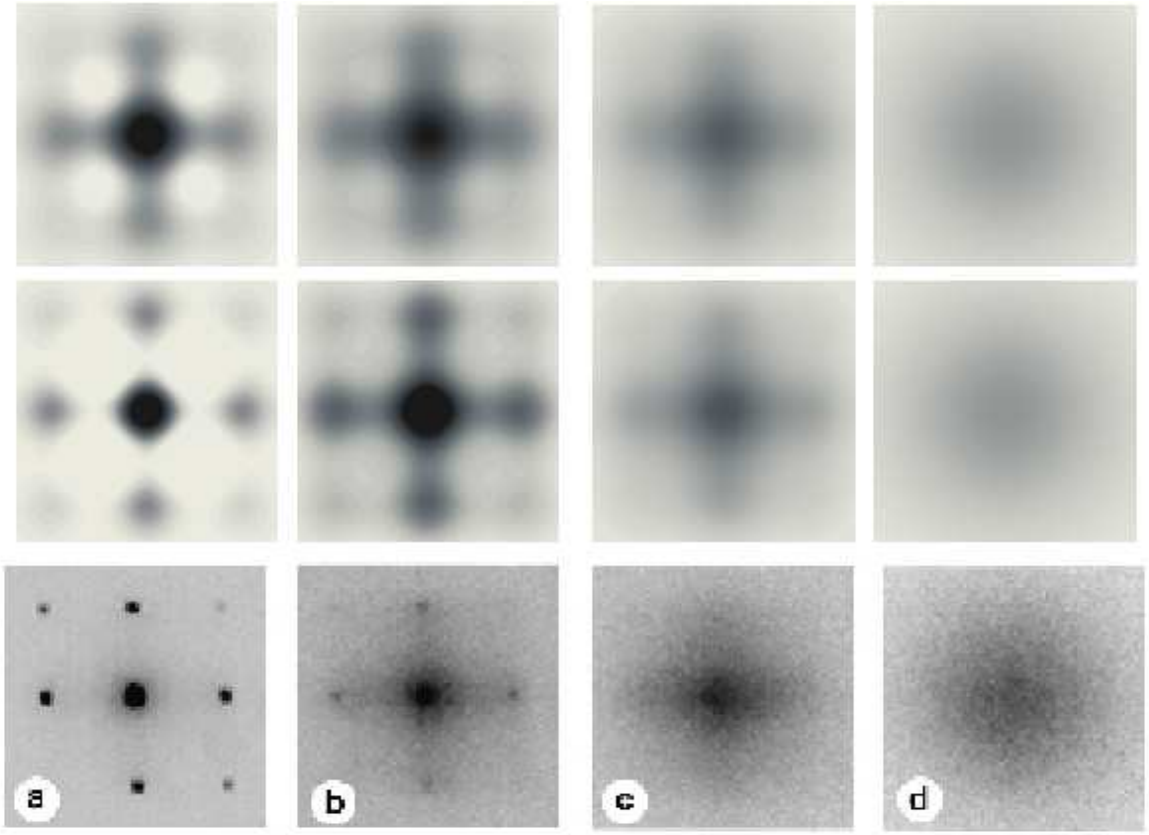
- Lowest orders:

$$G_1^{(0)}(0, i|j, 0) = \frac{\delta_{ij}}{\mathcal{Z}^{(0)}} \sum_n n e^{-\beta E_n}$$

$$G_1^{(1)}(0, i|j, 0) = \frac{J 2 \delta_{d(i,j),1}}{U \mathcal{Z}^{(0)2}} \sum_{n,k} \frac{n(n+1)}{(n-k+1)(k-n+1)} e^{-\beta(E_n + E_k)}$$

Time-of-flight pictures



first-order calculation ($T = 0$)

second-order calculation ($T = 0$)

experimental absorption pictures

(a) $V_0 = 8E_R$, (b) $V_0 = 14E_R$, (c) $V_0 = 18E_R$, and (d) $V_0 = 30E_R$

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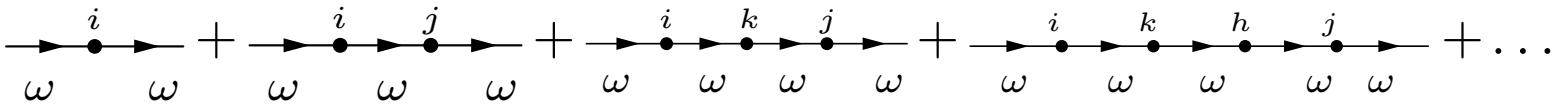
$\tilde{G}_1(\omega; i, j) =$ 

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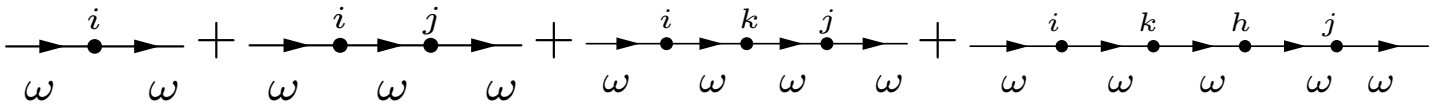
$\tilde{G}_1(\omega; i, j) =$ 

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- Summed most easily in Fourier space:

$$\tilde{G}_1^{(1)}(\omega, \mathbf{k}) = \frac{C_1^{(0)}(\omega)}{1 - J(\mathbf{k})\, C_1^{(0)}(\omega)}\,, \quad \tilde{G}_1^{(1)}(0, \mathbf{0}) = \frac{C_1^{(0)}(0)}{1 - 2DJC_1^{(0)}(0)}$$

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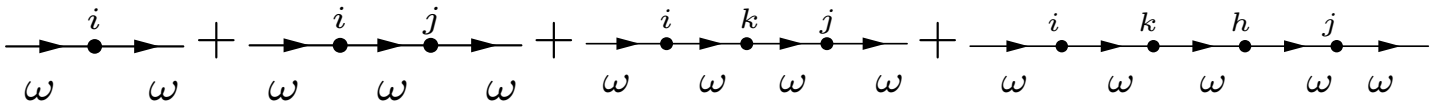
$\tilde{G}_1(\omega; i, j) =$ 

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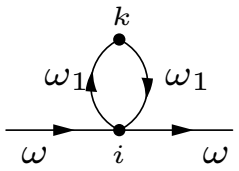
- Neglected contributions like 

vanish at least as $1/D$ for $D \to \infty$

Phase boundary

- Phase boundary given by:

$$2DJ_c = \frac{\sum_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n}\left(\frac{n+1}{E_{n+1}-E_n} - \frac{n}{E_n - E_{n-1}}\right)} \xrightarrow{T\to 0} = \frac{1}{\frac{n+1}{E_{n+1}-E_n} - \frac{n}{E_n - E_{n-1}}}$$

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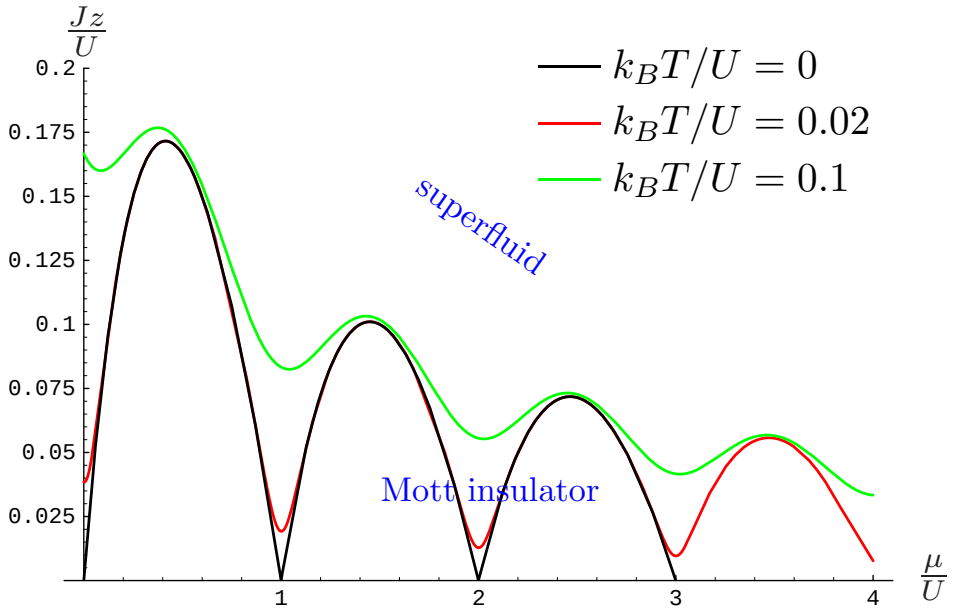
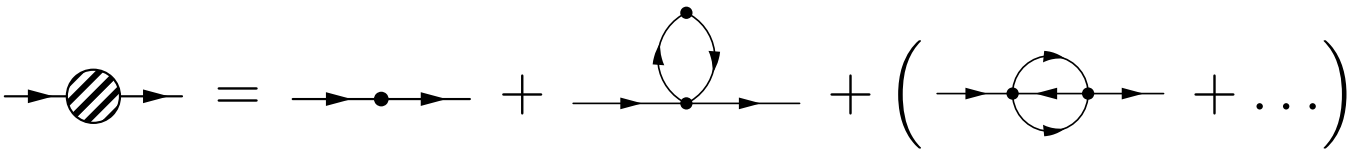
- Same result as obtained by mean-field theory ($z = 2D$):



Beyond mean field

- Replace  by sum over all one-particle irreducable diagrams:



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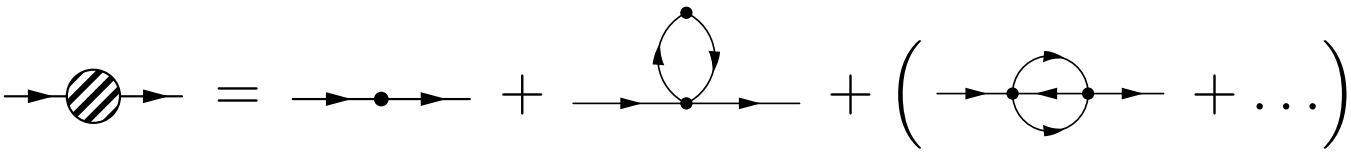

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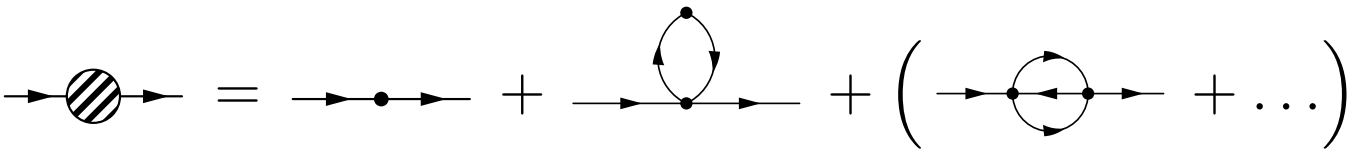

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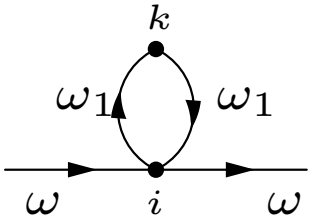
- Approximated by considering only the first two terms in 

Calculation of one-loop diagram

$$2D\delta_{i,j}J^2G_1^{(2B)}(\omega) =$$



$$= \frac{2D\delta_{i,j}}{\mathcal{Z}^{(0)2}}\Bigg(\frac{1}{U^2}\sum_{n,k} e^{-\beta(E_n+E_k)}$$

$$\times\Bigg\{\frac{(k+1)(n-1)n\left[k^2+2(n-1)^2-\mu^2+2k(2-2n-\mu)\right]}{(k-n+1)^2(k-2n+\mu)(1-n+\mu)^2}$$

$$+\ \text{7 more terms}\Bigg\} - C_1^{(0)}(\omega)^3$$

$$+\beta\Bigg\{\sum_{n,k}\left[\frac{(n+1)k}{k-n+1}+\frac{n(k+1)}{n-k+1}\right]\left[\frac{n+1}{n-\mu-i\omega}-\frac{n}{n-1-\mu-i\omega}\right]e^{-\beta(E_n+E_k)}$$

$$-C_1^{(0)}(\omega)\sum_{n,k}\left[\frac{(n+1)k}{k-n+1}+\frac{n(k+1)}{n-k+1}\right]e^{-\beta(E_n+E_k)}\Bigg\}\Bigg)$$

One-loop corrected phase boundary

- 2nd order resummed Green's function:

$$\tilde{G}_1^{(2)}(\omega, \mathbf{k} = \mathbf{0}) = \frac{C_1^{(0)}(\omega)}{1 - J2DC_1^{(0)}(\omega) + J^2 2DG_1^{(2B)}(\omega)/C_1^{(0)}(\omega)}$$

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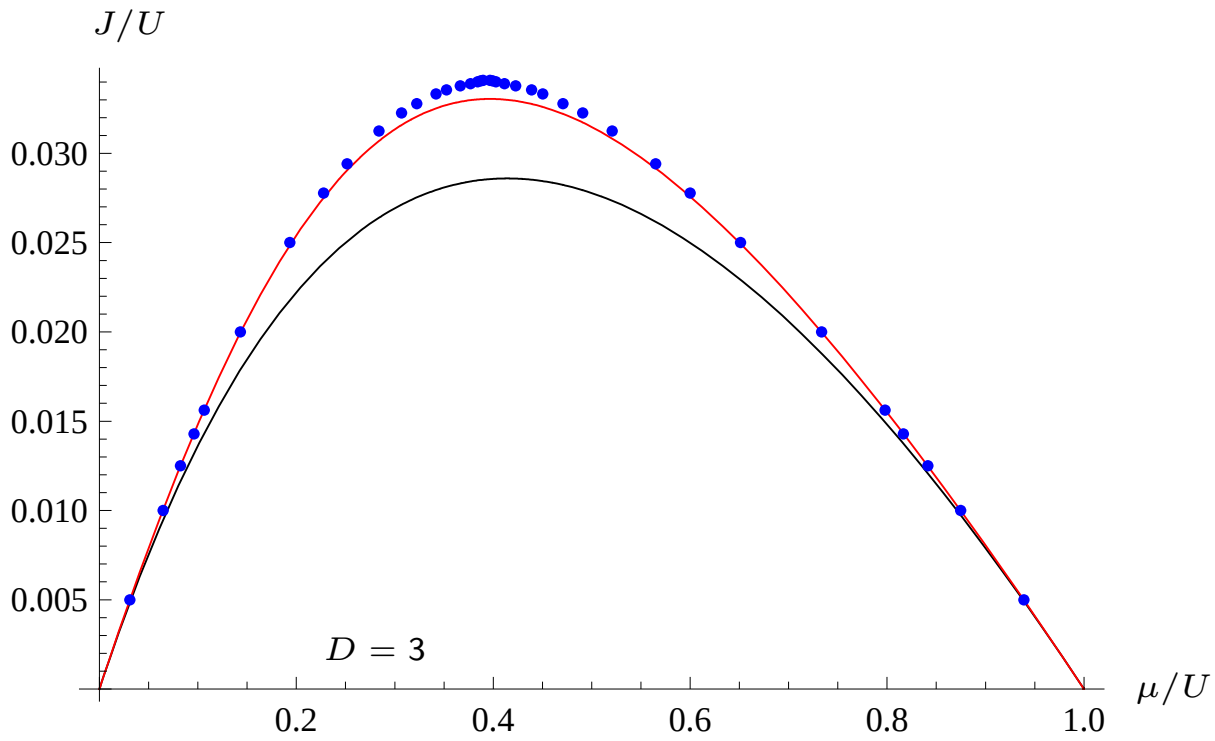
- Phase boundary

$$J_c = 1/\left\{C_1^{(0)}(0)D - \sqrt{2DG_1^{(2B)}(0)/C_1^{(0)}(0) + D^2 C_1^{(0)2(0)}}\right\}$$

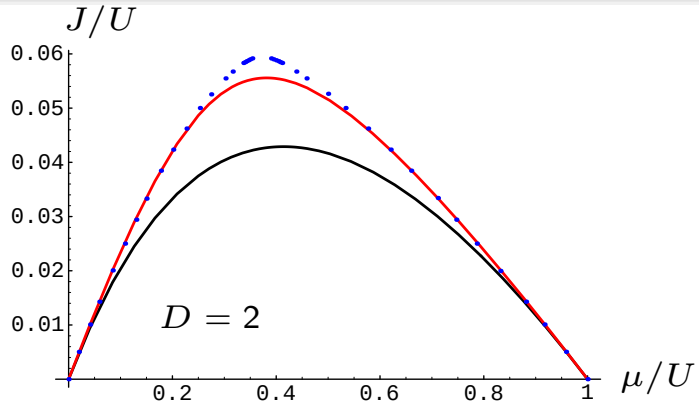
- In $T=0$ limit same result as E. Santos

Comparison with simulations for $T = 0$

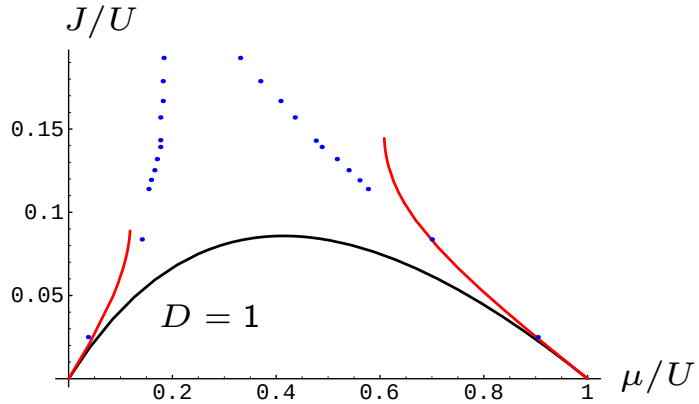


Capogrosso-Sansone et. al.
PRB **75**, 134302 (2007)

$n = 1$. Black: First order (Mean field)
Red: Second order

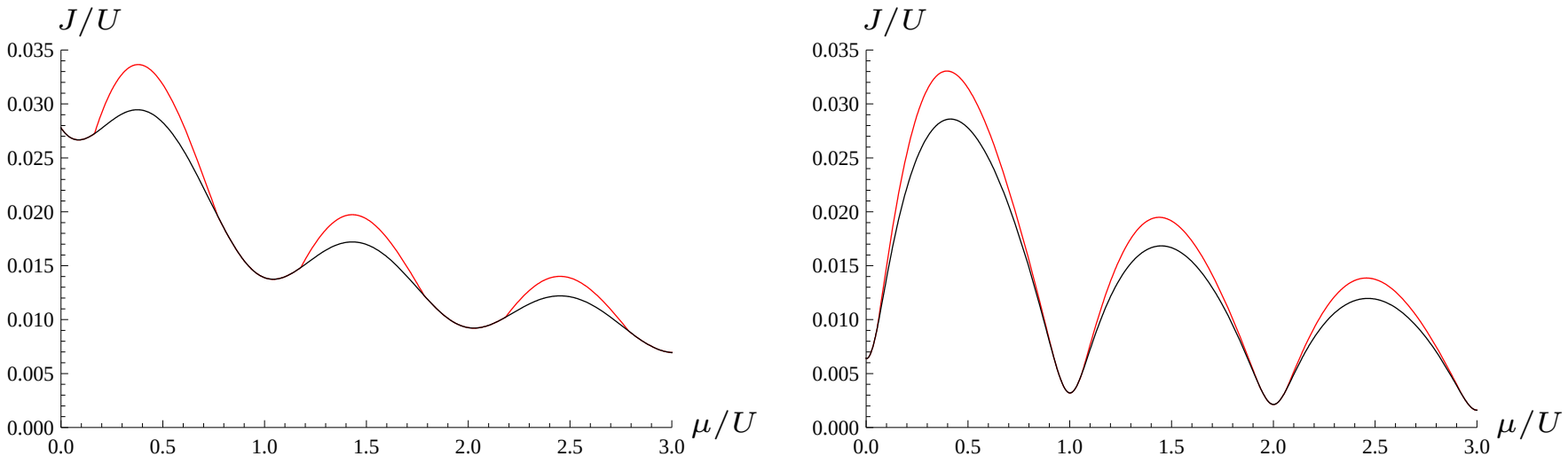


Capogrosso-Sansone et. al.
arXiv:0710.2703v3 (2007)



Niyaz, et. al.
PRB **44**, 7143 (1991)

Finite-temperature phase diagram



$D = 3$. Black: 1st order. Red: 2nd Order. Left: $T = 0.1\,U$. Right: $T = 0.02\,U$

- Temperature effects small at tip of lobe
- Second-order correction largest at zero temperature

Real-time Green's function

- Dynamic properties determined by retarded Green's function in real-time:

$$G_1(t', j'|, t, j) = \Theta(t - t')\frac{i}{\mathcal{Z}}\mathrm{Tr}\left\{e^{-\beta\hat{H}}\left[\hat{a}_{j,\mathsf{H}}(t), \hat{a}^{\dagger}_{j',\mathsf{H}}(t')\right]\right\}$$

- Can be obtained by analytic continuation of imaginary-time result. Easily done by replacing

$$i\omega_m \longrightarrow \omega + i\eta$$

- Zeroth order:

$$G_1^{(0)}(\omega; i, j) = \frac{\delta_{i,j}}{\mathcal{Z}^{(0)}}\sum_n\left[\frac{(n+1)}{E_{n+1} - E_n - \omega - i\eta} - \frac{n}{E_n - E_{n-1} - \omega - i\eta}\right]e^{-\beta E_n}$$

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- Dispersion relation of pairs:

$$\omega_{\mathrm{ph}}(\mathbf{k}) = \omega_1(\mathbf{k}) - \omega_2(\mathbf{k}) = \sqrt{U^2 - UJ(\mathbf{k})(4n+2) + J(\mathbf{k})^2}$$

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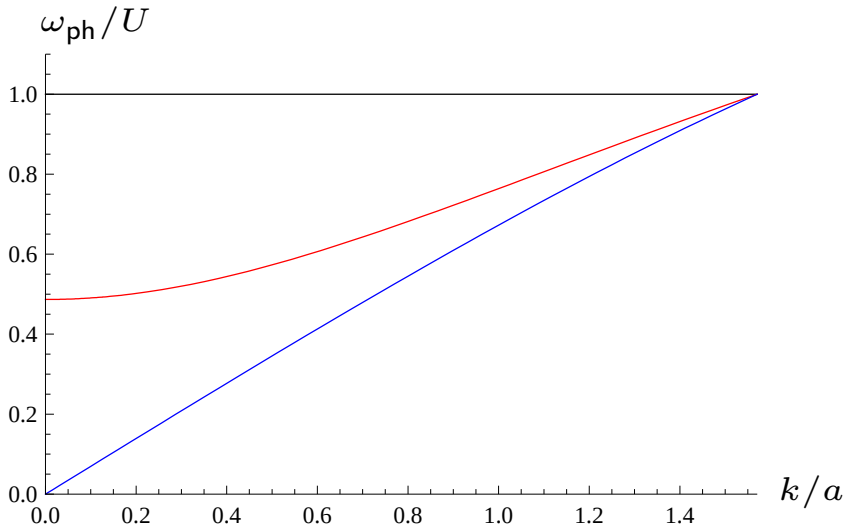
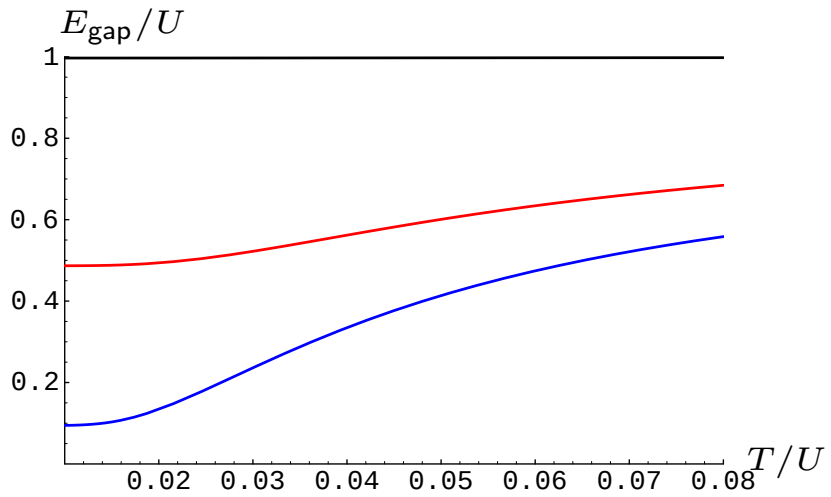


$n = 1$, $T = 0$. Black: $J = 0$

Red: $2DJ = 0.13\,U$

Blue: $2DJ = 2DJ_c = 0.172\,U$



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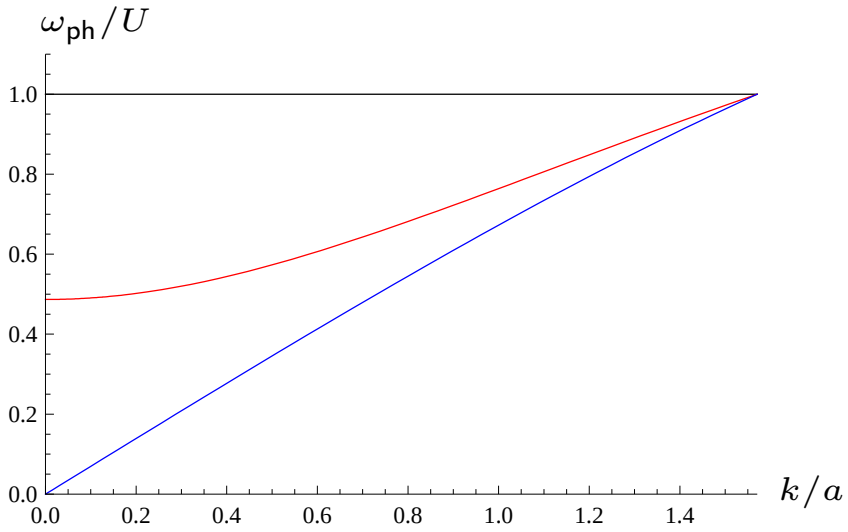

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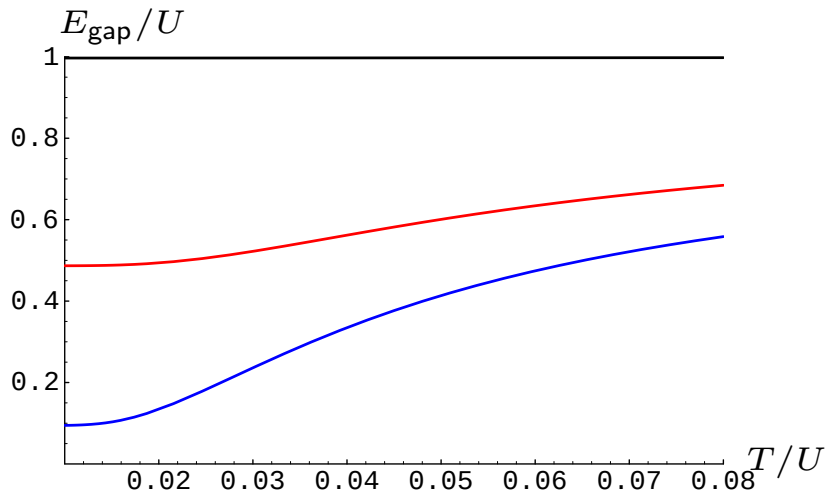

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- Gap vanishes when hopping reaches critical value.
  J_c: Hopping at tip of lobe
- Gap experimentally measurable. Could serve as thermometer.

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