

Quantum Phase Diagram of Bosons in Optical Lattices

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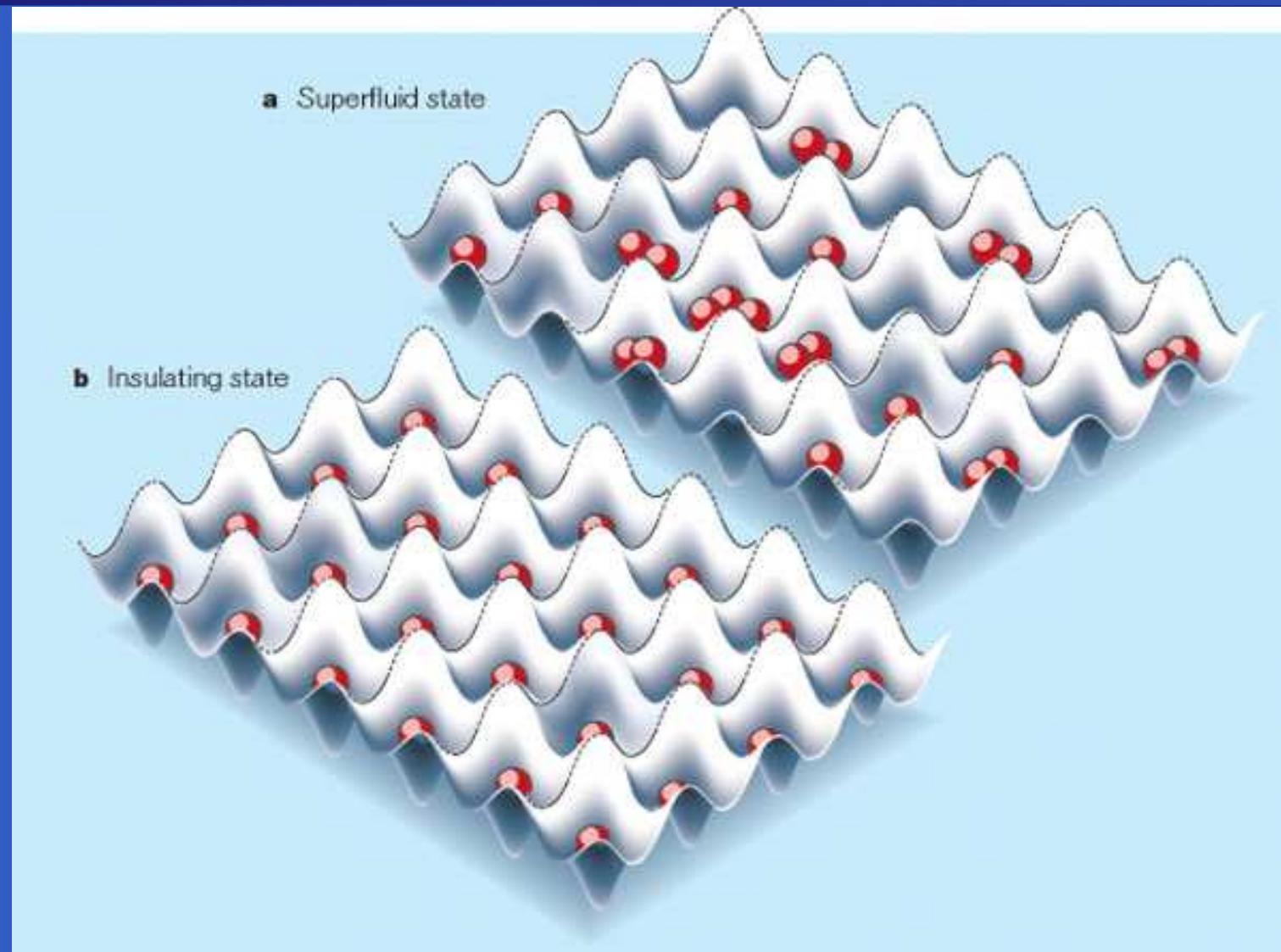


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Outline of the talk

1. Experimental facts
2. Second-quantized Hamiltonian
3. Mean-field theory
4. Corrections to mean-field theory
5. Second method
6. Perturbation theory
7. Results
8. Perspectives

1 - Experimental facts



2 - Second-quantized Hamiltonian

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

Wannier decomposition: $\hat{\psi}(\mathbf{x}) = \sum_i \hat{a}_i w(\mathbf{x} - \mathbf{x}_i)$

Bose-Hubbard Hamiltonian:

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

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

Matrix elements:

$$\begin{cases} t = - \int d^3x w^*(\mathbf{x}) \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right\} w(\mathbf{x}) \\ U = \frac{4\pi a \hbar^2}{m} \int d^3x |w(\mathbf{x})|^4 \end{cases}$$

3 - Mean-field theory

$$\sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j \rightarrow 2D \sum_i (\psi^* \hat{a}_i + \psi \hat{a}_i^\dagger - |\psi|^2)$$

Local Hamiltonian:

$$\hat{H}_{\text{MF}} = \sum_i \left[-2Dt \left(\psi^* \hat{a}_i + \psi \hat{a}_i^\dagger - |\psi|^2 \right) + \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i \right]$$

Partition function: $Z = \text{Tr} \left[e^{-\beta \hat{H}_{\text{MF}}(\psi^*, \psi)} \right] = e^{-\beta F_{\text{MF}}(\psi^*, \psi)}$

Self-consistency relations:

$$\begin{cases} \frac{\partial F_{\text{MF}}}{\partial \psi} = 0 \\ \frac{\partial F_{\text{MF}}}{\partial \psi^*} = 0 \end{cases} \implies \begin{cases} \langle \hat{a}_i^\dagger \rangle = \psi^* \\ \langle \hat{a}_i \rangle = \psi \end{cases}$$

4 - Corrections to mean-field theory

Introduction of smallness parameter:

$$\hat{H}(\eta, \psi^*, \psi) = \hat{H}_{\text{MF}}(\psi^*, \psi) + \eta \left[\hat{H}_{\text{BH}} - \hat{H}_{\text{MF}}(\psi^*, \psi) \right]$$

Partition function: $Z = \text{Tr} \left[e^{-\beta \hat{H}(\eta, \psi^*, \psi)} \right] = e^{-\beta F(\eta, \psi^*, \psi)}$

Extremization of free energy:

$$\begin{cases} \frac{\partial F}{\partial \psi} = 0 \\ \frac{\partial F}{\partial \psi^*} = 0 \end{cases} \implies \text{Interpretation within VPT}$$

4.1 - Procedure

1. Expansion in η defines level of approximation
 - Zeroth order: Mean-field phase diagram
 - First order: No shift of phase boundary
 - Second order: Quantum correction to phase boundary

2. Landau expansion:

$$F^{(N)}(\eta, \psi^*, \psi) = N_S \left[a_0^{(N)}(\eta) + a_2^{(N)}(\eta)|\psi|^2 + a_4^{(N)}(\eta)|\psi|^4 + \dots \right]$$

Here $a_{2p}^{(N)}(\eta)$ is truncated expansion in η up to order N of $a_{2p}(\eta)$:

$$\begin{cases} a_2(\eta) = (2Dt)^2(1-\eta)^2 \sum_{m=0}^{\infty} (-t\eta)^m \alpha_2^{(m)} + 2Dt(1-\eta) \\ a_{2p}(\eta) = (2Dt)^{2p}(1-\eta)^{2p} \sum_{m=0}^{\infty} (-t\eta)^m \alpha_{2p}^{(m)} \quad ; \quad p \neq 1 \end{cases}$$

4.2 - Phase diagram

Second-order phase transition $\iff a_4^{(N)}(\eta = 1) > 0$

Phase boundary: $a_2^{(N)}(\eta = 1) = 0$

General structure:

$$\begin{cases} a_2^{(0)}(\eta = 1) = \alpha_2^{(0)} t^2 + 2Dt \\ a_2^{(N)}(\eta = 1) = (-1)^N t^2 \left[\alpha_2^{(N)} t^N + \alpha_2^{(N-1)} t^{N-1} \right] ; \quad N \geq 1 \end{cases}$$

Phase boundary:

$$\begin{cases} t_c^{(0)} = -\frac{2D}{\alpha_2^{(0)}} \\ t_c^{(N)} = -\frac{\alpha_2^{(N-1)}}{\alpha_2^{(N)}} ; \quad N \geq 1 \end{cases}$$

4.3 - Explicit formulas

$$\begin{cases} \alpha_2^{(0)} = \frac{1+b}{\mu(b-1)} \\ \alpha_2^{(1)} = \frac{2D(1+b)^2}{\mu^2(b-1)^2} \\ \alpha_2^{(2)} = \frac{4D[D(b-3)(b+1)^3 - 3b(b-3+4b^2-2b^3)]}{(b-3)(b-1)^3\mu^3} \end{cases}$$

Here: $n = 1$ and $b = \mu/U$

$$\begin{cases} \frac{t_c^{(0)}}{U} = \frac{(1-b)b}{2D(b+1)} \\ \frac{t_c^{(1)}}{U} = \frac{(1-b)b}{2D(b+1)} \\ \frac{t_c^{(2)}}{U} = \frac{b(b-3)(b-1)(b+1)^2}{6b(b-3+4b^2-2b^3)-2D(b-3)(b+1)^3} \end{cases}$$

5 - Second method

Bose-Hubbard Hamiltonian with current:

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

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

Legendre transformation: $\Gamma(\psi^*, \psi) = \psi^* J + \psi J^* - F/N_s$

$$\frac{\partial \Gamma}{\partial \psi^*} = J \quad ; \quad \frac{\partial \Gamma}{\partial \psi} = J^*$$

Physical limit of vanishing current:

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

5.1 - Details

$$F(J^*, J) = F_0 + \sum_{n=1}^{\infty} c_{2n} |J|^{2n}$$

$$\Gamma(\psi^*, \psi) = -F_0 + \frac{1}{c_2} |\psi|^2 - 3 \frac{c_4}{c_2^4} |\psi|^4 + \dots$$

with: $c_{2p} = \sum_{n=0}^{\infty} (-t)^n \alpha_{2p}^{(n)}$

Remark: $\alpha_{2p}^{(n)}$ are the same used for the first method.

Phase boundary:

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

5.2 - Phase boundary

First order: $t_c^{(1)} = -\frac{\alpha_2^{(0)}}{\alpha_2^{(1)}}$

Remark: Identical to mean-field phase boundary.

Second order:

$$t_c^{(2)} = \frac{\bar{\alpha}_1}{2(\bar{\alpha}_2 - \bar{\alpha}_1^2)} \pm \frac{1}{2(\bar{\alpha}_2 - \bar{\alpha}_1^2)} \sqrt{\bar{\alpha}_1^2 - 4(\bar{\alpha}_1^2 - \bar{\alpha}_2)}$$

with: $\bar{\alpha}_1 = \frac{\alpha_2^{(1)}}{\alpha_2^{(0)}}$; $\bar{\alpha}_2 = \frac{\alpha_2^{(2)}}{\alpha_2^{(0)}}$

Note: Choose the smallest critical $t_c^{(2)}$.

6 - Perturbation theory

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$$

here $\hat{H} = \hat{H}_0 + \lambda \hat{V}$.

Perturbative series in λ :

$$|\Psi_n\rangle = \sum_{k=0}^{\infty} \lambda^k |\Psi_n^{(k)}\rangle \quad ; \quad E_n = \sum_{k=0}^{\infty} \lambda^k E_n^{(k)}$$

with: $E_n^{(k)} = \langle \Psi_n^{(0)} | \hat{V} | \Psi_n^{(k-1)} \rangle$

$$|\Psi_n^{(k)}\rangle = \sum_{m \neq n} |\Psi_m^{(0)}\rangle \frac{\langle \Psi_m^{(0)} | \hat{V} | \Psi_n^{(k-1)} \rangle}{E_n^{(0)} - E_m^{(0)}} - \sum_{l=1}^k E_n^{(l)} \sum_{m \neq n} |\Psi_m^{(0)}\rangle \frac{\langle \Psi_m^{(0)} | \Psi_n^{(k-l)} \rangle}{E_n^{(0)} - E_m^{(0)}}$$

6.1 - Diagrammatic notation

$$E_n^{(1)} = \langle \Psi_n^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle = \text{---●---}$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{1}{E_n^{(0)} - E_m^{(0)}} \langle \Psi_n^{(0)} | \hat{V} | \Psi_m^{(0)} \rangle \langle \Psi_m^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle = \text{---●---●---}$$

$$\begin{aligned} E_n^{(3)} &= \sum_{m_1 \neq n} \sum_{m_2 \neq n} \frac{1}{E_n^{(0)} - E_{m_1}^{(0)}} \frac{1}{E_n^{(0)} - E_{m_2}^{(0)}} \langle \Psi_n^{(0)} | \hat{V} | \Psi_{m_2}^{(0)} \rangle \\ &\quad \times \langle \Psi_{m_2}^{(0)} | \hat{V} | \Psi_{m_1}^{(0)} \rangle \langle \Psi_{m_1}^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle - \sum_{m_1 \neq n} \frac{1}{(E_n^{(0)} - E_{m_1}^{(0)})^2} \end{aligned}$$

$$\times \langle \Psi_n^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle \langle \Psi_n^{(0)} | \hat{V} | \Psi_{m_1}^{(0)} \rangle \langle \Psi_{m_1}^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle$$

$$= \text{---●---●---} - \text{---●---○---●---}$$

6.2 - Rules

- Each dot represents an interaction \hat{V} .
- The internal lines appearing between two consecutive dots are associated with the factor $\sum_{m \neq n} \frac{1}{(E_m^{(0)} - E_n^{(0)})^q} |\Psi_m^{(0)}\rangle\langle\Psi_m^{(0)}|$, and q is the number of lines linking the two given consecutive dots.
- If there is more than one line between two consecutive dots, each extra line is associated with an extra disconnected part of the diagram.
- The external lines are associated with the unperturbed bra and ket $\langle\Psi_n^{(0)}| \dots |\Psi_n^{(0)}\rangle$.

6.3 - More interaction terms

Example:

$$\hat{H} = \hat{H}_0 + \lambda \hat{V} + \sigma \hat{W}$$

$$\begin{cases} \hat{V} \rightarrow \bullet \\ \hat{W} \rightarrow \circ \end{cases}$$

$$\begin{aligned} E_n &= E_n^{(0)} + \lambda \text{---} \bullet \text{---} + \sigma \text{---} \circ \text{---} + \lambda\sigma \left(\text{---} \bullet \text{---} \circ \text{---} + \text{---} \circ \text{---} \bullet \text{---} \right) \\ &\quad + \lambda^2 \text{---} \bullet \text{---} \bullet \text{---} + \sigma^2 \text{---} \circ \text{---} \circ \text{---} + \dots \end{aligned}$$

Symmetries between diagrams if \hat{V} and \hat{W} are Hermitean:

$$\text{---} \bullet \text{---} \bullet \text{---} = \text{---} \circ \text{---} \bullet \text{---} \bullet \text{---} ; \quad \text{---} \bullet \text{---} \text{---} \bullet \text{---} = \text{---} \circ \text{---} \text{---} \circ \text{---}$$

6.4 - Lattice calculations

First approach:

$$\begin{aligned}\hat{H}(\eta, \psi^*, \psi) = & -t\eta \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j - 2Dt(1-\eta) \sum_i \left(\psi^* \hat{a}_i + \psi \hat{a}_i^\dagger - |\psi|^2 \right) \\ & + \sum_i \left[\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i \right]\end{aligned}$$

Second approach:

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

Note: Both Hamiltonians are essentially equivalent.

6.5 - Interaction terms in our case

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

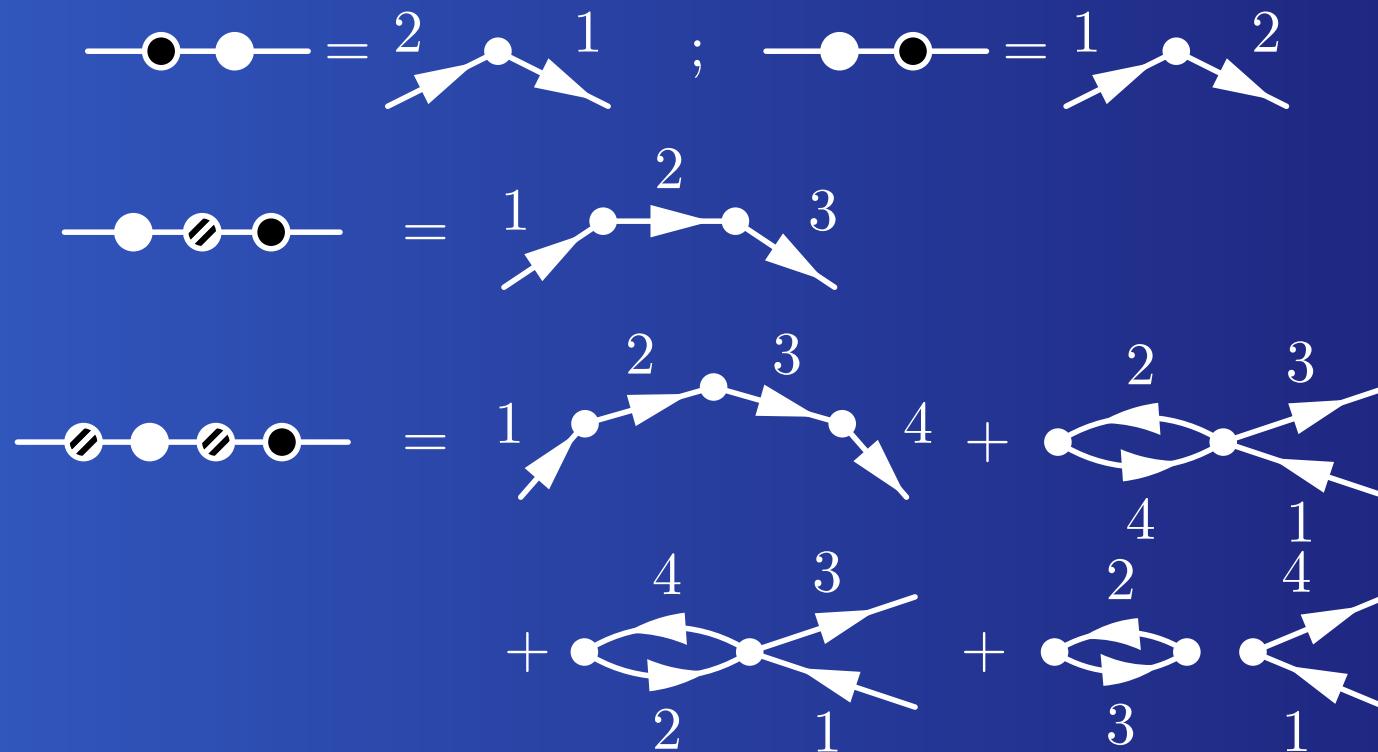
$$\begin{cases} \sum_i \hat{a}_i \rightarrow \bullet \\ \sum_i \hat{a}_i^\dagger \rightarrow \bullet \\ \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j \rightarrow \bullet\# \end{cases}$$

Ground-state energy:

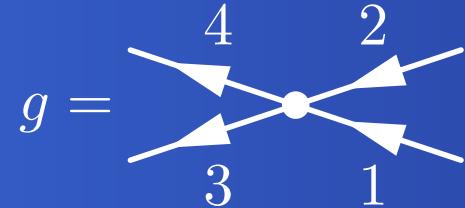
$$\begin{aligned} E_0 &= E_0^{(0)} + t^2 \text{---}\bullet\#\text{---} + |J|^2 \left(\text{---}\bullet\text{---}\bullet\text{---} + \text{---}\bullet\text{---}\bullet\text{---} \right) \\ &\quad + |J|^2 t \left(\text{---}\bullet\text{---}\bullet\#\text{---} + \text{---}\bullet\text{---}\bullet\#\text{---} + \text{---}\bullet\text{---}\#\text{---}\bullet \right. \\ &\quad \left. + \text{---}\bullet\#\text{---}\bullet\text{---} + \text{---}\#\text{---}\bullet\text{---} + \text{---}\#\text{---}\bullet\text{---} \right) + \dots \end{aligned}$$

6.6 - Individual processes

The previous diagrams can be split in their individual processes which are represented by arrow diagrams. For example:



6.7 - Evaluation

$$g = \text{Diagram} = N_s(n+1)(n+2) \frac{1}{(E_n^{(0)} - E_{n+1}^{(0)})^2} \frac{1}{E_n^{(0)} - E_{n+2}^{(0)}}$$


1. Create a particle at some site with N_s different possibilities:

$$g = N_s \left[\sqrt{n+1}/(E_n^{(0)} - E_{n+1}^{(0)}) \right] \dots$$

2. Create a second particle at the same position of the first:

$$g = N_s \left[\sqrt{n+1}/(E_n^{(0)} - E_{n+1}^{(0)}) \right] \left[\sqrt{n+2}/(E_n^{(0)} - E_{n+2}^{(0)}) \right] \dots$$

3. Annihilate one particle at the site of the two previously created particles:

$$g = N_s \left[\sqrt{n+1}/(E_n^{(0)} - E_{n+1}^{(0)}) \right] \left[\sqrt{n+2}/(E_n^{(0)} - E_{n+2}^{(0)}) \right] \left[\sqrt{n+2}/(E_n^{(0)} - E_{n+1}^{(0)}) \right] \dots$$

4. Annihilate the last particle:

$$g = N_s \left[\sqrt{n+1}/(E_n^{(0)} - E_{n+1}^{(0)}) \right] \left[\sqrt{n+2}/(E_n^{(0)} - E_{n+2}^{(0)}) \right] \left[\sqrt{n+2}/(E_n^{(0)} - E_{n+1}^{(0)}) \right] \sqrt{n+1}$$

6.8 - Coefficients

$$\alpha_2^{(0)} = 2 \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \end{array} 1 + 1 \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \end{array} 2$$

$$\alpha_2^{(1)} = 1 \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \\ | \quad | \\ \text{---} \end{array} 2 \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \end{array} 3 + 5 \text{ permutations}$$

$$\alpha_2^{(2)} = 1 \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \\ | \quad | \\ \text{---} \\ | \quad | \\ \text{---} \end{array} 2 \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \\ | \quad | \\ \text{---} \end{array} 3 \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \\ | \quad | \\ \text{---} \end{array} 4 + 23 \text{ permutations}$$

$$+ \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \\ | \quad | \\ \text{---} \end{array} 2 \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \\ | \quad | \\ \text{---} \end{array} 3 \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \\ | \quad | \\ \text{---} \end{array} 4 + 15 \text{ permutations}$$

$$+ \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \\ | \quad | \\ \text{---} \end{array} 4 \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \\ | \quad | \\ \text{---} \end{array} 1 \begin{array}{c} \text{---} \\ | \quad | \\ \text{---} \\ | \quad | \\ \text{---} \end{array} 4$$

$$+ 7 \text{ permutations}$$

6.9 - Explicit results

$$\alpha_2^{(0)} = \frac{b+1}{U(b-n)(b+1-n)}$$

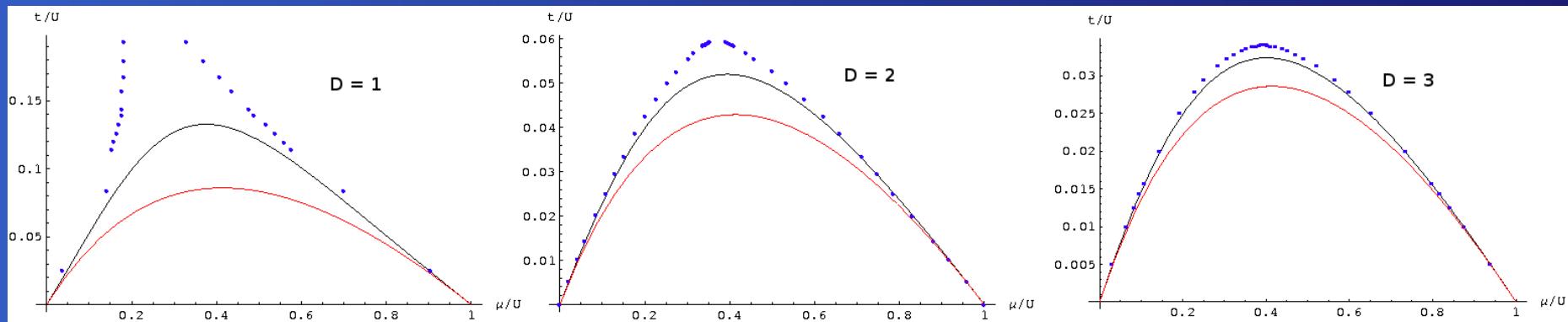
$$\alpha_2^{(1)} = \frac{2D(b+1)^2}{U^2(b-n)^2(b+1-n)^2}$$

$$\begin{aligned}\alpha_2^{(2)} &= 2D \left\{ 2D(b+1)^3(b-2-n)(b+3-n) + n(b-n)(b+1-n) \right. \\ &\quad \times (1+n)(4+3b+2n) \left[-3 - 2n + 2(b^2 + b - 2bn + n^2) \right] \left. \right\} \\ &/ [U^3(b-n-2)(b-n)^3(b+1-n)^3(b+3-n)]\end{aligned}$$

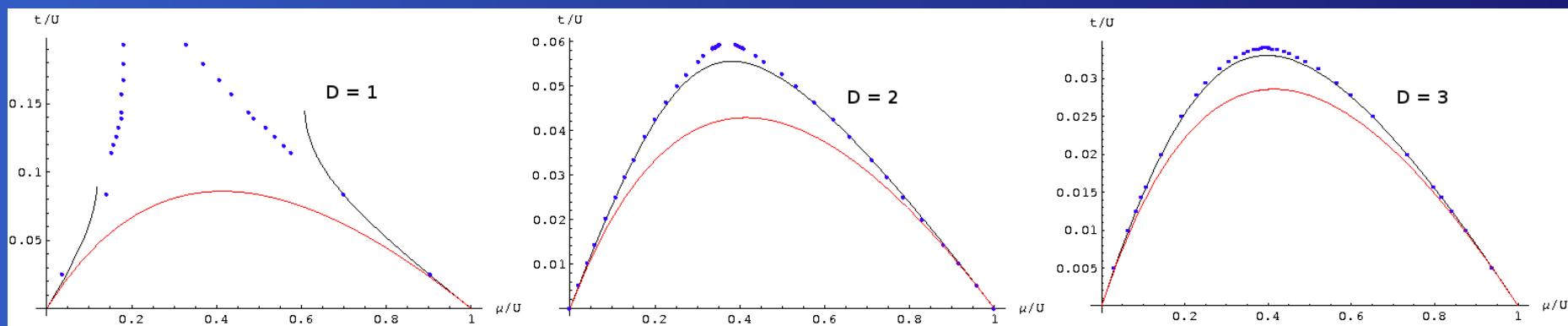
Here n is the number of particles at each site and $b = \mu/U$.

7 - Results

First Method:



Second method:



8 - Perspectives

- Automatization for higher orders
- Resummation
- Extension for $T \neq 0$
- Phase boundary from diverging Green's function