HIGH-ORDER STRONG-COUPLING EXPANSION FOR BOSE-HUBBARD MODEL

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Abstract

We apply the process-chain method [1,2] in order to calculate the quantum phase boundary between the Mott insulator and the superfluid phase for bosons in a hypercubic optical lattice within the strong-coupling method [3]. The respective results in 1d, 2d, and 3d, which are obtained up to 12th order and then extrapolated to infinite order, turn out to coincide almost with high-precision Quantum-Monte Carlo results. Finally, we show that these high-order strong-coupling results also follow from a high-order effective potential calculation [2,4,5].

High-order strong-coupling expansion

Bose-Hubbard model:

$$H = H' + H_0 , \quad H' = -t \sum_{\langle i,j \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i) , \quad H_0 = \sum_i \left[\frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - \mu \hat{n}_i \right] ,$$

where $\langle i,j \rangle$ represents nearest-neighbor sites, t denotes the hopping matrix element, $\hat{b}_i^\dagger (\hat{b}_i)$ creates (destroys) a bosonic particle on site i, U stand for the on-site repulsion, and μ is the chemical potential.

(I). Another form of Rayleigh-Schrödinger perturbation theory: Kato representation for the nth order perturbative contribution for the mth energy eigenvalue

$$E_m^{(n)} = \mathrm{Tr} \sum_{\alpha_l} S^{\alpha_1} H' S^{\alpha_2} H' ... H' S^{\alpha_{n+1}},$$

where

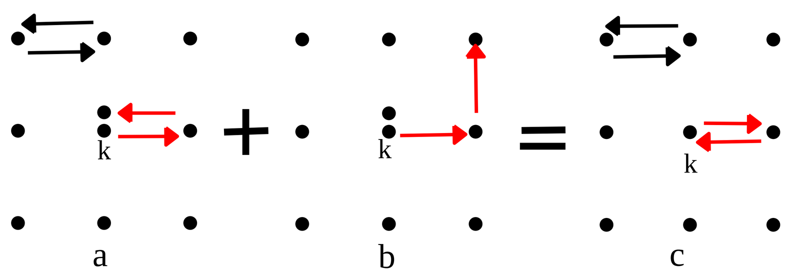
$$\sum_{l=1}^{n+1} \alpha_l = n-1, \alpha_l \geq 0, \qquad S^{\alpha_l} = \begin{cases} -|m\rangle\langle m| & \text{if } \alpha_l = 0 \\ \frac{|e\rangle\langle e|}{(E_m^0 - E_e^0)^{\alpha_l}} & \text{if } \alpha_l \neq 0. \end{cases}$$

Cyclic interchangeability of operators under the trace:

$$S^{\alpha_i} S^{\alpha_j} = \begin{cases} -S^0 & \alpha_i = \alpha_j = 0 \\ 0 & \alpha_i = 0, \alpha_j \neq 0 \text{ or } \alpha_i \neq 0, \alpha_j = 0 \\ S^{\alpha_i + \alpha_j} & \alpha_i \neq 0, \alpha_j \neq 0 \end{cases} \quad \Longrightarrow \quad \langle g | H' S^{\alpha_1'} H' ... S^{\alpha_{n-1}'} H' | g \rangle .$$

We obtain a number list called *Katolist*: $\langle \alpha_1 \alpha_2 ... \alpha_{n-1} \rangle \Longrightarrow (\alpha_1' \alpha_2' ... \alpha_{n-1}')$, e.g. $\langle 00120 \rangle = (012)$

(II). Generate the simplest arrow diagrams and their respective weights for each perturbative order. The problem of calculating the higher order strong-coupling results is that the ground state becomes degenerate when either a particle or a hole is added. As a consequence, we have to take into account all open diagrams:



The black processes (disconnected to site k) cancel with each other only red processes (connected to site k) need to be considered.

(III). Calculate perturbative energy contribution for each order, and obtain the coefficient $\beta_{u(d)}^{(i)}$ of the critical line by putting open diagram (b) plus close diagram (a) of additional particle (hole) state equal to close diagram (c) of the Mott insulator.

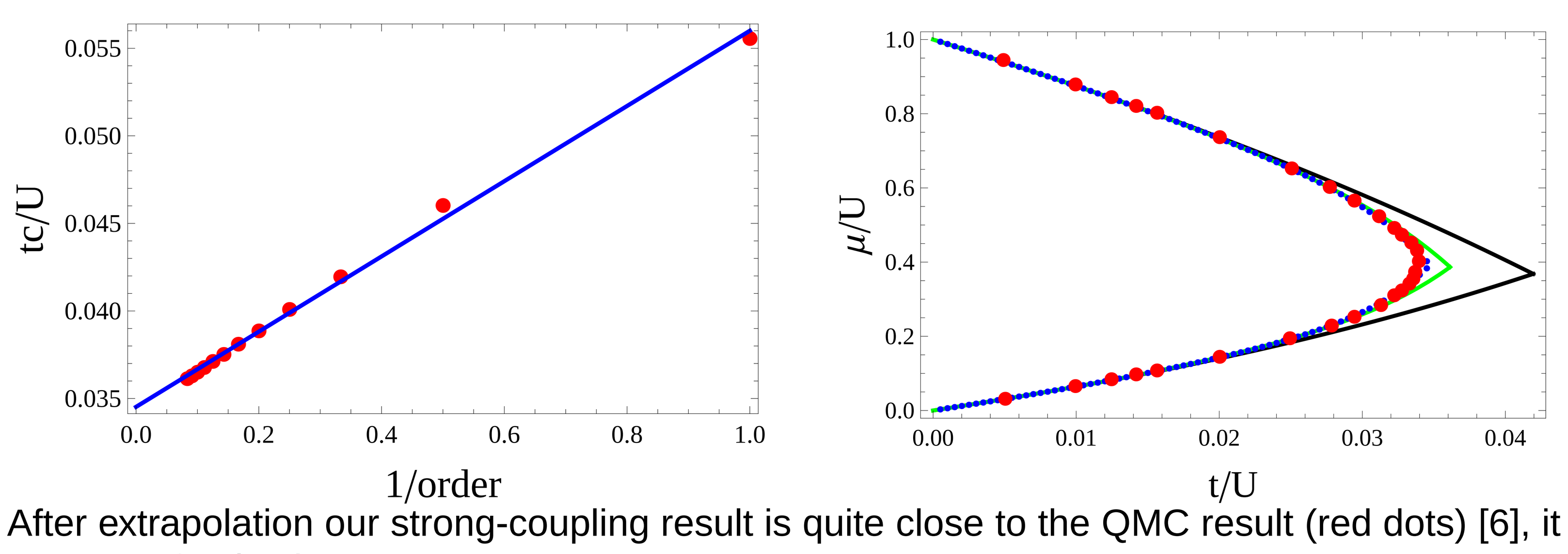
$$\text{particle}: \frac{\mu_u}{U} = 1 - \sum_i \beta_u^{(i)} \left(\frac{t}{U} \right)^i , \qquad \text{hole}: \frac{\mu_d}{U} = \sum_i \beta_d^{(i)} \left(\frac{t}{U} \right)^i .$$

Three-dimensional result

For 3d systems we obtain the upper and lower phase boundaries for the occupation number $n=1$ as follows:

i	1	2	3	4	5	6
$\beta_d^{(i)}$	6	36	720	10932	260400	4.92578E6
$\beta_u^{(i)}$	12	45	666	11904.75	244519	5.27784E6
i	7	8	9	10	11	12
$\beta_d^{(i)}$	1.27965E8	2.66526E9	7.30515E10	1.7065E12	4.53956E13	9.73239E14
$\beta_u^{(i)}$	1.21888E8	2.75967E9	7.22332E10	1.79457E12	3.92428E13	9.85176E14

Thus, the higher the order the closer is the strong-coupling phase boundary to the real phase boundary [6]. Extrapolating both for the critical point and for fixed μ we find that the extrapolation is well described with a linear fit as predicted in Ref. [3].



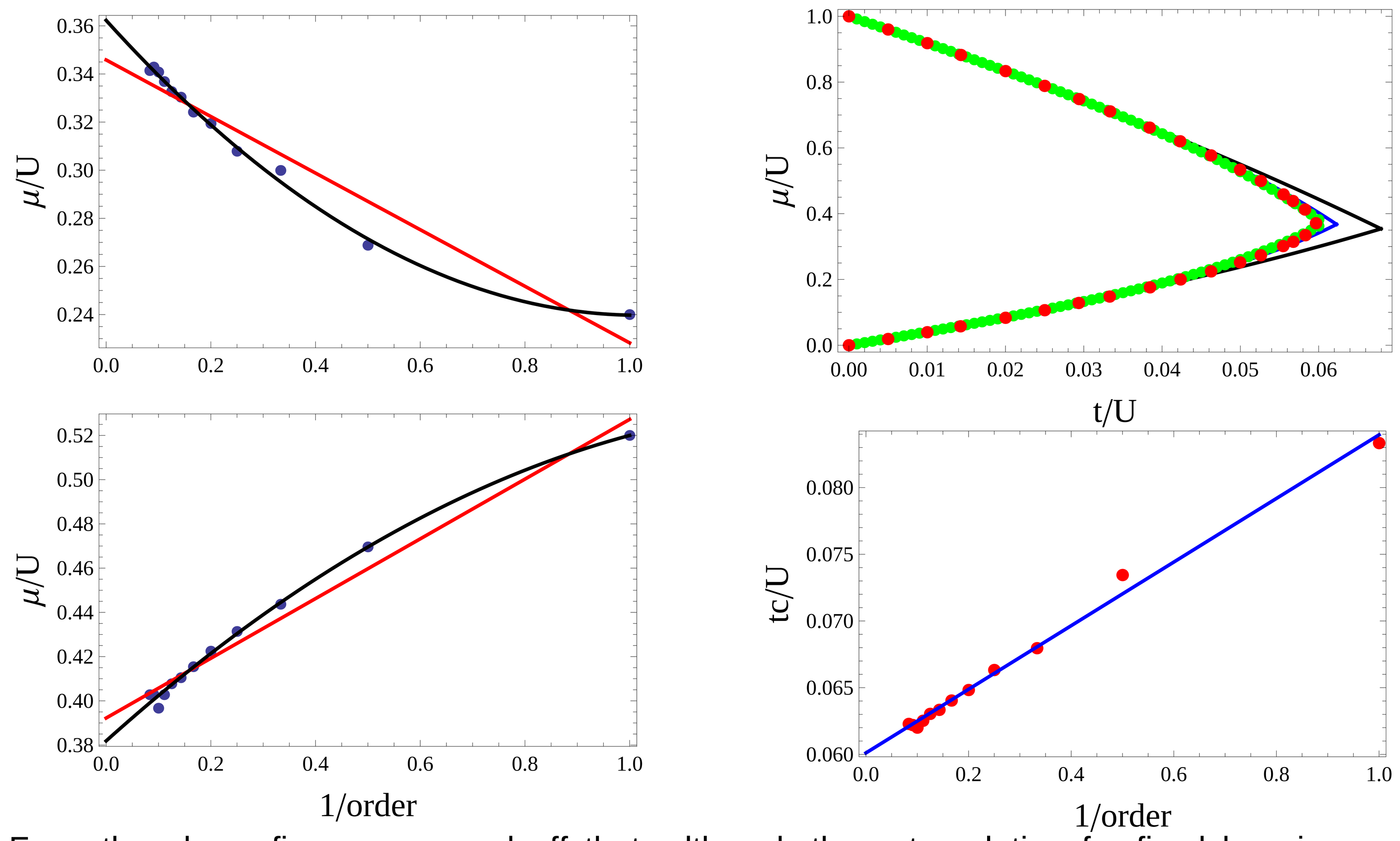
After extrapolation our strong-coupling result is quite close to the QMC result (red dots) [6], it has an error of only about one percent.

Two-dimensional result

For 2d systems higher order coefficients turn out to be negative

i	1	2	3	4	5	6
$\beta_d^{(i)}$	4	8	144	616	14832	101314
$\beta_u^{(i)}$	8	14	120	949.9	11447.4	150807
i	7	8	9	10	11	12
$\beta_d^{(i)}$	2.2195E6	1.37905E7	4.14857E8	6.51985E9	1.10675E11	-1.56698E12
$\beta_u^{(i)}$	1.77591E6	1.63398E7	4.8973E8	1.00904E10	-5.74011E10	-1.73184E12

so the higher-order results deviate slightly from the real phase boundary [7], which is unusual.



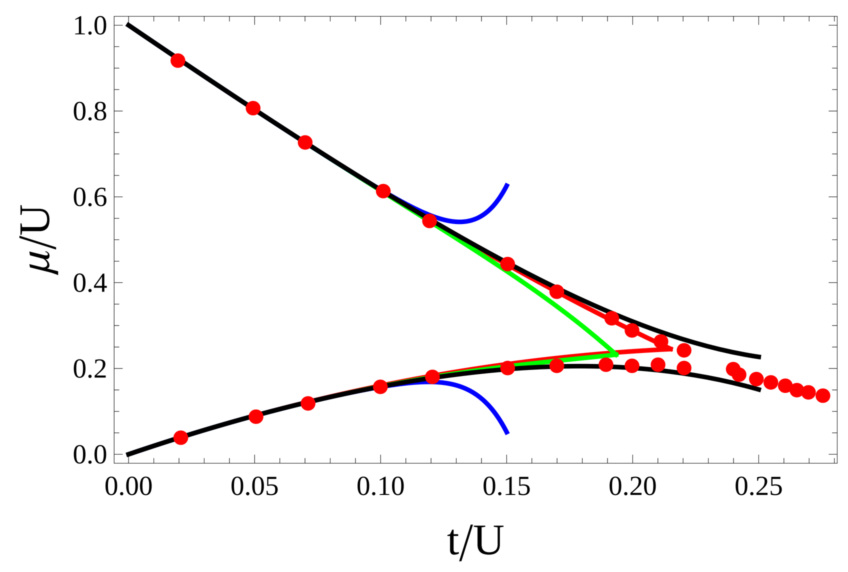
From the above figures we read off that, although the extrapolation for fixed hopping matrix element $t = 0.06U$ is rather quadratic than linear, the critical points for each order fit quite well with a linear extrapolation. Furthermore, due to the extrapolation we obtain a precise phase boundary result in comparison with QMC simulations (red dots) [7].

One-dimensional result

For 1d systems we yield

i	1	2	3	4	5	6
$\beta_d^{(i)}$	2	-4	0	-20	-21.3333	549.333
$\beta_u^{(i)}$	4	-1	-6	5.65	-95.0867	1772.91
i	7	8	9	10	11	12
$\beta_d^{(i)}$	-851.111	-51173.2	340065	7.65362E6	-8.63819E7	-9.30652E8
$\beta_u^{(i)}$	-2803.65	-124020	1.00836E6	1.41931E7	-2.51857E8	-5.02314E8

Thus, higher order perturbative results are even more weird than for 2d systems. This is illustrated by the 1d quantum phase diagram for $n=1$ where the strong-coupling results for 3rd (red), 5th (black), 6th (green), and 12th (blue) order are compared with DMRG results (red dots) [8,9]:



Although some higher order results do even not form a lobe, all results almost coincide for $\mu < 0.12$, so we can only consider these values as trustworthy. Note that the third-order result is quite close to the real phase boundary.

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