

High-order diagrammatic expansion around BCS

Polarized superfluid phase of the attractive Hubbard model

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[arXiv:2103.12038]

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*Polarized superfluid phase
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Polarized superfluid phase of the attractive Hubbard model

“Quantum 2021”

- superconductivity: Kamerlingh Onnes, 1911
- BCS theory: 1957
- 2021: BCS theory → exact

Unbiased approaches for fermionic \mathcal{N} -body problems

strongly interacting fermions: *solids & molecules, nuclei & neutron stars, QCD*

Challenge: large \mathcal{N} , thermo. lim. $\mathcal{N} \rightarrow \infty$

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analytics

1D, small \mathcal{N} , weakly correlated limits

Tensor network

1D: 😊

2D: harder (bond dimension $\rightarrow \infty$)

3D: ?

continuous space: ?

“bulk” Monte Carlo approaches

quantum
 d dim.

volume L^d

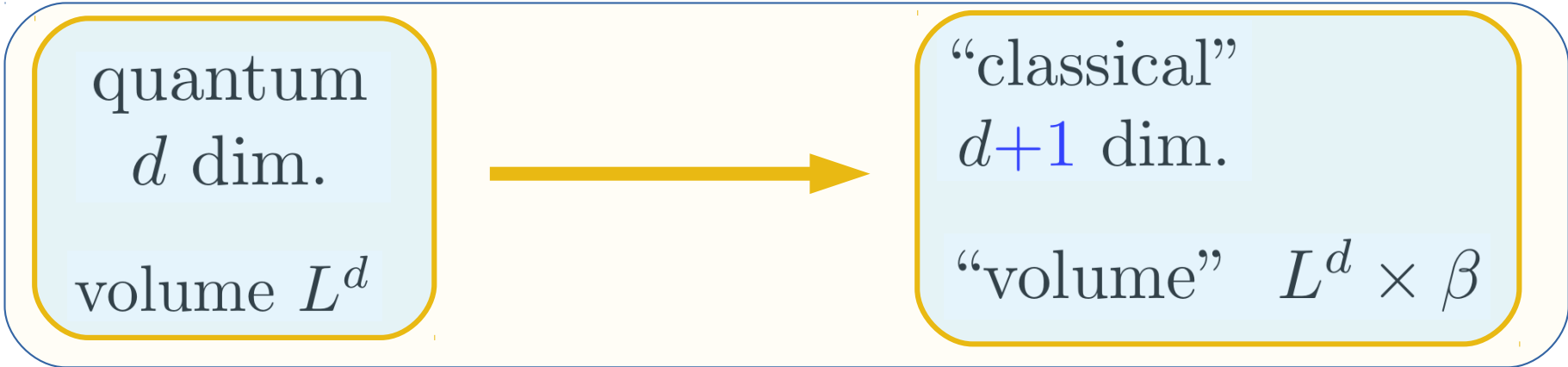


“classical”
 $d+1$ dim.

“volume” $L^d \times \beta$

- path integral $\mathbf{r}_1(\tau), \dots, \mathbf{r}_N(\tau)$
- **A**uxiliary **F**ield **Q**MC (*lattice QCD*)
- **D**eterminantal **D**iagrammatic **M**C (*CT-INT*)

“bulk” Monte Carlo approaches

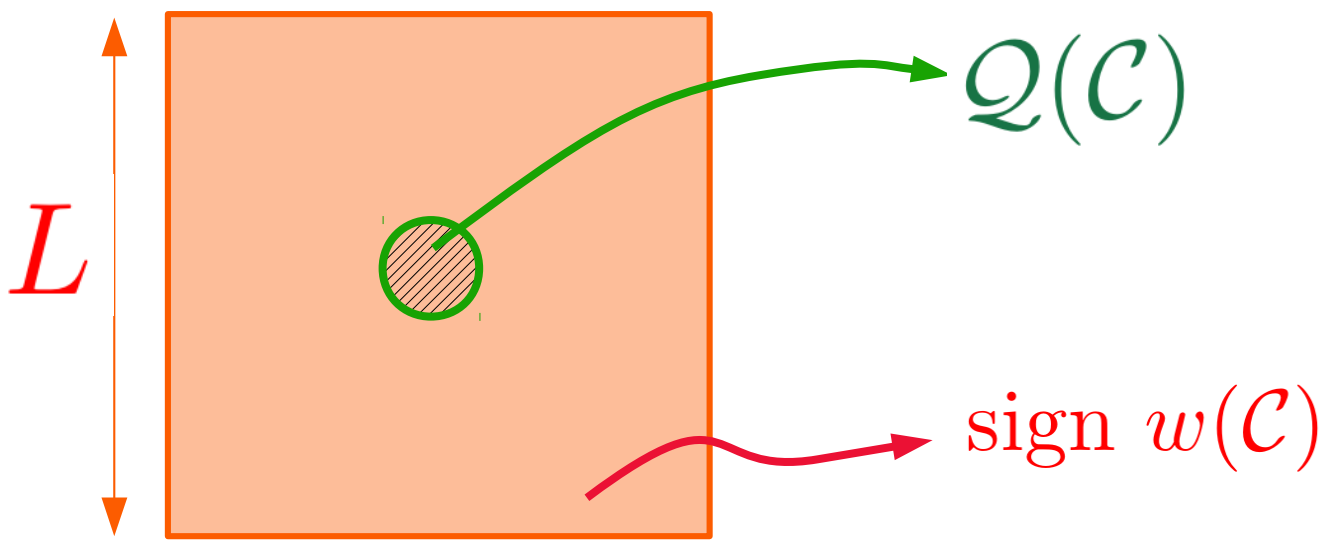


- path integral $\mathbf{r}_1(\tau), \dots, \mathbf{r}_N(\tau)$
- Auxiliary Field QMC (lattice QCD)
- Determinantal Diagrammatic MC (CT-INT)

except in special cases

fermion sign problem: $t_{\text{CPU}} \sim e^{\#\beta N}$

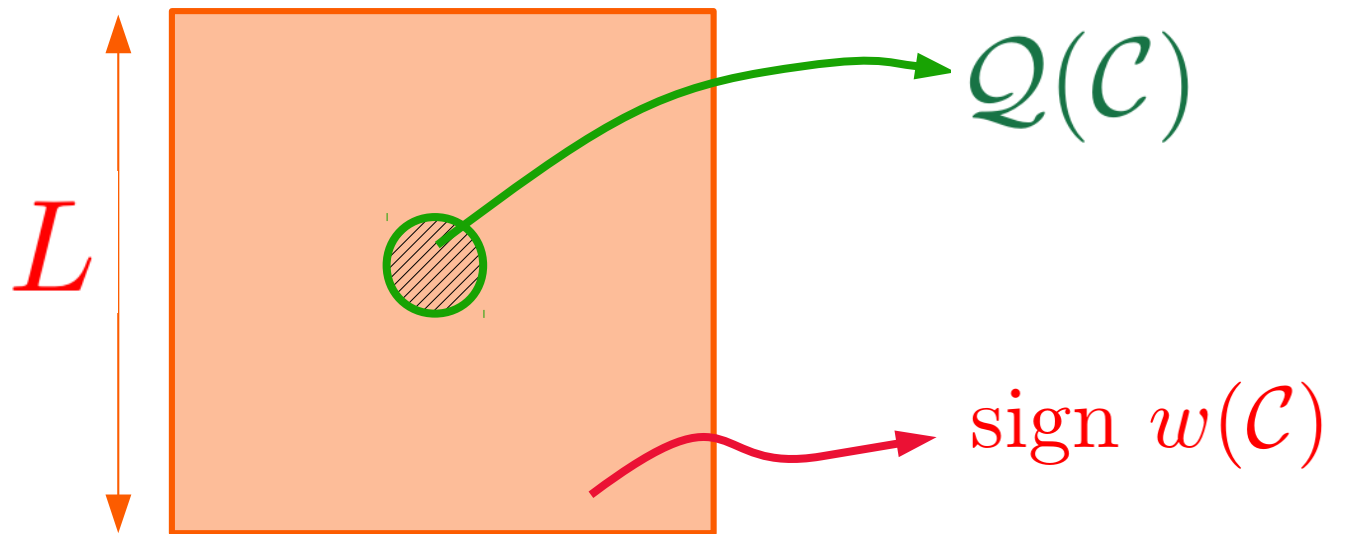
$$Q = \frac{\sum_c Q(c) w(c)}{\sum_c w(c)}$$



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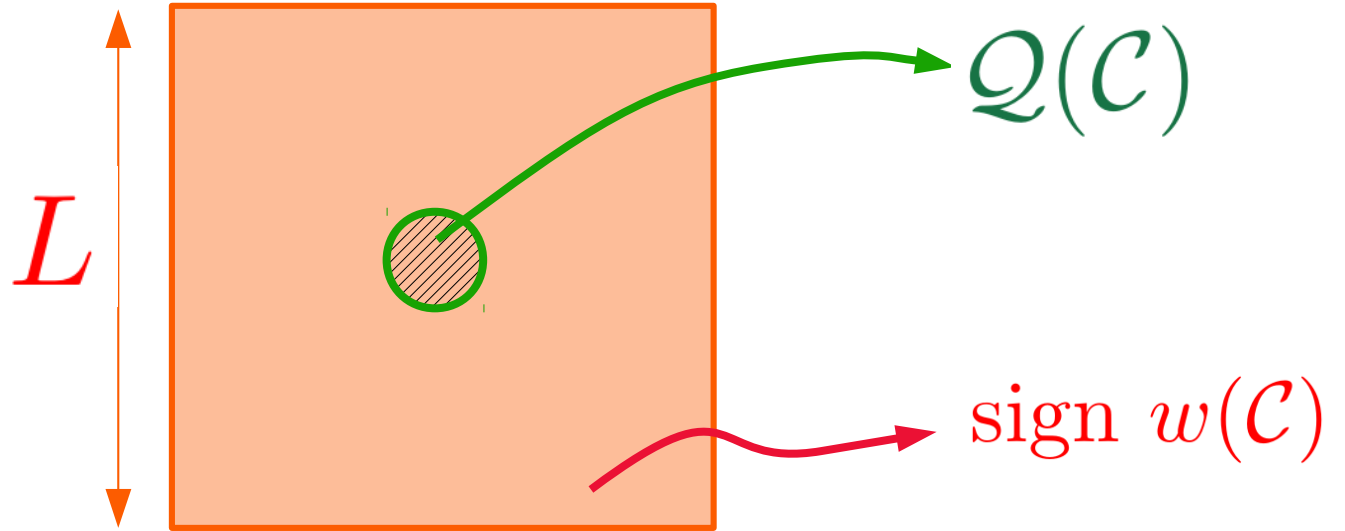
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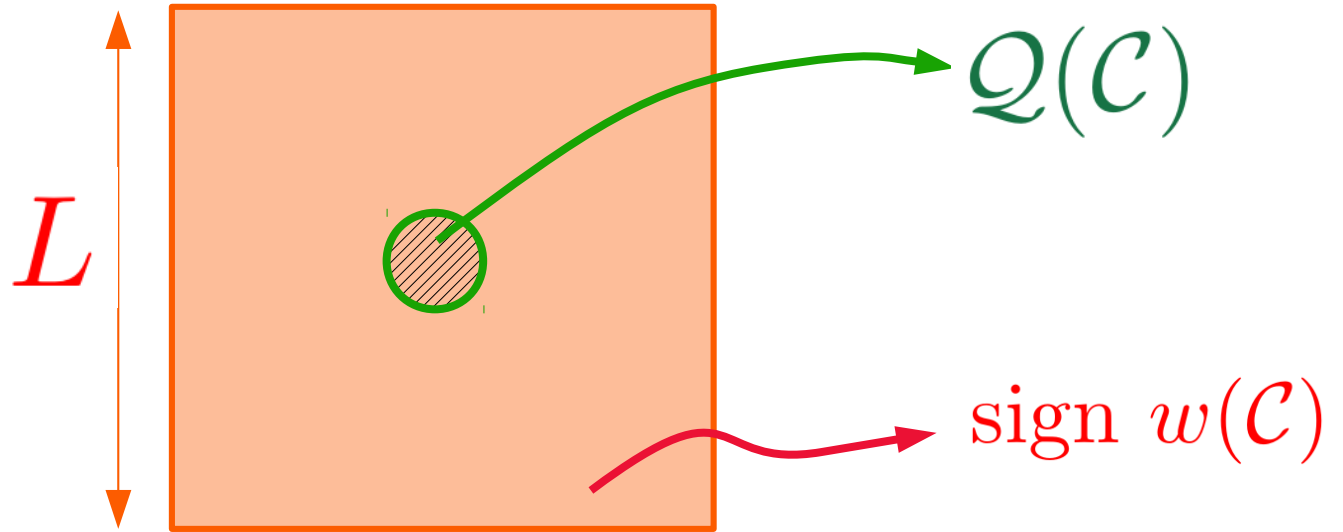
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3D XY-model, $T < T_c$.

$$\left. \begin{aligned} \langle \vec{S}(\vec{r}) \rangle &= \vec{0} \\ \lim_{\lambda \rightarrow \infty} \left(\lim_{L \rightarrow \infty} \langle \vec{S}(\vec{r}) \cdot \vec{S}(\vec{0}) \rangle \right) &= M^2 \end{aligned} \right\} \Rightarrow \boxed{\vec{S}(\vec{r}) \text{ and } \vec{S}(\vec{0}) \text{ CORRELATED}}$$

Broken-symmetry point of view:

$$\left[\begin{array}{l} \text{external field } \vec{h} \cdot \vec{u}_x \\ \langle \rangle := \lim_{h \rightarrow 0} \lim_{L \rightarrow \infty} \langle \rangle \end{array} \right.$$

$$\langle \vec{S}(\vec{r}) \rangle = M \cdot \vec{u}_x$$

$$\lim_{\lambda \rightarrow \infty} \langle \vec{S}(\vec{r}) \cdot \vec{S}(\vec{0}) \rangle = M^2 = \langle \vec{S}(\vec{r}) \rangle \cdot \langle \vec{S}(\vec{0}) \rangle$$

\Rightarrow UNCORRELATED

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sum all connected Feynman diagrams of order $N \leq N_{\max}$

truncation error $\epsilon_{\text{sys}} \xrightarrow{N_{\max} \rightarrow \infty} 0$

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flexibility of diagrammatic technique:

- change the *starting point* (order zero)
- reorganize expansion (use *dressed* propagators / vertices)
 \Rightarrow *non-perturbative*

\Rightarrow *low orders already ~ OK*

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fermionic sign helps:

strong cancellations between diagrams
 \Rightarrow ***large orders contributions reduced***

Diagrammatic MC with *connected diagrams*

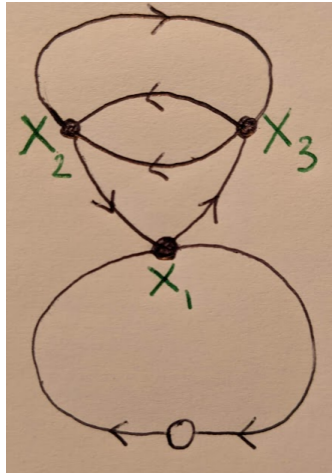
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$$S \rightsquigarrow S_\xi \quad \text{such that} \quad \begin{cases} S_{\xi=0} \text{ quadratic} \\ S_{\xi=1} = S \\ \xi \mapsto S_\xi \text{ analytic} \end{cases}$$

$$Q = \langle \hat{Q} \rangle_S \rightsquigarrow Q(\xi) = \langle \hat{Q} \rangle_{S_\xi} = \sum_{N=0}^{\infty} Q_N \xi^N$$

$$Q = Q(\xi = 1) = \sum_{N=0}^{\infty} Q_N \quad (\text{if series converges})$$

sum of all order-N *connected Feynman diag.*
 well-defined in thermo. limit $\mathcal{N} = \infty$



$$Q_N = \sum_{\text{connected topologies } \mathcal{T}} \int dX_1 \dots dX_N \underbrace{\mathcal{D}(\mathcal{T}; X_1 \dots X_N)}_{\substack{\longrightarrow 0 \\ |X_i| \rightarrow \infty}}$$

$$X := (\vec{r}, \tau) \\ \int dX := \sum_{\vec{r}} \int_0^\beta d\tau$$

Freedom in choosing S_0

- Mean-field • DMFT • Fully dressed G (“bold”)
- add field (bosonic): sum ladders (pp or ph)

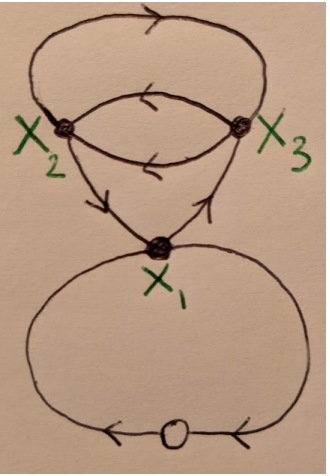
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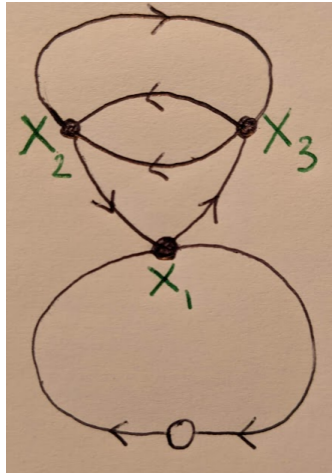
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• symmetry breaking



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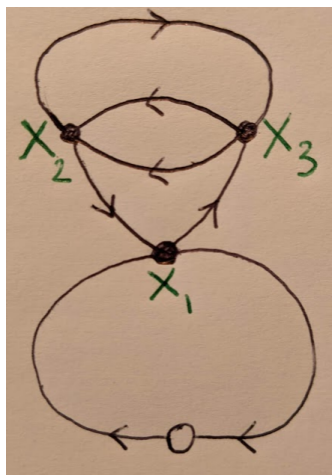
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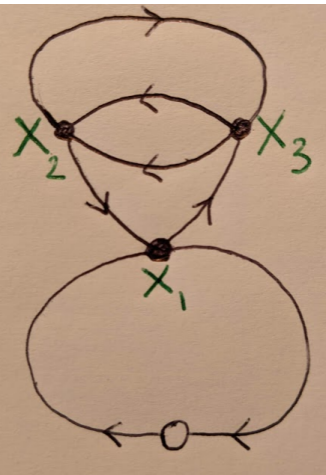


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Monte Carlo algorithms

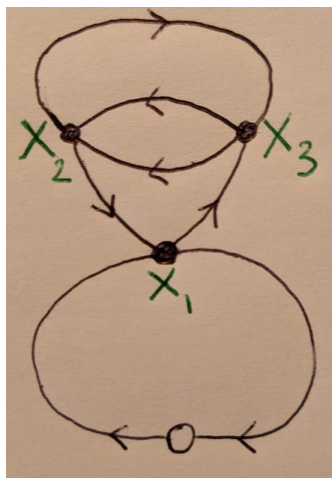
- DiagMC [Van Houcke *et al.* 2010]

configuration: $\mathcal{C} = (\mathcal{T}, X_1, \dots, X_N)$ probability: $P(\mathcal{C}) \propto |\mathcal{D}(\mathcal{T}; X_1 \dots X_N)|$

- CDet [Rossi 2017, Rossi *et al.* 2020]

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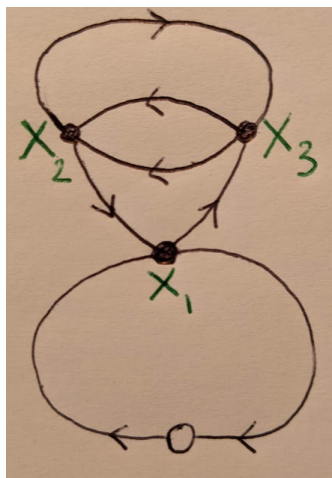
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- DiagMC [Prokof'ev & Svistunov 1998 & 2008 (bosonic & fermionic)
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see talks by
K. Van Houcke
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Real-time (Anderson impurity):

- “Keldysh Det” [Profumo *et al.* 2015]

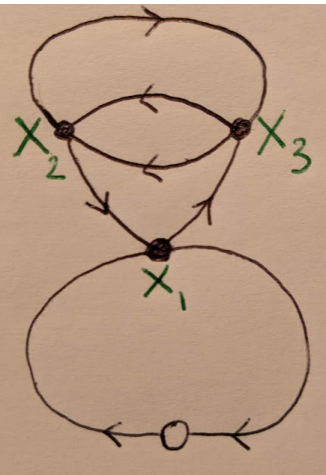
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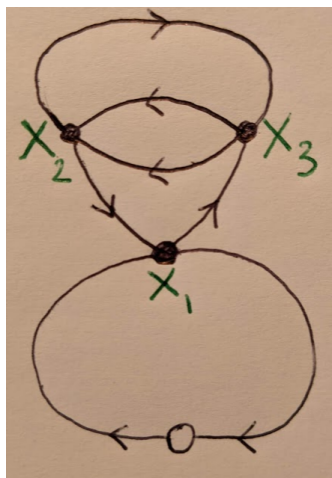
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Computational complexity

$$\bullet t_{\text{CPU}} \sim \begin{cases} (N!)^2 & (\text{DiagMC}) \\ e^{\#N} & (\text{CDet}) \end{cases}$$

- counteracted by convergence: $|a_N| \sim e^{-\#N}$

$$t(\epsilon) \sim \epsilon^{-\# \ln(\ln \epsilon^{-1})} \quad (\text{DiagMC}),$$

$$t(\epsilon) \sim \epsilon^{-\alpha} \quad (\text{CDet}).$$

where $\epsilon =$ total error
(statistical + truncation)

a hunting board of diagrammatic MC...

repulsive Hubbard model 2D square lattice
supercond. phase diagram (d- & p-wave) $T \rightarrow 0$ in Fermi-liq regime [Deng *et al.* 2015]
crossover to AF insulator at half-filling [Simkovic *et al.* 2020 ; Kim *et al.* 2020]
diagonal hopping \rightarrow pseudogap physics [Wu *et al.* 2017 ; Rossi *et al.* 2020]

graphene *Dirac liquid* $T=0$ [Tupitsyn & Prokof'ev 2017]

phonons+electrons with Coulomb interactions 3D cubic lattice
phonon spectrum (Kohn anomaly) [Tupitsyn *et al.* 2016]

unitary Fermi gas contact interactions, 3D c^0 space (cold atoms)
eq. of state, contact, non-Fermi-liq $n(k)$ [Van Houcke *et al.* 2012 ; Rossi *et al.* 2018]

electron gas Coulomb interactions, 3D c^0 space
static response, Fermi-liq params [Chen & Haule 2019 / 2020]

frustrated spins AF Heisenberg model, triangular & pyrochlore lattices
quantum \leftrightarrow classical correspondence [Kulagin *et al.* 2013 ; Huang *et al.* 2016]

(...) all in normal phases ($T > T_c$)

Haldane model 2D honeycomb , magnetic field
 $T=0$: *topological phases, magnetically ordered* [Tupitsyn & Prokof'ev 2019]

here: **superfluid / superconducting** phase

Hubbard model – 3D cubic lattice

$$H = H_{\text{kin}} - \sum_{\sigma} \mu_{\sigma} N_{\sigma} + H_{\text{int}}$$

$$H_{\text{kin}} = -t \sum_{\langle \mathbf{i}, \mathbf{j} \rangle \sigma} (c_{\mathbf{i}\sigma}^{\dagger} c_{\mathbf{j}\sigma} + h.c.)$$

$$H_{\text{int}} = U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \quad U < 0$$

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Diag. expansion in superfluid (superconducting) phase $\mathcal{O} := \langle c_{0\uparrow} c_{0\downarrow} \rangle$

unperturbed quadratic Hamiltonian:

$$H_0 = H_{\text{kin}} - \sum_{\sigma} \mu_{0,\sigma} N_{\sigma} + H_{\text{pair}}^{(\Delta_0)}$$

breaks U(1) symmetry

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$$Q(\xi) := \langle \hat{Q} \rangle_{H_{\xi}} \hat{=} \sum_{N=0}^{\infty} Q_N \xi^N$$

pressure: $P = -\Omega/L^3$, $\Omega = -T \ln \text{Tr} \exp(-\beta H)$

$$P(\xi) := \frac{T}{L^3} \ln \text{Tr} \exp(-\beta H_{\xi}) \hat{=} \sum_{N=0}^{\infty} P_N \xi^N$$

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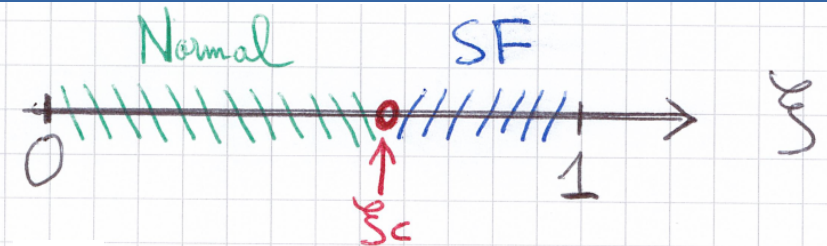
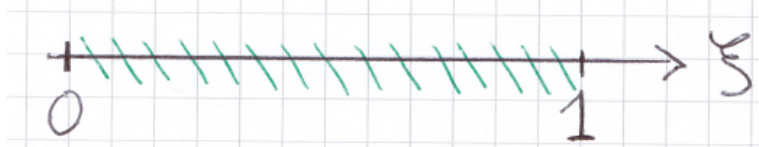
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$(1 - \xi) \Delta_0 \Leftrightarrow$ **symmetry breaking field**

$$H_{\xi} \ni (1 - \xi) H_{\text{pair}}^{(\Delta_0)} = H_{\text{pair}}^{((1-\xi)\Delta_0)}$$

unperturbed quadratic Hamiltonian:

$$H_0 = H_{\text{kin}} - \sum_{\sigma} \mu_{0,\sigma} N_{\sigma} + H_{\text{pair}}^{(\Delta_0)}$$

breaks U(1) symmetry

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Normal ("Para-SF")

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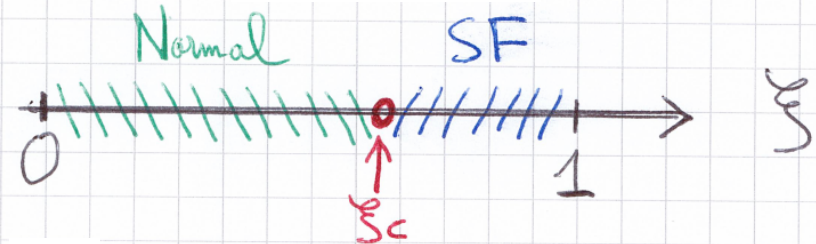
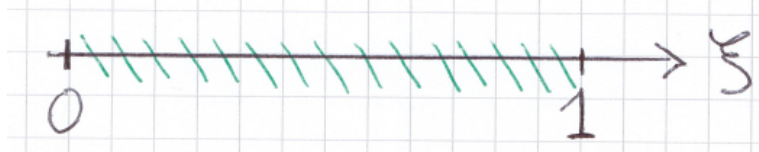
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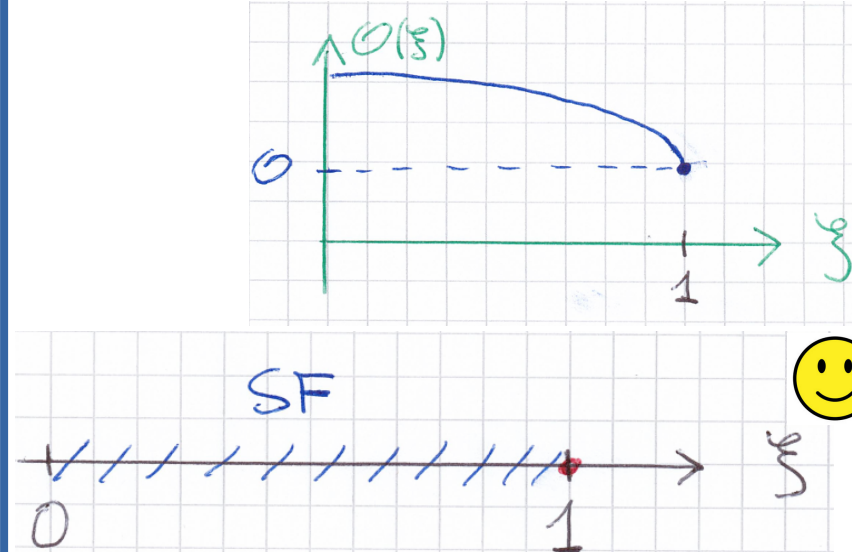
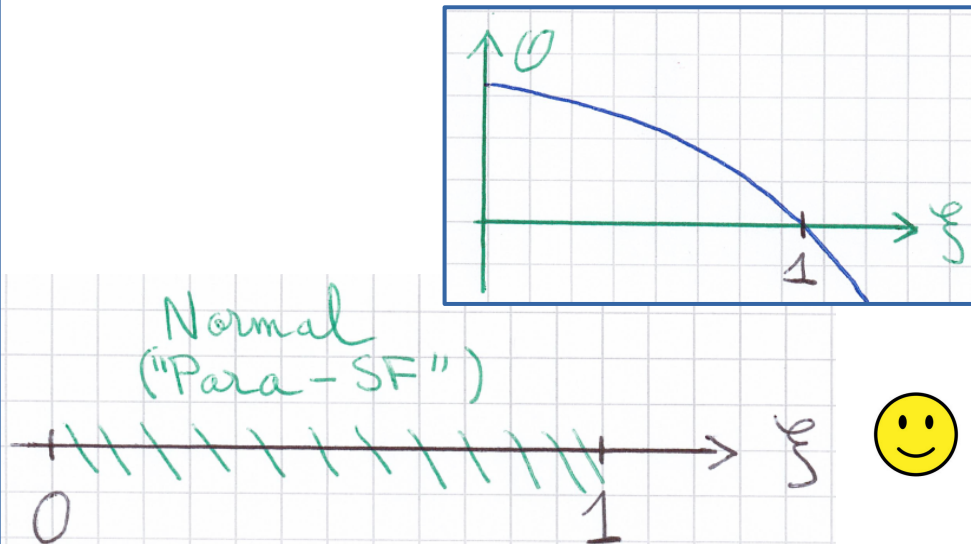
$T > T_c$

$T < T_c$

$\Delta_0 = 0$



$\Delta_0 > 0$



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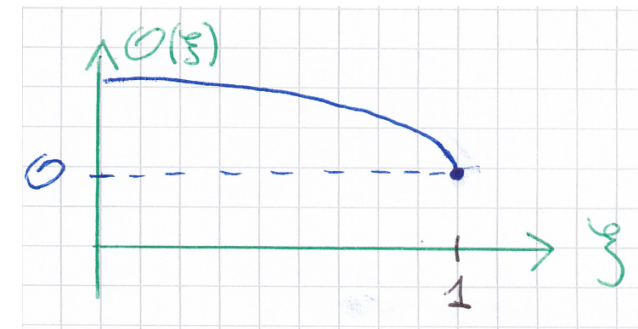
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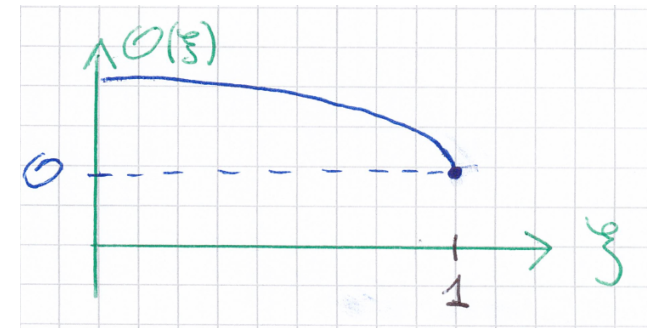
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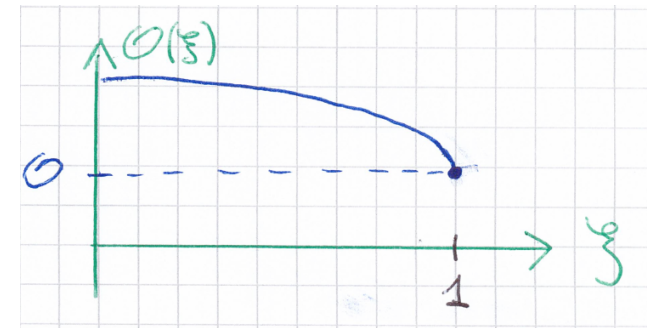
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order parameter : $\mathcal{O}(\xi) := \langle c_{\mathbf{0}\uparrow} c_{\mathbf{0}\downarrow} \rangle_{H_{\xi}} \xrightarrow{\xi \rightarrow 1^-} \mathcal{O} \neq 0$

spontaneous symmetry breaking – thermodynamic limit $L \rightarrow \infty$ before $\xi \rightarrow 1^-$

$$\mathcal{O}(\xi) = \sum_{N=0}^{\infty} \mathcal{O}_N \xi^N$$

$$\mathcal{O} = \mathcal{O}(\xi \rightarrow 1^-) = \sum_{N=0}^{\infty} \mathcal{O}_N$$

unperturbed quadratic Hamiltonian:

$$H_0 = H_{\text{kin}} - \sum_{\sigma} \mu_{0,\sigma} N_{\sigma} + H_{\text{pair}}^{(\Delta_0)}$$

breaks U(1) symmetry

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natural choice:
BCS mean-field theory

$$\mu_{0,\sigma} = \mu_{\sigma} - U \langle n_{\mathbf{0},-\sigma} \rangle_{H_0}$$

$$\Delta_0 = \Delta_{\text{MF}} := -U \langle c_{\mathbf{0}\uparrow} c_{\mathbf{0}\downarrow} \rangle_{H_0}$$

also $\Delta_0 \neq \Delta_{\text{MF}}$

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also $\Delta_0 \neq \Delta_{\text{MF}}$

$$O_0 = \text{diagram}$$

$$O_1 = \left[\begin{array}{l} \text{diagram} + \text{diagram} \\ \text{diagram} + \text{diagram} \end{array} \right] = 0 \text{ if } \Delta_0 = \Delta_{\text{MF}}$$

unperturbed quadratic Hamiltonian:

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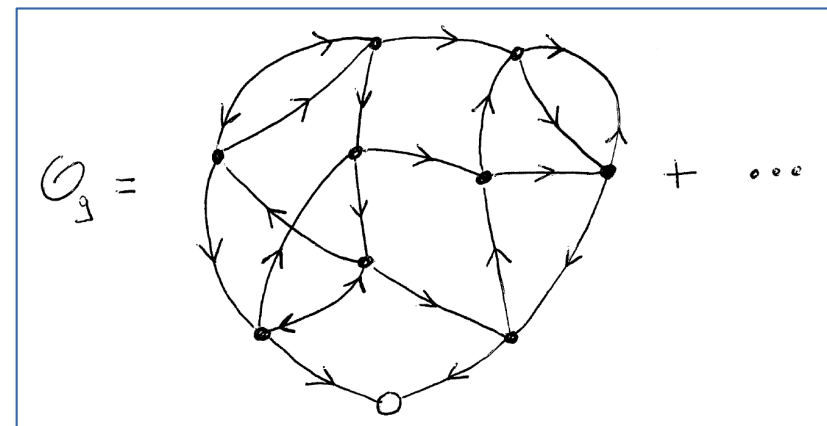
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also $\Delta_0 \neq \Delta_{\text{MF}}$

$$\mathcal{O}_0 = \text{[diagram: loop with two vertices and two arrows]} \\ \mathcal{O}_1 = \left[\begin{array}{l} \text{[diagram: loop with two vertices, two arrows, and a red dot]} \\ \text{[diagram: loop with two vertices, two arrows, and a red dot]} \\ \text{[diagram: loop with two vertices, two arrows, and a red dot]} \\ \text{[diagram: loop with two vertices, two arrows, and a red dot]} \end{array} \right] + \dots = 0 \text{ if } \Delta_0 = \Delta_{\text{MF}}$$



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also $\Delta_0 \neq \Delta_{\text{MF}}$

$O_0 =$ [diagram of a loop]

$O_1 =$ [diagram of two loops] + [diagram of a loop with a red 'x' and Δ_0]

$= 0$ if $\Delta_0 = \Delta_{\text{MF}}$

$O_1 =$ [lattice diagram with arrows] + ...

large distances : small contribution

broken symmetry

algorithm:

CDet [Rossi 2017]

with Nambu propagators

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with **Nambu propagators**

$$\begin{pmatrix} \mathcal{G}_{00}(X-X') & \mathcal{G}_{01}(X-X') \\ \mathcal{G}_{10}(X-X') & \mathcal{G}_{11}(X-X') \end{pmatrix} := - \begin{pmatrix} \langle T c_{\uparrow}^{\dagger}(X) c_{\uparrow}(X') \rangle_{H_0} & \langle T c_{\uparrow}^{\dagger}(X) c_{\downarrow}^{\dagger}(X') \rangle_{H_0} \\ \langle T c_{\downarrow}(X) c_{\uparrow}(X') \rangle_{H_0} & \langle T c_{\downarrow}(X) c_{\downarrow}^{\dagger}(X') \rangle_{H_0} \end{pmatrix}$$

algorithm: **CDet** [Rossi 2017] with **Nambu propagators**

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$$\mathcal{O}_N = -\frac{(-U)^N}{N!} \int dX_1 \dots dX_N \text{cdet}(A)$$

$$X = (\mathbf{i}, \tau)$$

$$\text{cdet}(A) = \det(A) - \sum (\text{disconnected diagrams})$$

*(recursively
3^N operations)*

$$A := \begin{pmatrix} 0 & \delta_{\text{sh}} & \dots & \mathcal{G}_{00}(X_1-X_N) & \mathcal{G}_{01}(X_1-X_N) & \mathcal{G}_{0\alpha}(X_1) \\ \delta_{\text{sh}} & 0 & \dots & \mathcal{G}_{10}(X_1-X_N) & \mathcal{G}_{11}(X_1-X_N) & \mathcal{G}_{1\alpha}(X_1) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \mathcal{G}_{00}(X_N-X_1) & \mathcal{G}_{01}(X_N-X_1) & \dots & 0 & \delta_{\text{sh}} & \mathcal{G}_{0\alpha}(X_N) \\ \mathcal{G}_{10}(X_N-X_1) & \mathcal{G}_{11}(X_N-X_1) & \dots & \delta_{\text{sh}} & 0 & \mathcal{G}_{1\alpha}(X_N) \\ \mathcal{G}_{\alpha'0}(-X_1) & \mathcal{G}_{\alpha'1}(-X_1) & \dots & \mathcal{G}_{\alpha'0}(-X_N) & \mathcal{G}_{\alpha'1}(-X_N) & \mathcal{G}_{\alpha'\alpha}(0) \end{pmatrix}$$

$$\delta_{\text{sh}} = 0 \text{ if } \Delta_0 = \Delta_{\text{MF}}$$

$$(\alpha = 1, \alpha' = 0)$$

algorithm: **CDet [Rossi 2017]** with **Nambu propagators**

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$$\mathcal{O}_N = -\frac{(-U)^N}{N!} \int dX_1 \dots dX_N \text{cdet}(A) \quad X = (\mathbf{i}, \tau)$$

$$\text{cdet}(A) = \det(A) - \sum (\text{disconnected diagrams}) \quad \left(\begin{array}{l} \text{recursively} \\ 3^N \text{ operations} \end{array} \right)$$

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$$\delta_{\text{sh}} = 0 \text{ if } \Delta_0 = \Delta_{\text{MF}} \quad (\alpha = 1, \alpha' = 0)$$

implementation: **Fast Feynman Diagrammatics** library [Rossi & Simkovic]
with **Many Configuration MC** [Simkovic & Rossi 2021]

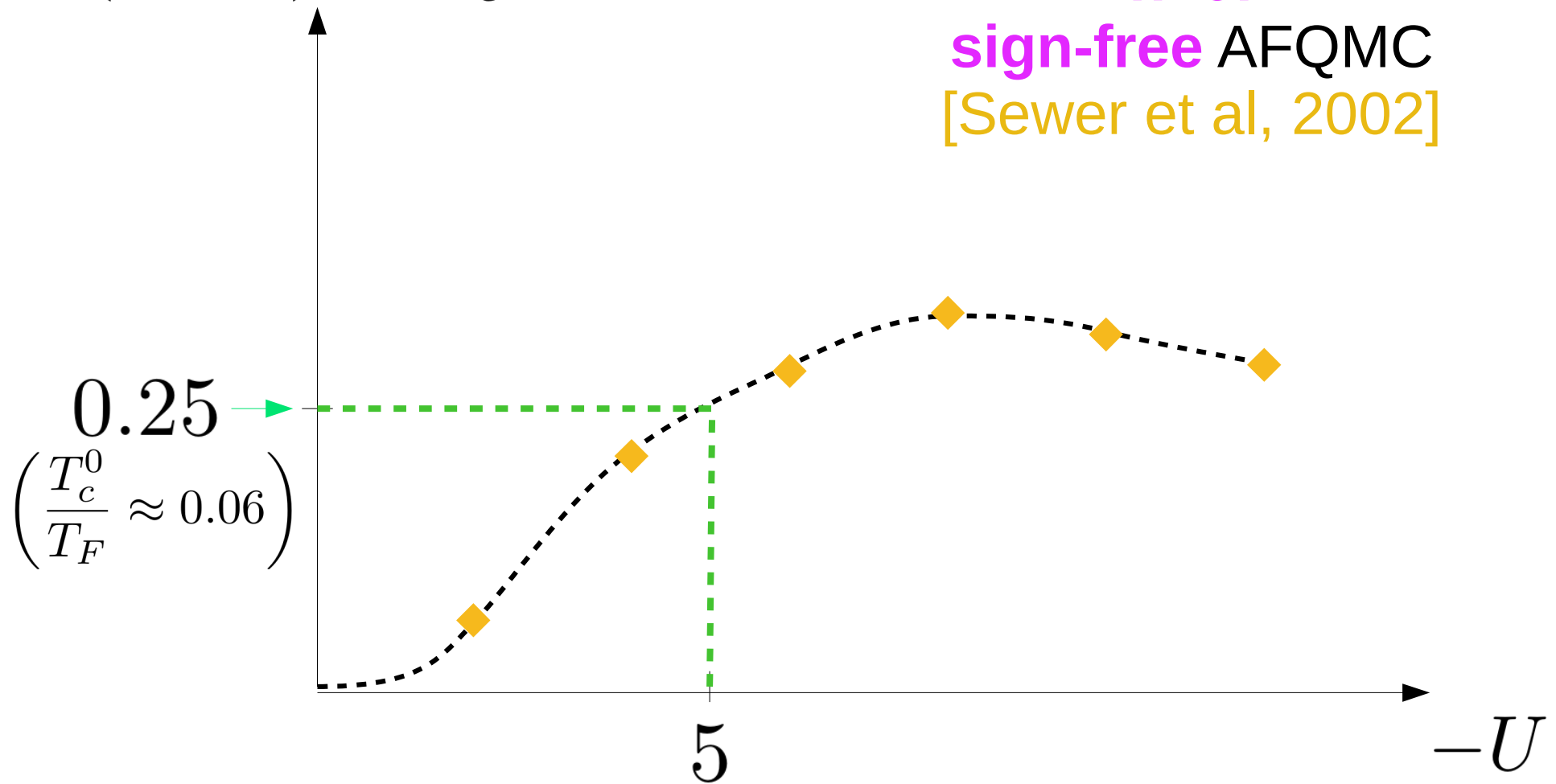
RESULTS

$$\mu_{\uparrow} = \mu + h, \quad \mu_{\downarrow} = \mu - h$$

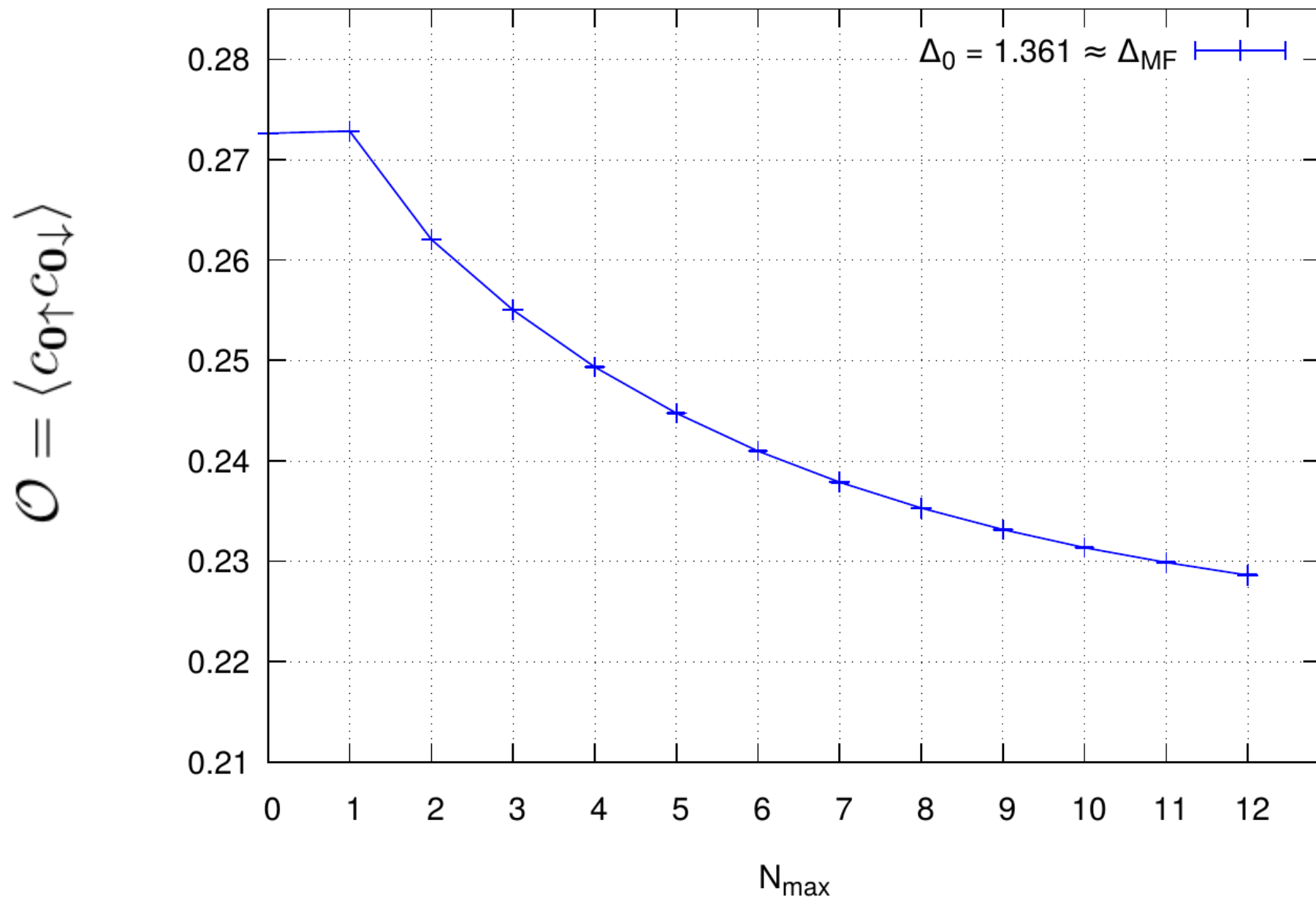
$$t \equiv 1, \quad U = -5$$

$$\mu = -3.38 \Rightarrow \langle n_{\uparrow} + n_{\downarrow} \rangle \simeq 0.5 \text{ (quarter filling)}$$

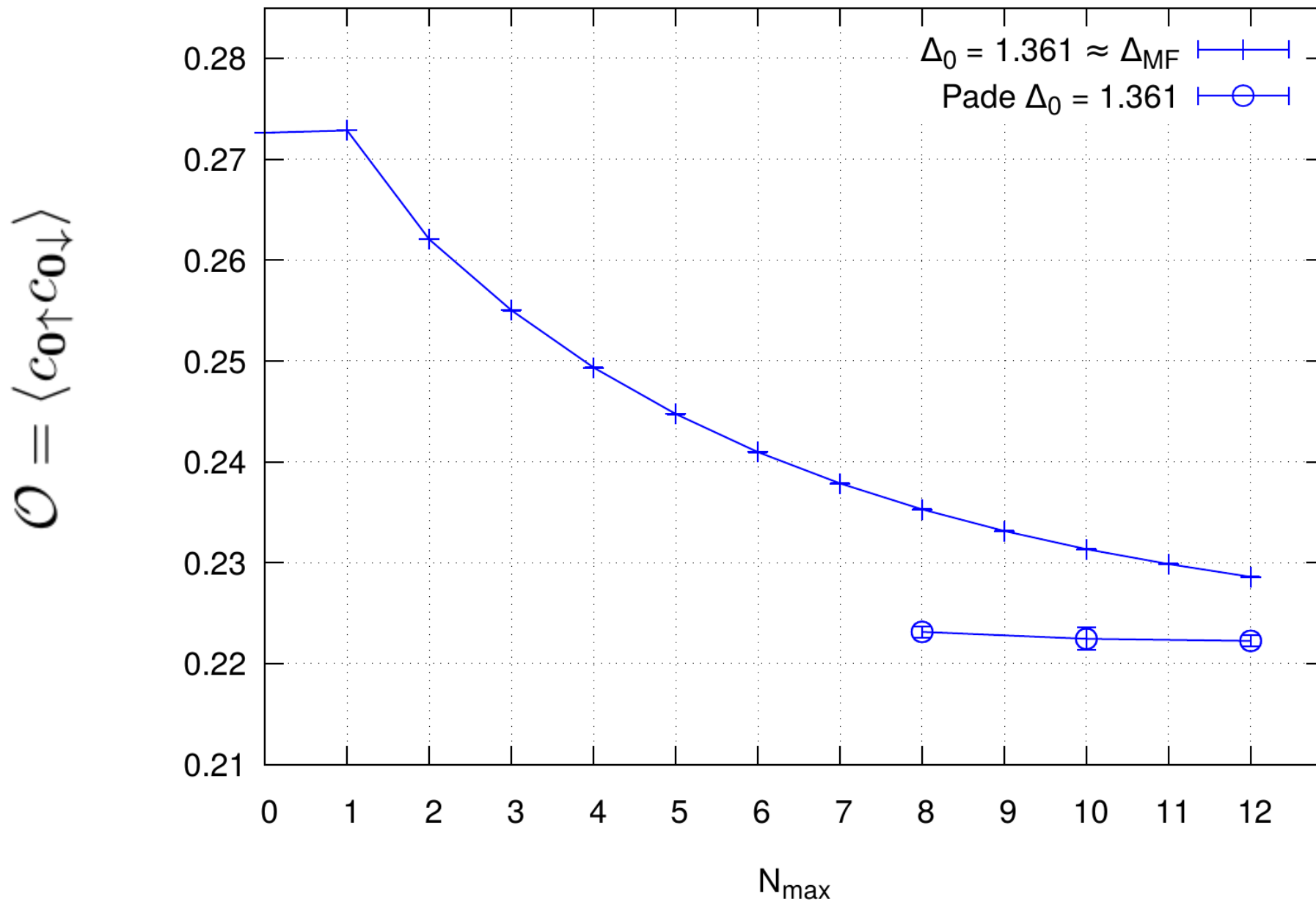
$$T_c(h = 0) =: T_c^0$$



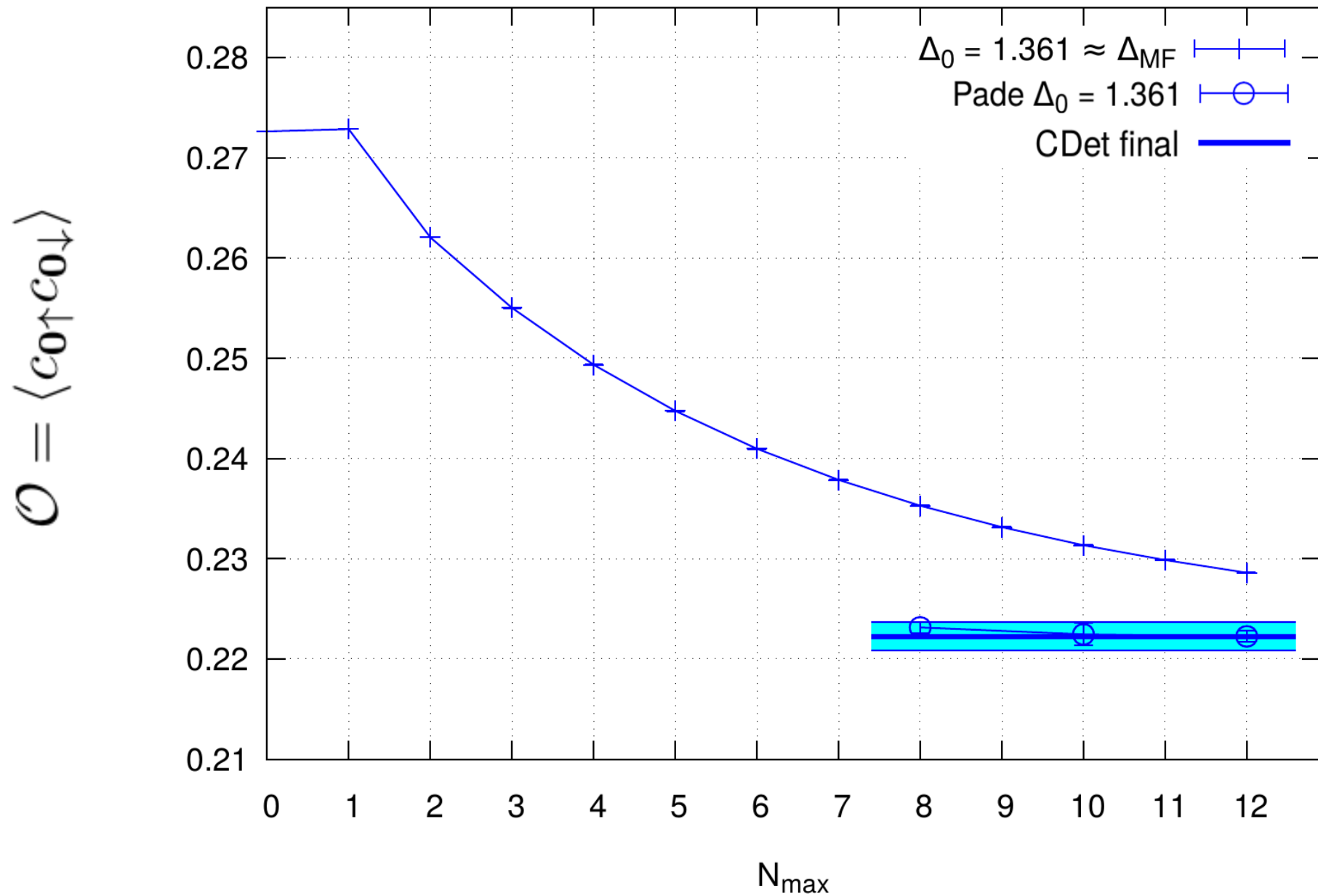
$$T = 1/8 \approx T_c^0/2, \quad h = 0$$



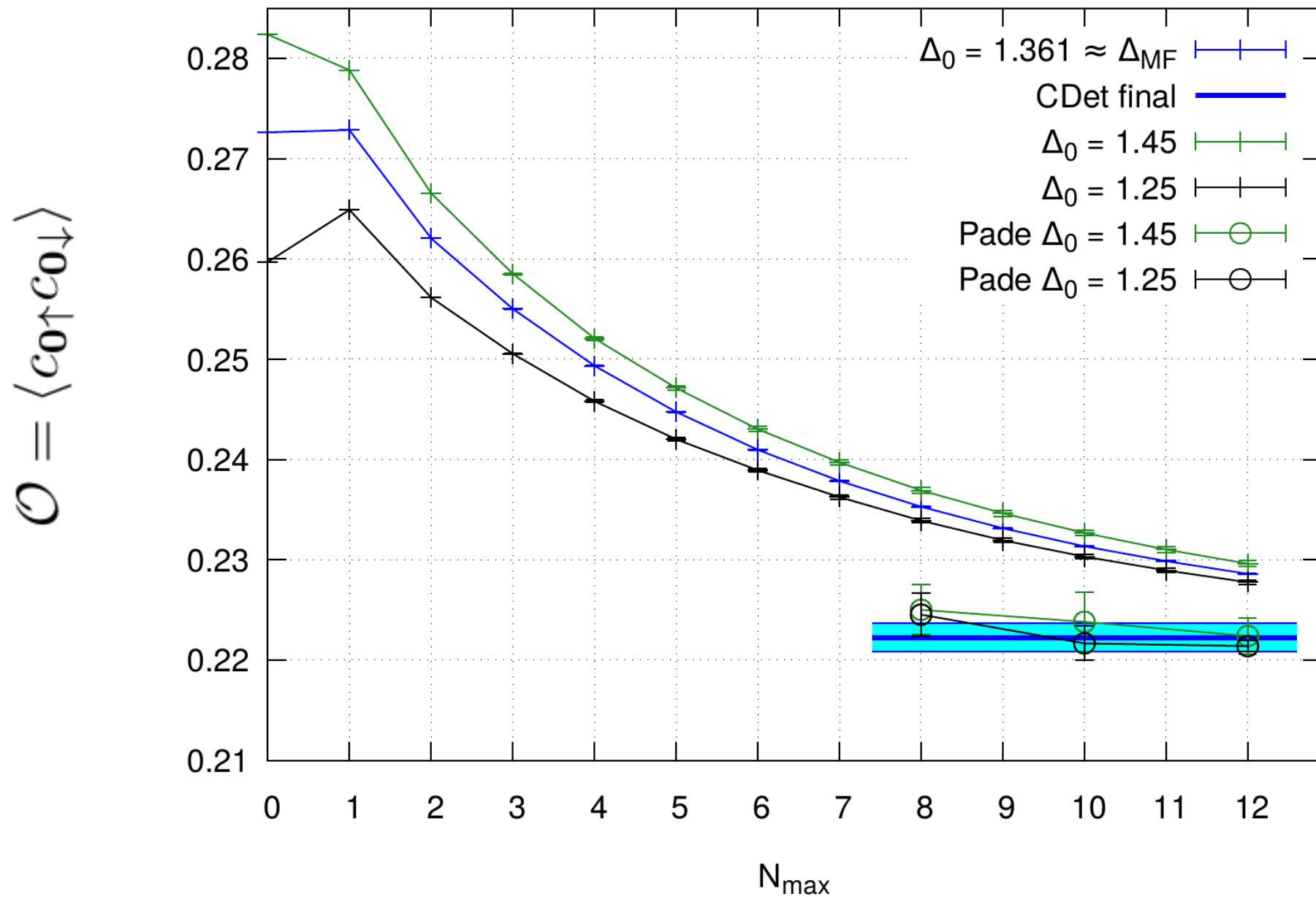
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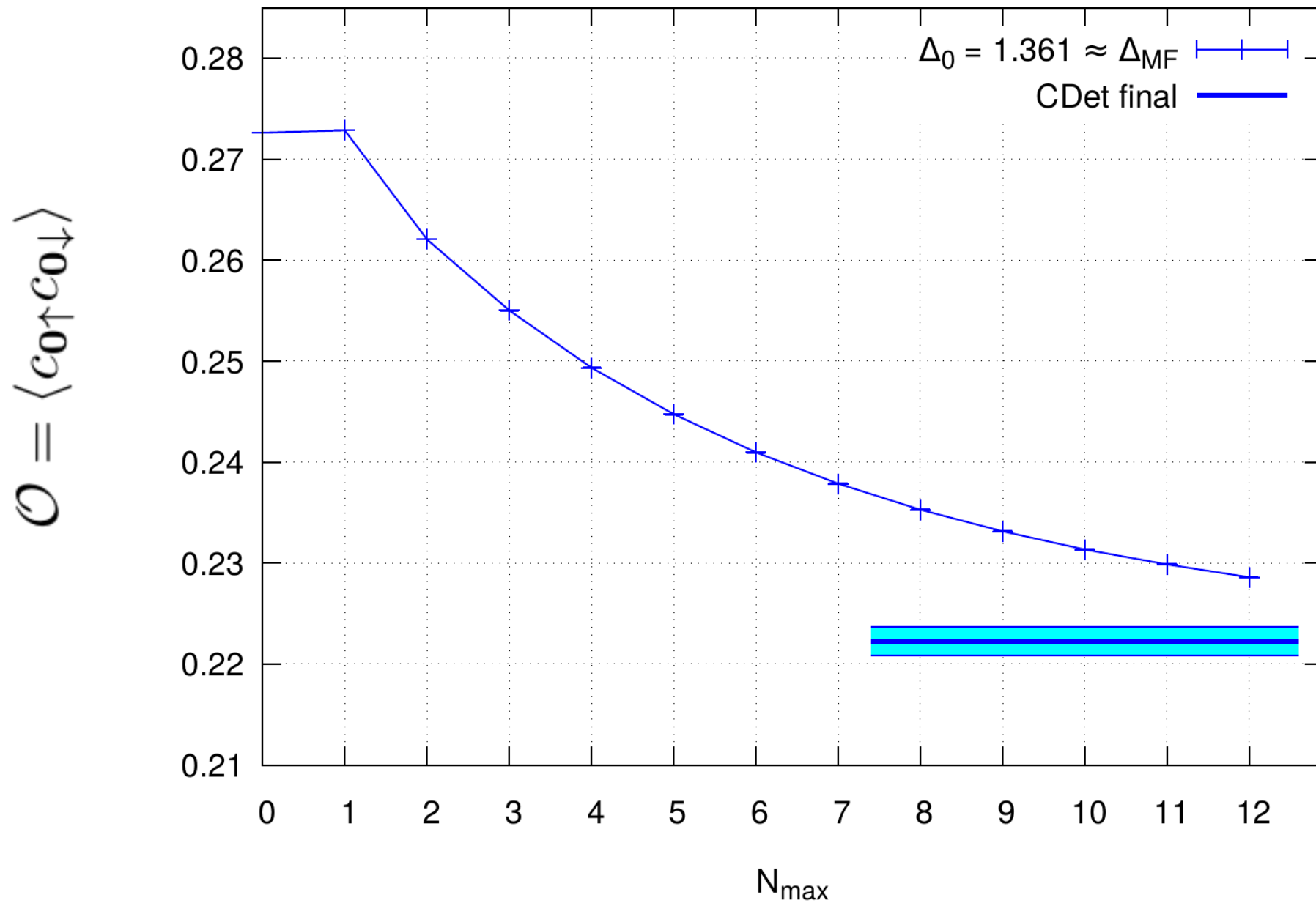
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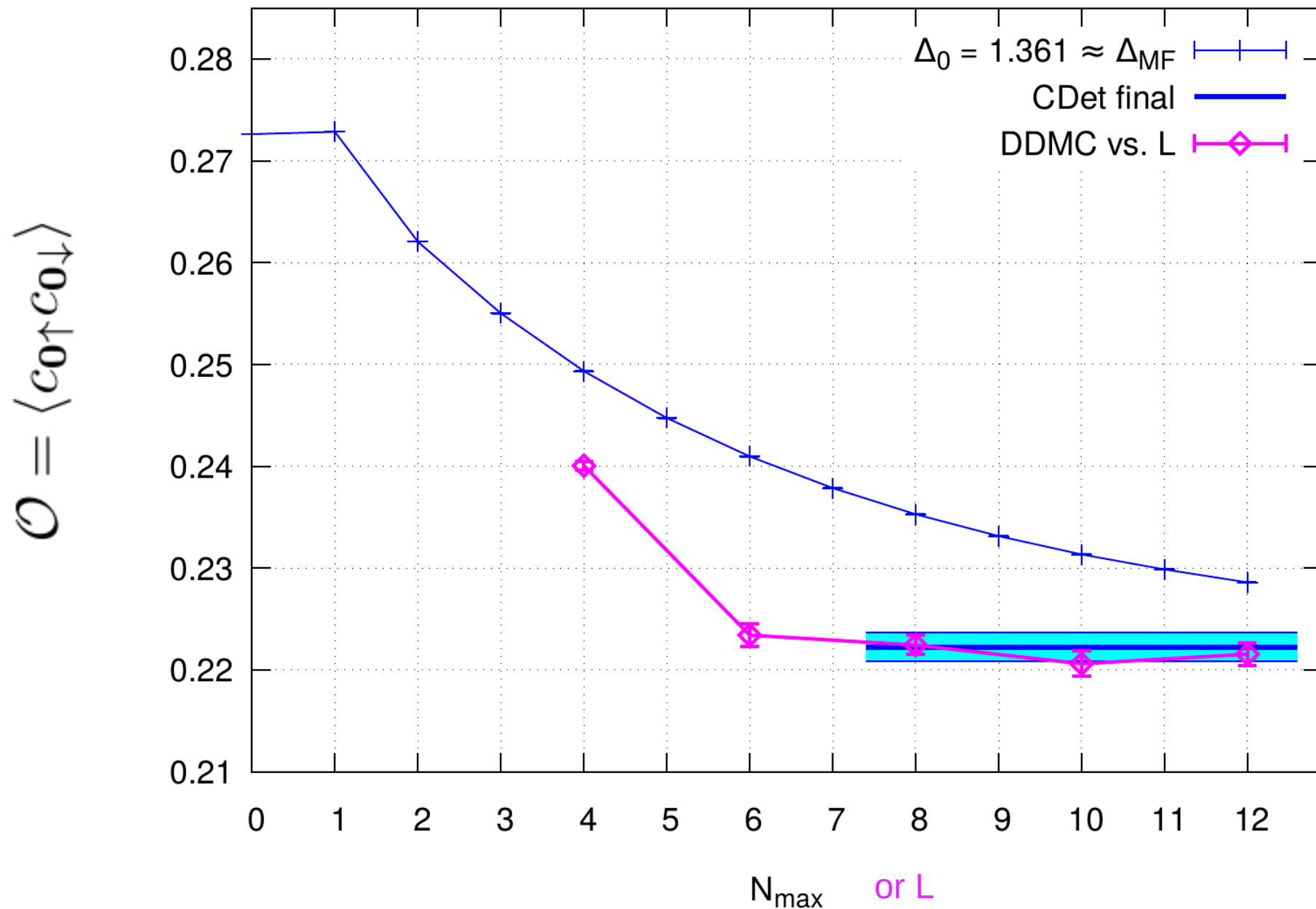


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benchmark vs.
Determinant Diagrammatic MC
[Burovski's code]



Polarized regime

$$h \neq 0 \quad \left(h \equiv \frac{\mu_{\uparrow} - \mu_{\downarrow}}{2} \right)$$

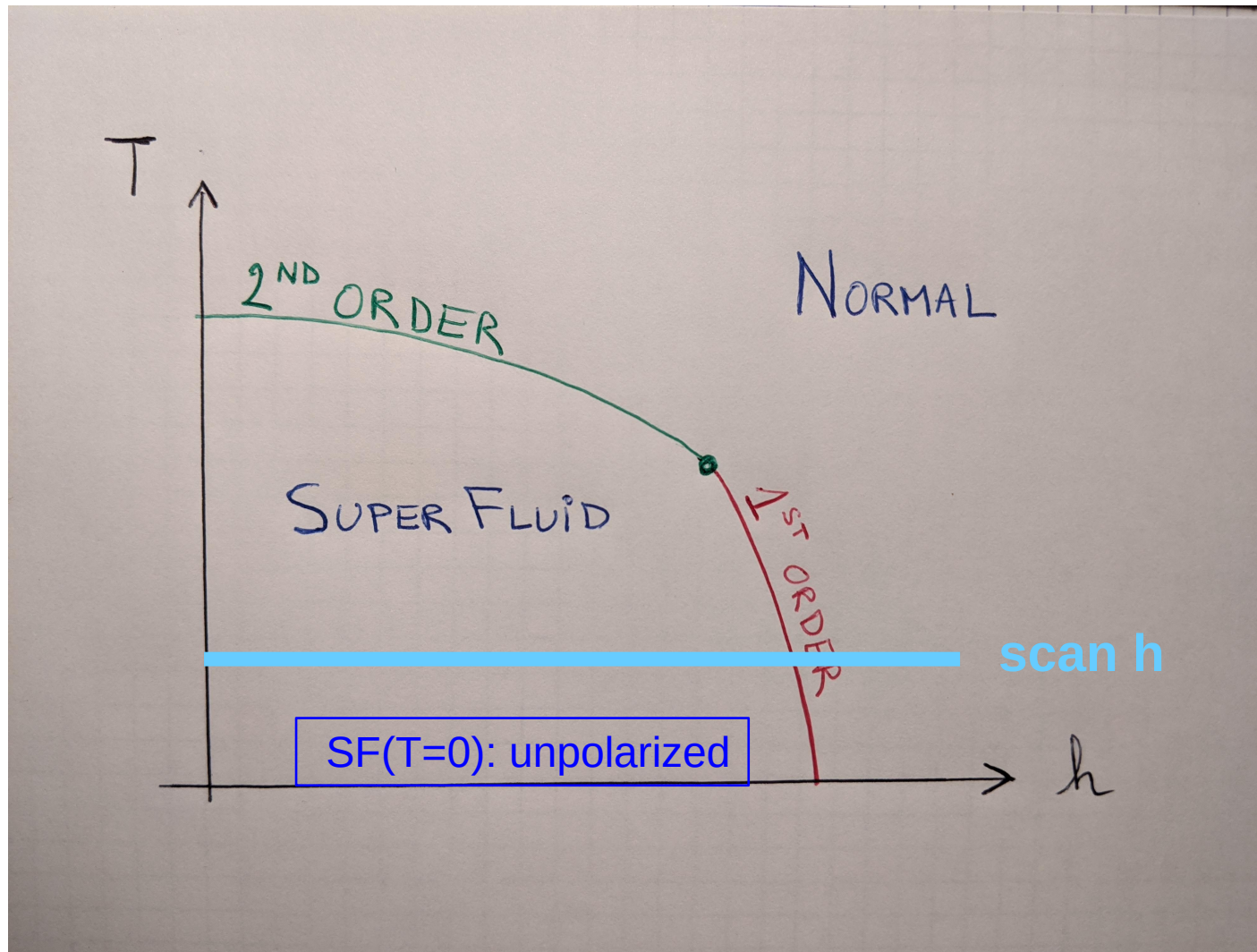
no unbiased results available (sign problem)

Polarized regime

$$h \neq 0 \quad \left(h \equiv \frac{\mu_{\uparrow} - \mu_{\downarrow}}{2} \right)$$

no unbiased results available (sign problem)

expected phase-diagram topology (U not very large & discarding FFLO)
from BCS-MF; DMFT [Dao *et al.* 2008; Koga & Werner 2010]
& cold-atom experiments in c^0 space [ENS & MIT, 2008-2010]

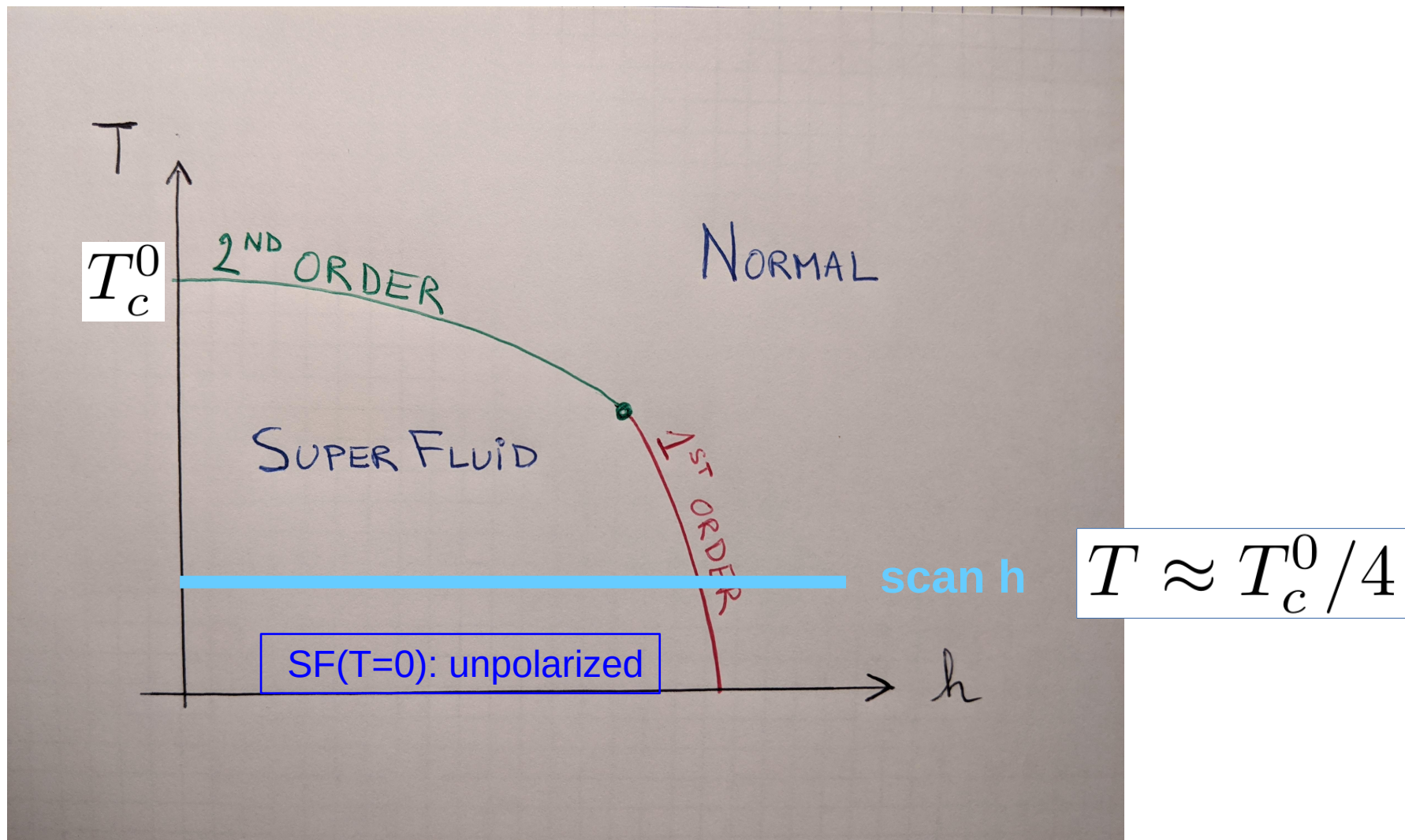


Polarized regime

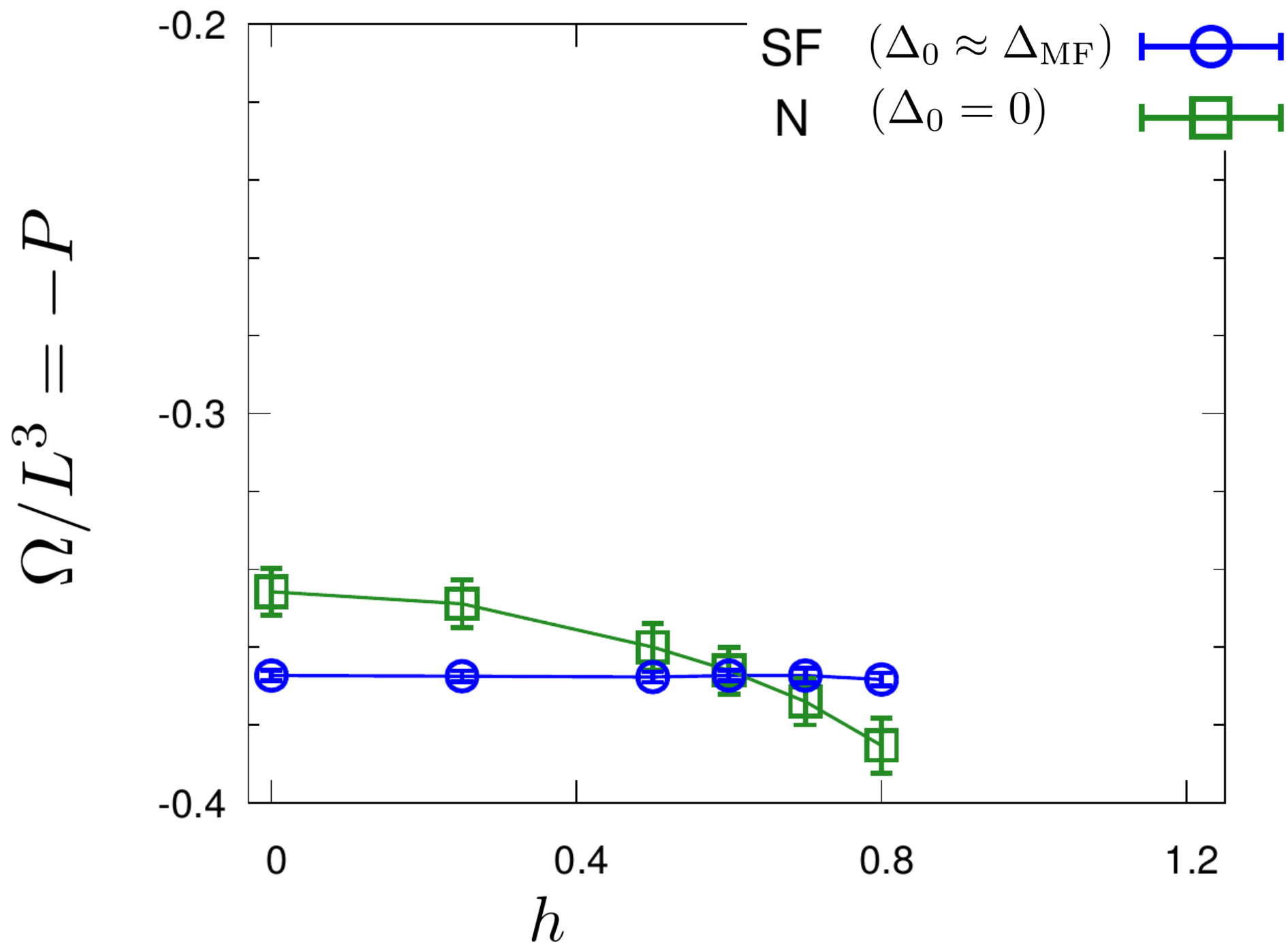
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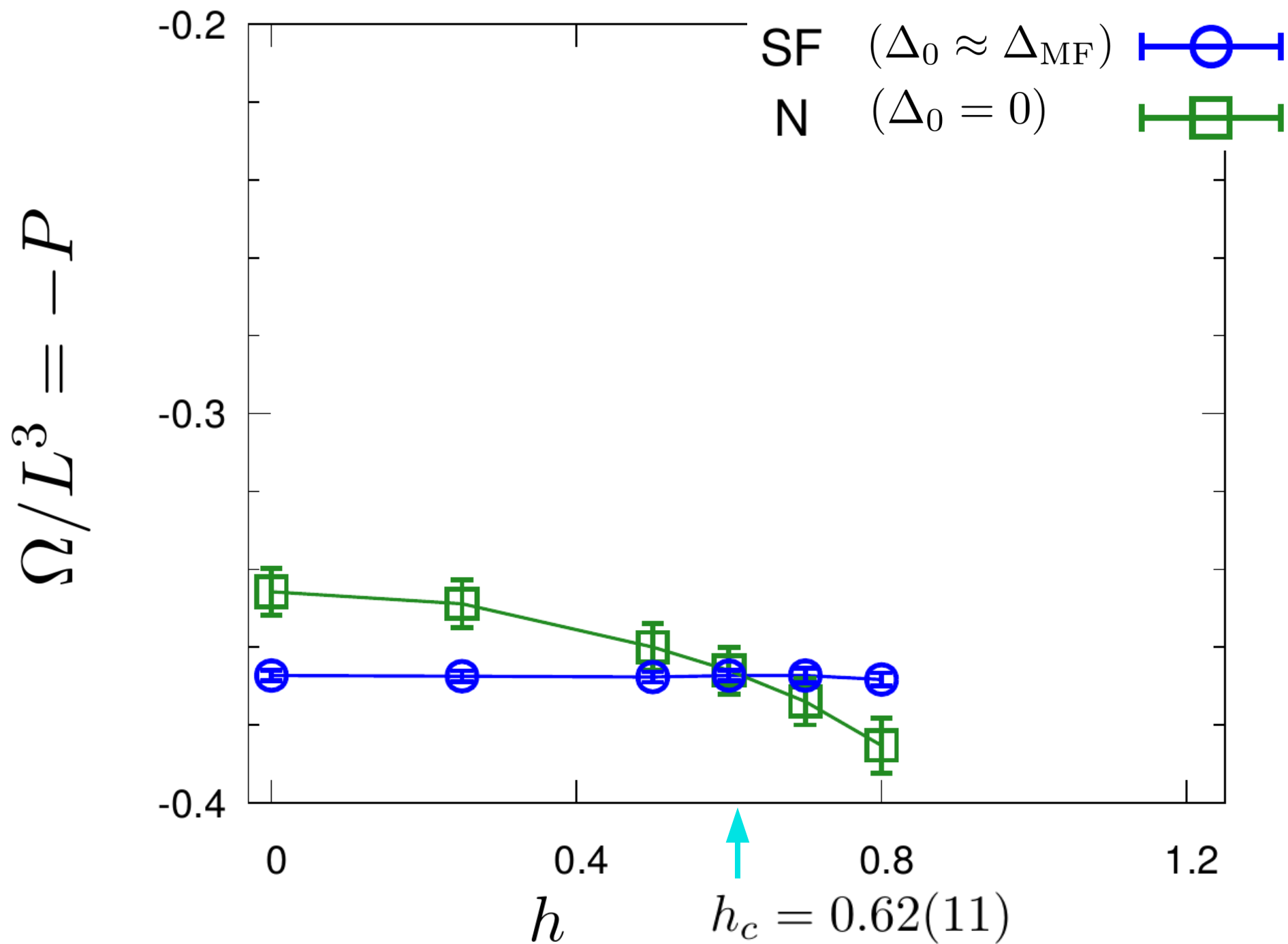
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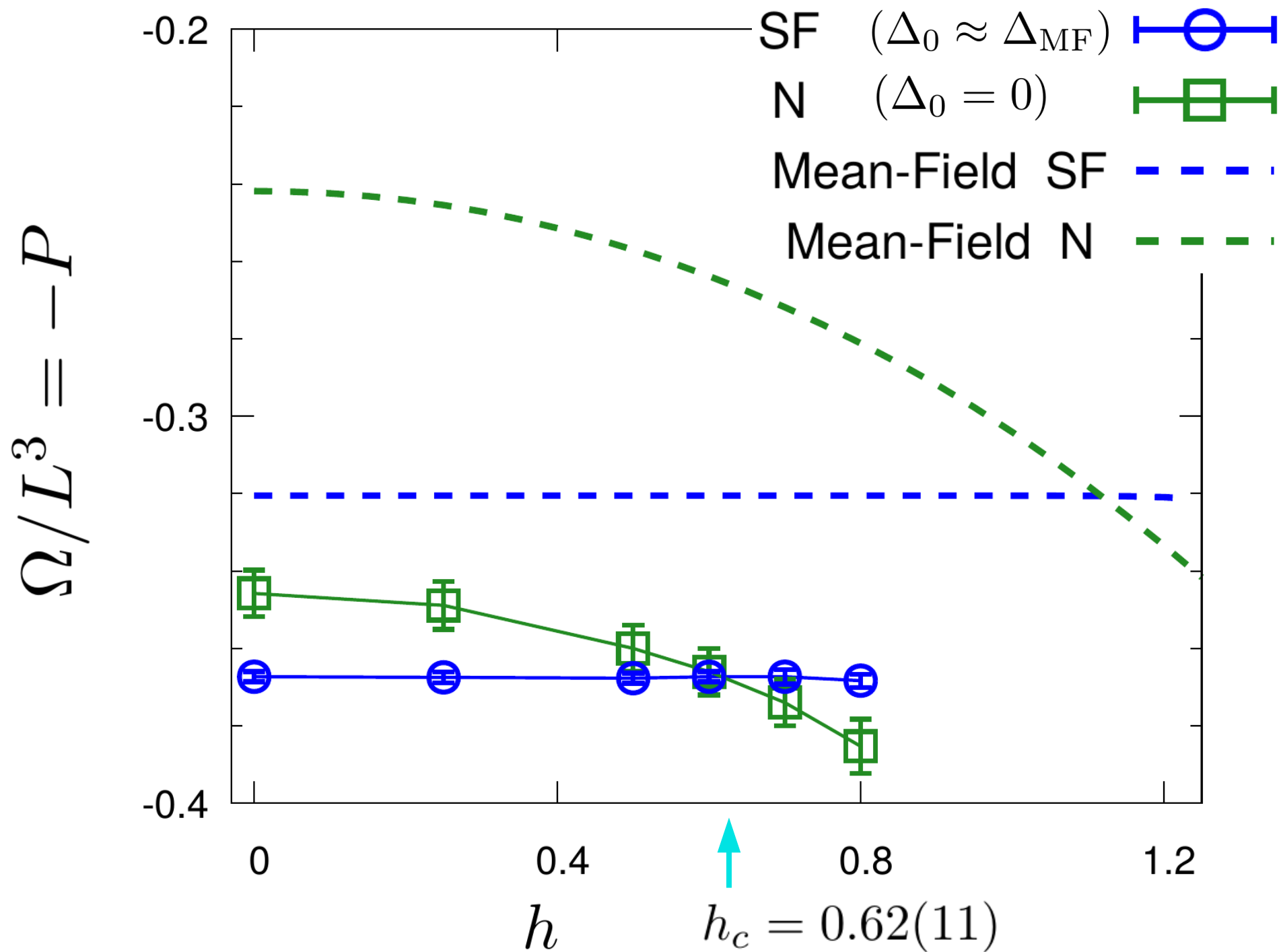
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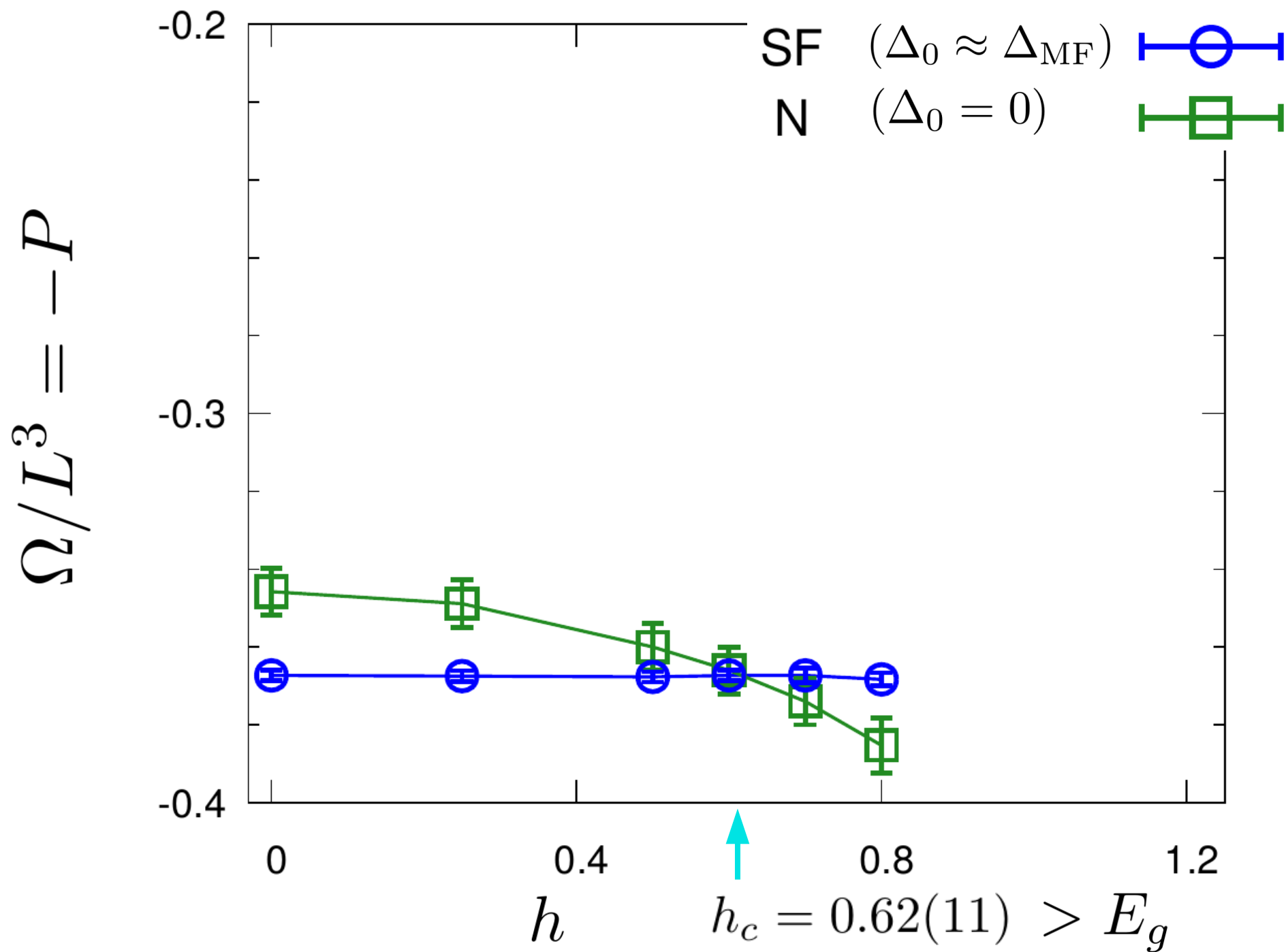
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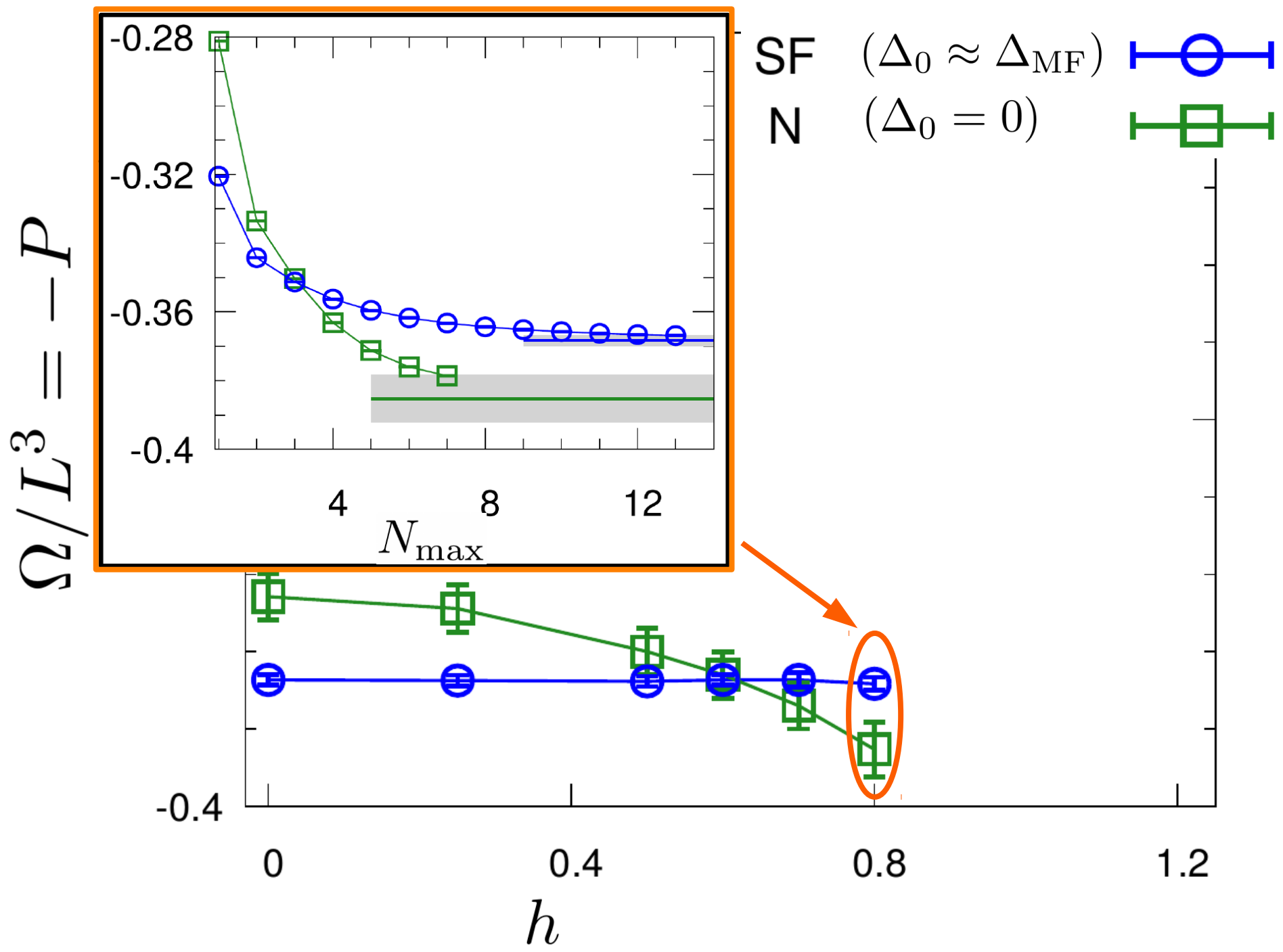
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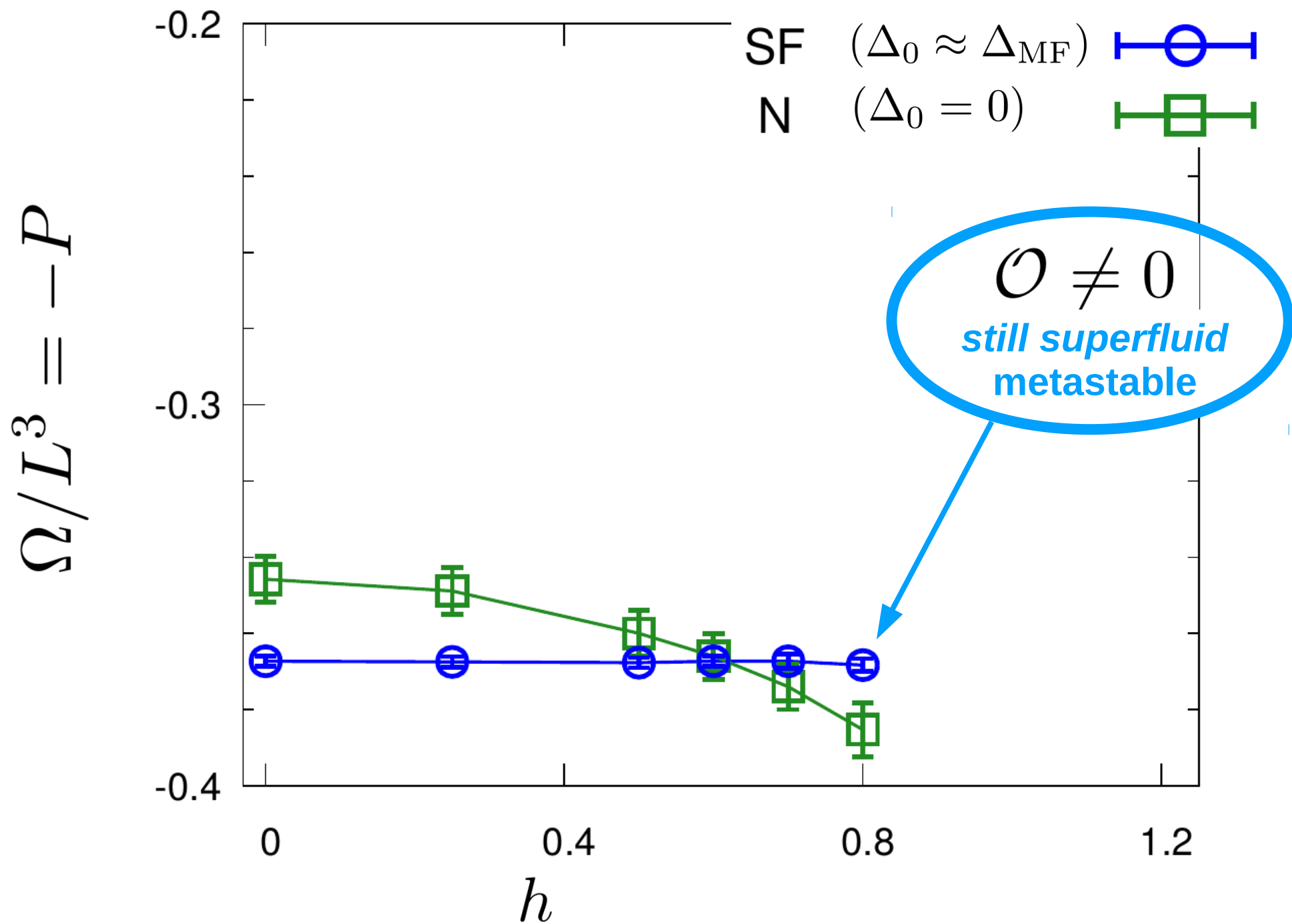
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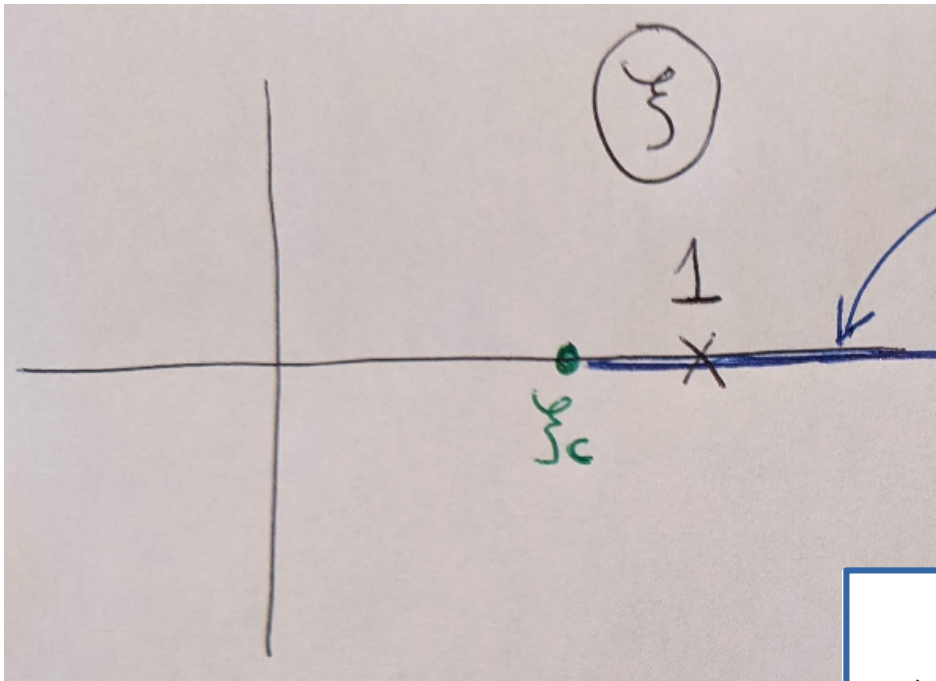


$$T = 1/16 \approx T_c^0/4$$



Metastable regime: *slowly* divergent series

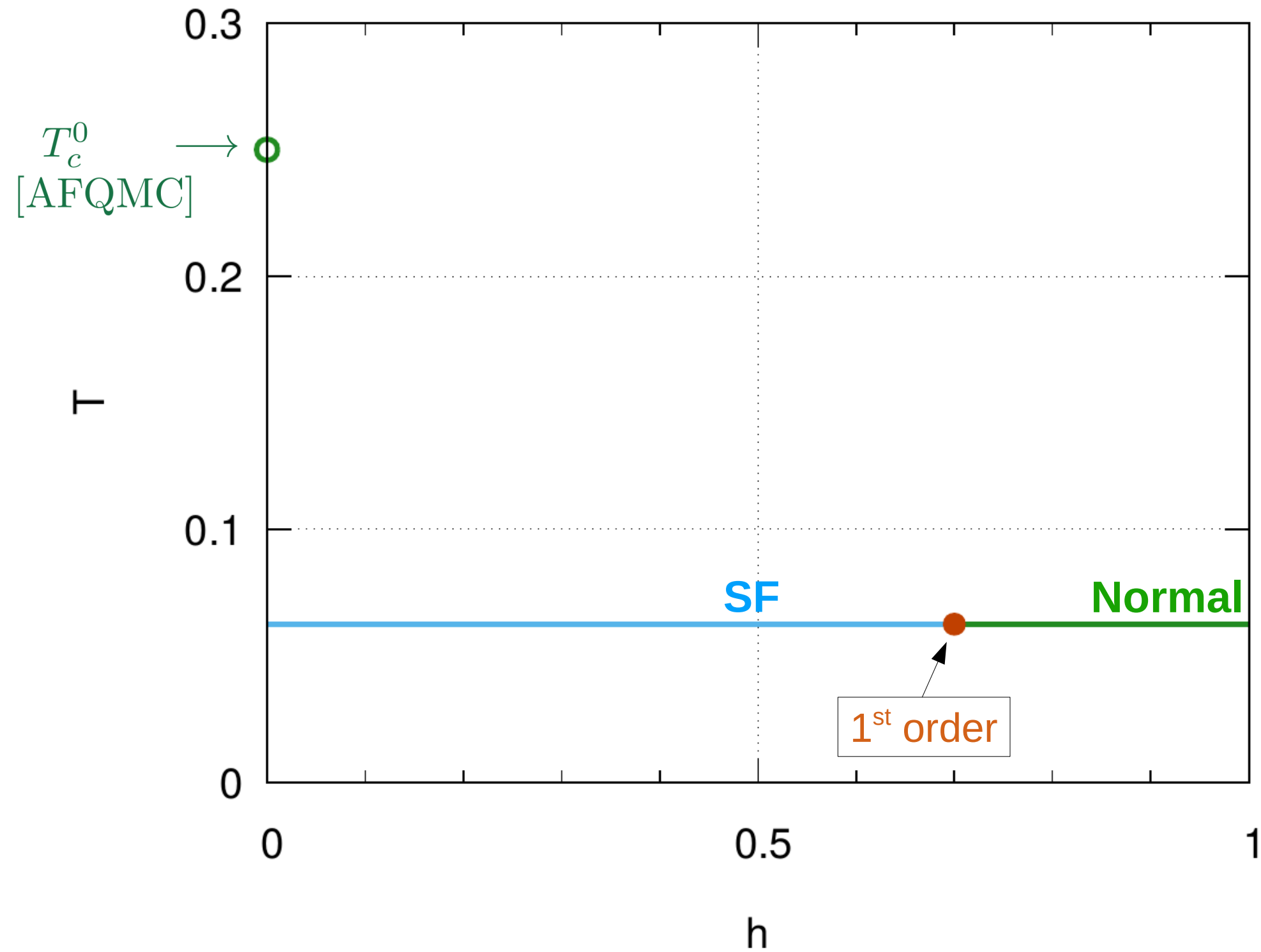
near (1st order) transition point
large energy barrier
→ *weak* essential singularity

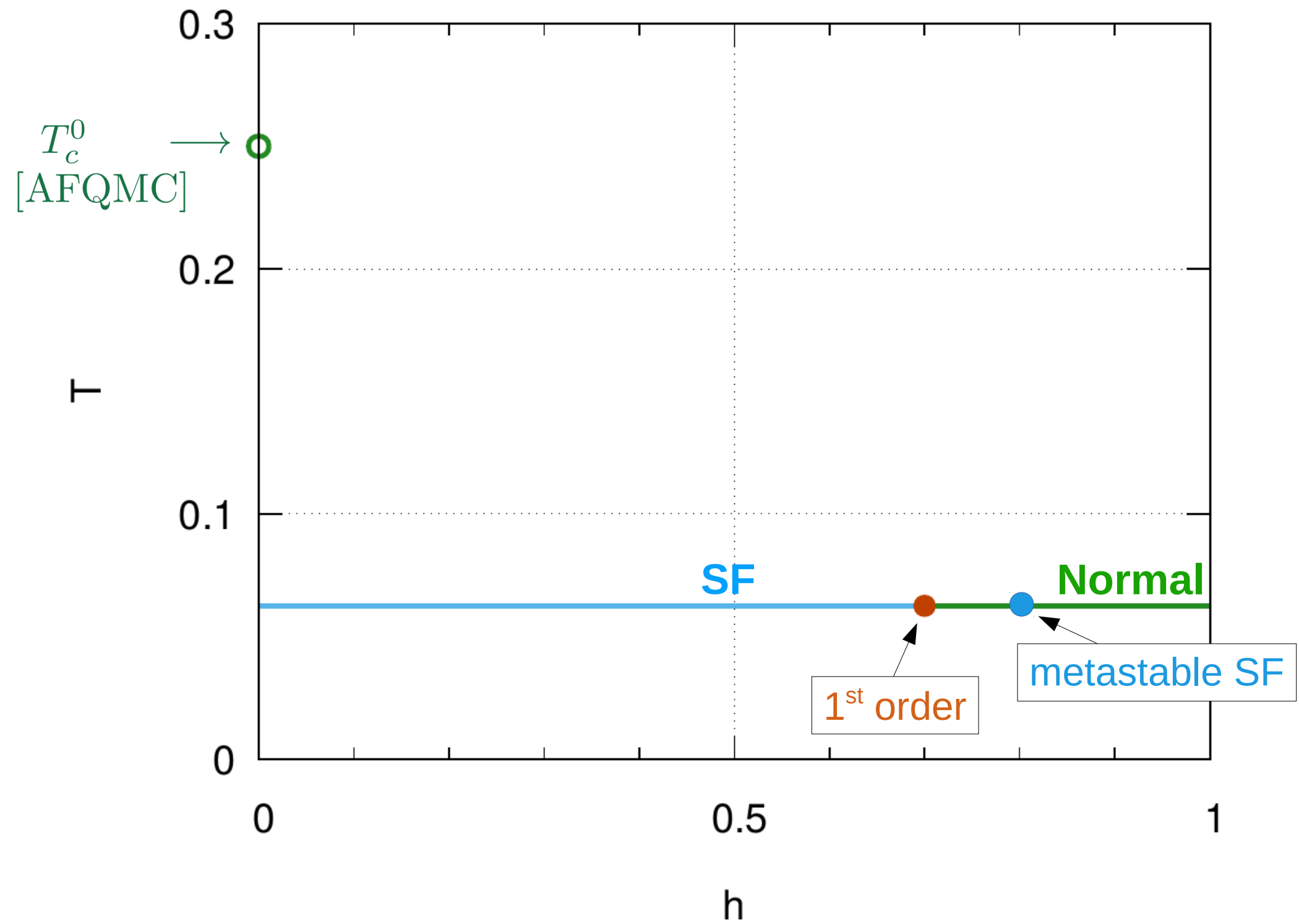


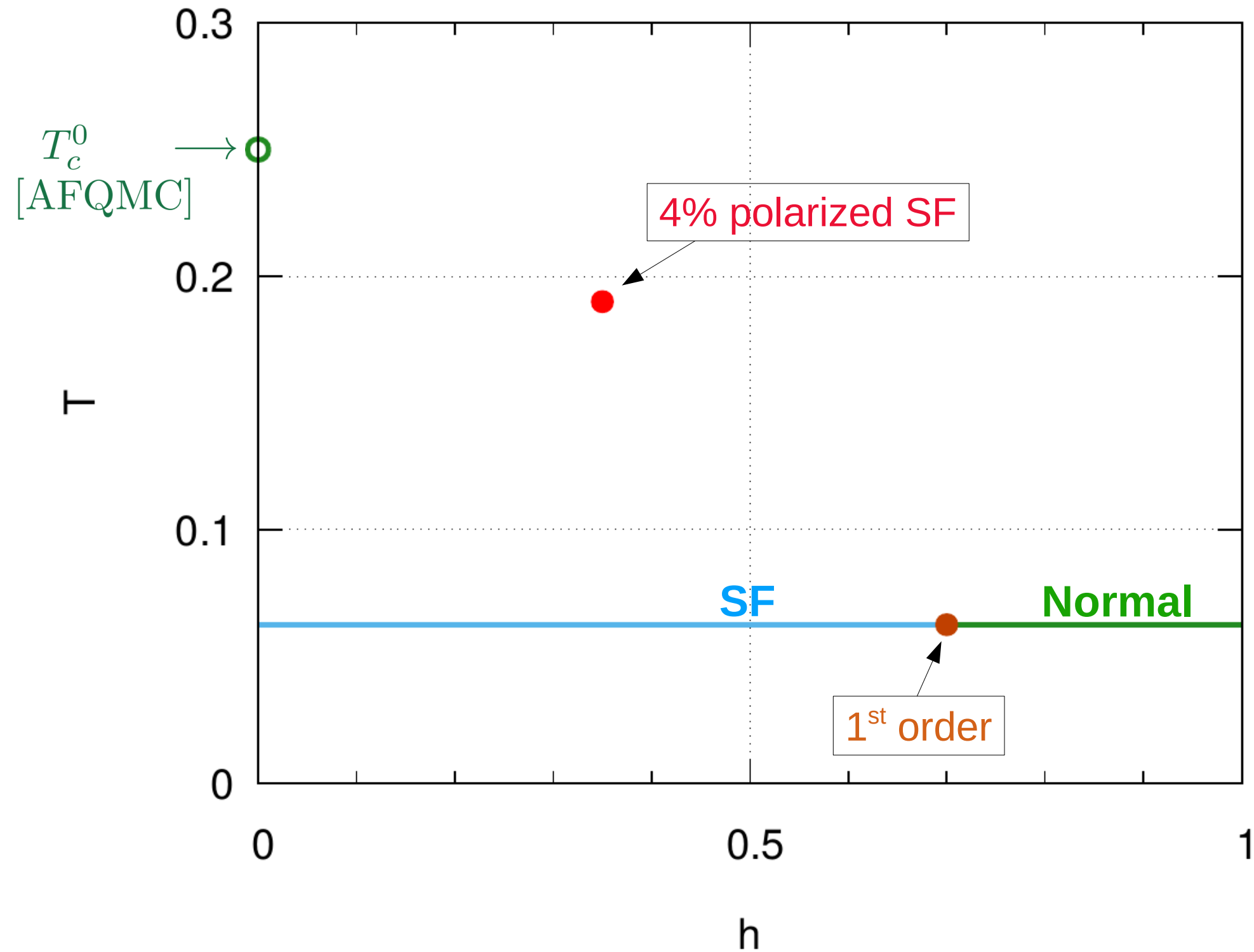
$$\text{Disc } Q(\xi) \underset{\xi \rightarrow \xi_c}{\sim} \exp\left(-\frac{\#}{|\xi - \xi_c|^{\#}}\right)$$

$$\Rightarrow Q_N \underset{N \rightarrow \infty}{\sim} \left(\frac{1}{\xi_c}\right)^N \exp(-\# N^a)$$

$$a < 1$$

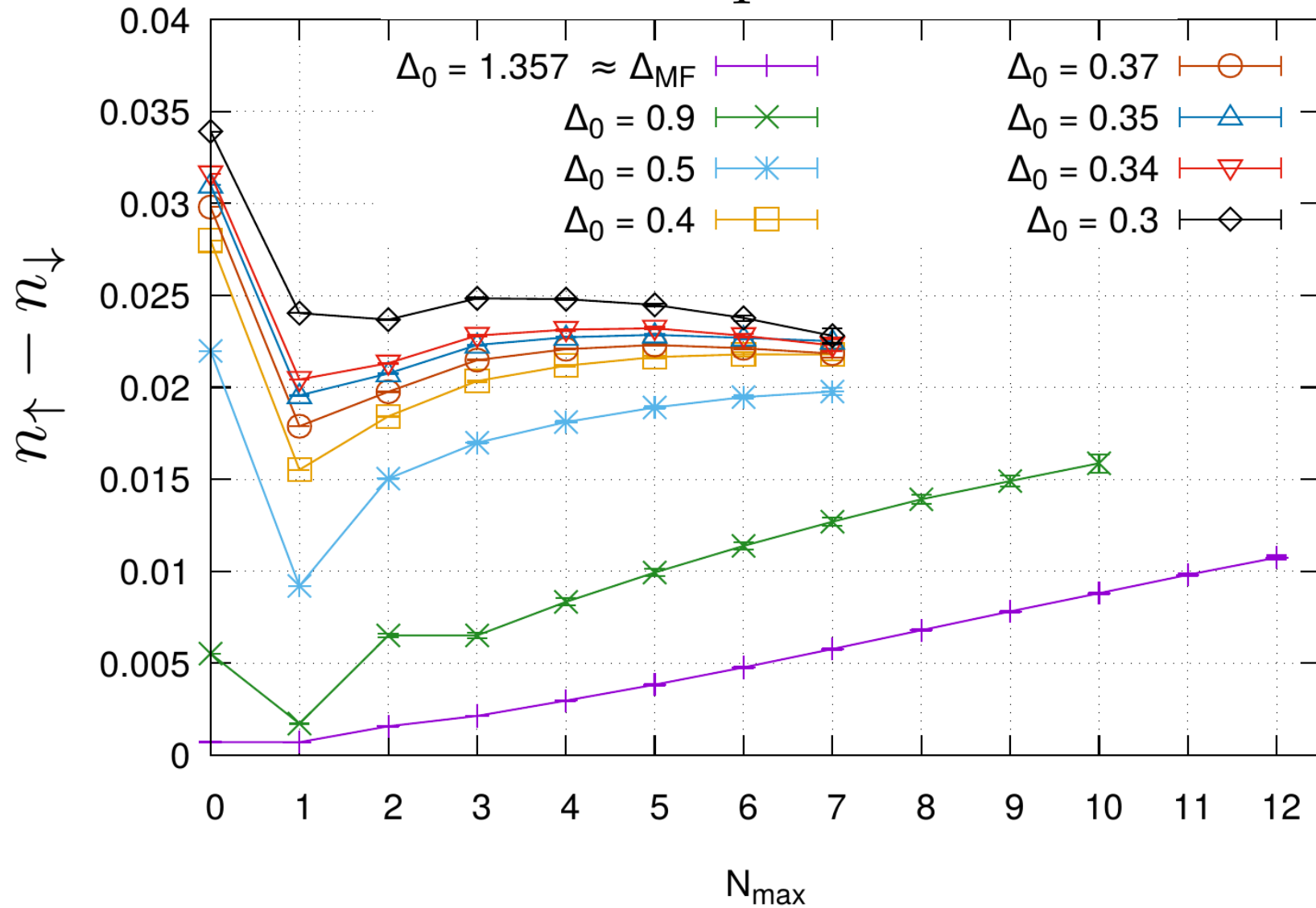






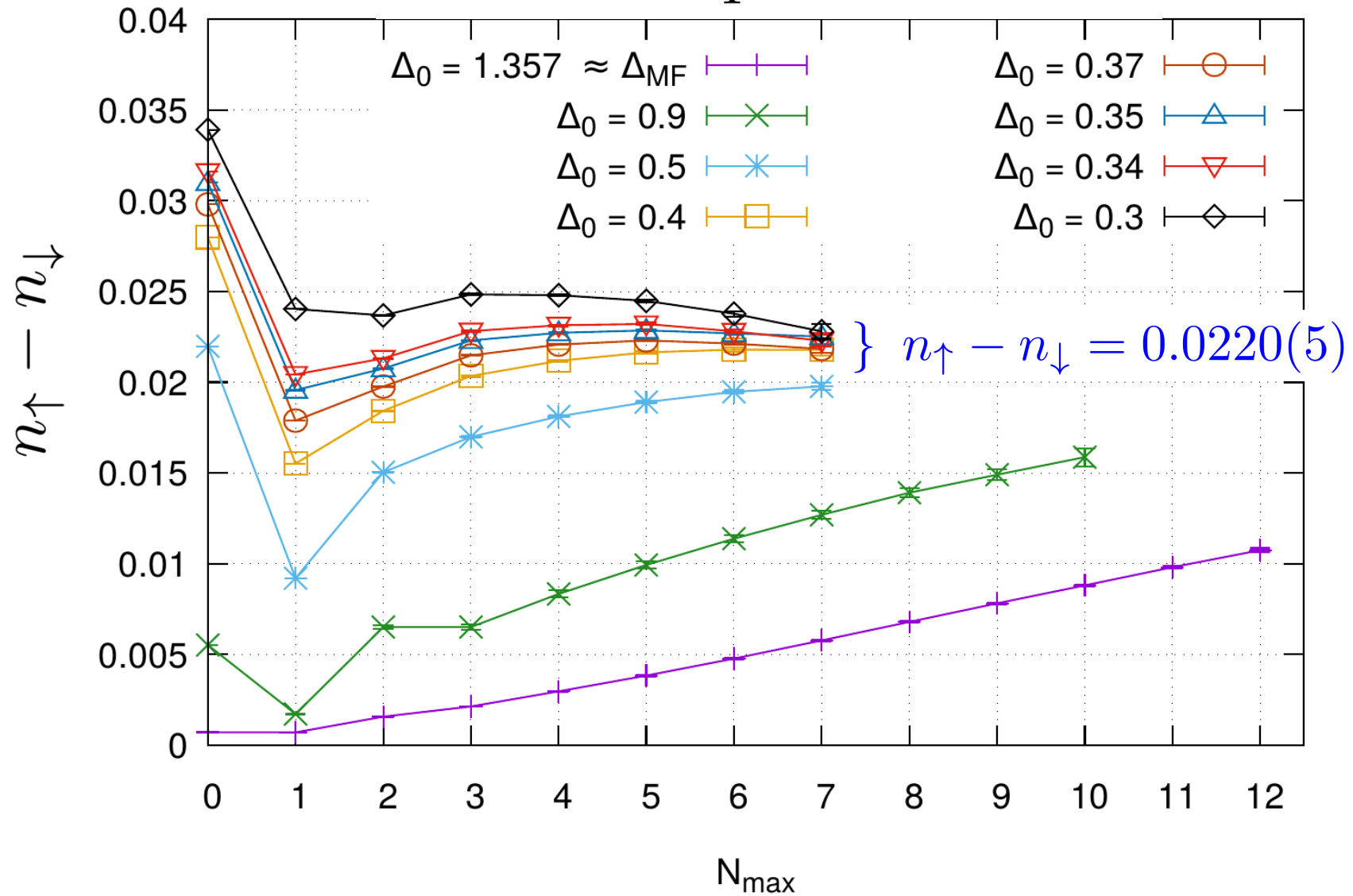
Polarized superfluid

$$T = 0.19 \approx \frac{3}{4} T_c^0, \quad h = 0.35$$



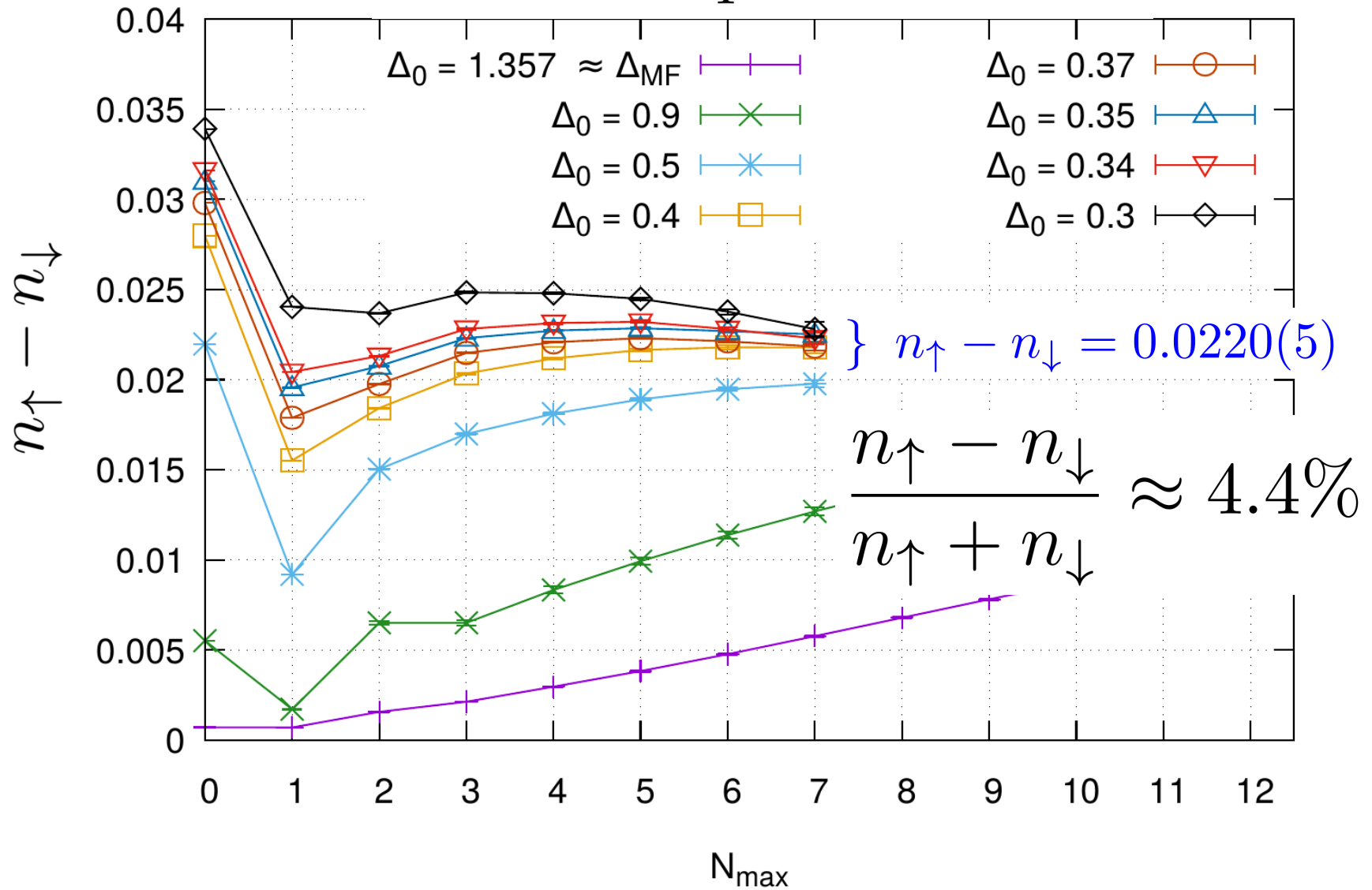
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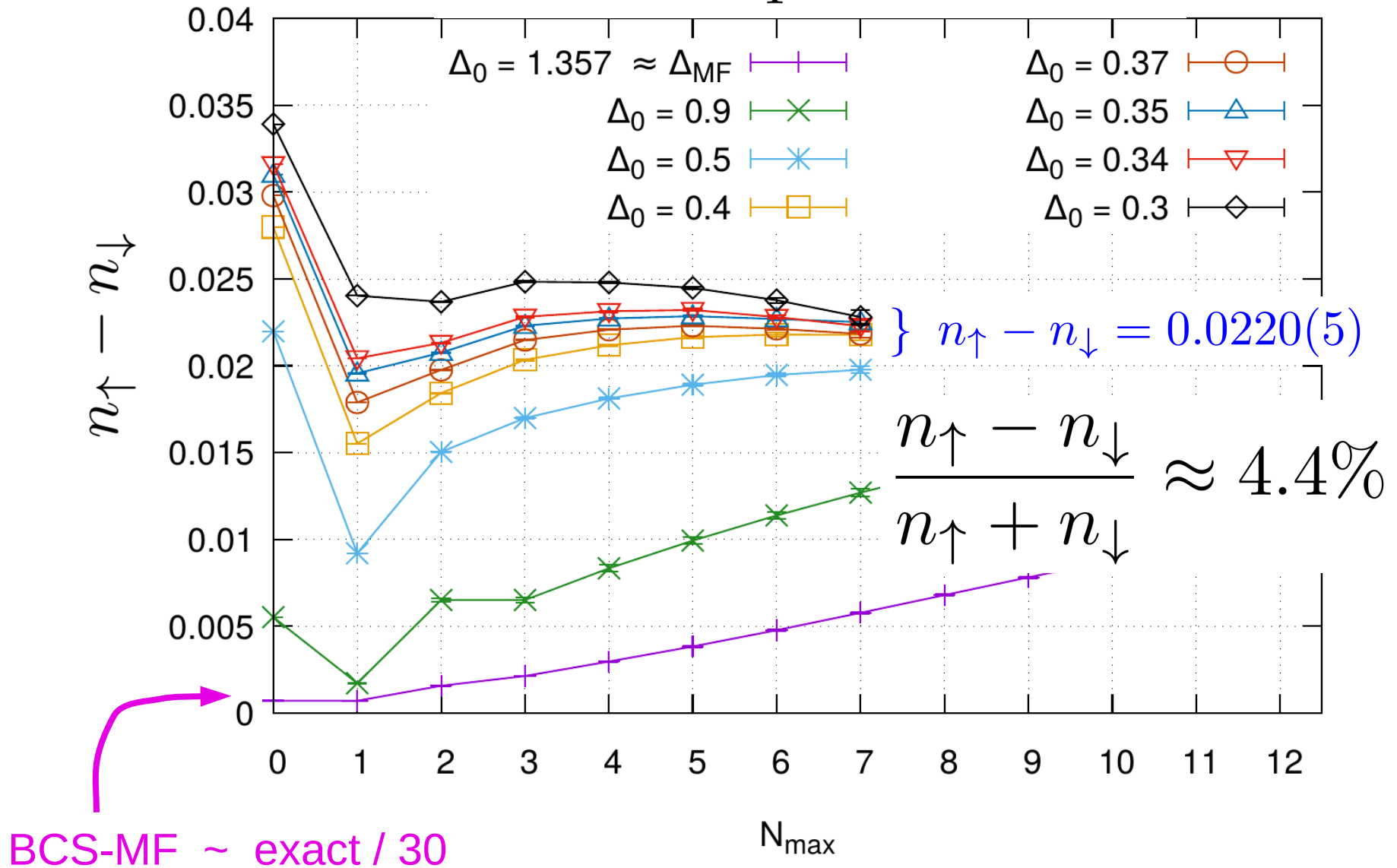
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Polarized superfluid

Quasi-particle description

$$H_{\text{eff}} = \sum_{\mathbf{k}} \sum_{\sigma=\pm 1} (E_{\mathbf{k}} - \hbar \cdot \sigma) \underbrace{b_{\mathbf{k},\sigma}^+ b_{\mathbf{k},\sigma}}_{\text{Fermionic}}$$

\rightarrow $\boxed{\hbar\text{-independent}}$

\uparrow $[b_{\mathbf{k},\sigma}; N_{\uparrow} - N_{\downarrow}] = \sigma \cdot b_{\mathbf{k},\sigma}$

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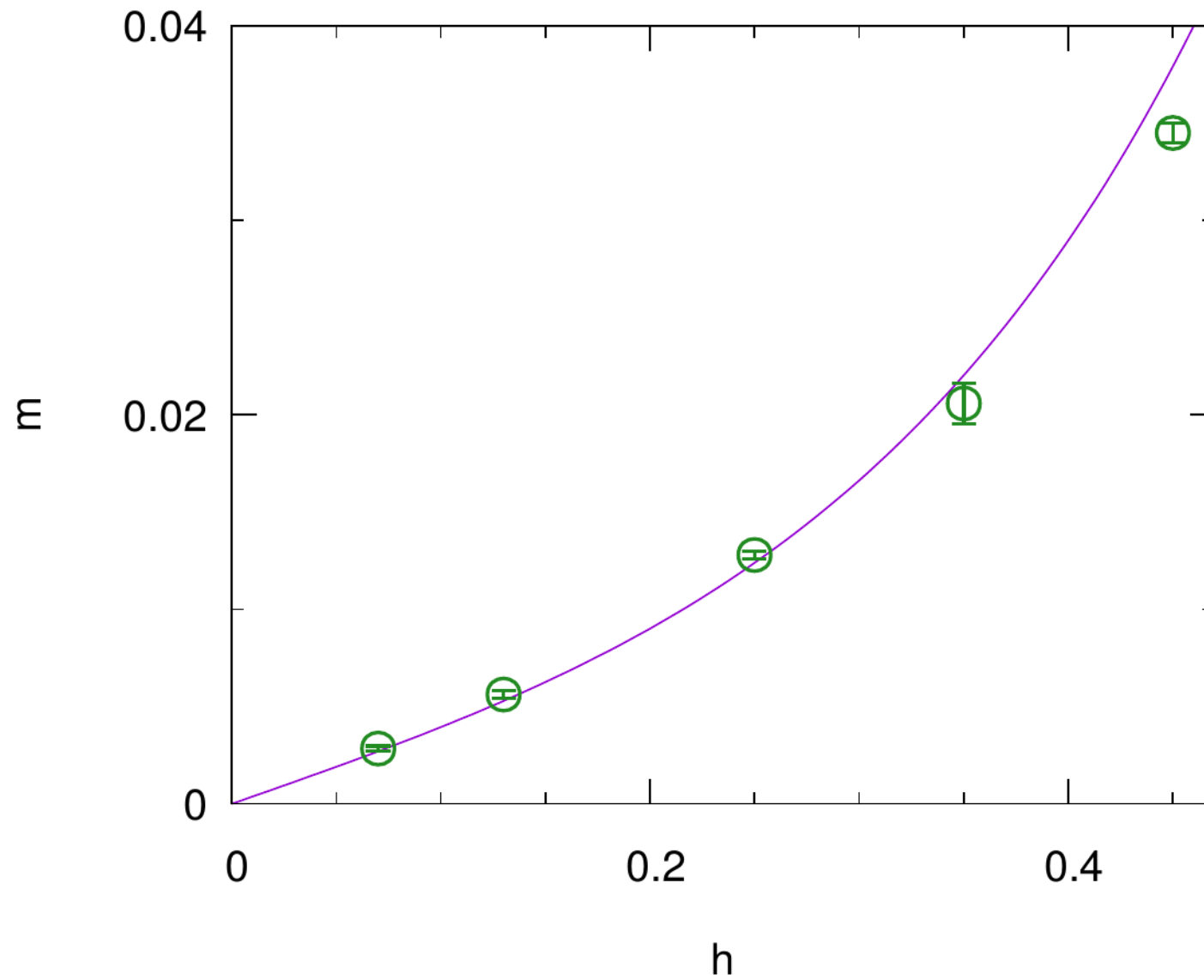
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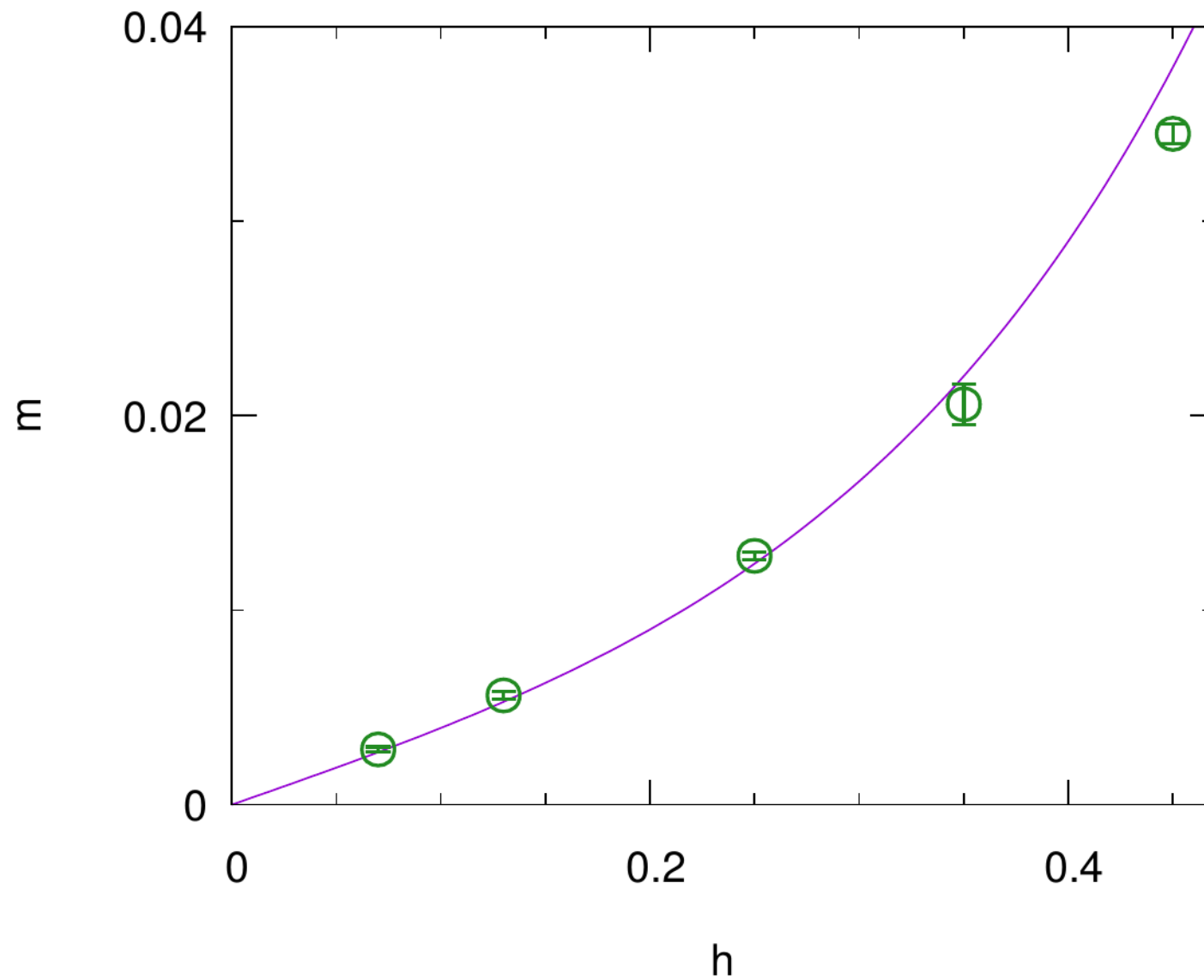
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$$E_{\mathbf{k}} \geq E_g \quad (\text{gap})$$
$$\Rightarrow n_{\text{qp}}(T) < e^{-\beta E_g}$$



$$\text{Fit: } m = m_{qp} \cdot (e^{\beta h} - e^{-\beta h})$$

$$m_{qp} \approx 0,0036$$



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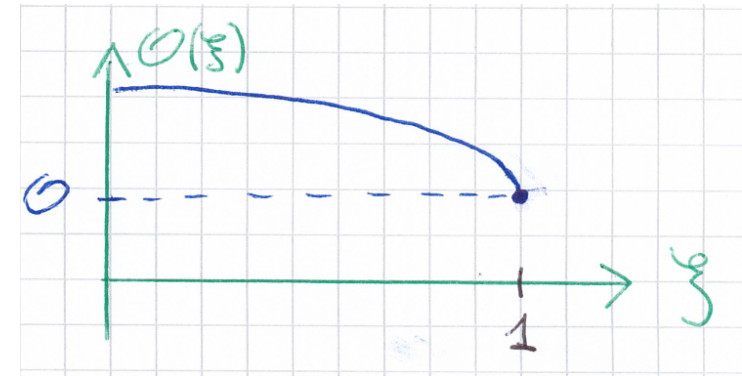
$$m_{qp} \approx 0,0036 \Rightarrow E_g < 1,07$$

Large-order behavior of SF expansion

$(1 - \xi) \Leftrightarrow$ **symmetry
breaking
field**

Goldstone singularity [Patashinskii-Pokrovskii / Brézin-Wallace, 1973]

$$\mathcal{O}(\xi) \underset{\xi \rightarrow 1^-}{=} \mathcal{O} + \text{cst} \sqrt{1 - \xi} + \dots \quad (T < T_c)$$



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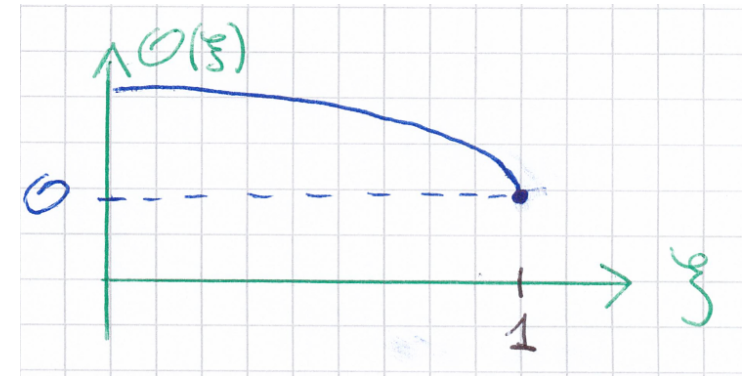
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SF stiffness



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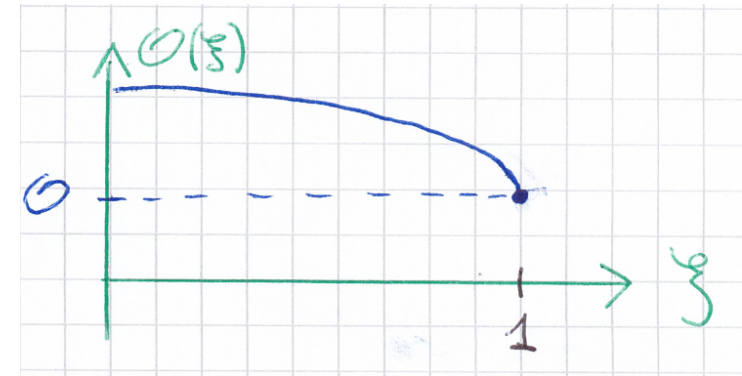
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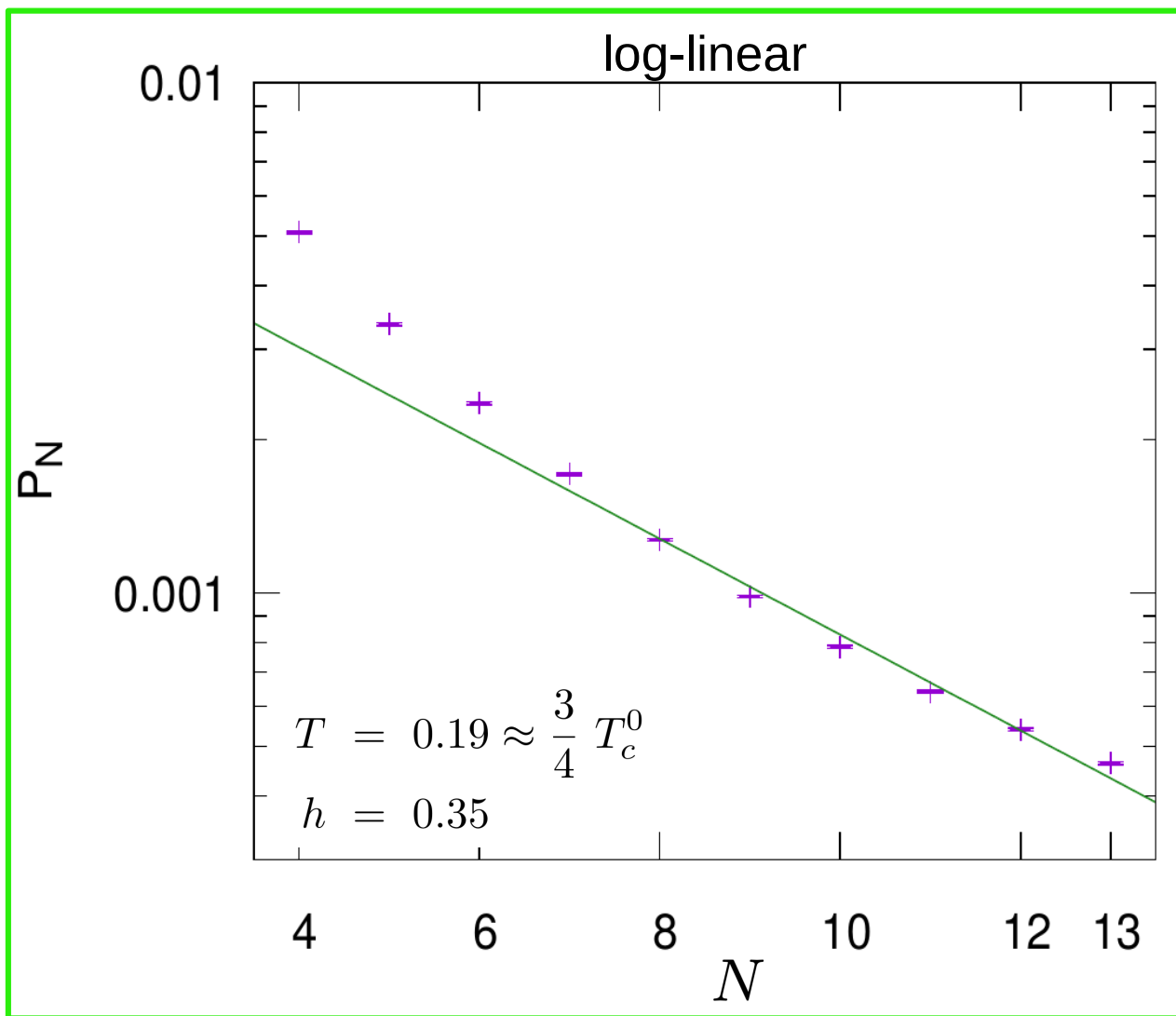
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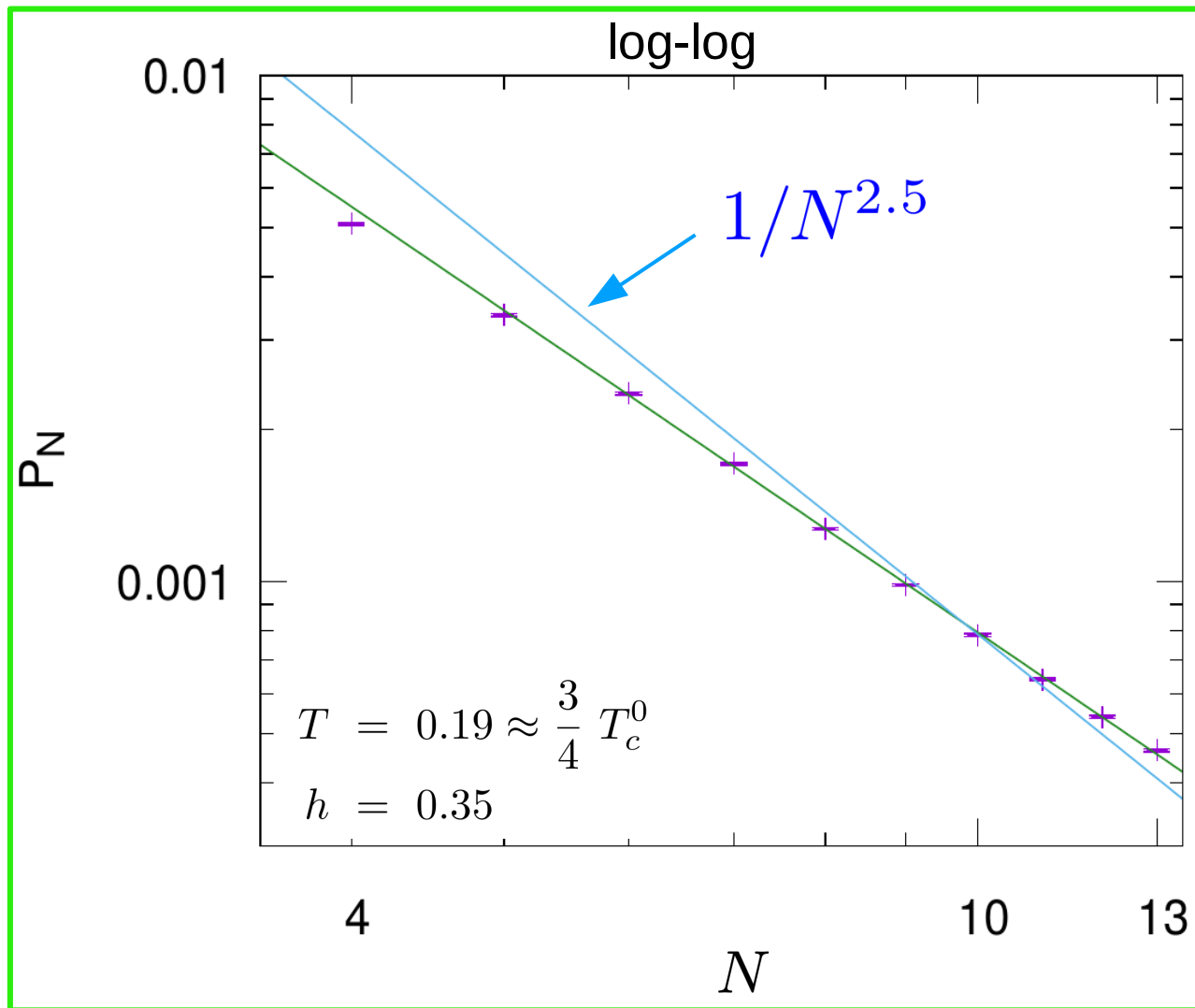
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OUTLOOK

- bare vertex $U \rightarrow$ **ladders** [CDet, Normal: Simkovic *et al.* 2020]
→ strong coupling
polarized SF at $T=0$? (gapless SF, “breached-pair phase”)

- **FFLO?** MF: yes

$$H_0 \ni \sum_{\vec{i}} \Delta_0(\vec{i}) c_{\vec{i},\uparrow}^+ c_{\vec{i},\downarrow}^+ + h.c.$$

- **2D:** BKT, algebraic order

- d-wave
supercond. phase:

$$H_0 \ni \sum_{\vec{k}} \Delta_0(\vec{k}) a_{\vec{k},\uparrow}^+ a_{-\vec{k},\downarrow}^+ + h.c.$$

- **c^0 space:** unitary gas

- filling $\rightarrow 0$

- directly in c^0 :

zero convergence radius, but resumable
as in Normal phase [Rossi *et al.* 2018] ?

- **nuclear phys:** expansion around Hartree-Fock-Bogolioubov (\sim BCS-MF)
yields promising results already at $N_{\max} = 3$ [Tichai *et al.* 2018]

our suggestion: MC in *position*-representation
[\neq Li-Wallenberger-Gull 2020]