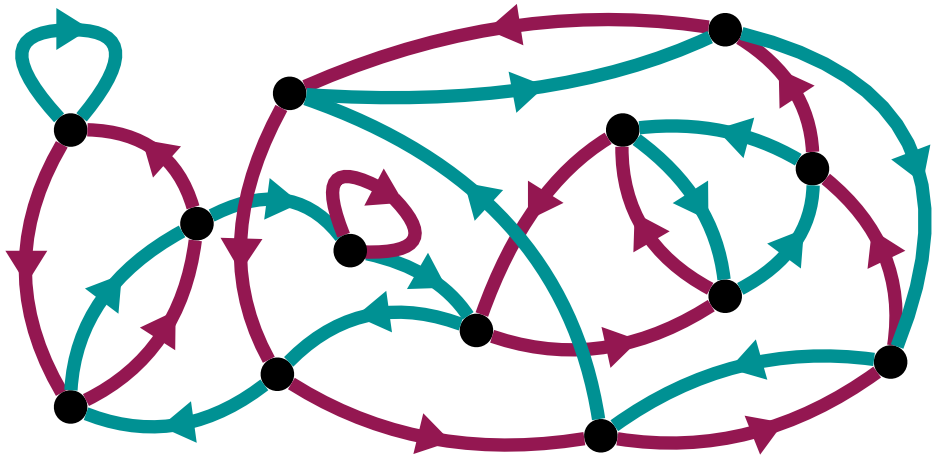
Diagrammatic Monte Carlo for the Hubbard model



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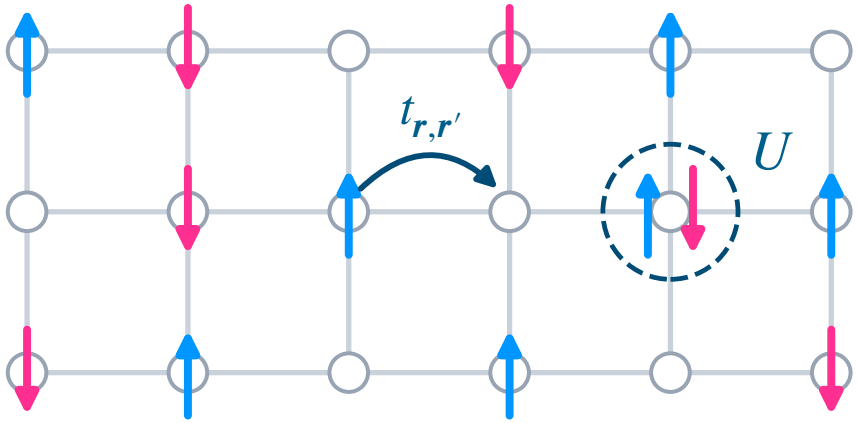
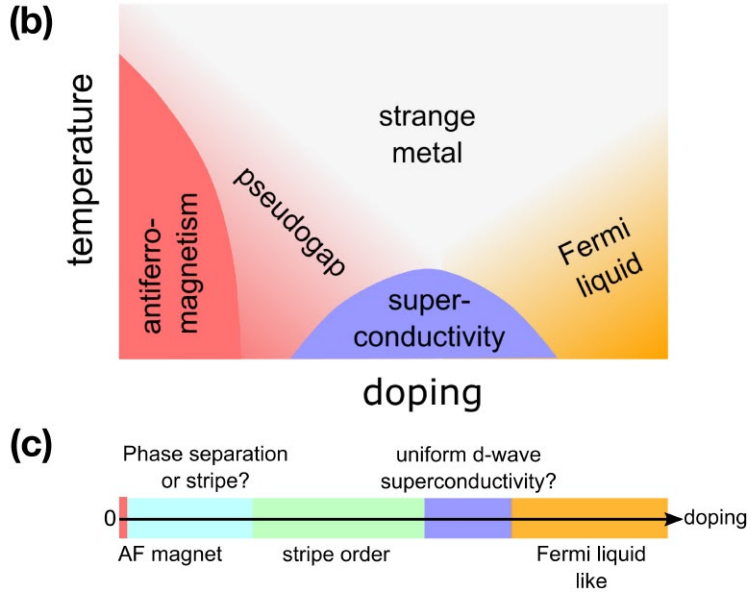
1
Introduction

The Hubbard model

$$\hat{H}_{\text{phys}} = -\mu \sum_{\sigma,\boldsymbol{r}} \hat{n}_\sigma(\boldsymbol{r}) - \sum_{\sigma,\boldsymbol{r},\boldsymbol{r}'} t_{\boldsymbol{r},\boldsymbol{r}'}\, \hat{c}^\dagger_\sigma(\boldsymbol{r})\hat{c}_\sigma(\boldsymbol{r}') + U \sum_{\boldsymbol{r}} \hat{n}_\uparrow(\boldsymbol{r})\, \hat{n}_\downarrow(\boldsymbol{r})$$

spin $\sigma \in \{\uparrow, \downarrow\}$ on lattice sites $\boldsymbol{r}$



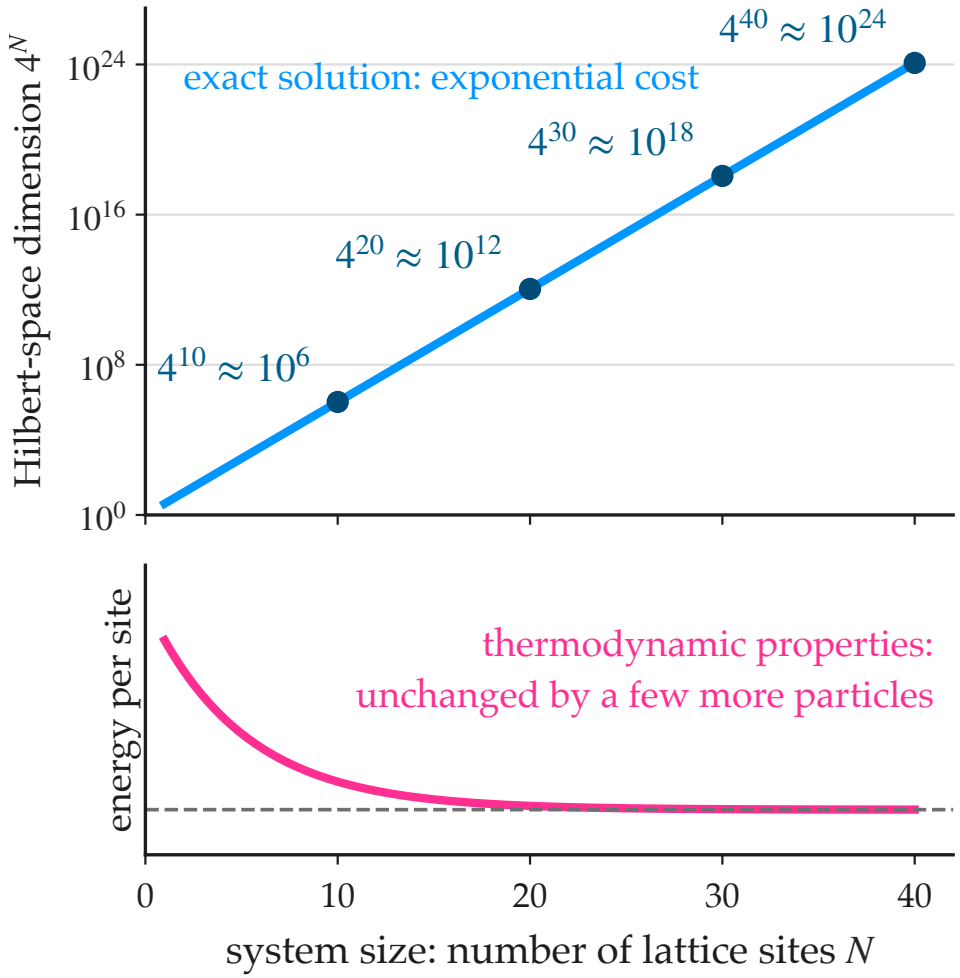


Two of many proposed phase diagrams [3]

Hotly debated phase diagram: High Tc SC?

[1] J. Hubbard, Proc. R. Soc. Lond. A 276, 238 (1963); [2] D. P. Arovas, E. Berg, S. A. Kivelson, and S. Raghu, Annu. Rev. Condens. Matter Phys. 13, 239 (2022); [3] M. Qin, T. Schäfer, S. Andergassen, P. Corboz, and E. Gull, Annu. Rev. Condens. Matter Phys. 13, 275 (2022)

An information paradox



Most of the exponentially-large wave function does not lead to any observable physical effect

Evaluating directly physical observables avoides the exponential scaling

Quantum vs Diagrammatic Monte Carlo (DiagMC)

Quantum Monte Carlo

$$\langle O \rangle = \frac{A}{Z}, \qquad A, Z \sim e^{\#\text{Volume/Temperature}}$$

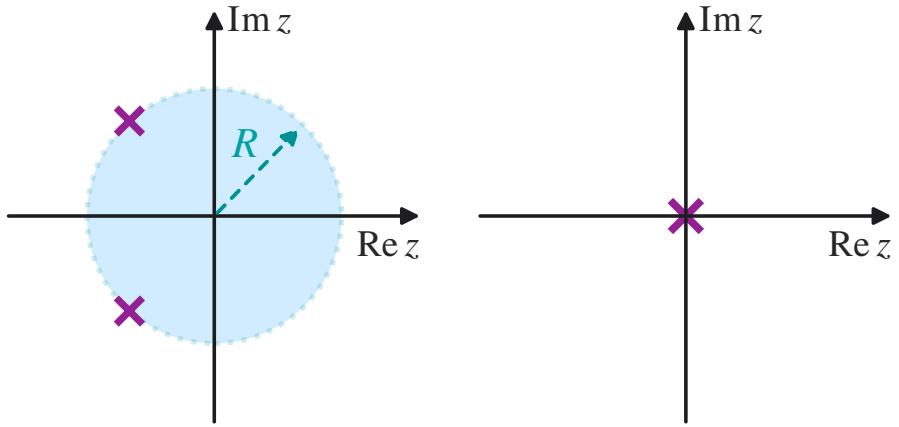
sampling both A and Z → sign problem

Diagrammatic Monte Carlo

$$\langle O \rangle = O_0 + O_1 + O_2 + \dots$$

O_j intensive: no sign problem by definition

Cancellations *help*



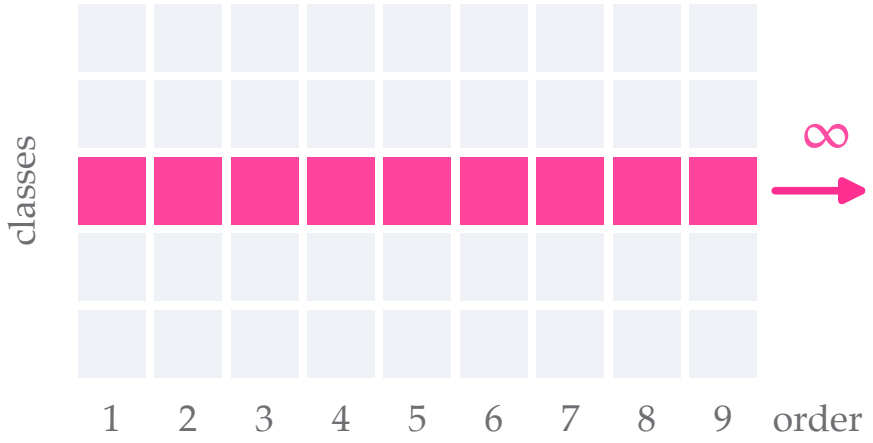
fermions: $R > 0$ bosons: $R = 0$ (generically)

(at least in some regions of the phase diagram)

Polynomial complexity for fermions

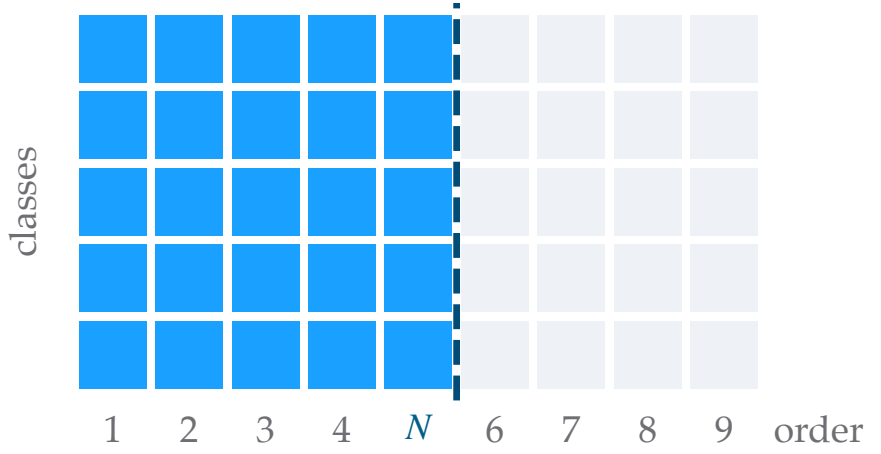
Standard perturbative approaches vs DiagMC

Conventional perturbation theory



limited subset of diagrams resummed to infinite order

Diagrammatic Monte Carlo

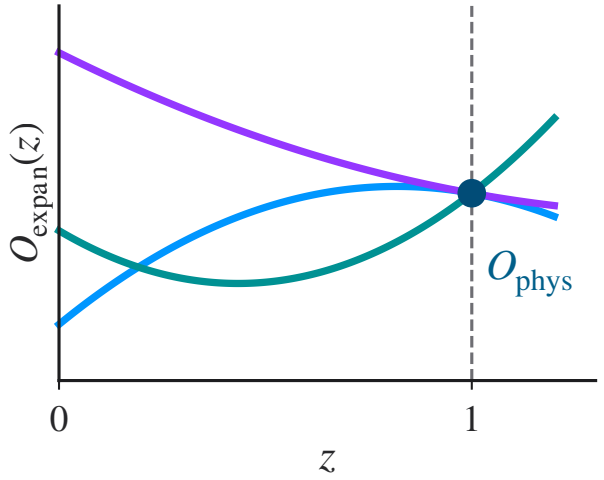


all diagrammatic contributions up to a chosen order N

Systematic way to control the reliability of the final result

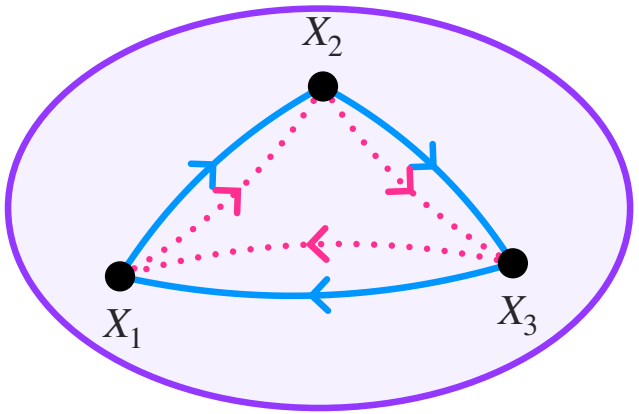
The DiagMC workflow

1 *Choosing* the expansion → **2 *Computing* the expansion** → **3 *Summing* the expansion**



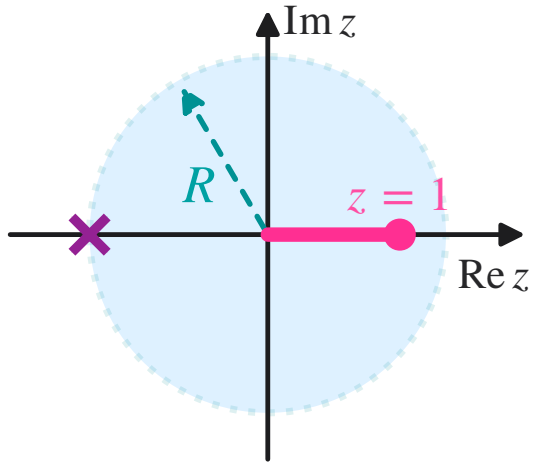
$$O_{\mathrm{expan}}(z)$$

diagrammatic renormalization and beyond



$$O_{\mathrm{expan}}(z) = \sum_{n=0}^{N} z^n \; O_{\mathrm{expan},n}$$

summing all diagrams to high orders

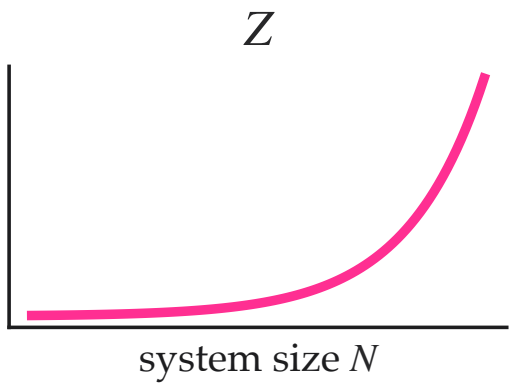


$$O_{\mathrm{phys}} = O_{\mathrm{expan}}(z = 1)$$

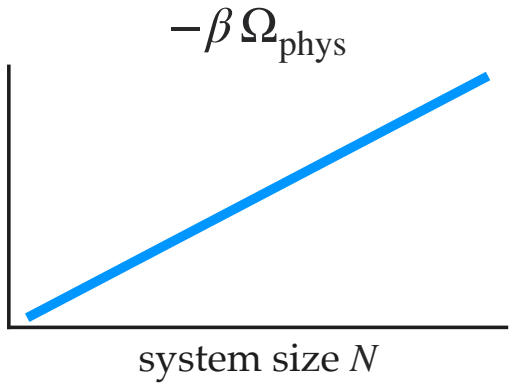
convergence, singularities and resummation

2
Notation and theoretical setup

Physical quantities and definition of **expansion**



exponential of an extensive quantity



extensive

$$Z = \mathrm{Tr}\; e^{-\beta \hat{H}_{\rm phys}}$$

$$\Omega_{\rm phys} = -\frac{1}{\beta}\log Z$$

*Abstract definition of **expansion***

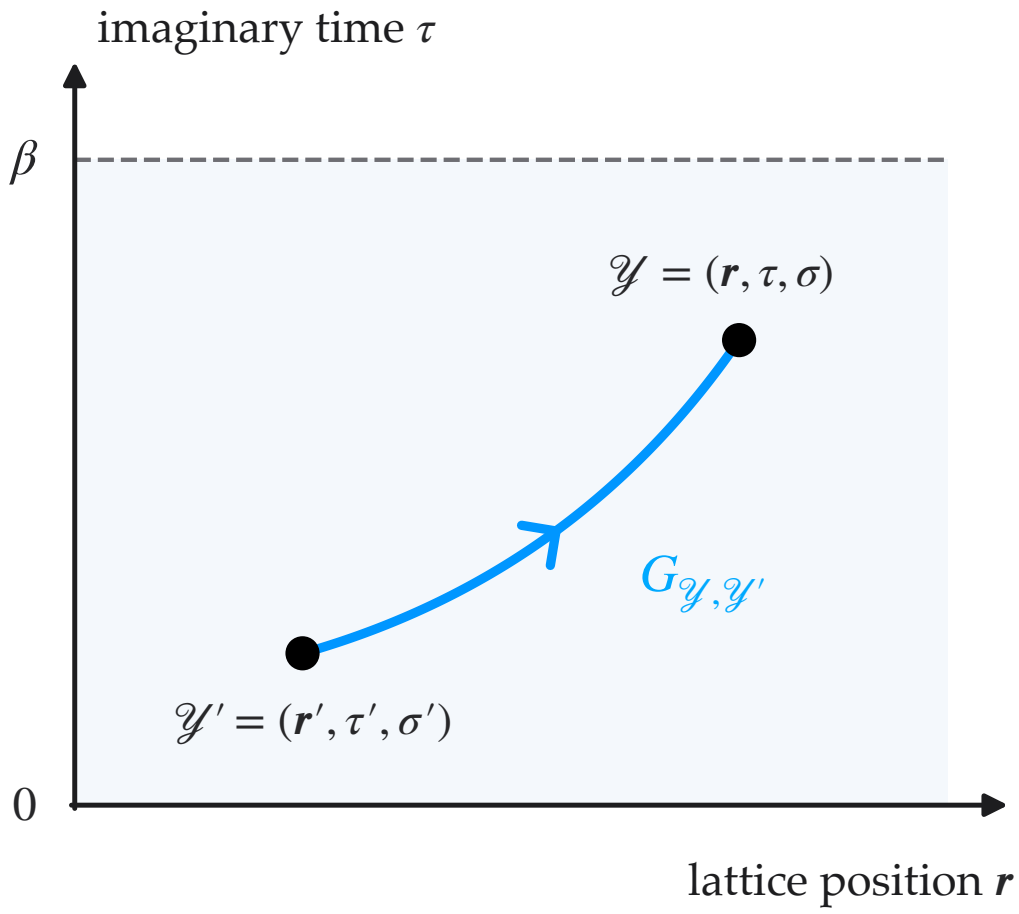
$\Omega_{\rm expan}(z)$: expansion function such that:

$$\Omega_{\rm phys} = \Omega_{\rm expan}(z=1)$$

$z \in \mathbb{C}$: effective coupling constant

Unphysical apart from $z = 1$

Imaginary-time formalism and Green's function



$$X = (\boldsymbol{r}, \tau), \qquad \tau \in [0, \beta]$$

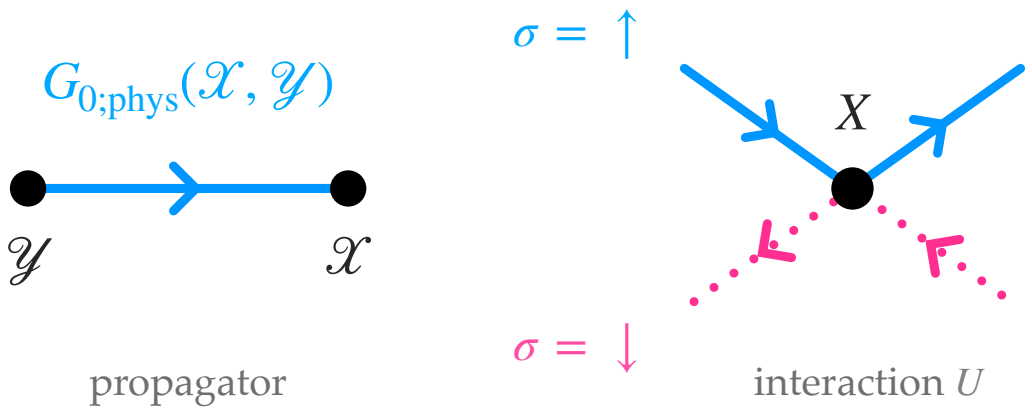
$$\mathcal{X} = (\boldsymbol{r}, \tau, \sigma)$$

$$G_{\text{phys};\mathcal{Y},\mathcal{Y}'} = -\frac{1}{Z}\text{Tr}\left[e^{-\beta \hat{H}_{\text{phys}}} \hat{T}\left(\hat{c}(\mathcal{Y})\hat{c}^{\dagger}(\mathcal{Y}')\right)\right]$$

$$G_{0;\text{phys}} = G_{\text{phys}}\Big|_{U=0}$$

Spacetime formalism is general and flexible

Diagrams and functional integral formalism



Grassmann integral:

$$S_{\mathrm{phys}} = -\langle\varphi\,|\,G^{-1}_{0;\mathrm{phys}}\,|\,\varphi\rangle + U\int dX\,(\bar{\varphi}_\uparrow\bar{\varphi}_\downarrow\varphi_\downarrow\varphi_\uparrow)(X)$$

$$\Omega_{\mathrm{phys}} = -\frac{1}{\beta}\log\int\mathscr{D}[\varphi,\bar{\varphi}]\;e^{-S_{\mathrm{phys}}}$$

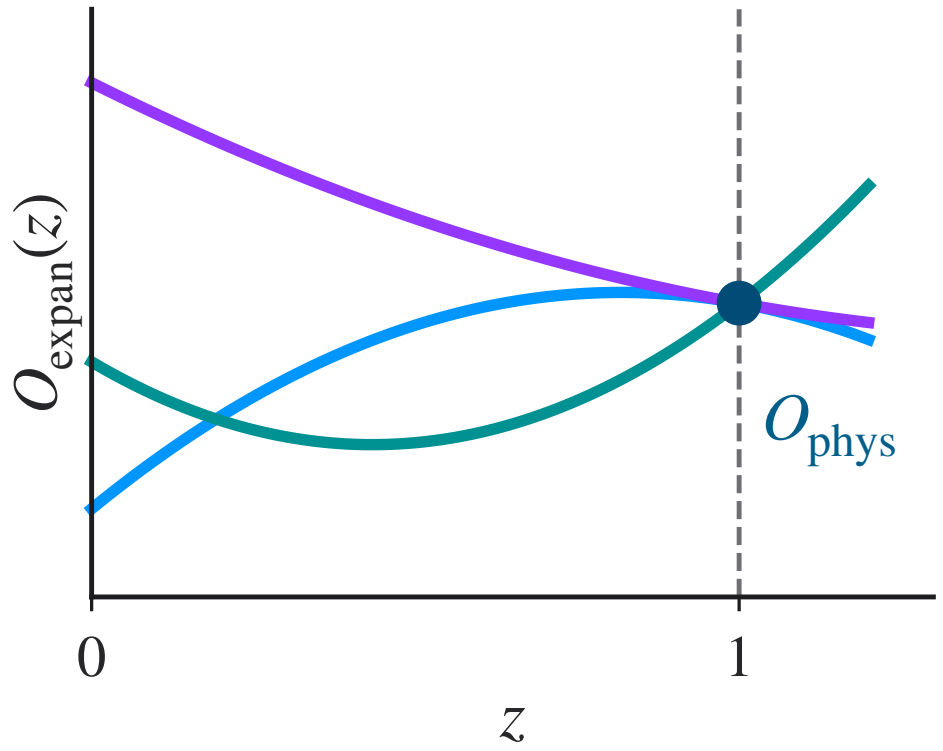
Useful for diagrammatics and for renormalization.

no quantum operators, no time ordering!

3

Choosing the expansion: diagrammatic renormalization and beyond

A purely-functional formalism to describe renormalization



Choice of expansion crucial for both qualititative and quantitative reasons

3.1 Bare-expansion functionals

$$S_{\mathrm{bare}}[G_0, V]$$

↓

3.2 Shifted-action expansions

$$S_{\mathrm{expan}}(z) := S_{\mathrm{bare}}[G_0(z), V(X) = z\,U]$$

bare expansion · α-shift · symmetry breaking · bosonic shifts

↓

3.3 Why full one-particle renormalization can converge to the wrong answer

[1] R. Rossi, F. Werner, N. Prokof'ev, and B. Svistunov, Phys. Rev. B 93, 161102(R) (2016); [2] R. Rossi, F. Šimkovic, and M. Ferrero, EPL 132, 11001 (2020)

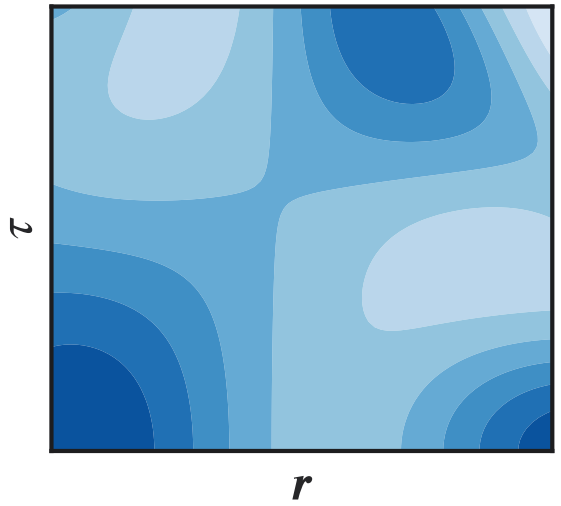
Bare-expansion functionals

$$S_{\text{phys}} = -\langle \varphi \,|\, G^{-1}_{0;\text{phys}} \,|\, \varphi \rangle + U \int dX \, (\bar{\varphi}_\uparrow \bar{\varphi}_\downarrow \varphi_\downarrow \varphi_\uparrow)(X)$$

$$S_{\text{bare}}[G_0, V] := -\langle \varphi \,|\, G_0^{-1} \,|\, \varphi \rangle + \int dX \; V(X) \; (\bar{\varphi}_\uparrow \bar{\varphi}_\downarrow \varphi_\downarrow \varphi_\uparrow)(X)$$

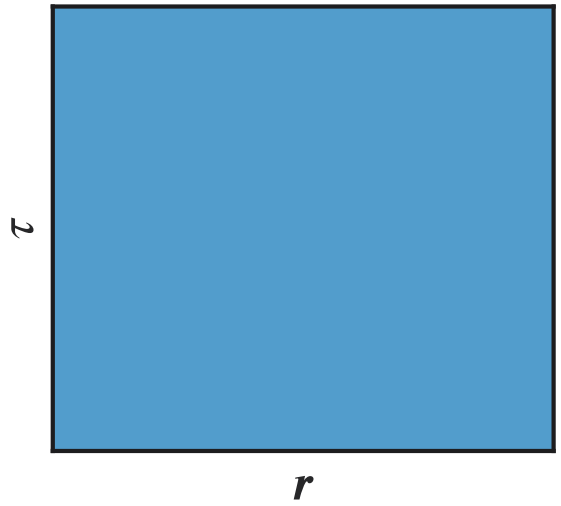
General bare functional

$V(X)$



Physical choice

$V(X) = U$

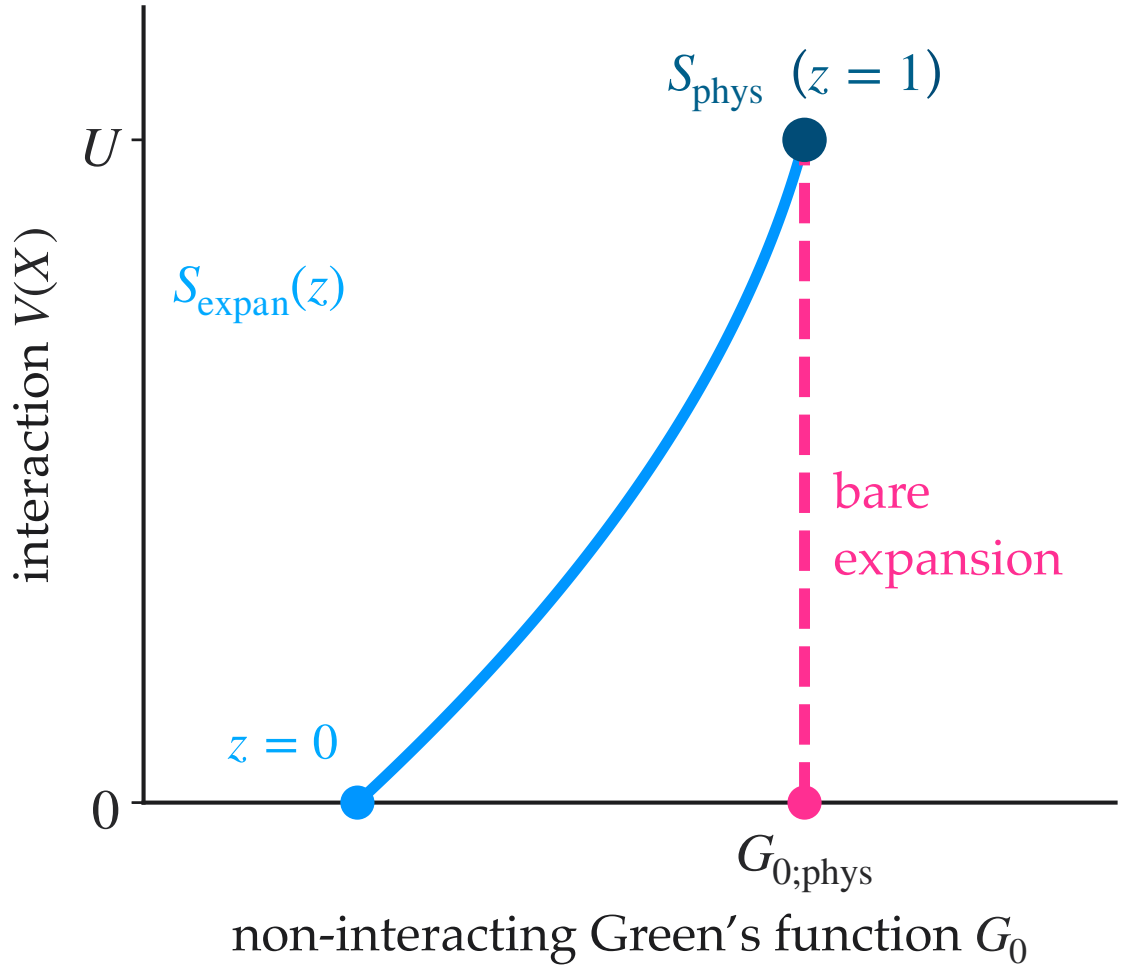


retrieving the physical action

$$S_{\text{bare}}[G_0 = G_{0;\text{phys}}, V(X) = U] = S_{\text{phys}}$$

A natural formalism for renormalization

General formalism for fermionic renormalization



shifted action

$$S_{\text{expan}}(z) := S_{\text{bare}}[G_0(z), V(X) = z\,U]$$

$$G_0(z = 1) = G_{0;\text{phys}}, \qquad S_{\text{expan}}(z = 1) = S_{\text{phys}}$$

the bare expansion

$$S_{\text{bare-ex}}(z) := S_{\text{bare}}[G_{0;\text{phys}}, V(X) = z\,U]$$

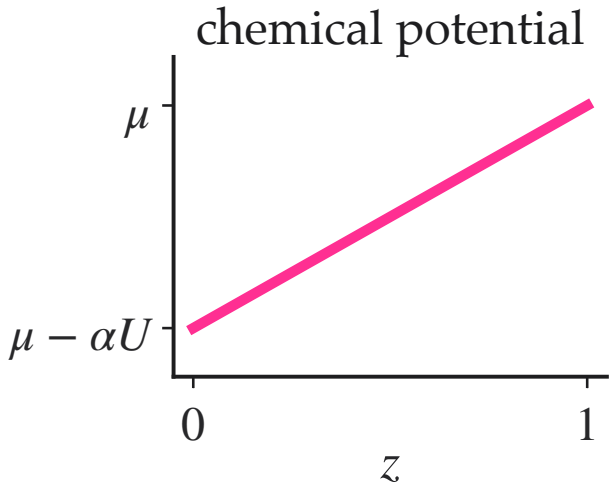
$O_{\text{expan}}(z)$ **computed with** $S_{\text{expan}}(z)$

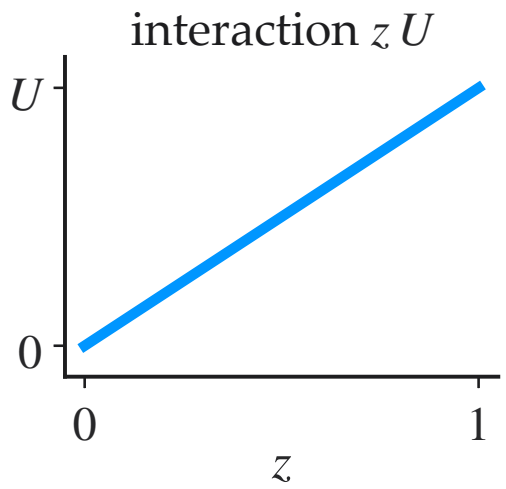
satisfies $O_{\text{expan}}(z = 1) = O_{\text{phys}}$

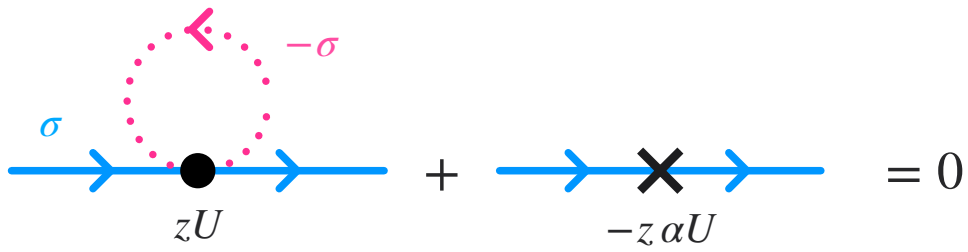
[1] R. Rossi, F. Werner, N. Prokof'ev, and B. Svistunov, Phys. Rev. B 93, 161102(R) (2016); [2] R. Rossi, F. Šimkovic, and M. Ferrero, EPL 132, 11001 (2020)

Linearly-shifted actions I: the α-shift expansion

$$\hat{H}_{\alpha\text{-sh}}(z) = \hat{H}_{\text{phys}} + (1-z)\,\alpha\,U \sum_{\boldsymbol{r},\sigma} \hat{n}_\sigma(\boldsymbol{r}) - (1-z)U \sum_{\boldsymbol{r}} \hat{n}_\uparrow(\boldsymbol{r})\hat{n}_\downarrow(\boldsymbol{r})$$







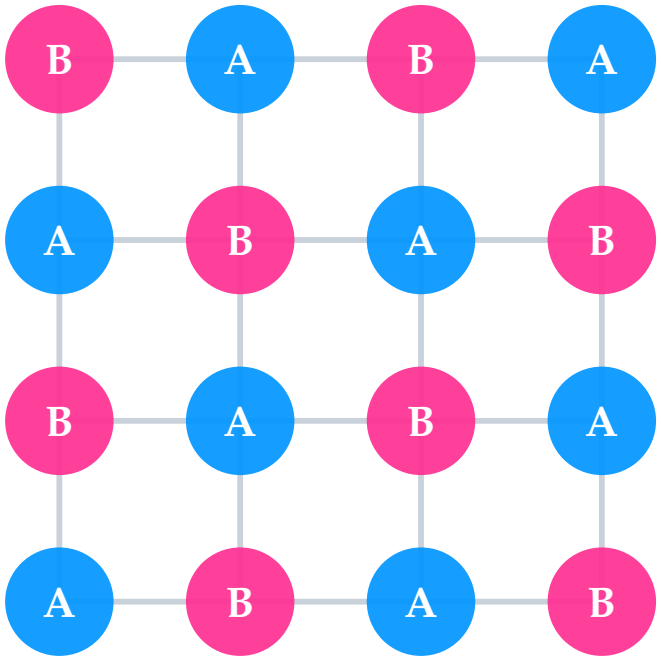
tadpole diagrams eliminated for $\alpha = n_0/2$

$O_{\text{expan}}(z)$ **depend on** α**, but** $O_{\text{expan}}(z=1) = O_{\text{phys}}$ **must be** α**-independent**

Linearly-shifted actions II: symmetry breaking terms

Example: AF phase

$$v_\sigma(\boldsymbol{r}) = \alpha\, U + \gamma\, U\, s_\sigma(\boldsymbol{r})$$



$$s_\uparrow(\boldsymbol{r}) = +1 \text{ on } A,\ -1 \text{ on } B$$

$$s_\downarrow(\boldsymbol{r}) = -s_\uparrow(\boldsymbol{r})$$

Bare expansion cannot work in symmetry-broken phase.

Solution: break symmetry

$$\hat{H}_{\alpha\gamma\text{-sh}}(z) = \hat{H}_{\text{phys}} + (1-z)\sum_{\boldsymbol{r},\sigma} v_\sigma(\boldsymbol{r})\,\hat{n}_\sigma(\boldsymbol{r}) - (1-z)U\sum_{\boldsymbol{r}} \hat{n}_\uparrow(\boldsymbol{r})\hat{n}_\downarrow(\boldsymbol{r})$$

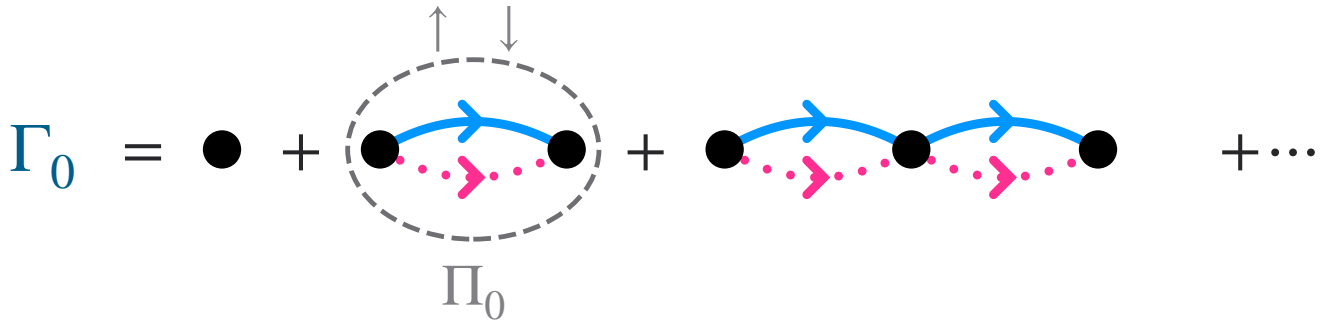
Quadratic at $z = 0$, physical at $z = 1$

Necessary to converge!

[1] G. Spada, R. Rossi, F. Šimkovic, R. Garioud, M. Ferrero, K. Van Houcke, and F. Werner, arXiv:2103.12038 (2021); [2] R. Garioud, F. Šimkovic, R. Rossi, G. Spada, T. Schäfer, F. Werner, and M. Ferrero, Phys. Rev. Lett. 132, 246505 (2024)

Linearly-shifted actions III: bosonic shifts

$$S_{\text{expan}}(z) = -\langle \varphi \,|\, G_0^{-1}(z) \,|\, \varphi \rangle - \int_{X,Y} \bar{\eta}(X)\eta(Y) W_0^{-1}(X,Y)(z) + \sqrt{z} \int_X (\bar{\eta}\varphi_\uparrow \varphi_\downarrow + \text{c.c.})(X)$$

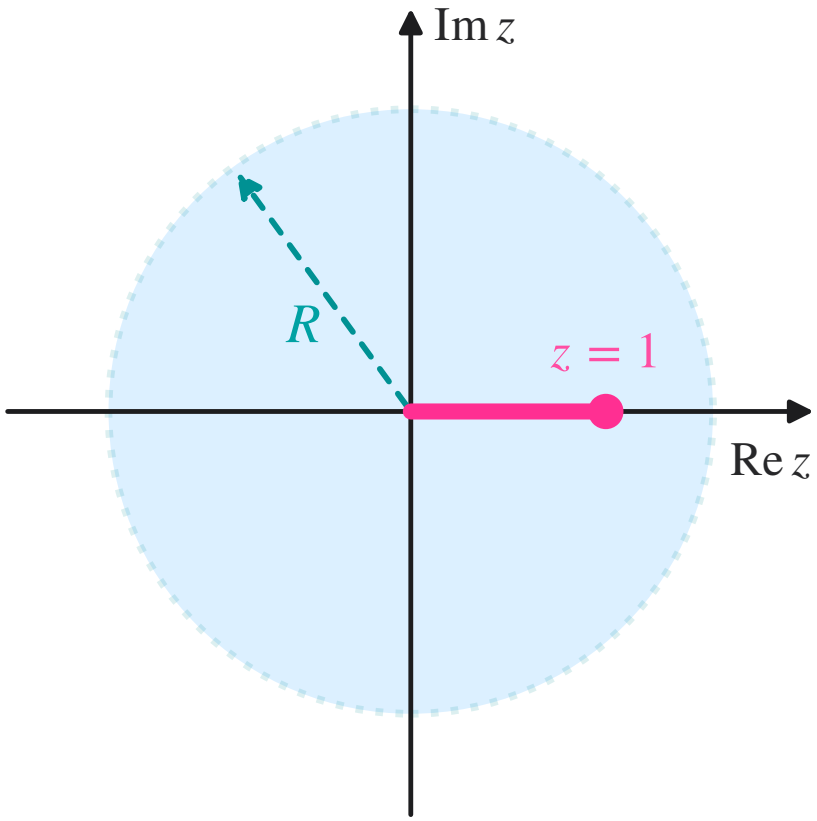


$$W_0^{-1}(z) = \Gamma_0^{-1} + z\Pi_0$$

all particle-particle bubble diagrams are eliminated

Example of renormalization beyond the one-particle channel

Why full one-particle renormalization can converge to the wrong answer



strictly inside the radius of convergence:
misleading convergence ruled out

Fully-self-consistent schemes can create unphysical singularities AND a misleading convergence

Fully-self-consistent expansions I: full chemical-potential renormalization

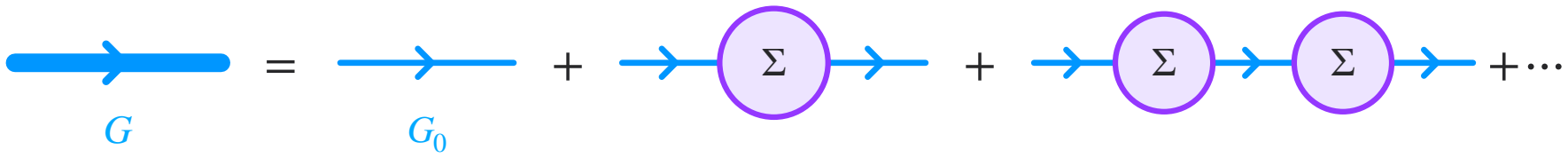
$$\mu(z) \qquad \text{such that} \qquad n(z) = n$$

$\mu(z)$ real chemical potential → **no problem!**

E. Kozik, M. Ferrero, and A. Georges, Phys. Rev. Lett. 114, 156402 (2015)

Fully-self-consistent expansions II: one-particle renormalization

$$G_0(z) \qquad \text{such that} \qquad G(z) = G$$

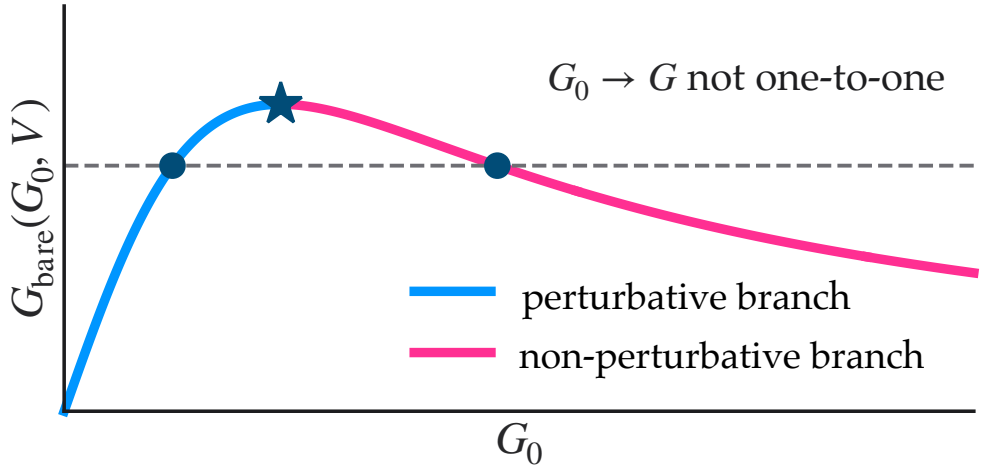


$$G^{-1} = (G_{0;\text{bold}}[G, V])^{-1} - \Sigma_{\text{bare}}[G_{0;\text{bold}}[G, V], V]$$

$$\Sigma_{\text{bold}}[G, V] := \Sigma_{\text{bare}}[G_{0;\text{bold}}[G, V], V]$$

Solved order-by-order in V -> **skeleton Feynman diagrams**

Non-invertibility of the mapping G0 → G and misleading convergence



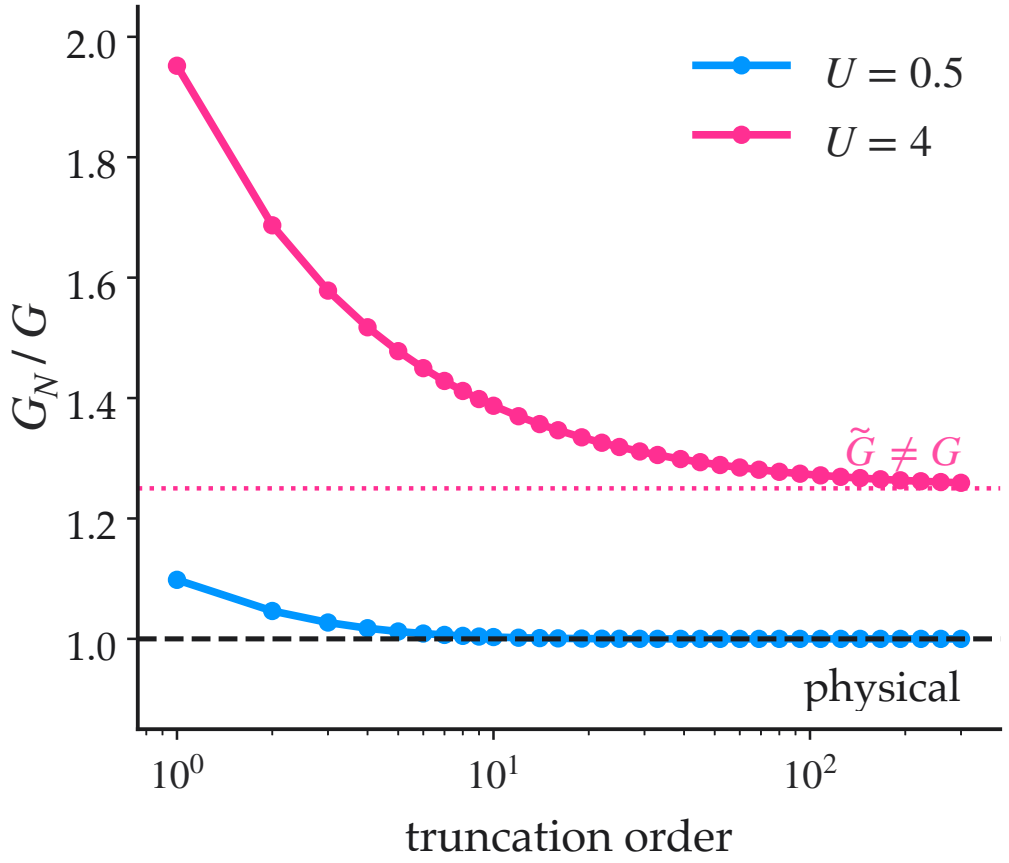
0-D Hubbard model

$$\Sigma_{\mathrm{bold}}(G, V) = \frac{-1 \pm \sqrt{1 + 4\,VG^2}}{2G}$$

No physical phase transition

artificial singularity at large-enough U

Misleading convergence:

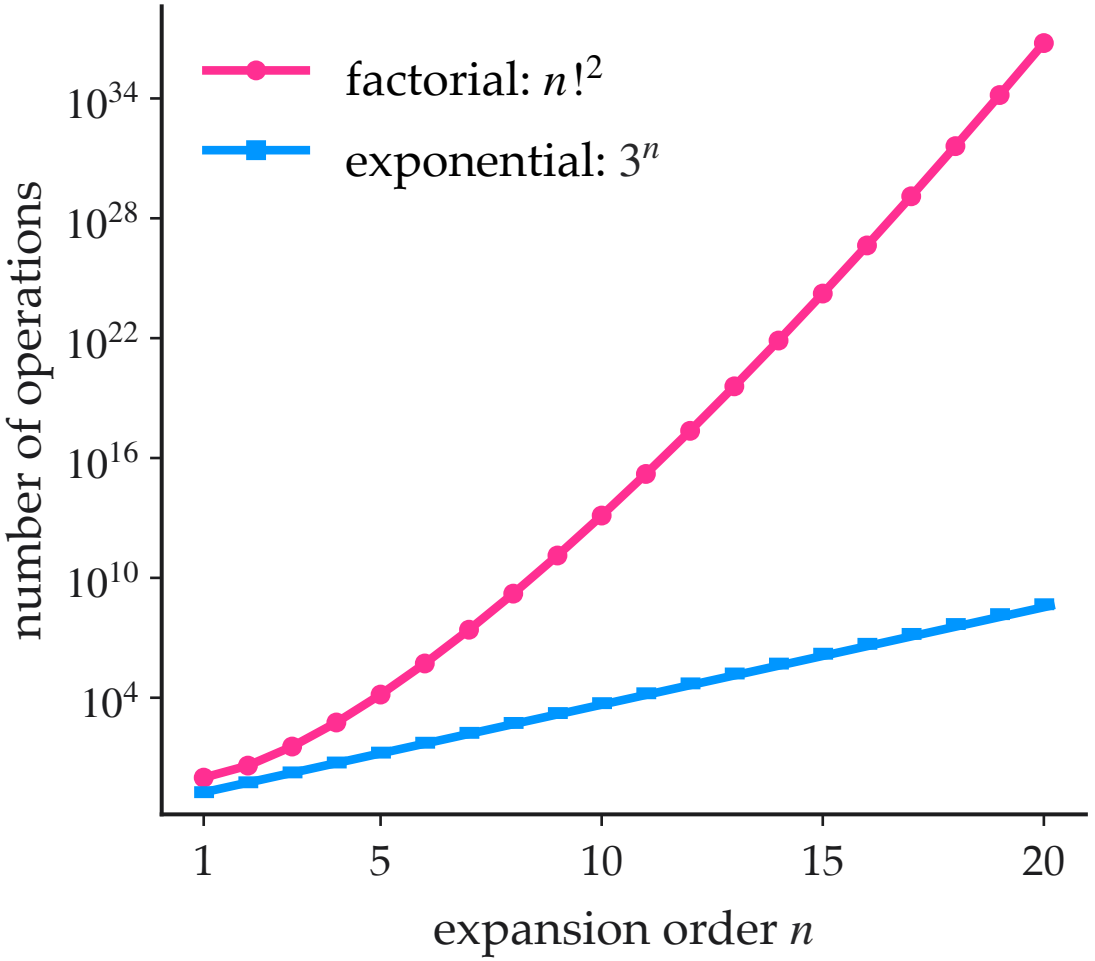


R. Rossi and F. Werner, J. Phys. A: Math. Theor. 48, 485202 (2015)

4

Computing the expansion: summing all diagrams to high orders

The efficient computation of the expansion coefficients



3 main strategies to evaluate the coefficients:

(i) **enumerate** all Feynman diagrams one-by-one

(ii) **sample** Feynman-diagram topologies [1–4]

(iii) **sum** over all symmetrized diagram topologies

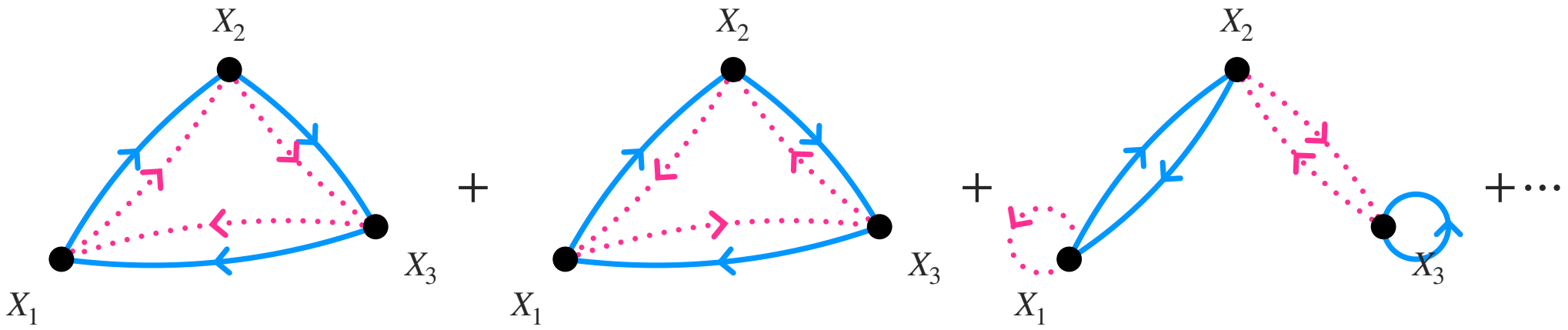
Summing all connected Feynman diagrams is NP-hard

but exponential algorithms are still much better than enumeration

[1] N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. Lett. 99, 250201 (2007); [2] K. Van Houcke, E. Kozik, N. Prokof'ev, and B. Svistunov, Physics Procedia 6, 95 (2010); [3] E. Kozik, K. Van Houcke, E. Gull, L. Pollet, N. Prokof'ev, B. Svistunov, and M. Troyer, EPL 90, 10004 (2010); [4] N. Prokof'ev, "Diagrammatic Monte Carlo", in E. Pavarini, E. Koch, and S. Zhang, eds., Many-Body Methods for Real Materials, Modeling and Simulation Vol. 9, Forschungszentrum Jülich (2019)

Symmetrized sum of all connected Feynman diagrams

$$O_{\text{expan},n} = \frac{1}{n!} \int dX_1 \ldots dX_n \; V(X_1) \ldots V(X_n) \; O_{\text{expan}}(\{X_1, \ldots, X_n\}) \Big|_{V(X)=U}$$



$O_{\text{expan}}(\{X_1, \ldots, X_n\})$: sum of **all** connected Feynman diagrams with fixed vertex positions, **symmetrized** over the vertex positions

Symmetrizing diagrams over vertex positions is important

Third order, at half filling: the two contributions cancel exactly

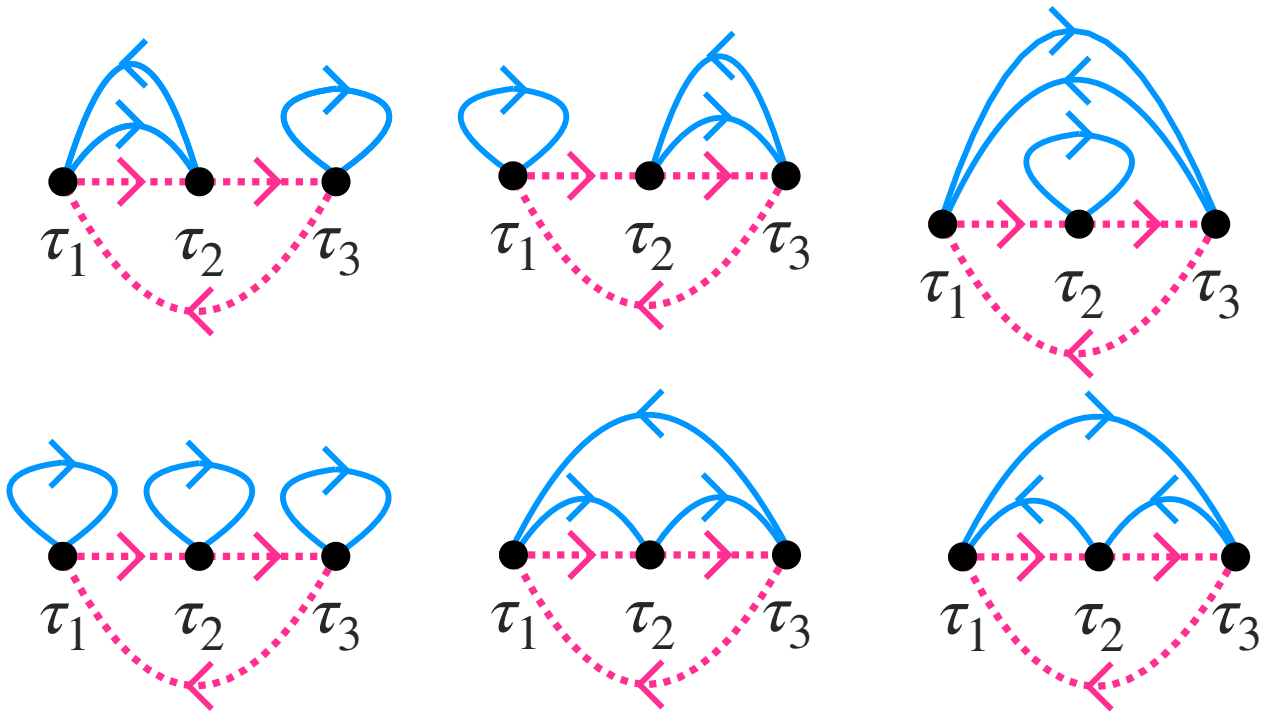
$$\hat{H} = -\mu\hat{N}, \qquad \mu(z) = z$$

$$F(z) = -\frac{1}{\beta}\log(1 + e^{\beta z})$$

$$F_{2n+1} = 0, \qquad n \geq 1$$

Cancellations inside this single Feynman diagram:
perfect for odd n, still exponential for even n

Summing over all Feynman-diagram topologies is important



$$\hat{H}(z) = -\sum_{\sigma} \mu_\sigma \hat{n}_\sigma + z\, U \hat{n}_\uparrow \hat{n}_\downarrow$$

limit $\beta\mu_\downarrow \to -\infty$

$$F_n = -\frac{(-\beta U)^n}{\beta\, n!} \frac{e^{\beta\mu_\downarrow}}{1 + e^{-\beta\mu_\uparrow}} + O(e^{2\beta\mu_\downarrow})$$

$n!$ Feynman diagrams, same absolute contribution, $F_n \sim 1/n!$:

factorial cancellations between topologies

Wick's theorem → sum of all symmetrized connected+disconnected diagrams

$$(-1)^m \langle \varphi(\mathcal{X}_1)\bar{\varphi}(\mathcal{Y}_1)\ldots\varphi(\mathcal{X}_m)\bar{\varphi}(\mathcal{Y}_m)\rangle_{S_{\text{bare}}[G_0,0]} = \sum_{\sigma\in S_m} \text{sign}\ \sigma \prod_{j=1}^{m} G_0(\mathcal{X}_j, \mathcal{Y}_{\sigma_j}) = \det \mathbb{G}_0$$

$$\det \begin{vmatrix} G_{11} & G_{12} & G_{13} & G_{14} \\ G_{21} & G_{22} & G_{23} & G_{24} \\ G_{31} & G_{32} & G_{33} & G_{34} \\ G_{41} & G_{42} & G_{43} & G_{44} \end{vmatrix}$$

$$G_{jk} = G_0(\mathcal{X}_j, \mathcal{Y}_k)$$

one permutation σ: $\text{sign}\,\sigma \prod_j G_{j\sigma_j}$

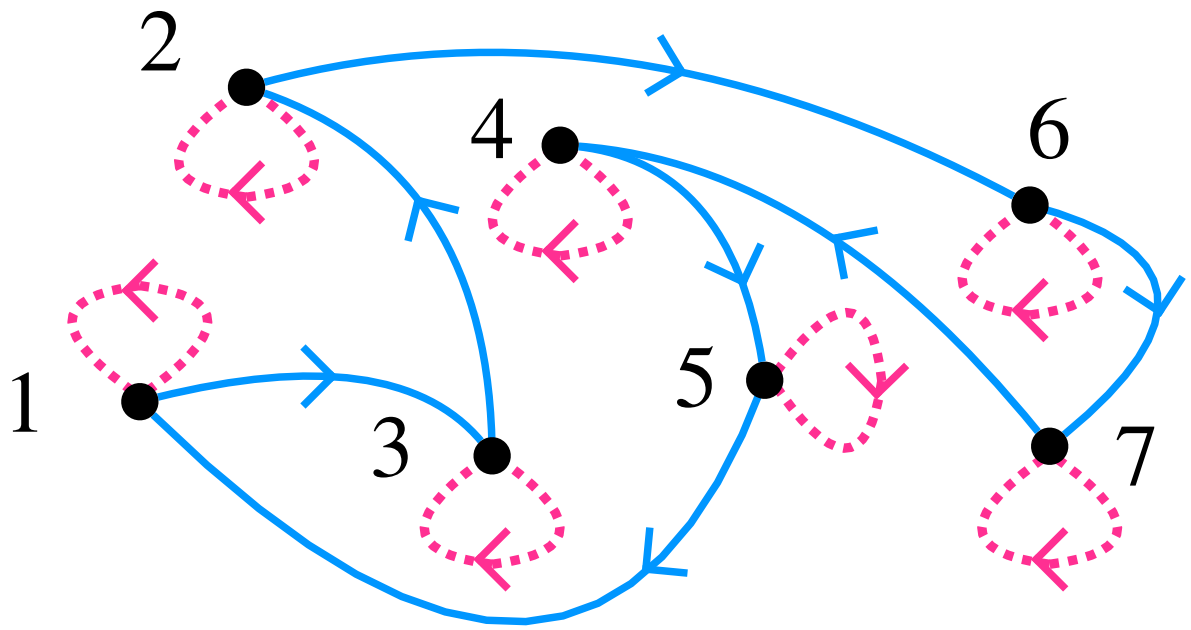
$n!$ diagrams, symmetrized over $n!$ permutations of the vertices, in $O(n^3)$ time.

Not well-defined in the thermodynamic limit:

we need to remove disconnected diagrams

[1] A. N. Rubtsov, V. V. Savkin, and A. I. Lichtenstein, Phys. Rev. B 72, 035122 (2005); [2] E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, and P. Werner, Rev. Mod. Phys. 83, 349 (2011)

Summing all connected Feynman diagrams is NP-hard



One Feynman diagram at order n: $G_{0;\uparrow}$ lines and trivial tadpole lines for $G_{0;\downarrow}$.

$$G_{0;\downarrow,jk} = \delta_{jk}$$

$$\left(\prod_{j=1}^{n} G_{0;\downarrow;jj}\right) \sum_{\eta \in H_n} \prod_{j=1}^{n} G_{0;\uparrow;j\eta_j}$$

the Hamiltonian cycle polynomial

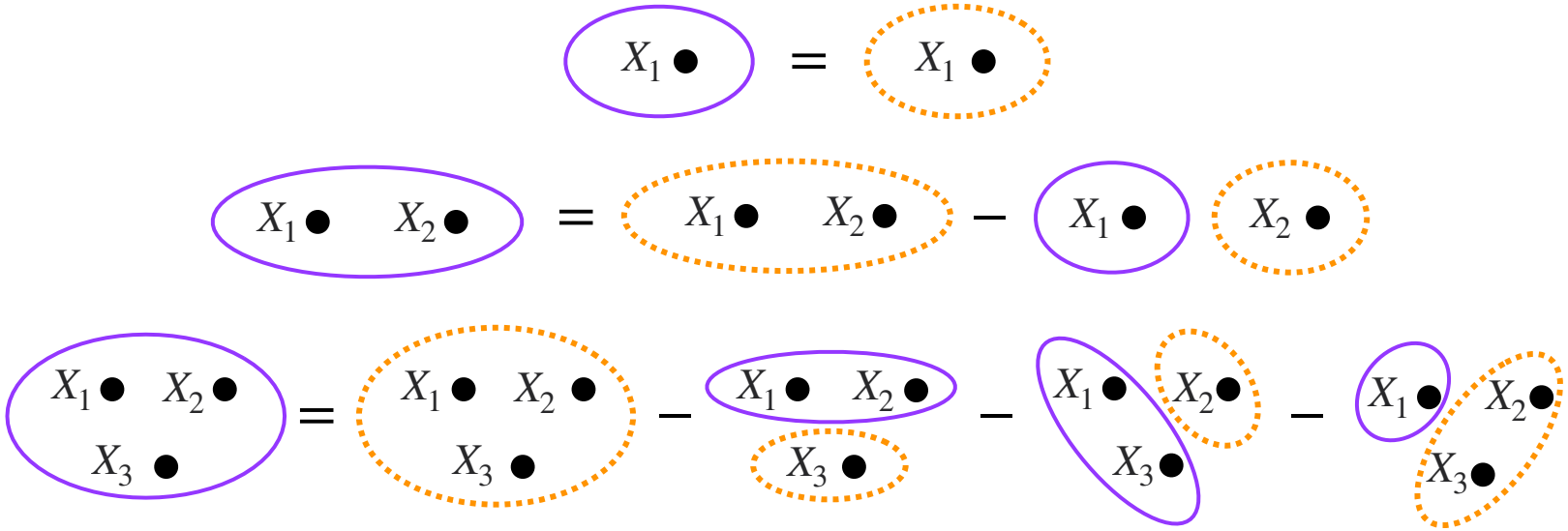
Hamiltonian cycle problem: NP-complete [1–3];
Held-Karp algorithm: $O(n^2 2^n)$.

no generic polynomial-time algorithm

[1] R. M. Karp, in R. E. Miller and J. W. Thatcher, eds., Complexity of Computer Computations (Plenum, New York, 1972), pp. 85–103; [2] M. Held and R. M. Karp, J. Soc. Indust. Appl. Math. 10, 196 (1962); [3] R. Bellman, J. ACM 9, 61 (1962)

The connected determinant approach

$$\tilde{\Omega}_{\text{bare}} := \log \tilde{Z}_{\text{bare}}$$



$O(3^n)$

$O(n^2 2^n)$ with fast subset convolution

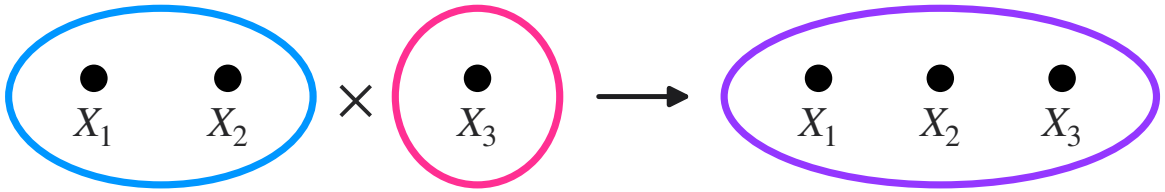
orange: $\tilde{Z}(S)$, all diagrams; violet: $\tilde{\Omega}(S)$, connected

$$\tilde{\Omega}(S) = \tilde{Z}(S) - \sum_{S' \subsetneq S \setminus \{X_1\}} \tilde{\Omega}(\{X_1\} \cup S')\, \tilde{Z}(S \setminus S' \setminus \{X_1\})$$

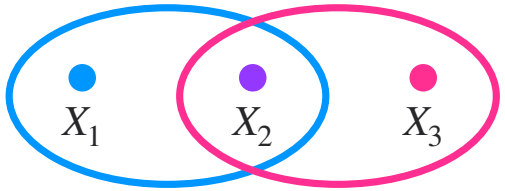
Removing disconnected diagrams recursively

R. Rossi, Phys. Rev. Lett. 119, 045701 (2017)

Algebraic formulation: nilpotent polynomials



$\eta_1\eta_2\,\eta_3 = \eta(\{X_1, X_2, X_3\})$



0

$\eta_1\eta_2\;\eta_2\eta_3 = 0$

$$\eta_j^2 = 0, \qquad \eta_j\eta_k = \eta_k\eta_j$$

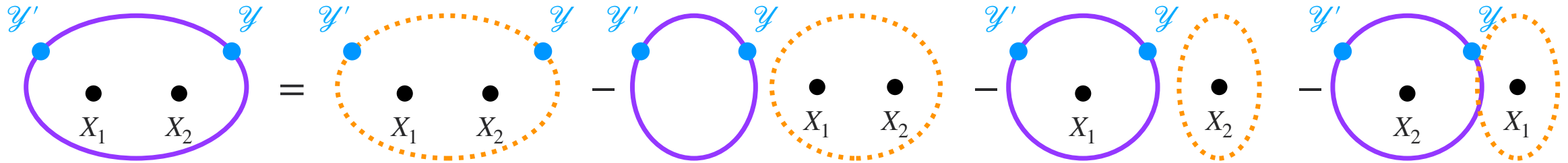
$$F[V = V_\eta] = \sum_{S\subseteq\{X_1,\ldots,X_n\}} F(S)\;\eta(S)$$

$$\tilde{\Omega}[[\boldsymbol{\eta}]] = \log \tilde{Z}[[\boldsymbol{\eta}]]$$

Grand-potential connected diagrams = logarithm of a nilpotent polynomial

Bare-expansion functional for the Green's function

$$G_{\text{bare};\mathcal{Y},\mathcal{Y}'}[[\eta]] = \frac{A_{\text{bare};\mathcal{Y},\mathcal{Y}'}[[\eta]]}{\tilde{Z}_{\text{bare}}[[\eta]]}$$



violet: $G_{\mathcal{Y},\mathcal{Y}'}(S)$ (connected); orange: $A_{\mathcal{Y},\mathcal{Y}'}(S)$, $\tilde{Z}(S)$ (connected + disconnected)

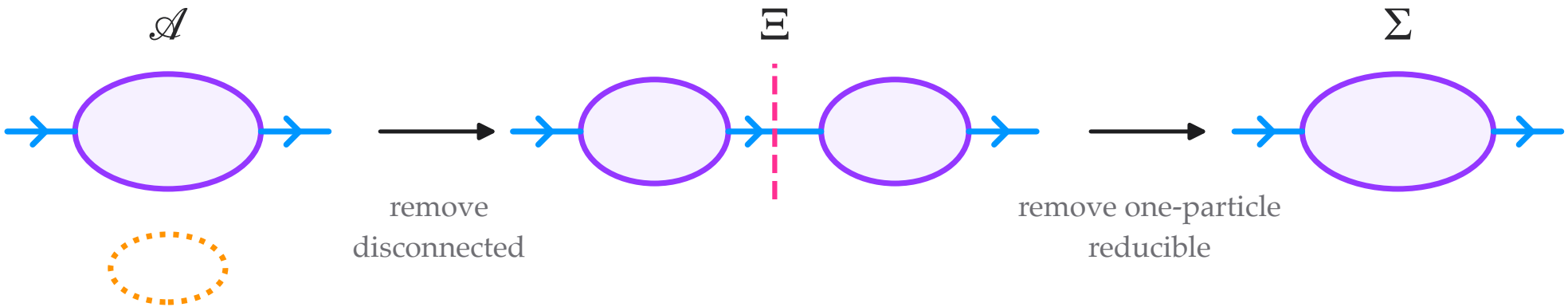
$$G_{\mathcal{Y},\mathcal{Y}'}(S) = A_{\mathcal{Y},\mathcal{Y}'}(S) - \sum_{S' \subsetneq S} G_{\mathcal{Y},\mathcal{Y}'}(S')\ \tilde{Z}(S \setminus S')$$

Connected diagrams for the Green's function:

just a nilpotent polynomial division

Self-energy

$$\tilde{Z}_{\text{bare}}[G_0](S) = (-1)^{|S|} \det \mathbb{G}_{0;\uparrow}(S) \det \mathbb{G}_{0;\downarrow}(S)$$



$$\boldsymbol{\Sigma}[[\boldsymbol{\eta}]]\ \boldsymbol{\rho}[[\boldsymbol{\eta}]] = \boldsymbol{\Xi}[[\boldsymbol{\eta}]]$$

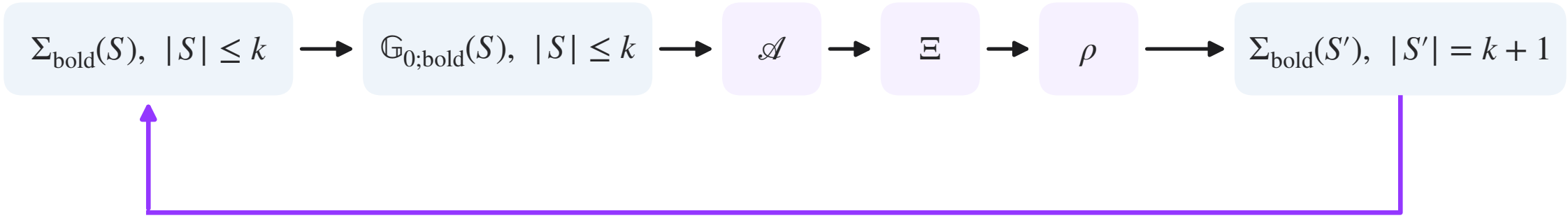
2^n determinants and adjugates: $O(n^3 2^n)$; elimination: $O(n^2 3^n)$

Direct self-energy evaluation

F. Šimkovic, R. Rossi, A. Georges, and M. Ferrero, Science 385, ade9194 (2024)

One-particle renormalization

$$G_{0;\mathrm{bold}}[G,V]^{-1} = G^{-1} + \Sigma_{\mathrm{bold}}[G,V]$$



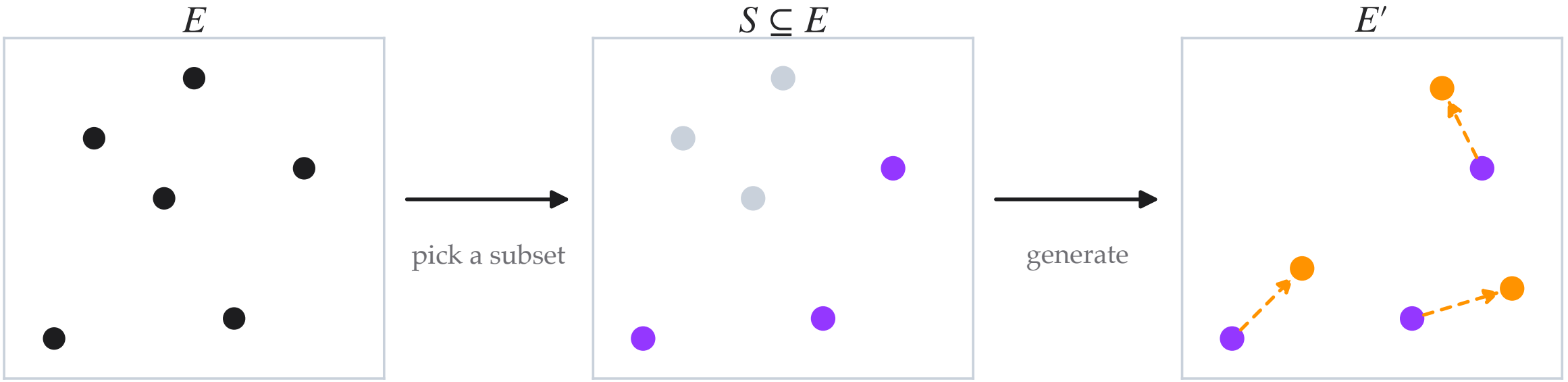
$k \to k+1$: operations in the ring of nilpotent polynomials

$O(n^3 4^n)$, much better than the $O(n^2 (n!)^2)$ naive enumeration; $O(n^3 3^n)$ [Kozik 2024]

identical to the bare algorithm, in the ring of nilpotent polynomials

E. Kozik, Nature Communications 15, 7916 (2024)

Sampling vertex positions with Many-Configuration Markov-Chain Monte Carlo



$$p_{\mathrm{eq}}(E) = \frac{\sum_{S \subseteq E} p_{\mathrm{gen}}(E \setminus S \,|\, S)\ \lambda_{|S|}\ \ |O(S)|}{\mathcal{N}_n}$$

Detailed balance at the level of each subset S:

all configurations S as possible updates

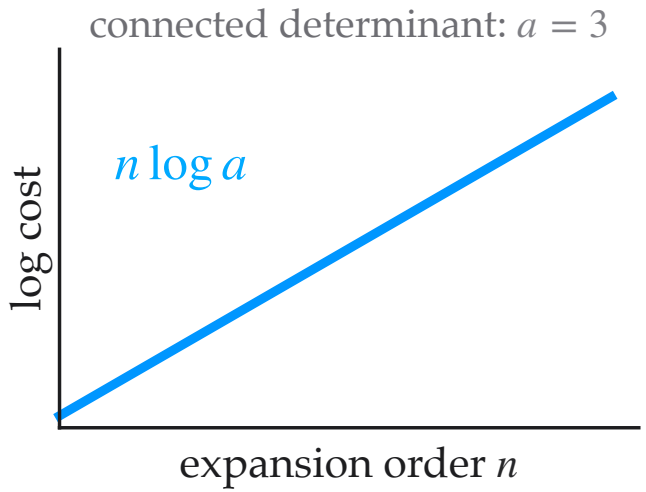
F. Šimkovic and R. Rossi, arXiv:2102.05613

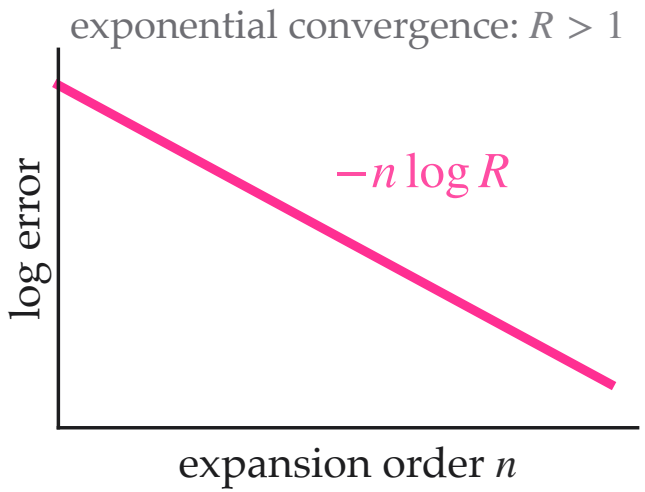
5

Summing the expansion: convergence, singularities and resummation

Finite radius of convergence and polynomial complexity

Bare expansion: a non-zero radius of convergence for all non-zero temperature [1].





radius of convergence $R > 1$

$$t(\epsilon) \sim \epsilon^{-\alpha}$$

$$\alpha = \frac{\log a}{\log R}$$

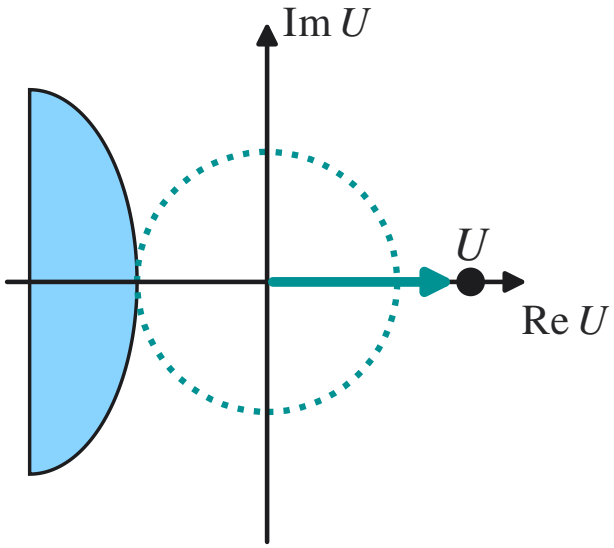
Fermionic quantum matter on the lattice at finite temperature [2]:

Polynomial-time algorithm, at least in a finite region of the phase diagram

[1] G. Benfatto, A. Giuliani, and V. Mastropietro, Ann. Henri Poincaré 7, 809 (2006); [2] R. Rossi, N. Prokof'ev, B. Svistunov, K. Van Houcke, and F. Werner, EPL 118, 10004 (2017)

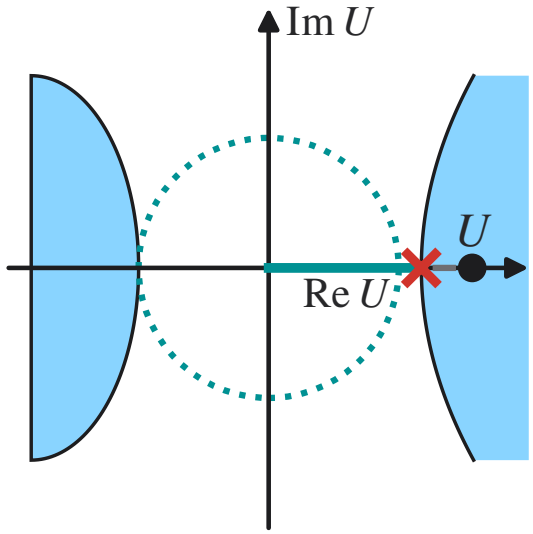
For positive real U, several scenarios are possible

First: no additional singularity



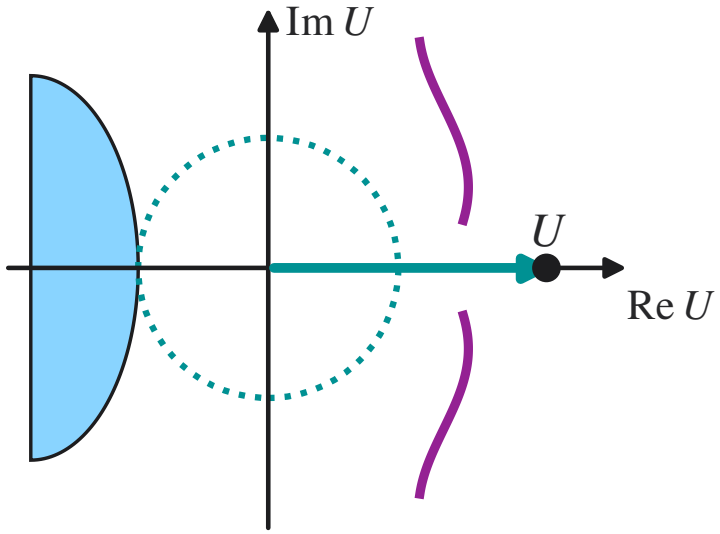
analytic continuation

Second: a physical phase transition



different phase of matter

Third: nearby complex singularities

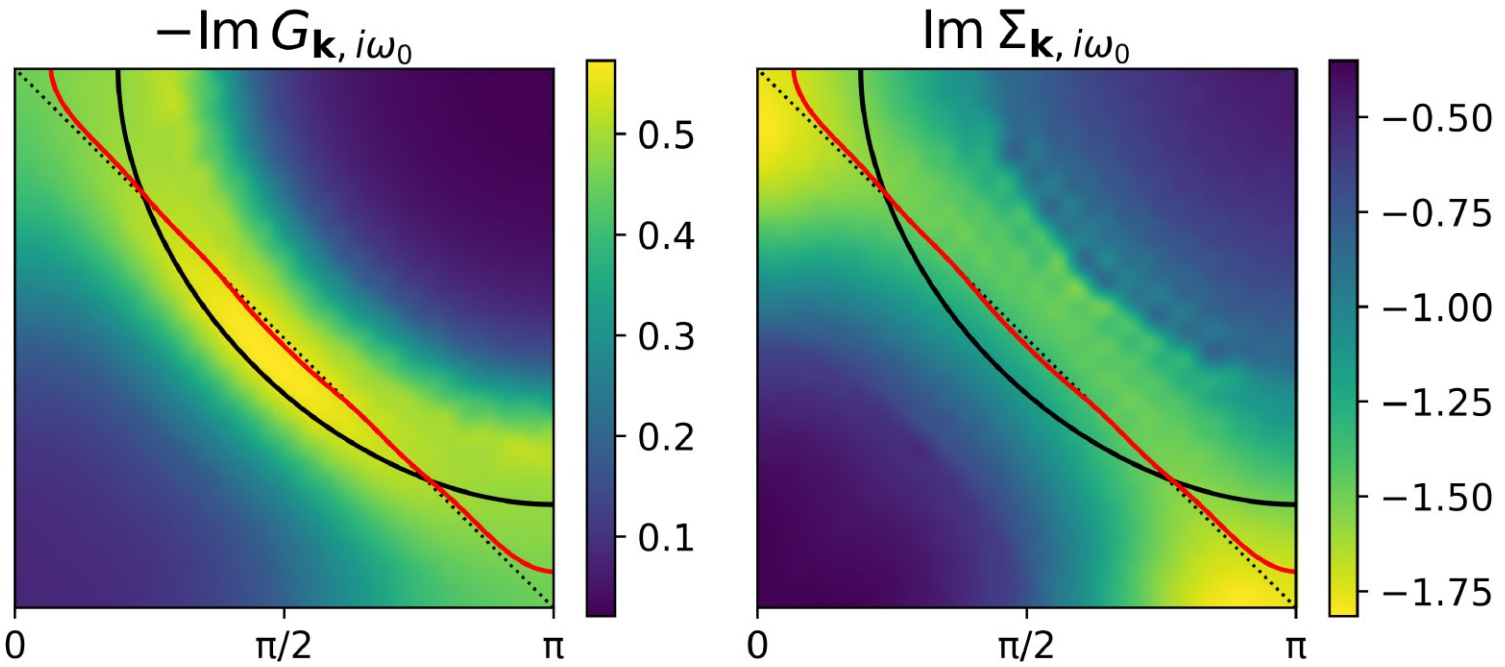


analytic continuation,
strong crossover

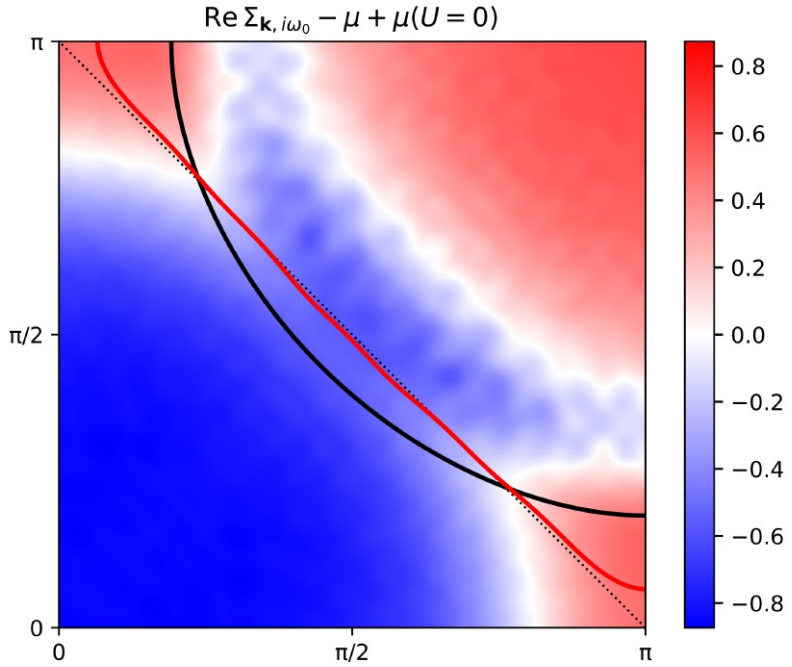
Analytic continuation remains possible

Results

Interaction-enhanced nesting: the Fermi-Hubbard model



CDet at fixed density, half filling, $U/t = 5.75$, $t'/t = -0.3$, $T/t = 1/7$, 60×60 lattice, ninth order; black: non-interacting FS; red: $E_k = 0$

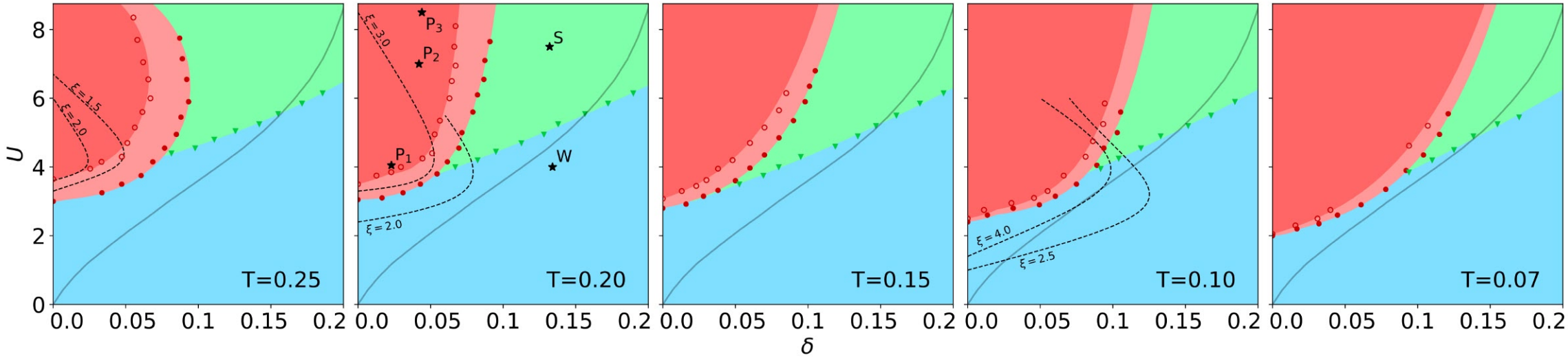


dispersion renormalization, strongest near the antinodes

Half filled t-t' Hubbard: pseudogap and nesting of the FS

R. Rossi, F. Šimkovic IV, M. Ferrero, A. Georges, A. M. Tsvelik, N. V. Prokof'ev, and I. S. Tupitsyn, Phys. Rev. Research 6, L032058 (2024)

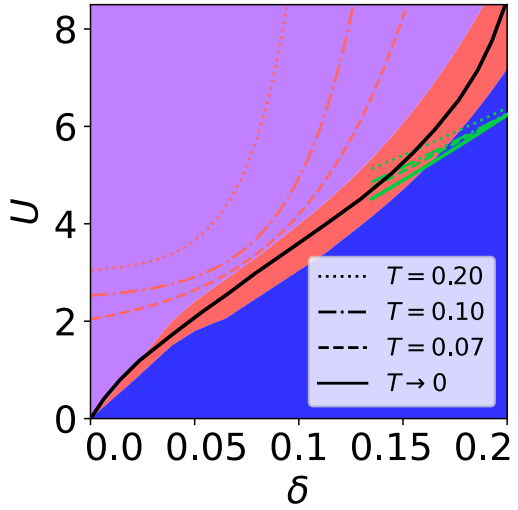
Origin and fate of the pseudogap in the doped Hubbard model



Doping δ, interaction U, from $T = 0.25$ to $T = 0.07$; dashed lines: constant spin correlation length

weakly correlated metal strongly correlated metal pseudogap

PG extrapolates to the stripe phase of zero T AFQMC

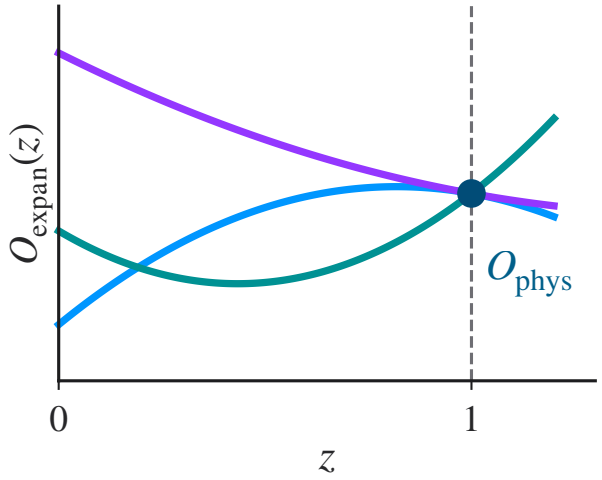


F. Šimkovic, R. Rossi, A. Georges, and M. Ferrero, Science 385, ade9194 (2024)
H. Xu, H. Shi, E. Vitali, M. Qin, and S. Zhang, *Phys. Rev. Research* 4, 013239 (2022)

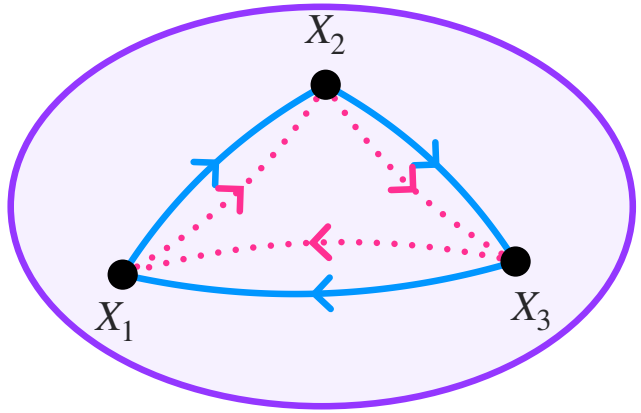
6
Conclusions

Conclusions

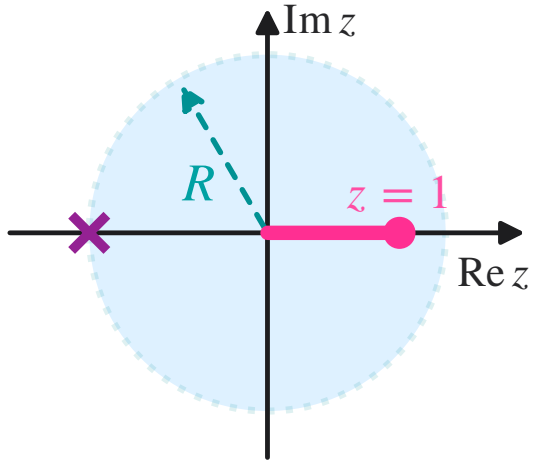
1 *Choosing* the expansion → **2 *Computing* the expansion** → **3 *Summing* the expansion**



the choice of the diagrammatic expansion



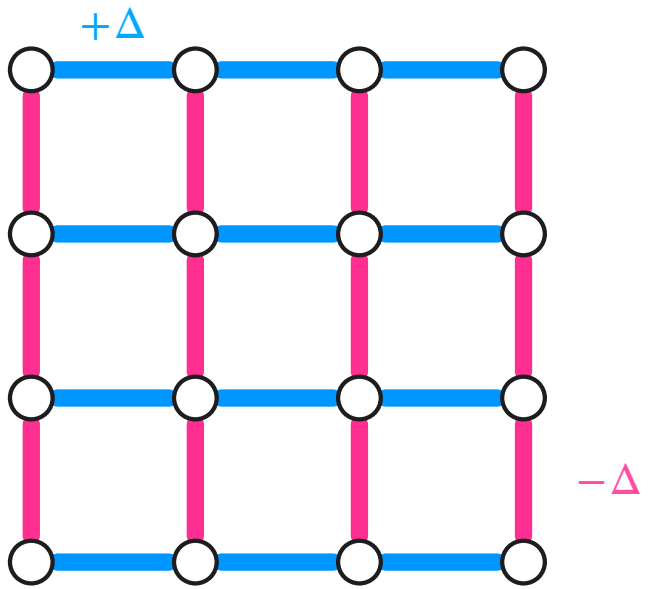
how to efficiently evaluate Feynman diagrams



how to sum the resulting series

CDet/DiagMC offers a numerically-exact solution of the finite-temperature Hubbard model (pseudogap, long and strong correlation crossovers…) at least in some parameter regimes

Outlook: broken-symmetry phases and new expansions



$$\Delta_{\boldsymbol{r},\boldsymbol{r}\pm\hat{x}} = +\Delta, \quad \Delta_{\boldsymbol{r},\boldsymbol{r}\pm\hat{y}} = -\Delta$$

$d_{x^2-y^2}$: $\Delta_{\boldsymbol{k}} \propto \cos k_x - \cos k_y$

Broken-symmetry phases

$$\hat{H}_{\Delta\text{-sh}}(z) = \hat{H}_{\text{phys}} + (1-z)\sum_{\boldsymbol{r},\boldsymbol{r}'} \Delta_{\boldsymbol{r},\boldsymbol{r}'}\left(\hat{c}^\dagger_\uparrow(\boldsymbol{r})\hat{c}^\dagger_\downarrow(\boldsymbol{r}') + \text{h.c.}\right) - (1-z)U\sum_{\boldsymbol{r}} \hat{n}_\uparrow(\boldsymbol{r})\hat{n}_\downarrow(\boldsymbol{r})$$

d-wave formalism: quadratic at $z = 0$, physical at $z = 1$

New renormalization schemes

New starting points and strong-coupling descriptions

[1] G. Spada, R. Rossi, F. Šimkovic, R. Garioud, M. Ferrero, K. Van Houcke, and F. Werner, arXiv:2103.12038 (2021);
[2] R. Garioud, F. Šimkovic, R. Rossi, G. Spada, T. Schäfer, F. Werner, and M. Ferrero, Phys. Rev. Lett. 132, 246505 (2024)