High-precision numerical solution of the Fermi polaron problem and large-order behavior of its diagrammatic series

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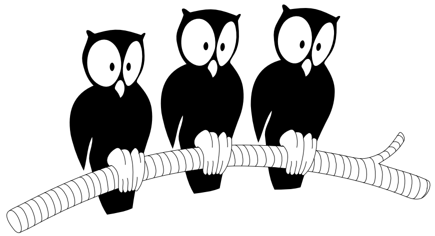
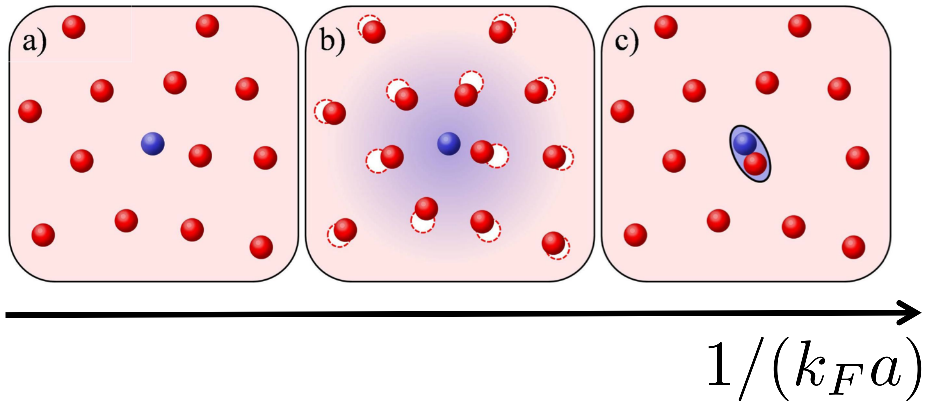
In collaboration with Riccardo Rossi (EPFL) and Félix Werner (LKB-ENS)



Institut Pascal, September 16, 2021

Fermi Polaron (polarized Fermi gas) = mobile impurity immersed in a Fermi sea



<u>Cold-atom experiment:</u>

Schirotzek, Wu, Sommer, Zwierlein (2009)

Yan, Patel, Mukherjee, Fletcher, Struck, Zwierlein (2019)

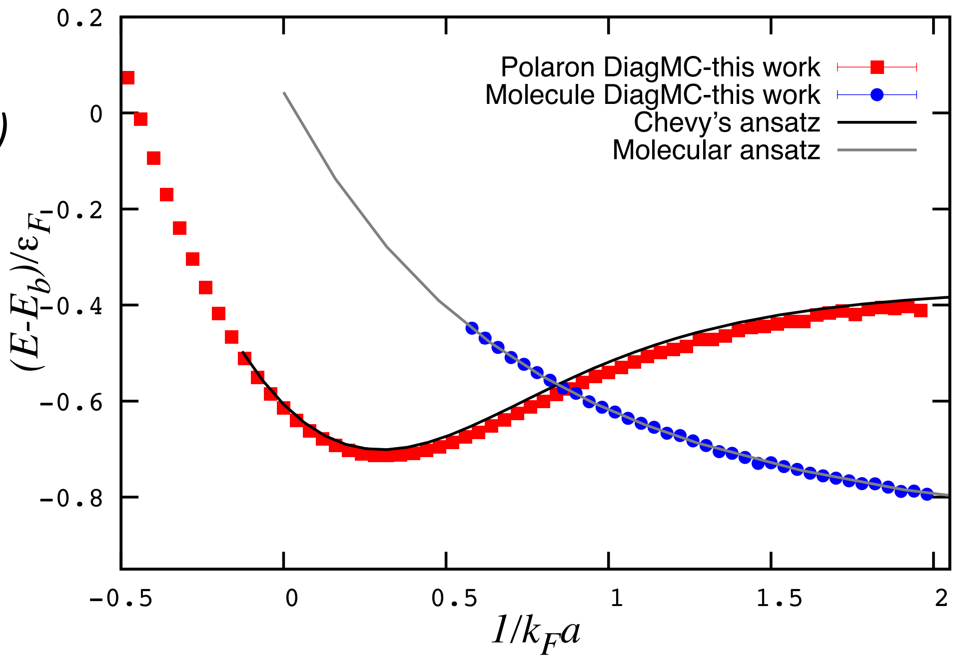
<u>Diagrammatic Monte Carlo for the polaron:</u>

Prokof'ev & Svistunov (PRB 2008)

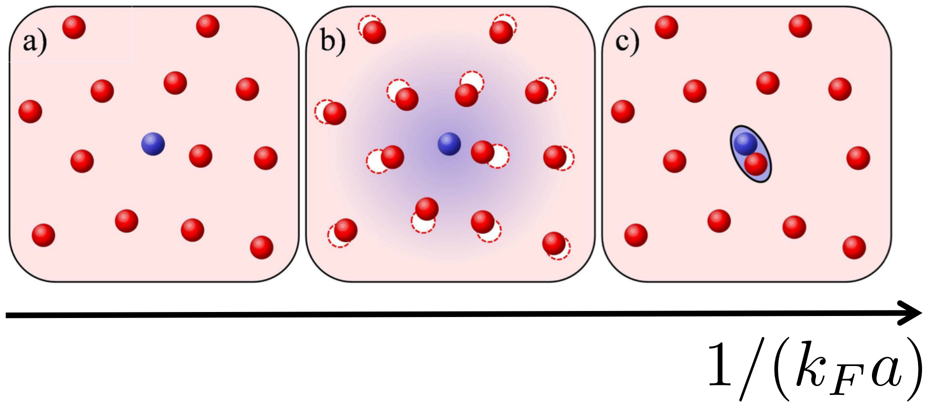
Vlietinck, Ryckebusch, Van Houcke (PRB 2013)

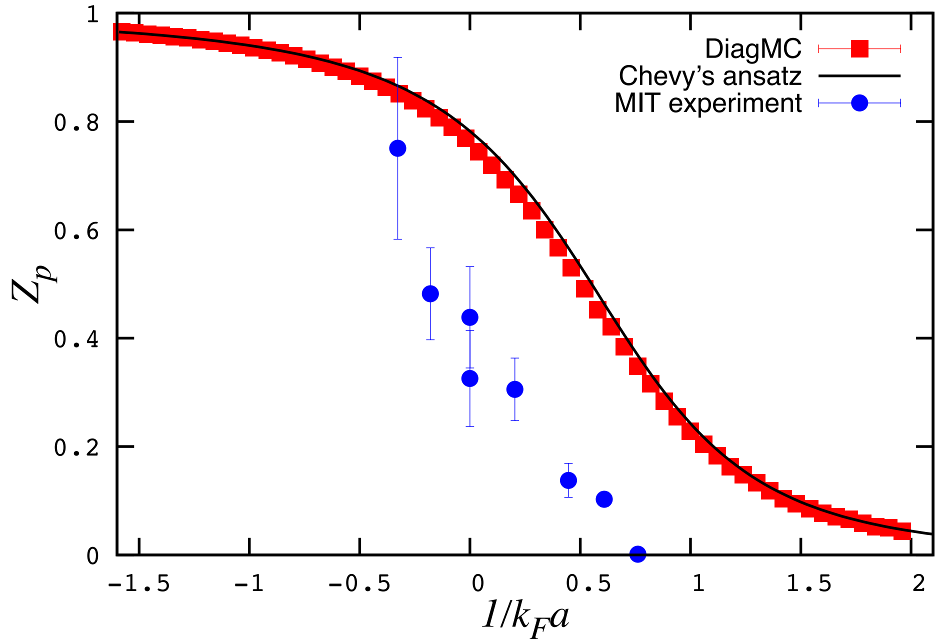
Kroiss, Pollet (PRB 2015)

Goulko, Mishchenko, Prokof'ev, Svistunov (PRA 2016)



Fermi Polaron (polarized Fermi gas) = mobile impurity immersed in a Fermi sea





Polaron residue:

$$Z_p = |\langle \Psi_{\text{polaron}} | \mathbf{0}_\downarrow, FS(N_\uparrow) \rangle|^2$$

Vlietinck, Ryckebusch, Van Houcke (PRB 2013)

Model and diagrams:

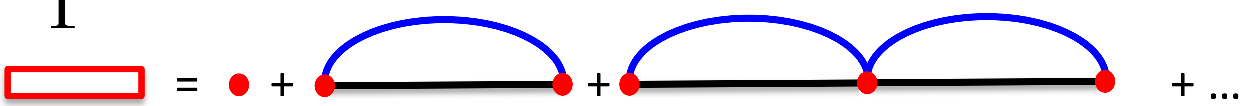
$$H = \frac{p^2}{2m} + H_{\text{Fermi sea}} + \int V(\mathbf{r} - \mathbf{r}')n(\mathbf{r}')d\mathbf{r}'$$

Lattice model (for ultraviolet regularization):

$$H = \sum_{\sigma} \int_{[-\frac{\pi}{b}, \frac{\pi}{b}]^3} \frac{d^3k}{(3\pi)^3} \frac{\hbar^2 k^2}{2m} c_\sigma^\dagger(\mathbf{k}) c_\sigma(\mathbf{k}) + g_0 \sum_{\mathbf{r}} b^3 n_\uparrow(\mathbf{r}) n_\downarrow(\mathbf{r})$$

$$\frac{1}{g_0} = \frac{m}{4\pi\hbar^2 a} - \int_{[-\frac{\pi}{b}, \frac{\pi}{b}]^3} \frac{d^3k}{(3\pi)^3} \frac{m}{\hbar^2 k^2}$$

Γ^0



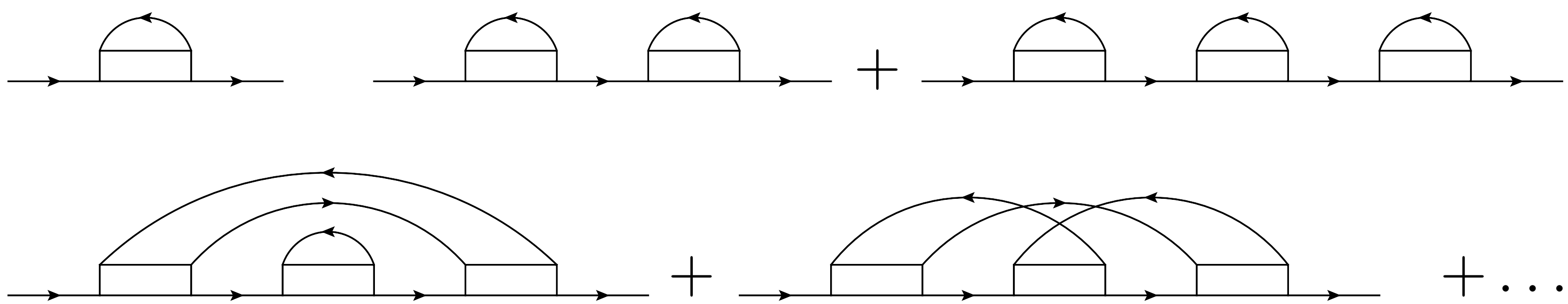
Continuum limit: $b \longrightarrow 0$

$g_0(b)$ such that a fixed

$\Rightarrow \Gamma^0$ depends only on a

(Universal)

$G(p, \tau) =$



$$a_N = \sum_{\text{topologies } \mathcal{T}} \int dX_1 \ldots dX_N \; \mathcal{D}(\mathcal{T}; X_1 \ldots X_N)$$

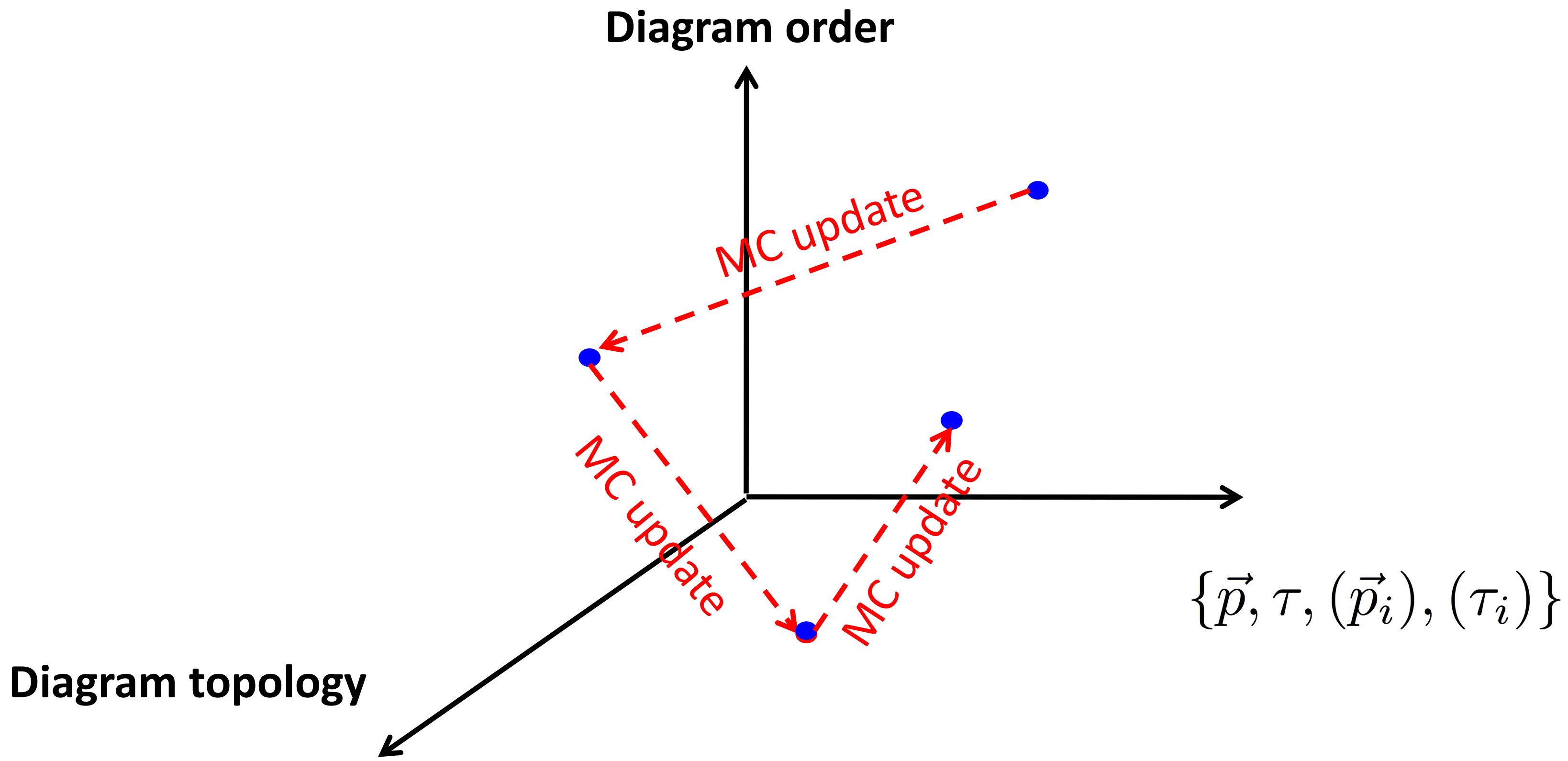
$$X = (\vec{p}, \tau)$$

$$\int dX = \int d\vec{p} \int_0^\beta d\tau$$

<u>DiagMC for the polaron</u> [Prokof'ev & Svistunov, PRB 2008]

Configuration: $\mathcal{C} = (\mathcal{T}, X_1, \ldots, X_N)$

Probability: $P(\mathcal{C}) \propto |\mathcal{D}(\mathcal{T}; X_1, \ldots, X_N)|$



$$a_N = \sum_{\text{topologies } \mathcal{T}} \int dX_1 \dots dX_N \; \mathcal{D}(\mathcal{T}; X_1 \dots X_N)$$

$$X = (\vec{r}, \tau)$$

$$\int dX = \sum_{\vec{r}} \int_0^\beta d\tau$$

CDet [Rossi PRL 2017]

configuration: $\mathcal{C} = (X_1, \dots, X_N)$

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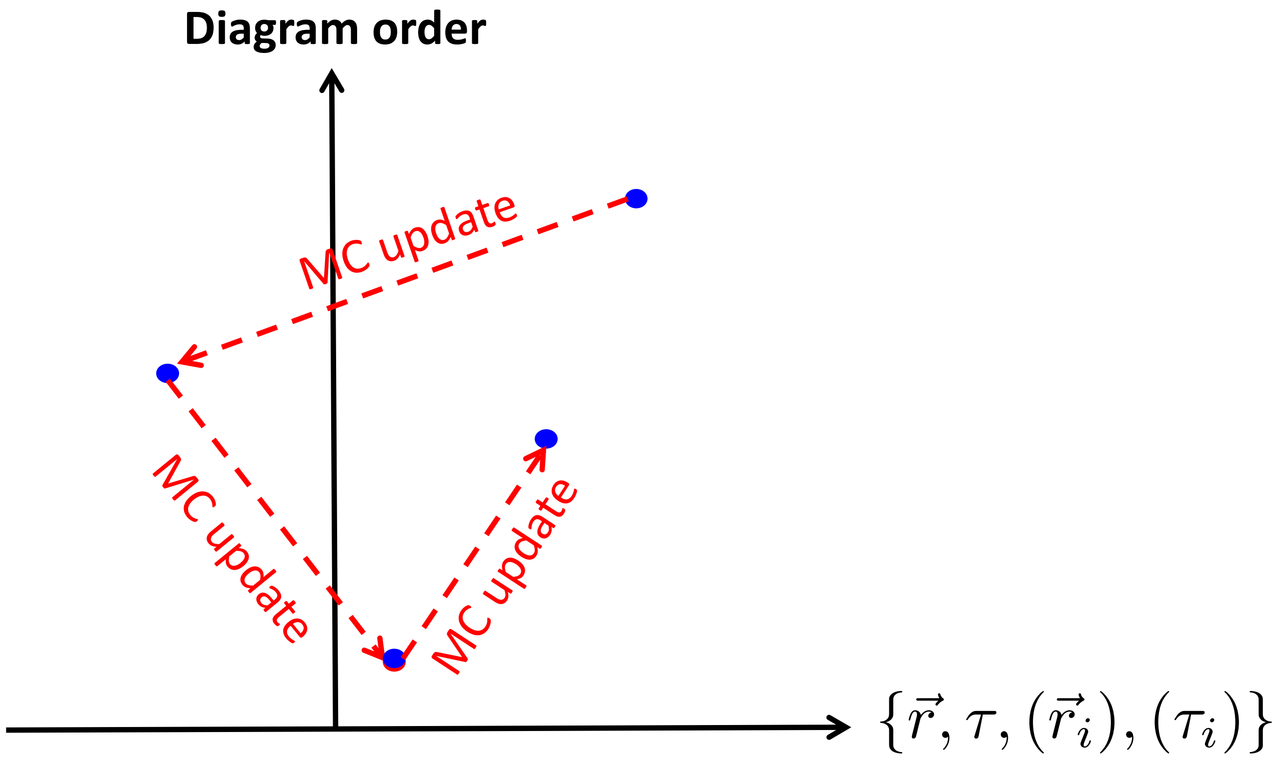
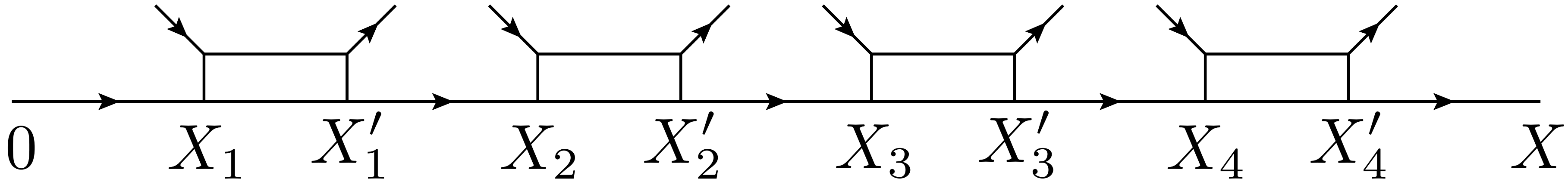


Calculation of the N-th order contribution to G



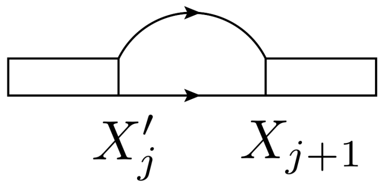
Set of spacetime points: $V_n = \{X_1, X_1', \ldots, X_n, X_n'\}$ with $X_i = (\mathbf{r}_i, \tau_i)$

$$G_N(X) = \int dX_1 \ldots \int dX_N' \; B(V_N, X) \; S_N(V_N)$$

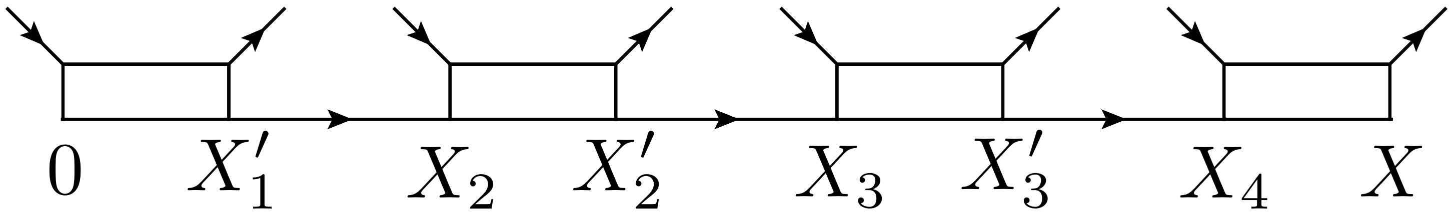
$$B(V_N, X) = G_\downarrow^0(X_1) \; \Gamma^0(X_1' - X_1) \; G_\downarrow^0(X_2 - X_1') \; \Gamma^0(X_2' - X_2) \ldots \; \Gamma^0(X_N' - X_N) \; G_\downarrow^0(X - X_N')$$

$$S_N(V_N) = \det[A(V_N)]$$

$$A_{i,j} = G_\uparrow^0(X_i - X_j') \quad \longrightarrow \quad A_{i,j} = \begin{cases} G_\uparrow^0(X_i - X_j') & \text{if } i \neq j+1 \; , \\ 0 & \text{if } i = j+1 \; . \end{cases}$$



Calculation of the N-th order contribution to Self-energy



Set of spacetime points: $V_n = \{X_1, X_1', \ldots, X_n, X_n'\}$ with $X_1 \equiv 0$, $X_N' \equiv X$

$$\Sigma_N(X) = \int dX_1' \int dX_2 \ldots \int dX_N \; \tilde{B}(V_N) \; \tilde{S}(V_N)$$

$$\tilde{B}(V_N) = \Gamma^0(X_1') \; G^0_\downarrow(X_2 - X_1') \; \times \; \Gamma^0(X_2' - X_2) \ldots \; \Gamma^0(X - X_N)$$

$$\tilde{S}_n(V_n) = S_n(V_n) - \sum_{k=1}^{n-1} \tilde{S}_k(V_k) \; S_{n-k}(V_n \setminus V_k) \qquad \text{for } n = 1, \ldots N.$$

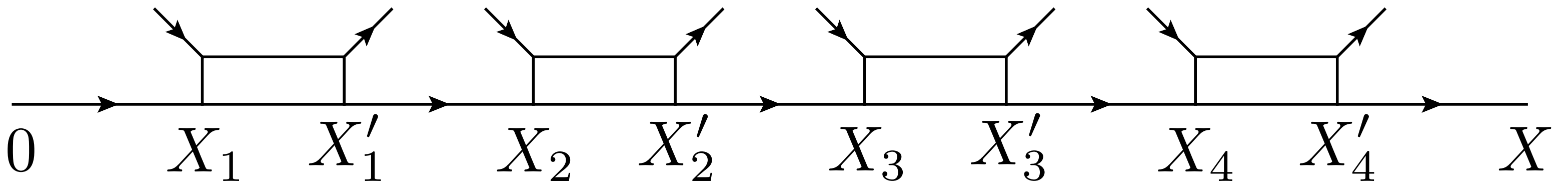
$$S_N(V_N) = \det[A(V_N)]$$

Computational cost? Polynomial: $\sum_{n=1}^{N} \sum_{k=1}^{n} k^3 \sim N^5$

Monte Carlo updates:

A configuration: (V_N, X)

Weight of a configuration: $W(V_N, X) = |B(V_N, X) S(V_N)| \; C_N \; e^{\Delta\mu\tau}$



Propagators at short time and distance:

$$G^0_\downarrow(\Delta\mathbf{r}, \Delta\tau) \sim \frac{1}{(\Delta\tau)^{3/2}} \; e^{-\frac{m}{2\Delta\tau}(\Delta\mathbf{r})^2}$$

$$\Gamma^0(\Delta\mathbf{r}, \Delta\tau) \sim \frac{1}{(\Delta\tau)^2} e^{-\frac{m}{\Delta\tau}(\Delta\mathbf{r})^2}$$

(i) Position shift:

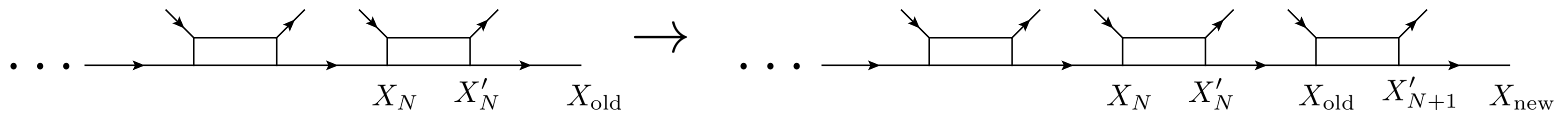
$$\Delta\mathbf{r}_{\mathrm{old}} \;\rightarrow\; \Delta\mathbf{r}_{\mathrm{new}}$$

(ii) Time shift:

$$\Delta\tau_{\mathrm{old}} \;\rightarrow\; \Delta\tau_{\mathrm{new}}$$

(i) Add

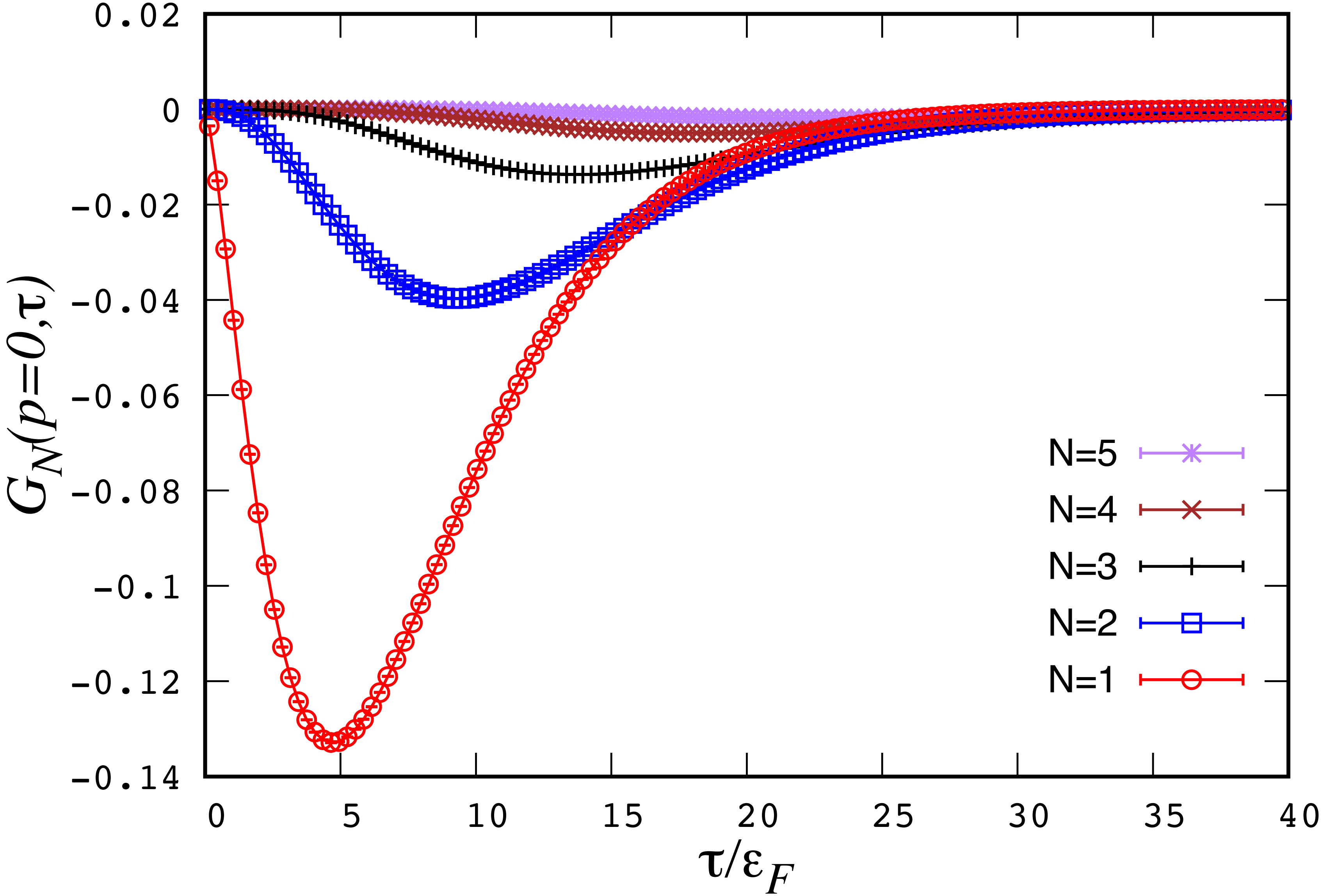
$$(V_N, X_{\mathrm{old}}) \quad \rightarrow \quad (V_{N+1}, X_{\mathrm{new}})$$



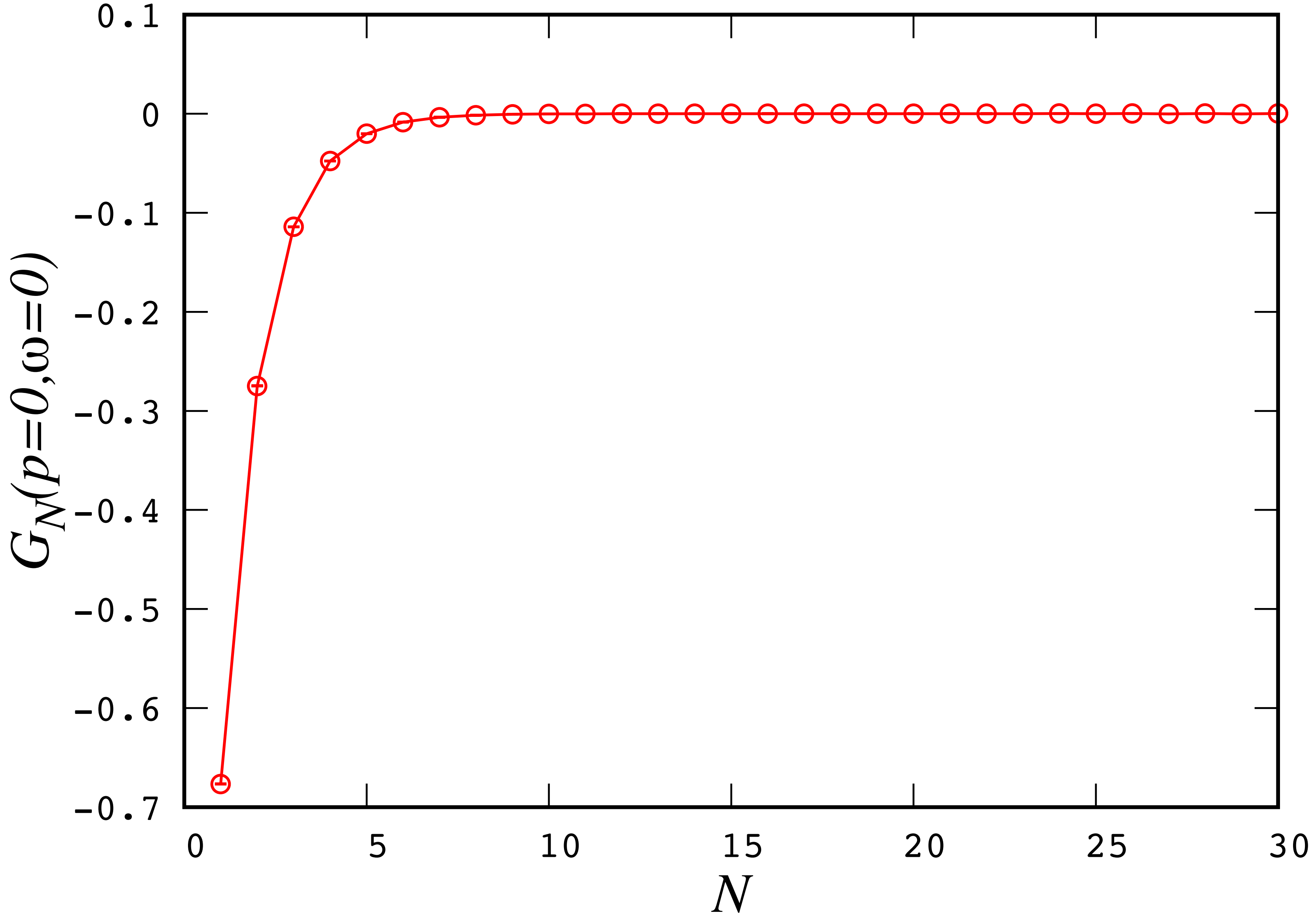
(ii) Remove

Green's function

$$k_F a = \infty$$



Green's function $k_F a = \infty$



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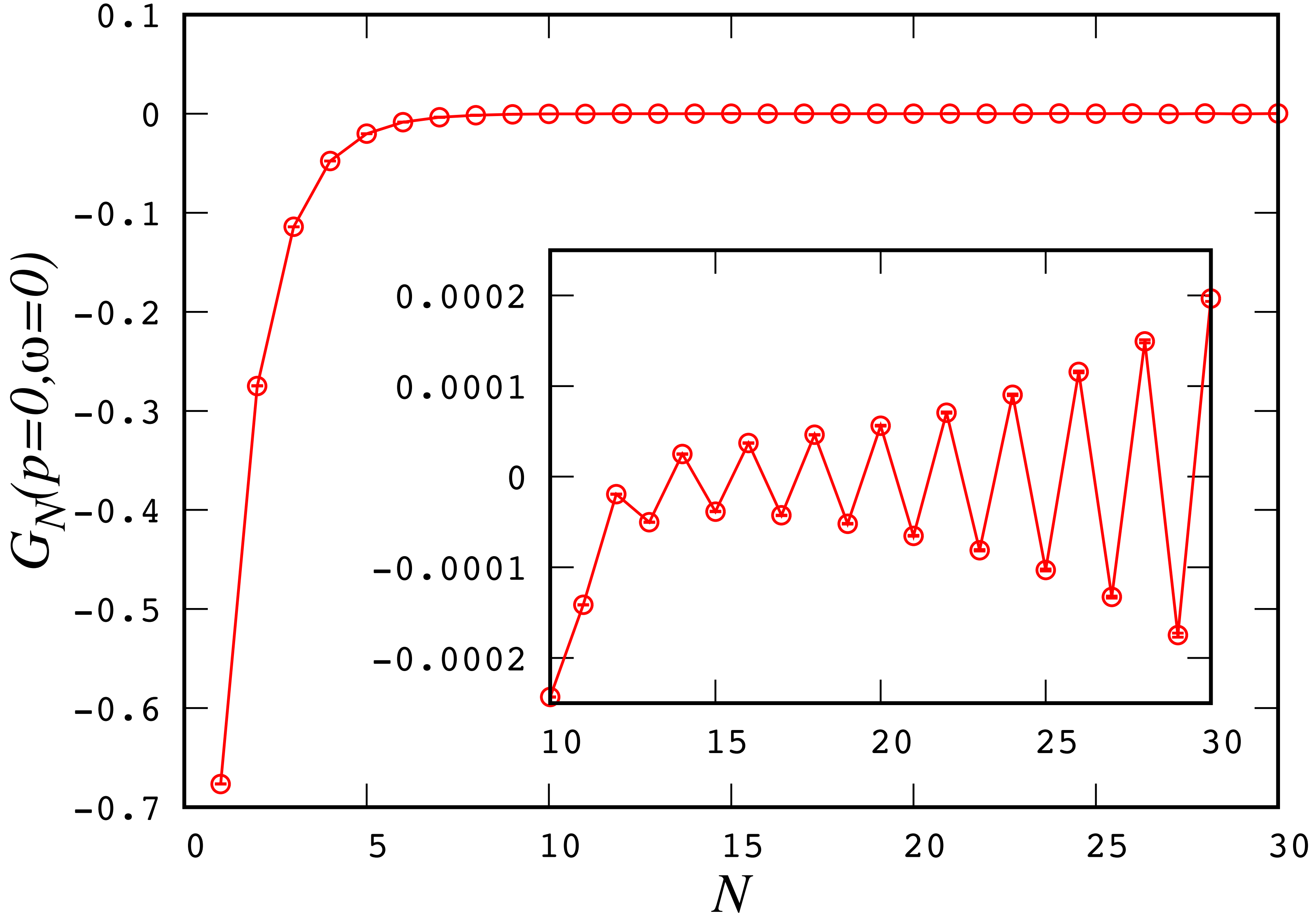
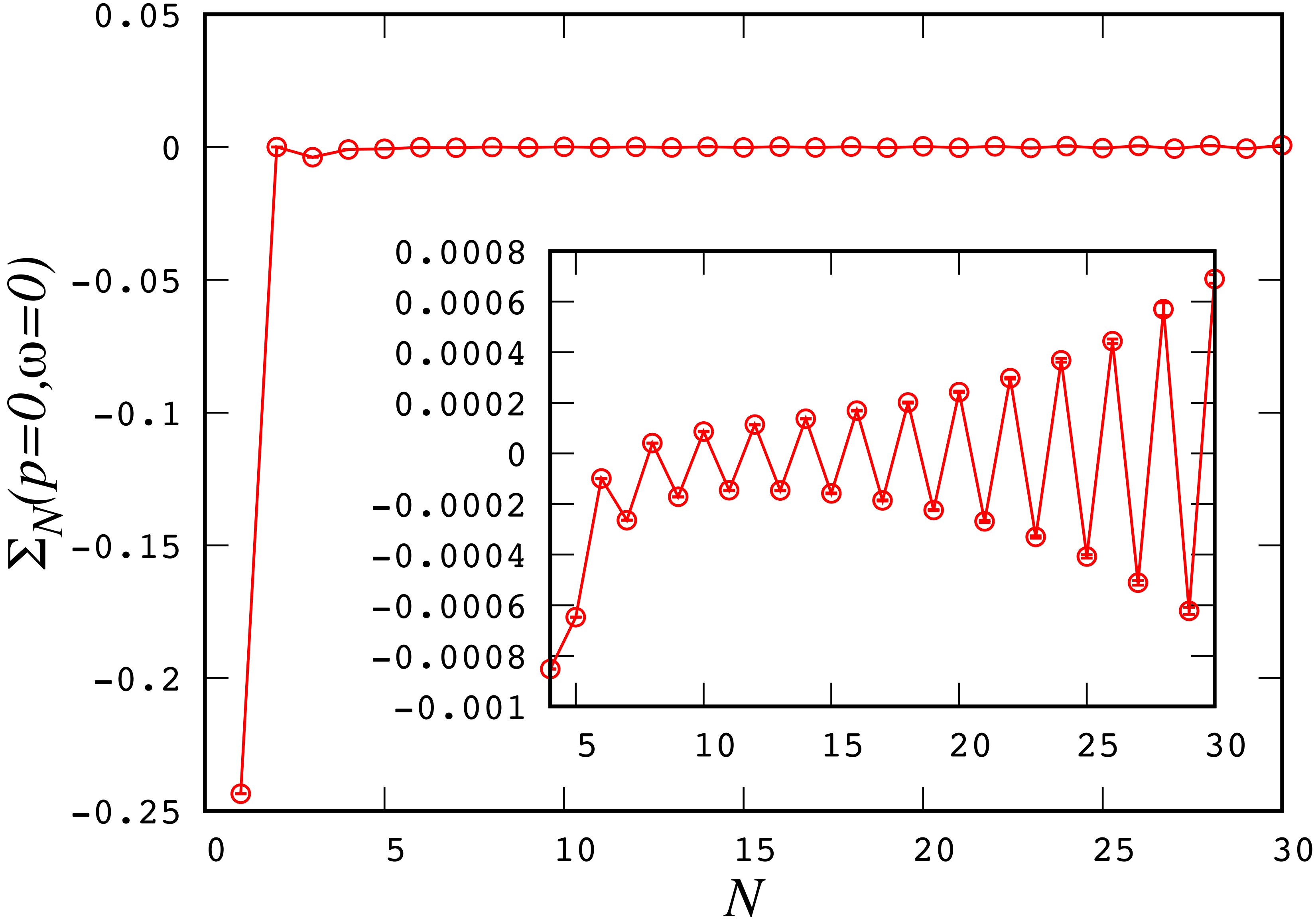
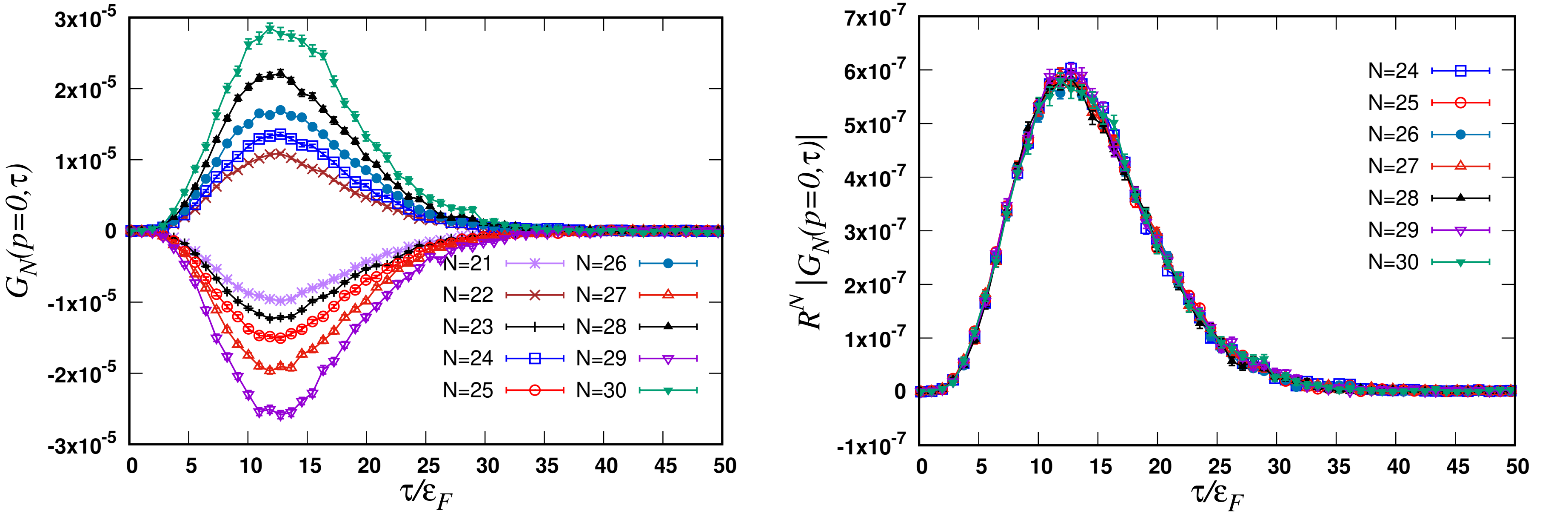


Self-energy

$$k_F a = \infty$$



Diagrammatic series has finite radius of convergence



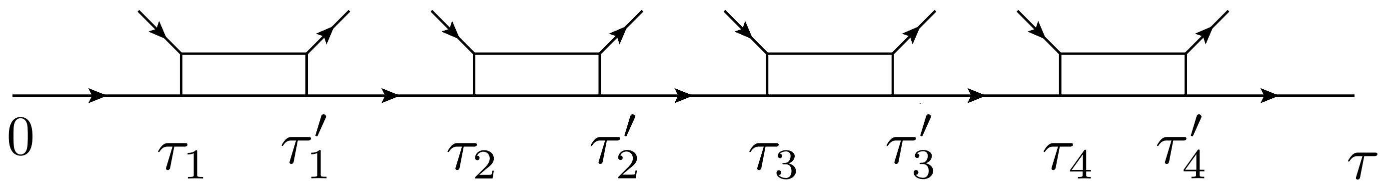
$$G_N(\mathbf{p}=0,\tau) = \frac{F(\tau)}{(-R)^N}$$

$$\text{at } k_F a = \infty : \quad R = 0.878(2)$$

Where does this asymptotic behavior come from?

Large-order behavior of the diagrammatic series:

A naive estimate due to time ordering of the vertices in the backbone:



$$\mathcal{D}_N = \int_0^{\tau_1'} d\tau_1 \int_0^{\tau_2} d\tau_1' \ldots \int_0^{\tau_N'} d\tau_N \int_0^{\tau} d\tau_N' = \frac{\tau^{2N}}{(2N)!}$$

Typical time of each backbone line: $\Delta\tau(N)$

$$2N\Delta\tau(N) \sim \tau \;\Rightarrow\; \Delta\tau(N) \ll \tau$$

$$\mathcal{D}_N = \left(\frac{\tau}{2N}\right)^{2N}$$

So sum of all diagrams of order $N \sim \tau^{2N}/N!$

Goulko, Mishchenko, Prokof'ev, Svistunov (PRA 2016)

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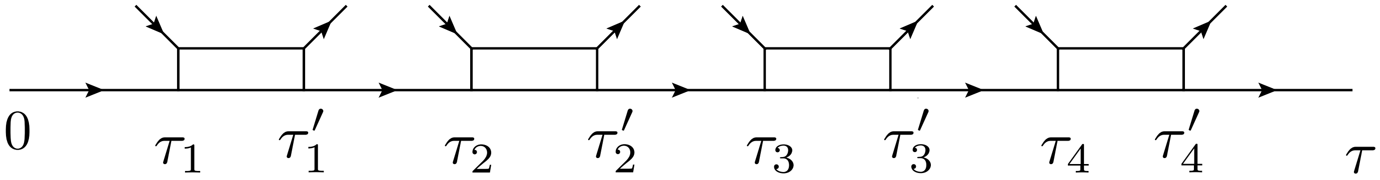

$$\int_0^{\tau_1'} d\tau_1 \int_0^{\tau_2} d\tau_1' \ldots \int_0^{\tau_N'} d\tau_N \int_0^{\tau} d\tau_N' = \frac{\tau^{2N}}{(2N)!}$$

So sum of all diagrams of order $N \sim \tau^{2N}/N!$

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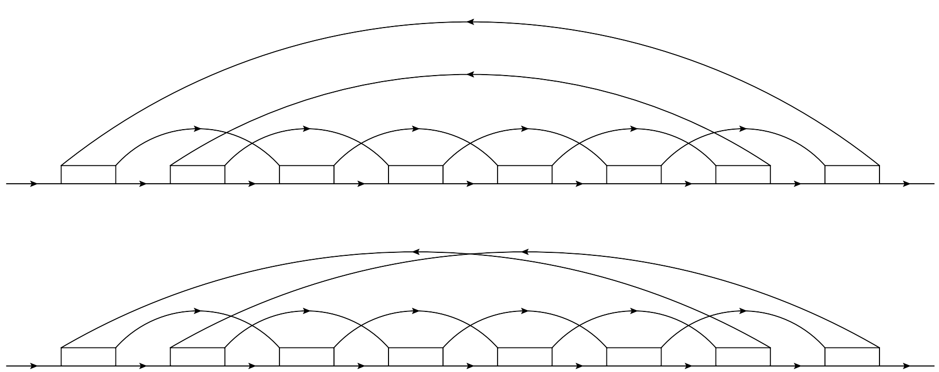
Rigorous bound with UV momentum cut-off (for vacuum $\Gamma^v(\mathbf{p},\tau) = -\frac{4\pi}{m^{3/2}\sqrt{\pi\tau}}\, e^{-(\frac{p^2}{4m}-\mu-\varepsilon_F)\tau}$):

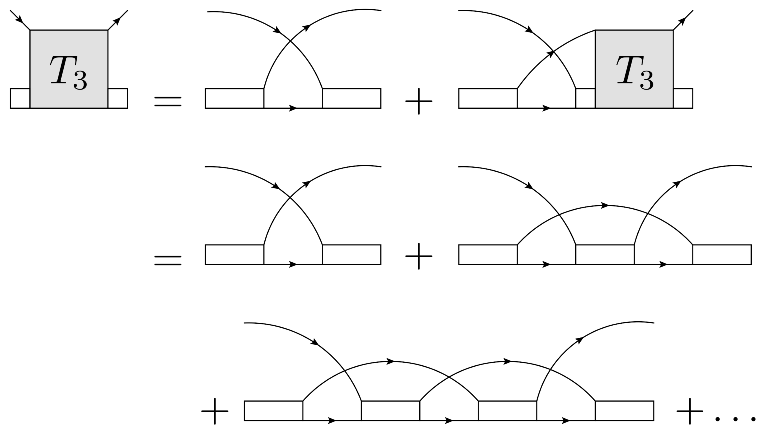
$$|G_N| \leq \alpha \frac{C^N\ p_c^{3N} \tau^{\frac{3N}{2}}}{(N/2-1)!} \sim \frac{1}{\sqrt{N!}}$$

So, convergence breaks down to the ultraviolet behavior.

Note that some classes do converge: $G_N = (G_\downarrow^0)^N (\Sigma_1)^N G_\downarrow^0 \sim 1/(N!)^{3/2}$

Two diagrams with the same behavior:





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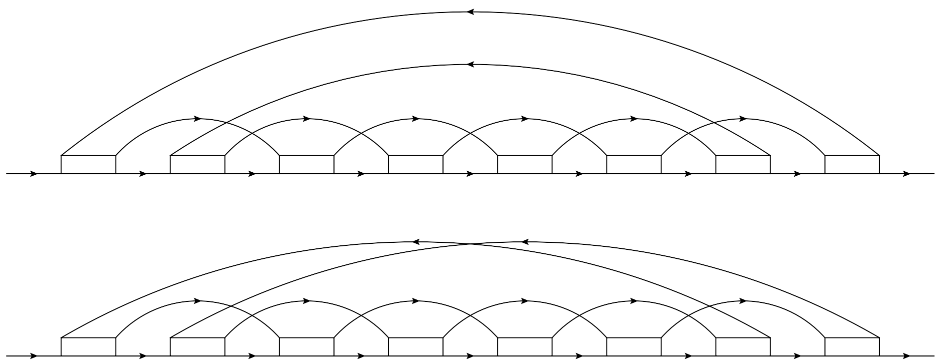
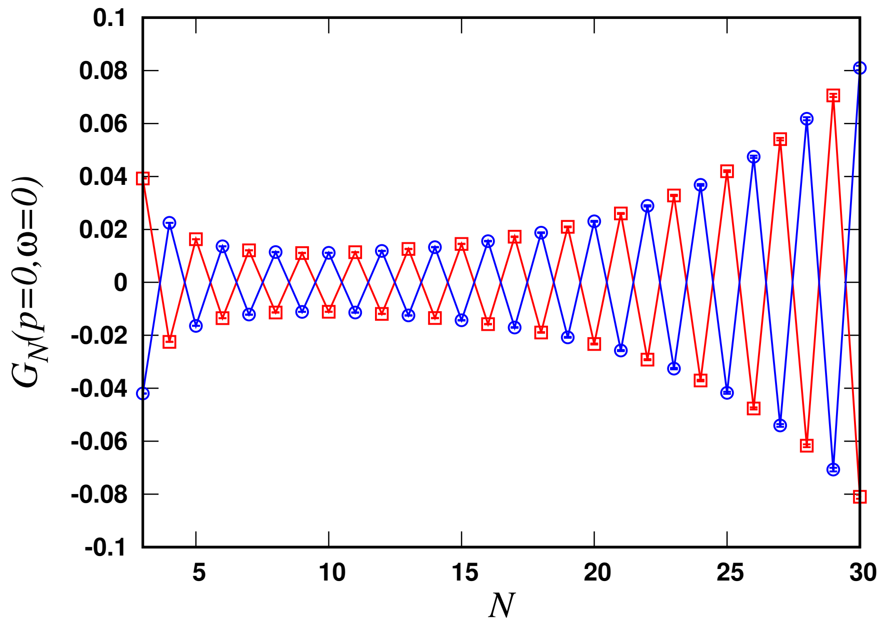
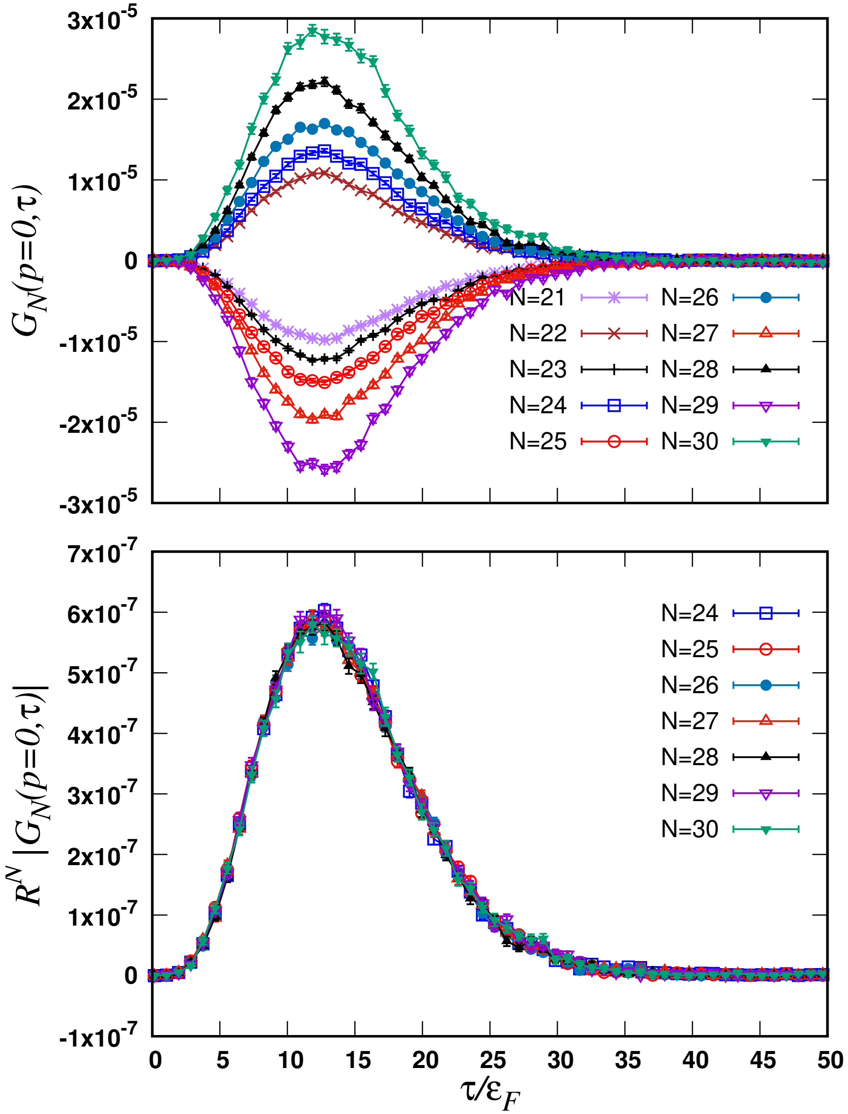
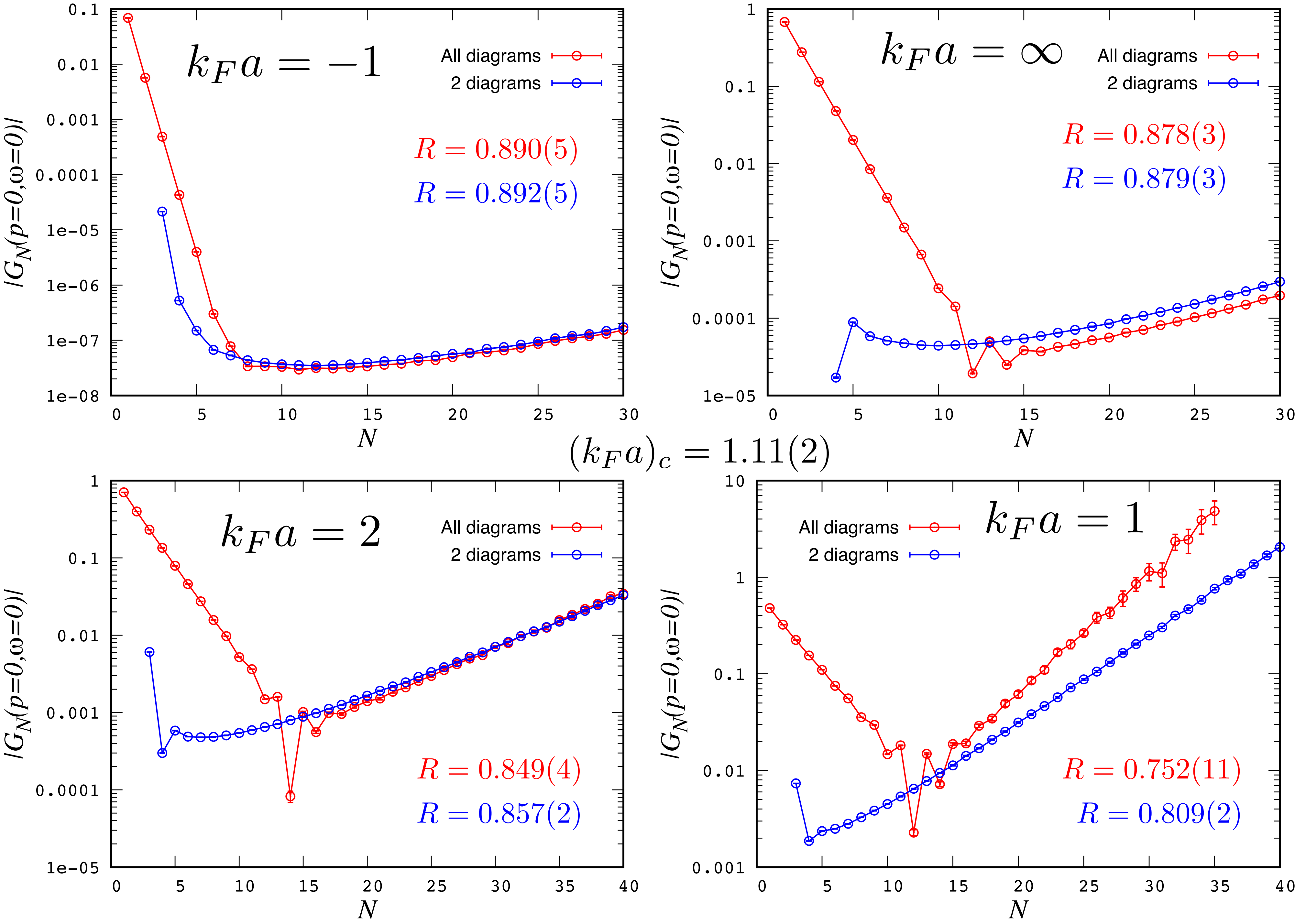




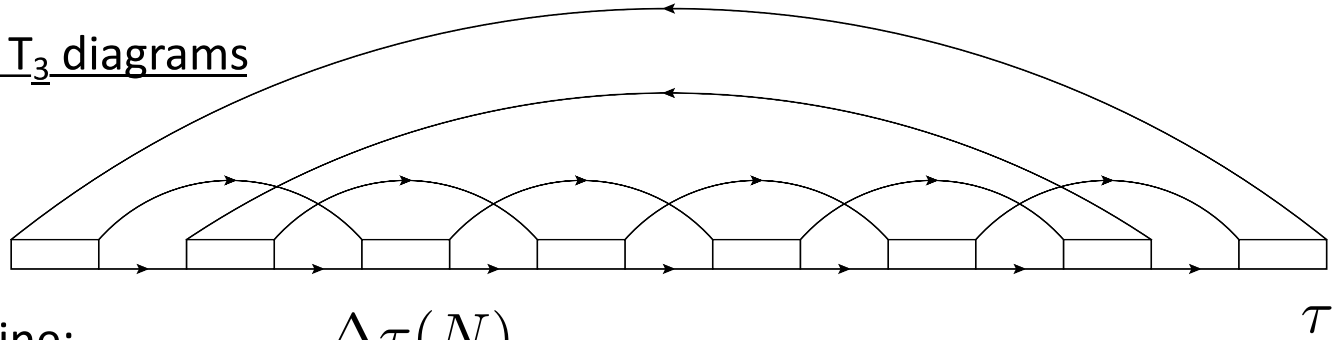


$$\text{at } k_F a = \infty : \quad R = 0.878(2)$$



$k_F a = -1$
All diagrams
2 diagrams
$R = 0.890(5)$
$R = 0.892(5)$
$|G_N(p=0,\omega=0)|$
N
$k_F a = \infty$
$R = 0.878(3)$
$R = 0.879(3)$
$(k_F a)_c = 1.11(2)$
$k_F a = 2$
$R = 0.849(4)$
$R = 0.857(2)$
$k_F a = 1$
$R = 0.752(11)$
$R = 0.809(2)$

Power-counting argument for T_3 diagrams



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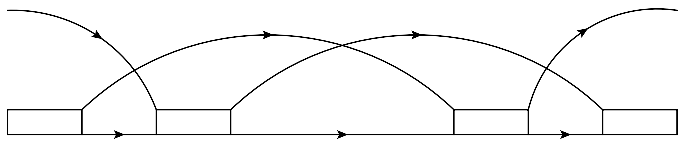
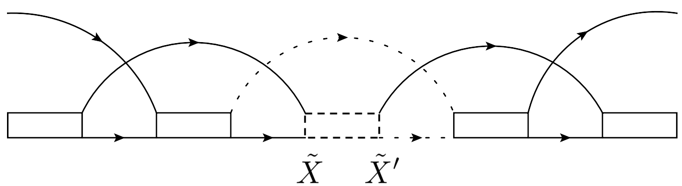
Propagators at short time and distance:

$$G^0_\downarrow(r,\tau) \sim \frac{1}{\tau^{3/2}}\; e^{-\frac{m}{2\tau}r^2}$$

$$\Gamma^0(r,\tau) \sim \frac{1}{\tau^2} e^{-\frac{m}{\tau}r^2}$$

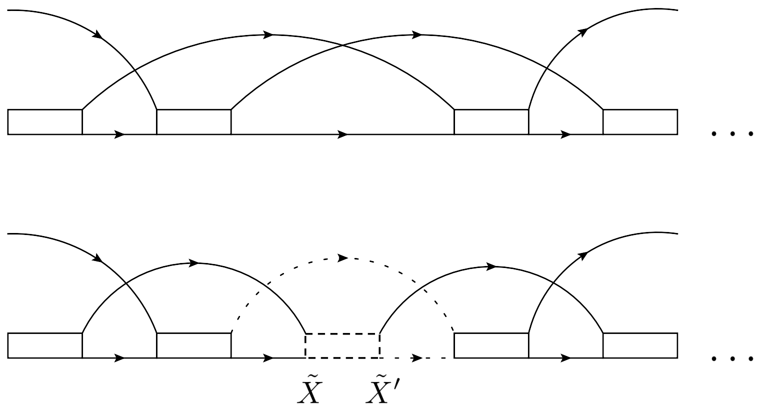
$\Sigma^N_{(1\ \mathrm{diagram})} = \dots$  $\dots$

$\Sigma^{N+1}_{(1\ \mathrm{diagram})} = \dots$  $\dots$

Power-counting argument

$$\Sigma^{N}_{(1\ \text{diagram})} = \dots$$

$$\Sigma^{N+1}_{(1\ \text{diagram})} = \dots$$



$$\frac{\Sigma^{(N+1)}_{(1\ \text{diagram})}}{\Sigma^{(N)}_{(1\ \text{diagram})}} \sim \underbrace{\int d\tilde{X}}_{(\Delta\tau)^{1+\frac{3}{2}}} \; \underbrace{\int d\tilde{X}'}_{(\Delta\tau)^{1+\frac{3}{2}}} \; \underbrace{G^0}_{\frac{1}{(\Delta\tau)^{\frac{3}{2}}}} \; \underbrace{G^0}_{\frac{1}{(\Delta\tau)^{\frac{3}{2}}}} \; \underbrace{\Gamma^0}_{\frac{1}{(\Delta\tau)^{2}}}$$

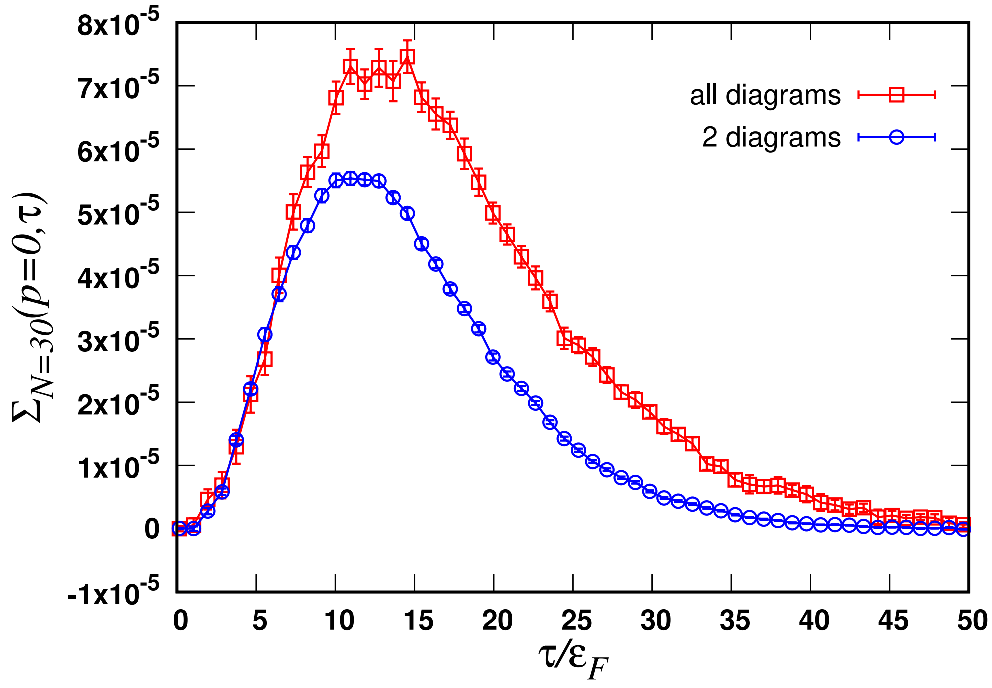
exponential dependence in N: $\Sigma^{(N)}_{(1\ \text{diagram})} \propto (-R)^{-N}$

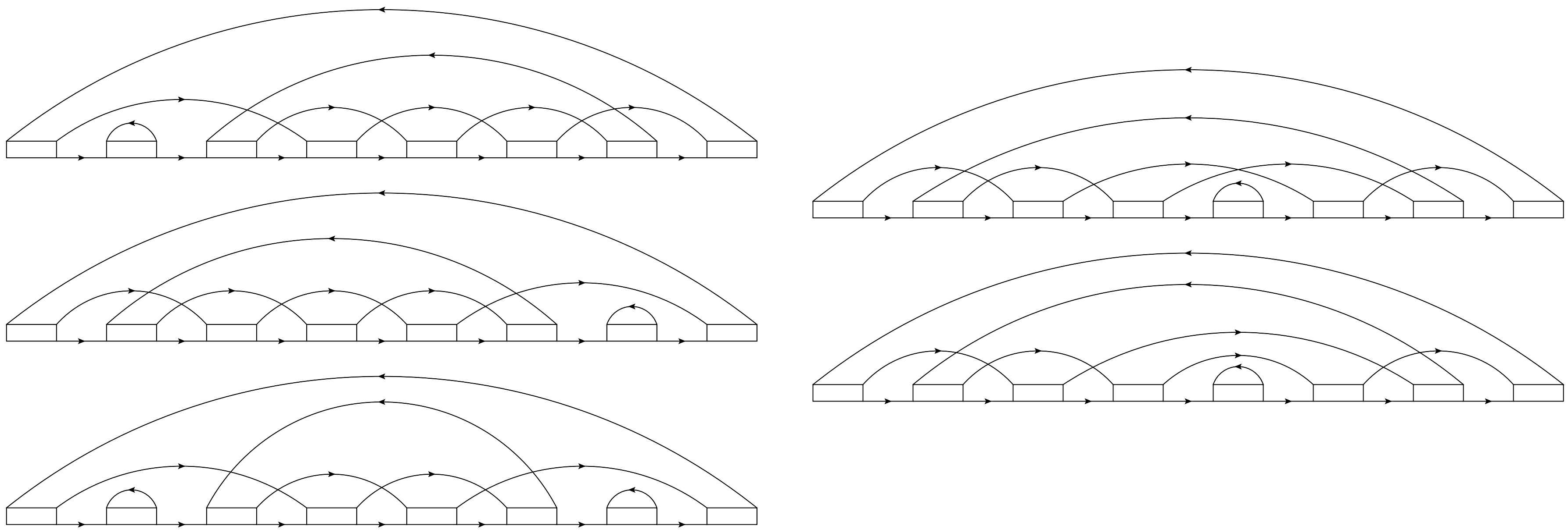
$$G^{(N)}_{(1\ \text{diagram})} \propto (-R)^{-N}$$

Time-dependence at large order:

$$G_N(\mathbf{p}=0,\tau) = \frac{F(\tau)}{(-R)^N}$$

$$F_{(2\ \mathrm{diagrams})}(\tau) \neq F_{\mathrm{all}}(\tau) \equiv F(\tau)$$





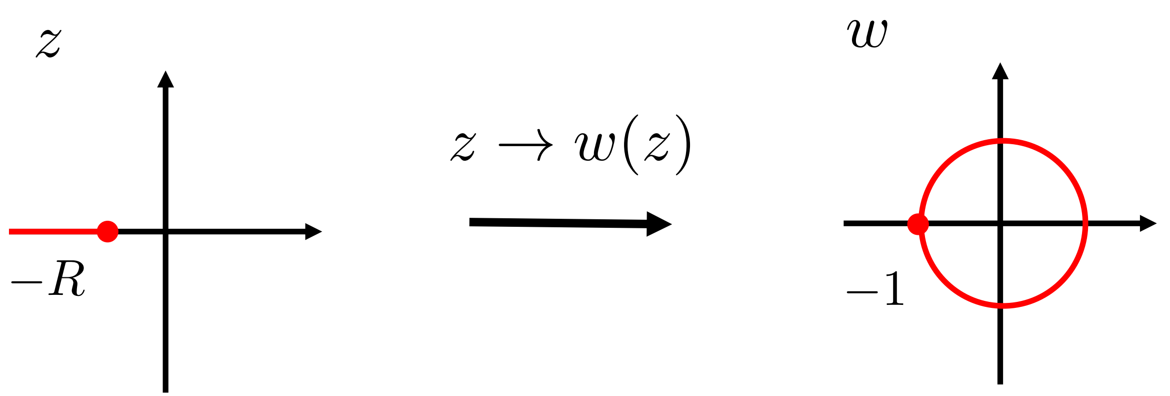
Resummation of diagrammatic series:

Formal power series: $$\Sigma(z) = \sum_{N=0}^{+\infty} \Sigma_N z^N \quad \text{with} \quad \Sigma_N \underset{N\to\infty}{\sim} (-1)^N R^{-N}$$

Conformal mapping: $z \to w(z)$ with $$z(w) = \frac{Aw}{(1-w)^\alpha}$$

$$w(z=0)=0$$
$$w(z=+\infty)=1$$
$$w(z=-R)=-1 \quad \Rightarrow \quad A = 2^\alpha R$$

$\underline{\alpha = 2:}$



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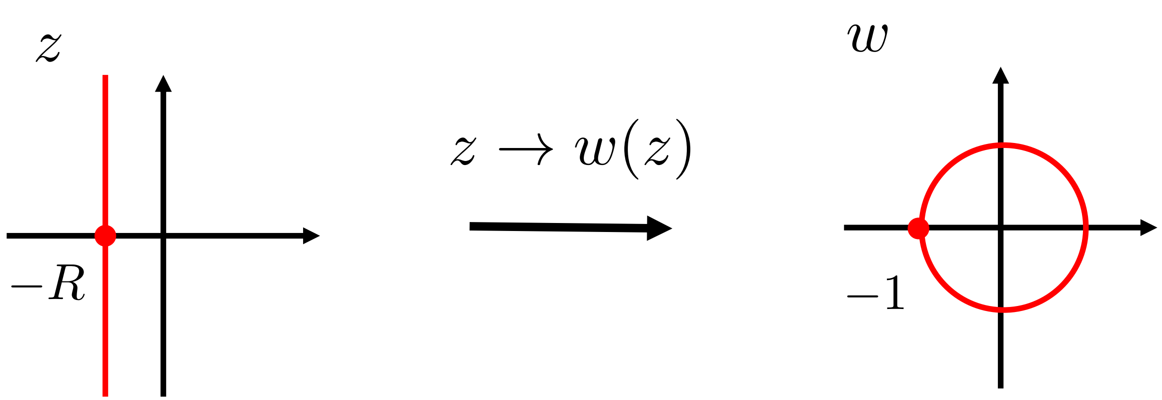
$\alpha = 1:$



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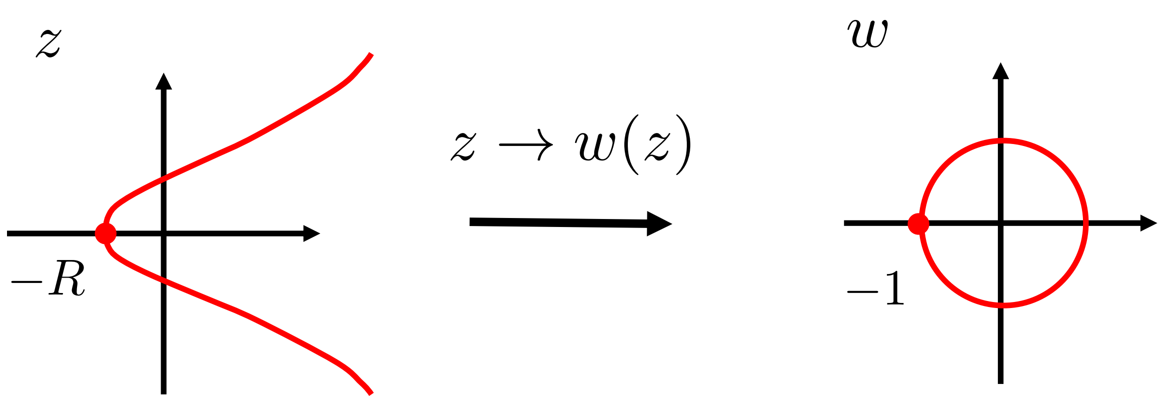
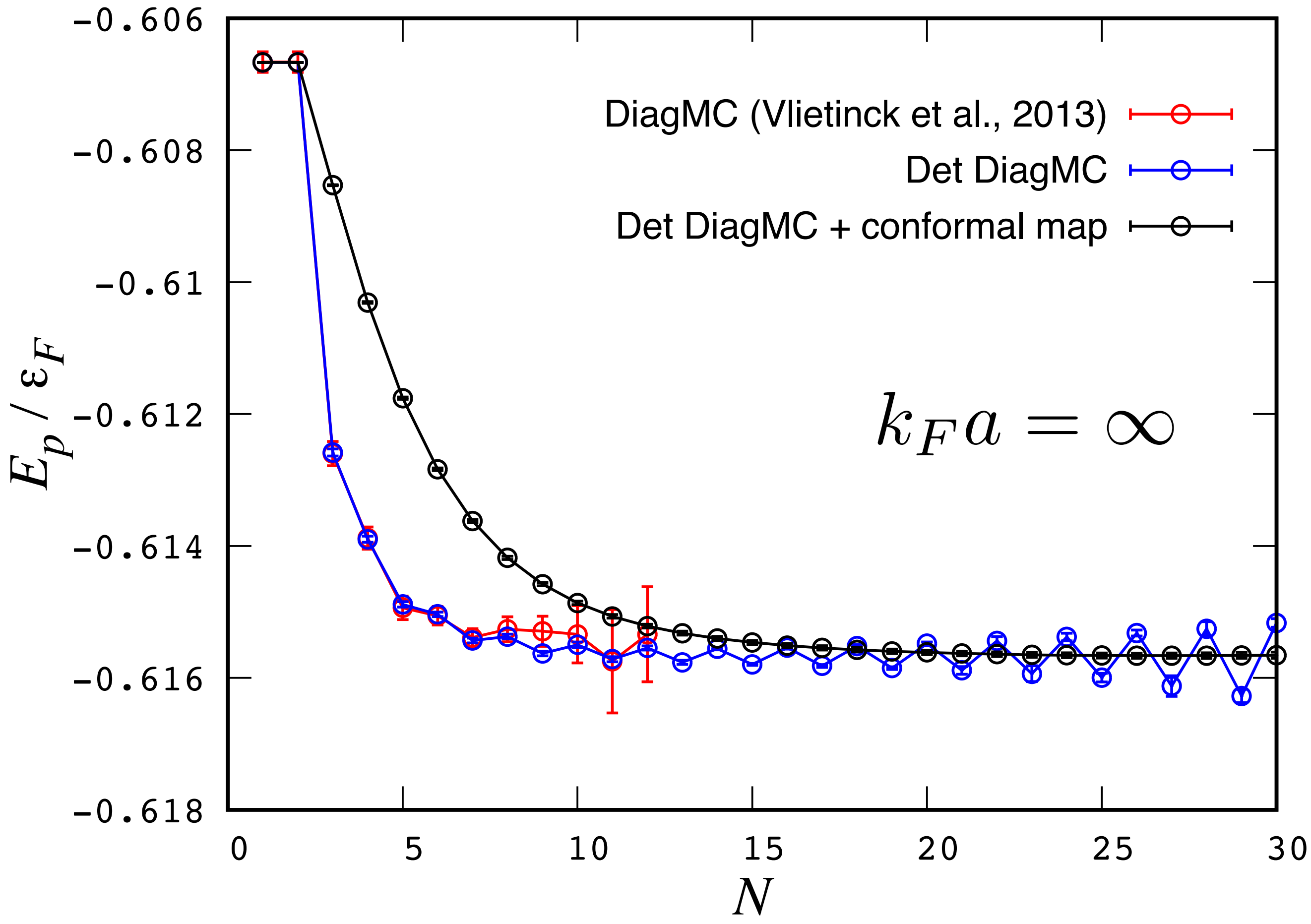
$\alpha = 1/2$:



Polaron energy from self-energy: $E_p = \Sigma(\mathbf{p} = 0, \omega = 0, \mu = E_p)$



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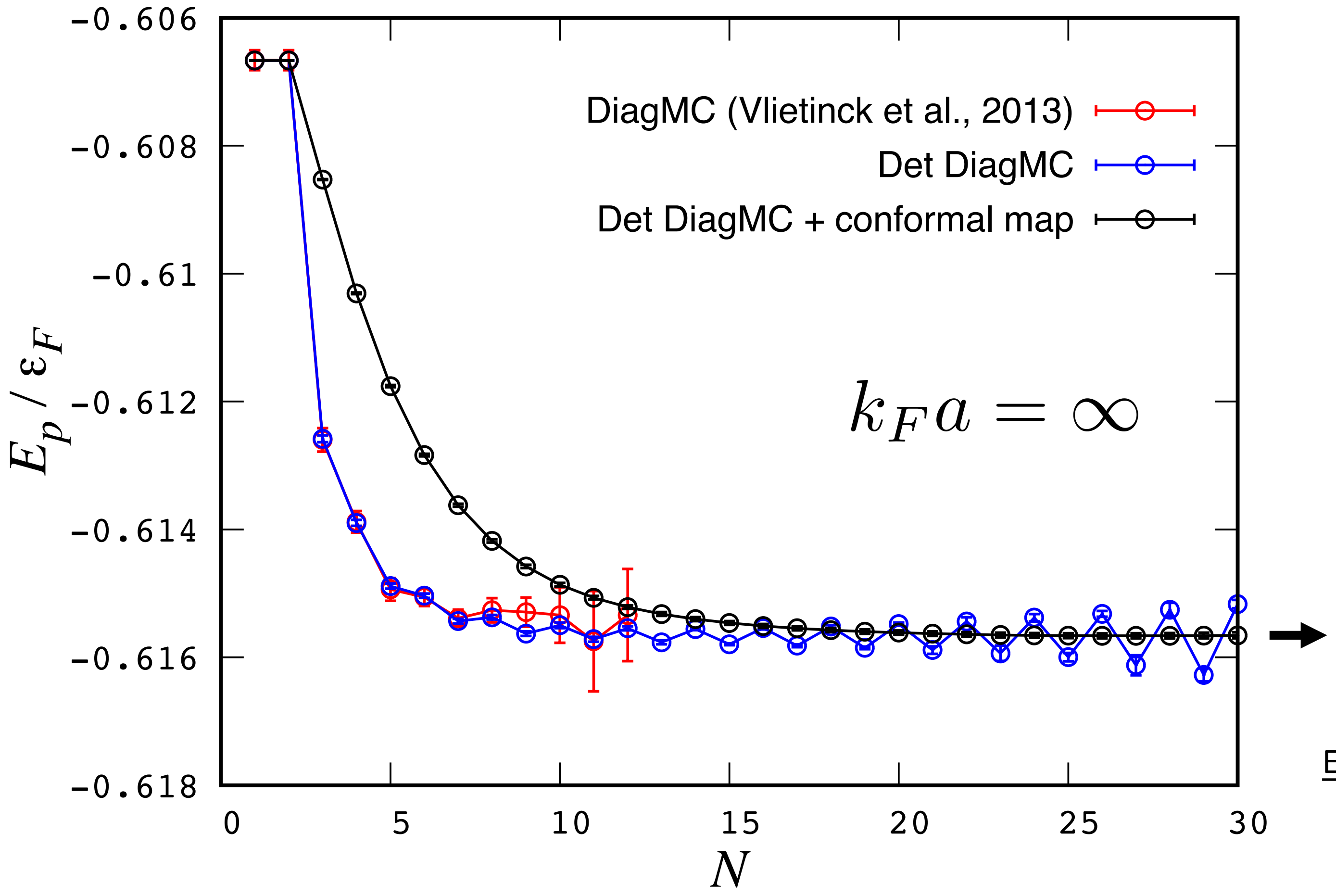


$\rightarrow E_p/\epsilon_F = -0.61565(4)$

Experiment (Zwierlein, MIT):

$E_p/\epsilon_F = -0.60(5)$

-0.61565(4)	this work
-0.607	one particle-hole variational ansatz [15, 16]
-0.615(3)	diagrammatic Monte Carlo [32, 33]
-0.6156	two particle-hole variational ansatz [84]
-0.615(1)	diagrammatic Monte Carlo [34]
-0.622(9)	lattice quantum Monte Carlo [92]
-0.60(5)	experiment [9]

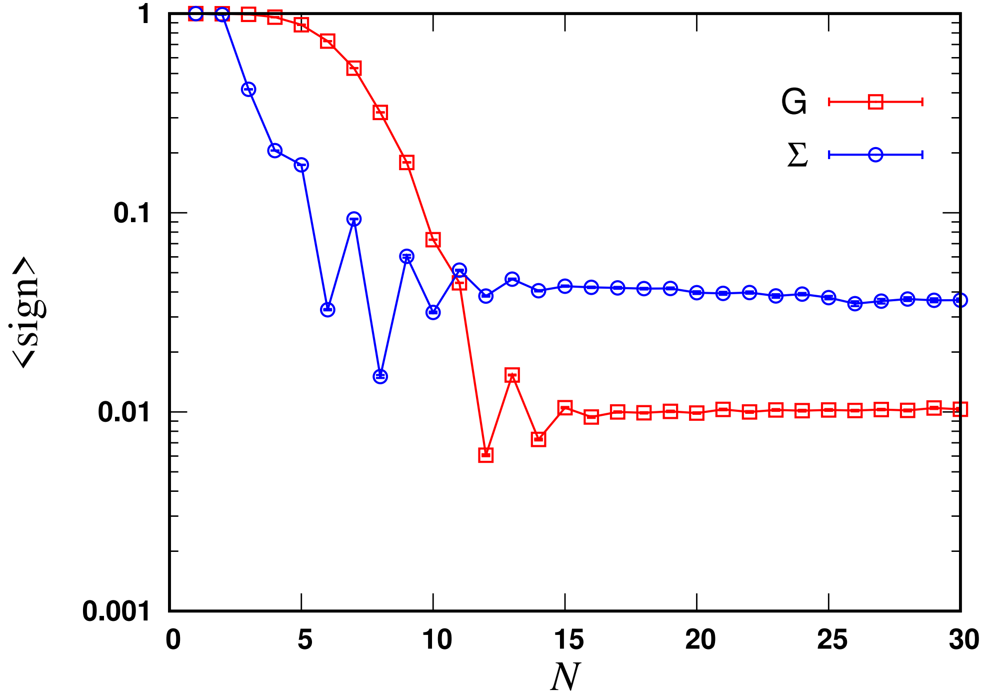
Chevy, Phys. Rev. A 74, 063628 (2006).
Prokof'ev, Svistunov, PRB 77, 125101 (2008).
Combescot, Giraud, PRL 101, 050404 (2008).
Vlietinck, Ryckebusch, VH, PRB 87, 115133 (2013).
Bour, Lee, Hammer, Meißner, PRL 115, 185301 (2015)
Yan et al., PRL 122, 093401 (2019).

Average sign corresponding to MC process at order N and algorithm efficiency

$$\sum_{N=1}^{\infty} a_N \quad \text{With} \quad a_N = \int dV_N \; W(V_N)$$

$$z_N = \int dV_N \; |W(V_N)|$$

$$\langle \text{sign} \rangle_N = \frac{a_N}{z_N}$$



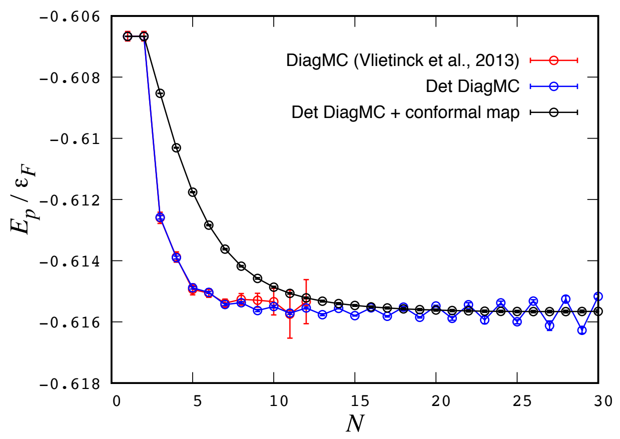
Computational complexity for PDET:

$$t = \mathcal{O}(1/\epsilon^{\nu})$$

Conclusions

- CDet for polaron: PDet

  KVH, Werner, Rossi, Phys. Rev. B **101**, 045134 (2020).

- 

- Large order: $G_N(\mathbf{p}=0,\tau) = \dfrac{F(\tau)}{(-R)^N}$

Finite density:

$$a_N \sim (N!)^{1/5}$$

Rossi, Ohgoe, VH, Werner PRL **121**, 130405 (2018)

Outlook

- Mass-imbalanced polaron (+halon physics)
- N+1 few-fermion problem
- Polaron at finite T
- Polaron: real-time calculations?
- Full understanding of large-order behavior?