

Revisiting the properties of an impurity in a Fermi liquid

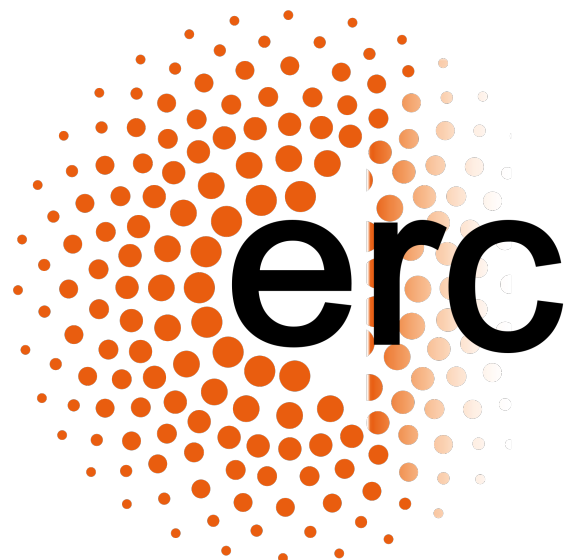
Status report

Lode Pollet

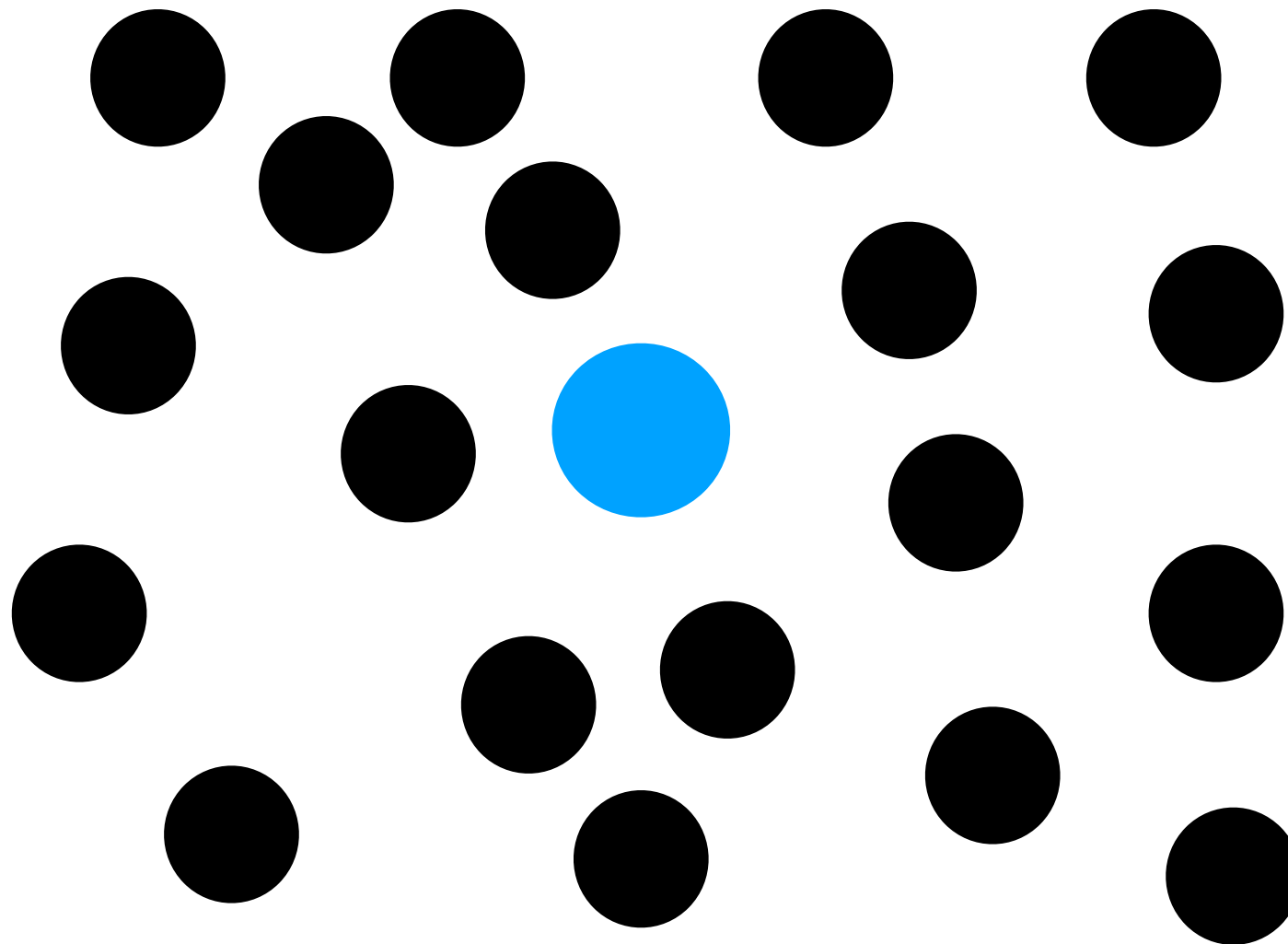
Stefan Wittlinger (LMU Munich)

Nikolay Prokof'ev (UMass)

Andrey Mishchenko (RIKEN, Japan)



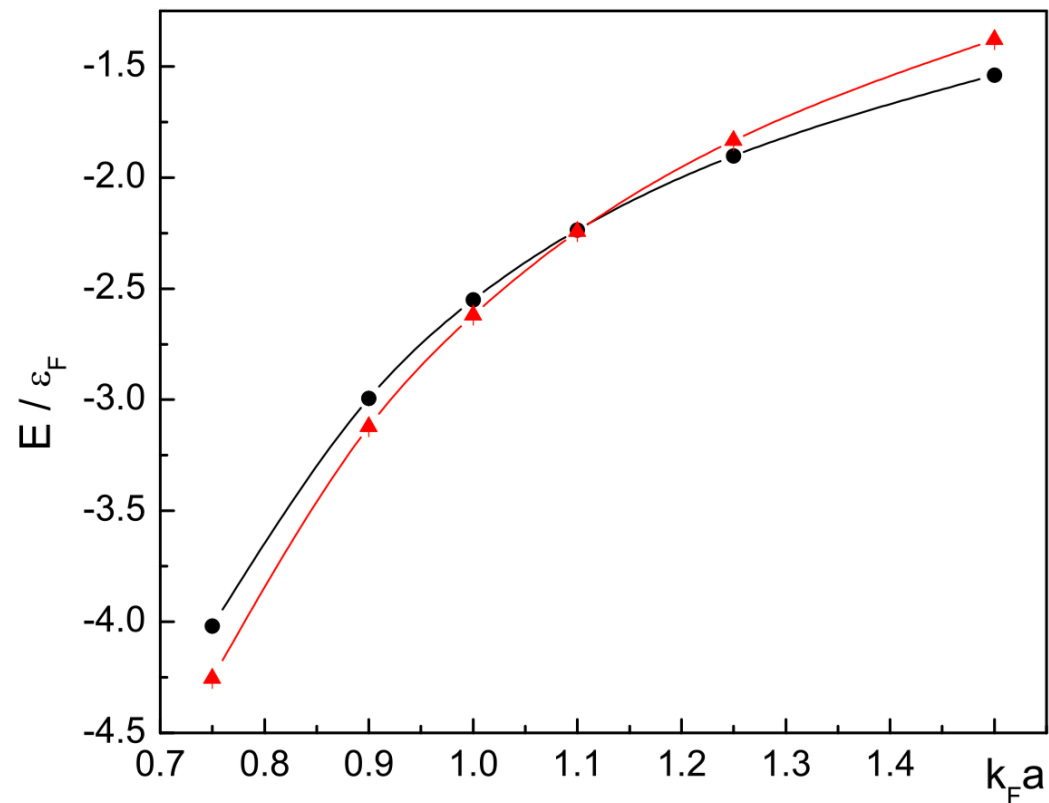
Fermi polaron



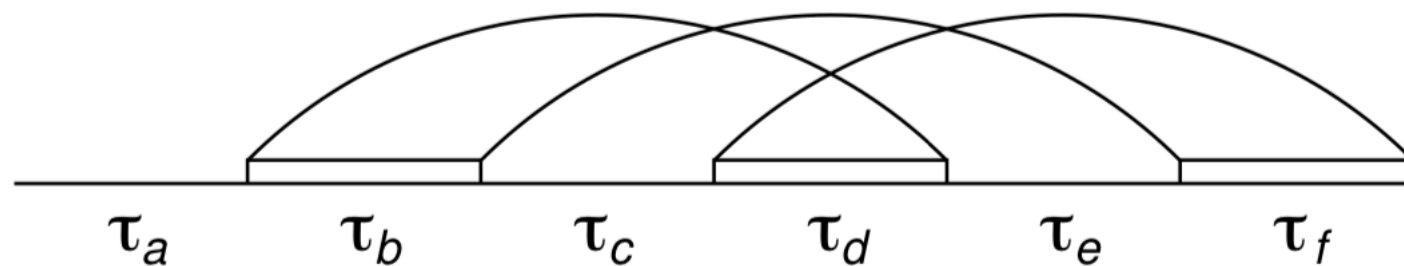
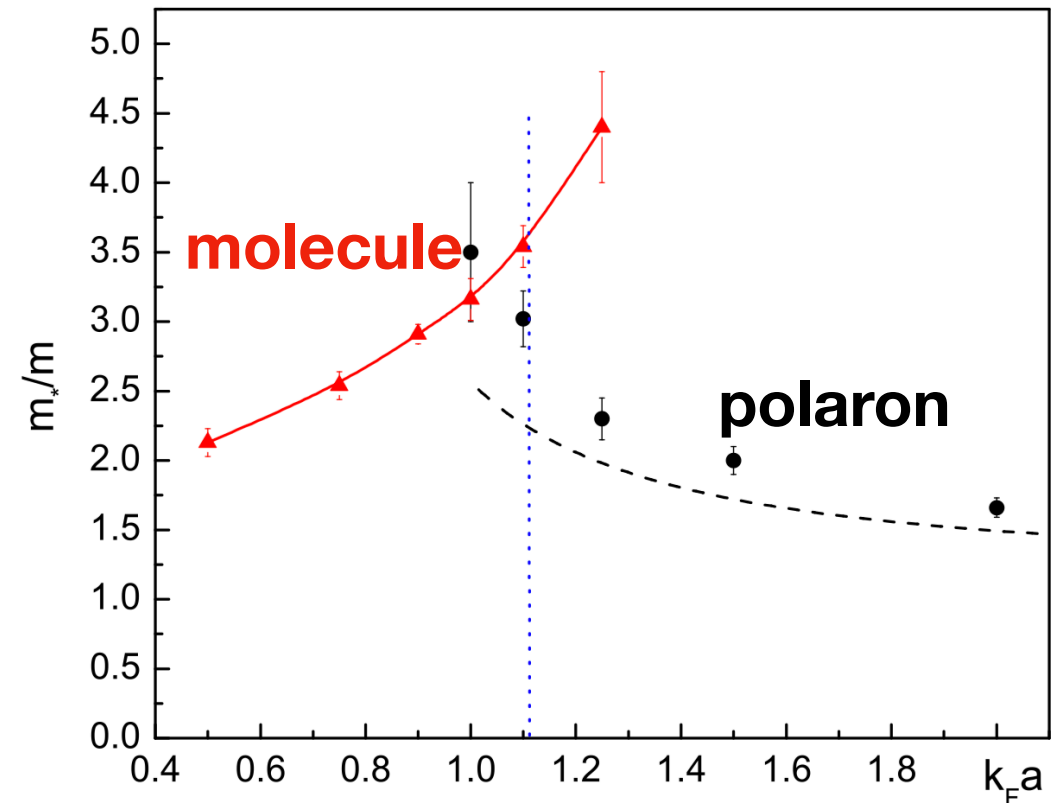
How does a particle move in a fermionic reservoir?

resonant Fermi polaron

polaron - molecule transition



effective mass



N. V. Prokof'ev and B. V. Svistunov
Phys. Rev. B **77**, 125101 (2008)

ions in He-3: experiments

$$M_{\text{ion}} \sim 100 - 200 m_{^3\text{He}}$$

cf. orthogonality catastrophe

$$T_F = \frac{p_F^2}{2m} \gg T_0 = \frac{p_F^2}{2M}$$

can be positively or
negatively charged

$$T_F \sim 5\text{K}$$

problem is in strong
coupling regime:

$$g = p_F^2 \sigma_{\text{tr}} / (3\pi^2) \gg 1$$

$$\Gamma = T_0 g \gg T_0$$

overdamped already at $T \gg T_0$

ions in He-3: experiments

this is Anderson
orthogonality physics

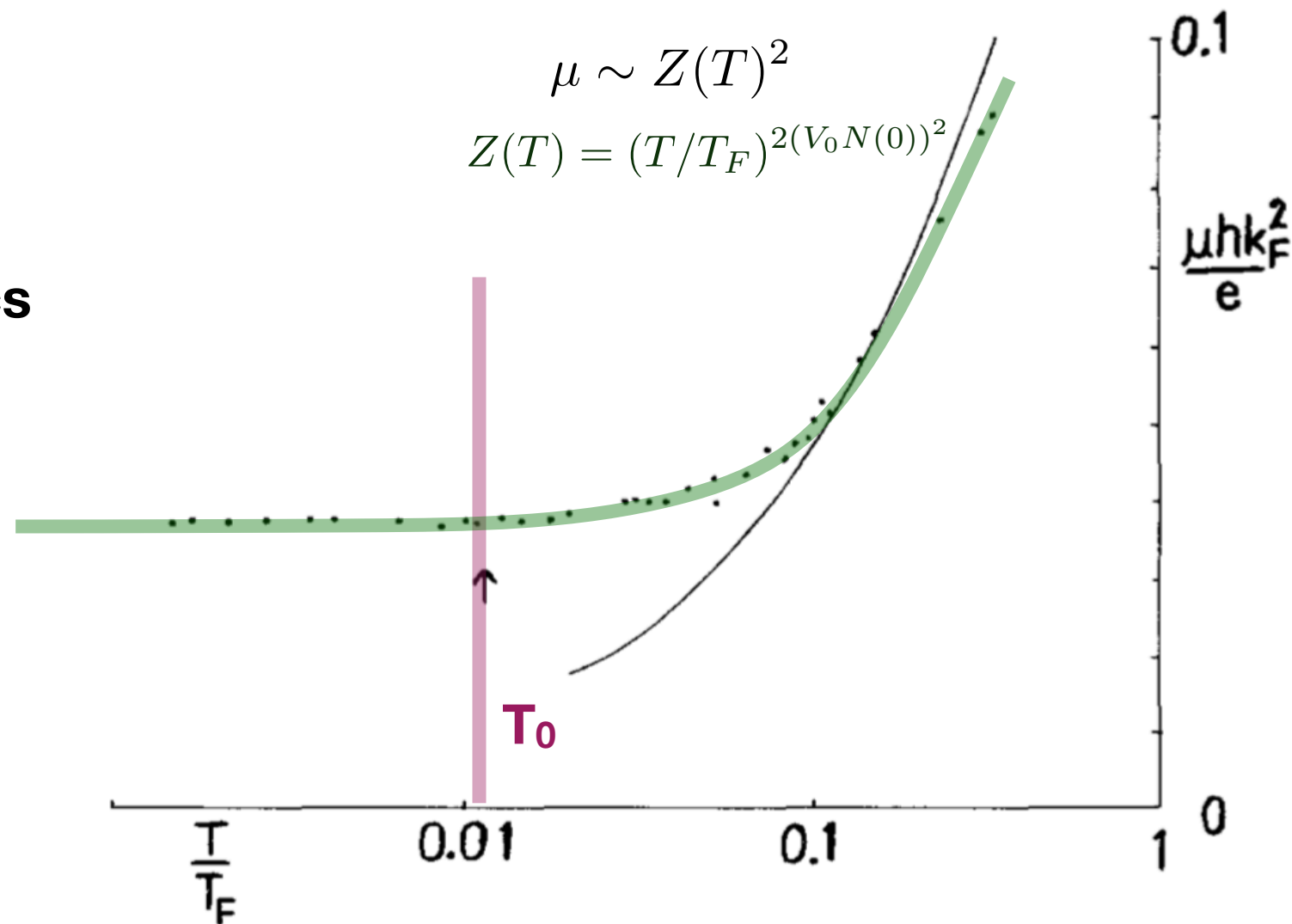


Fig. 3. Mobility of a negative ion for $T > T_0 = 10$ mK. The solid line

J. Kondo and T. Soda, JLTTP 50, p 21 (1983);

M. Kuchnir, P. R. Roach, and J.B. Ketterson, Phys. Rev. A 2, 262 (1970).

ions in He-3: experiments

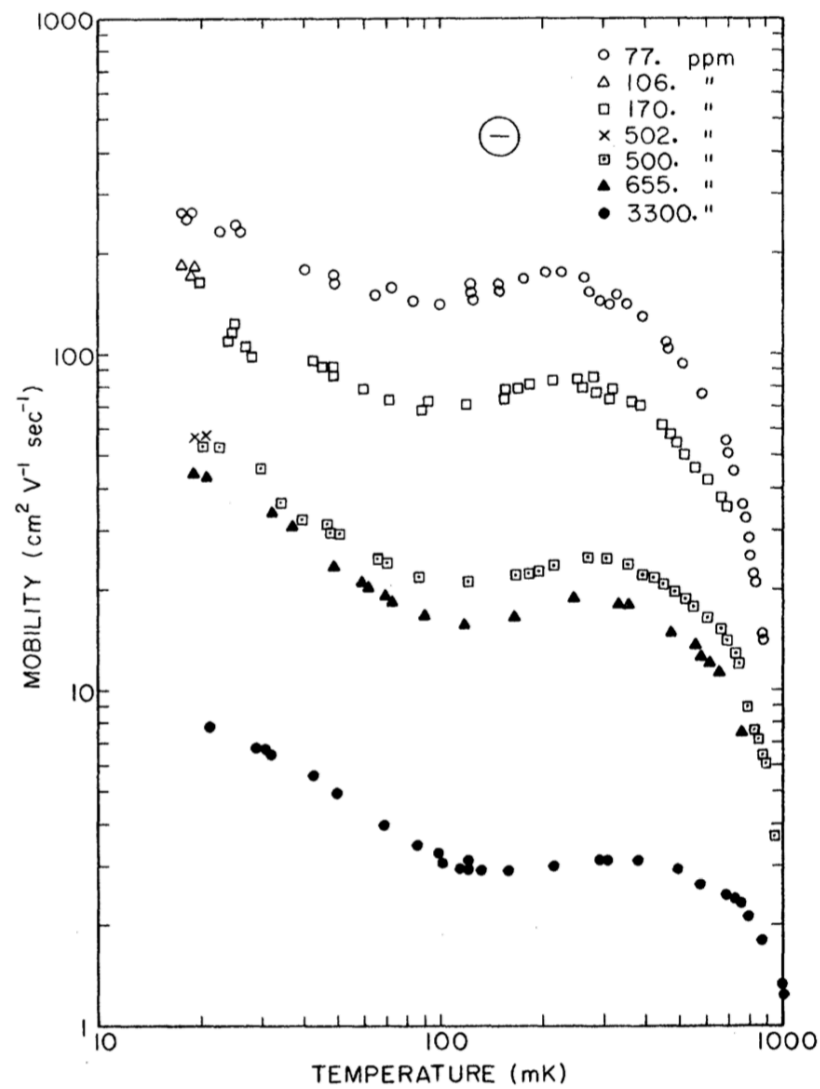


FIG. 3. Temperature dependence of the negative-ion mobility for several ^3He - ^4He solutions.

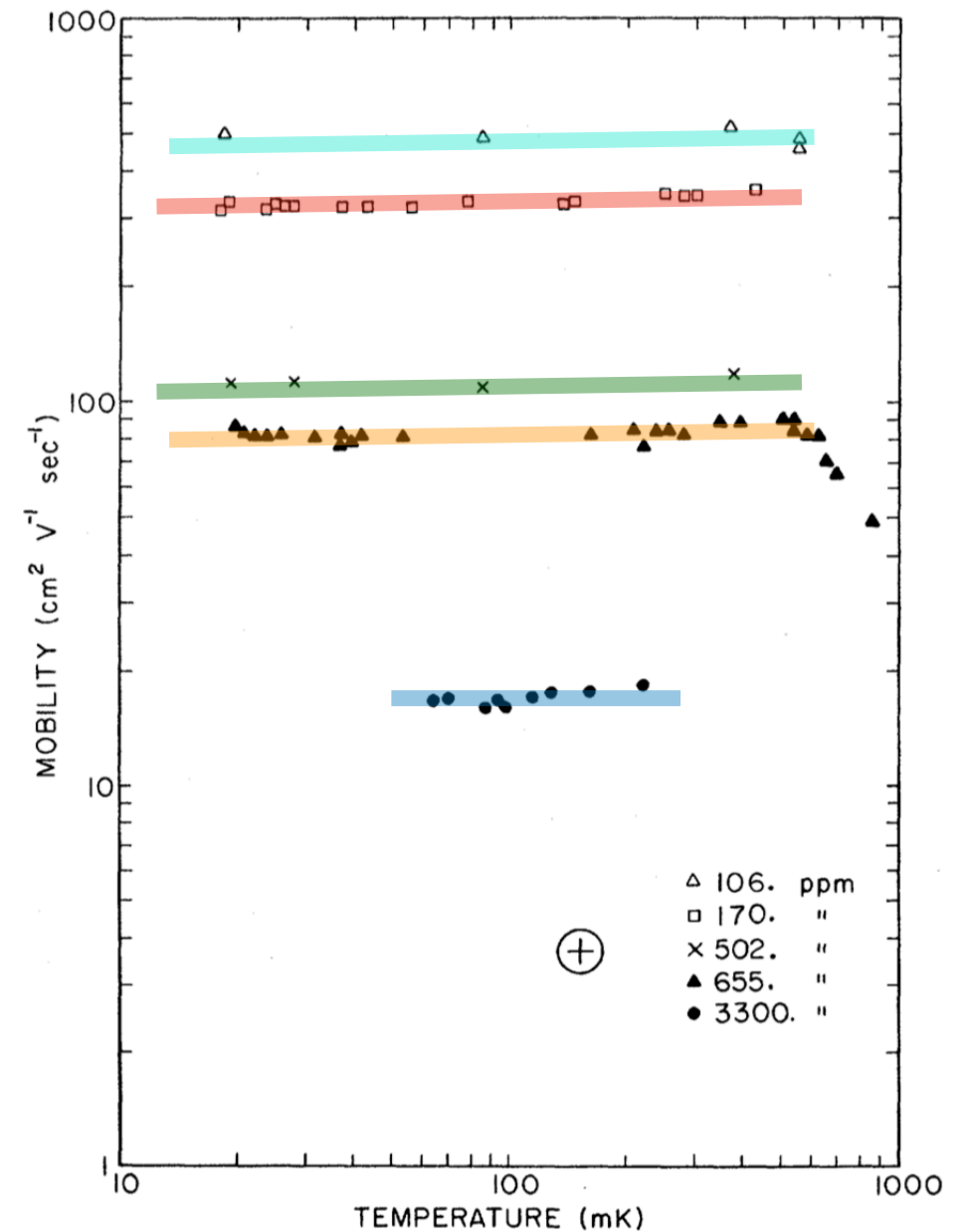


FIG. 4. Temperature dependence of the positive-ion mobility for several ^3He - ^4He solutions.

ions in He-3: experiments

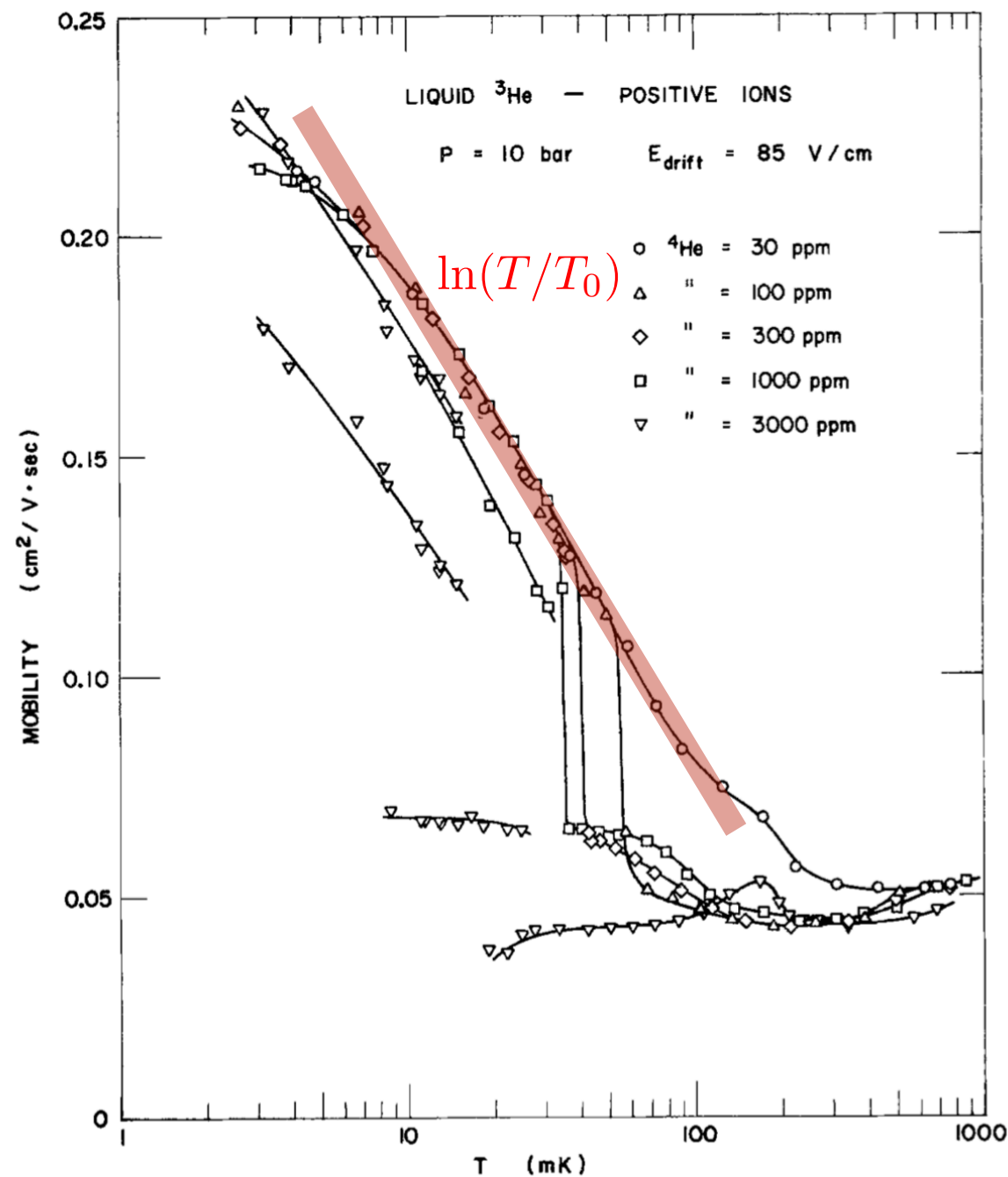


Fig. 5. The temperature dependence of the **positive-ion** mobility in liquid ³He at a pressure of 10 bar for various values of the ⁴He impurity content.

for negative ions
the mobility
remains constant
down to T_c

P. R. Roach, J. B.
Ketterson and P. D. Roach,
JLTP 34, p 169 (1978)

mobility beyond quasiparticles

Drude theory $\mu/e = \frac{1}{M} \frac{1}{-i\omega + \Gamma}$

describes diffusive motion for $\omega < \Gamma$

experimental observation : μ and Γ remain constant to temperatures $T \ll \Gamma$

At odds with the Mott-Ioffe-Regel limit: $\ell \gg \lambda_T$ or $\tau(T) \gg 1/T$

- **Interpreting Γ as the (constant) scattering rate at these low T is hence problematic because M should then remain constant as well**

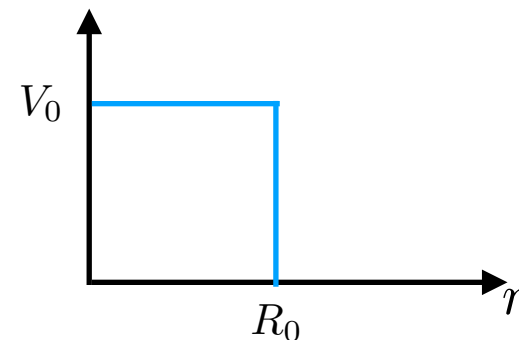
- **if $\tau(T) \gg 1/T$ remains obeyed, then the effective mass $M^* \propto M\Gamma/T$**

such that the DC mobility remains constant, $\mu(0) \sim \frac{1}{M\Gamma} \propto \frac{\tau(T)}{M^*}$

potential

**we use a soft-sphere potential:
amplitude V_0 , range R_0**

$$V(r) = V_0 \theta(R_0 - r)$$



s-wave scattering length:

$$a_{3D}^0 = R_0 \left(1 - \frac{\tanh mV_0 R_0}{mV_0 R_0} \right)$$

we are however interested in the case when many (~ 40) phase shifts contribute. Then the precise shape of the potential is probably irrelevant in understanding the strong-coupling regime

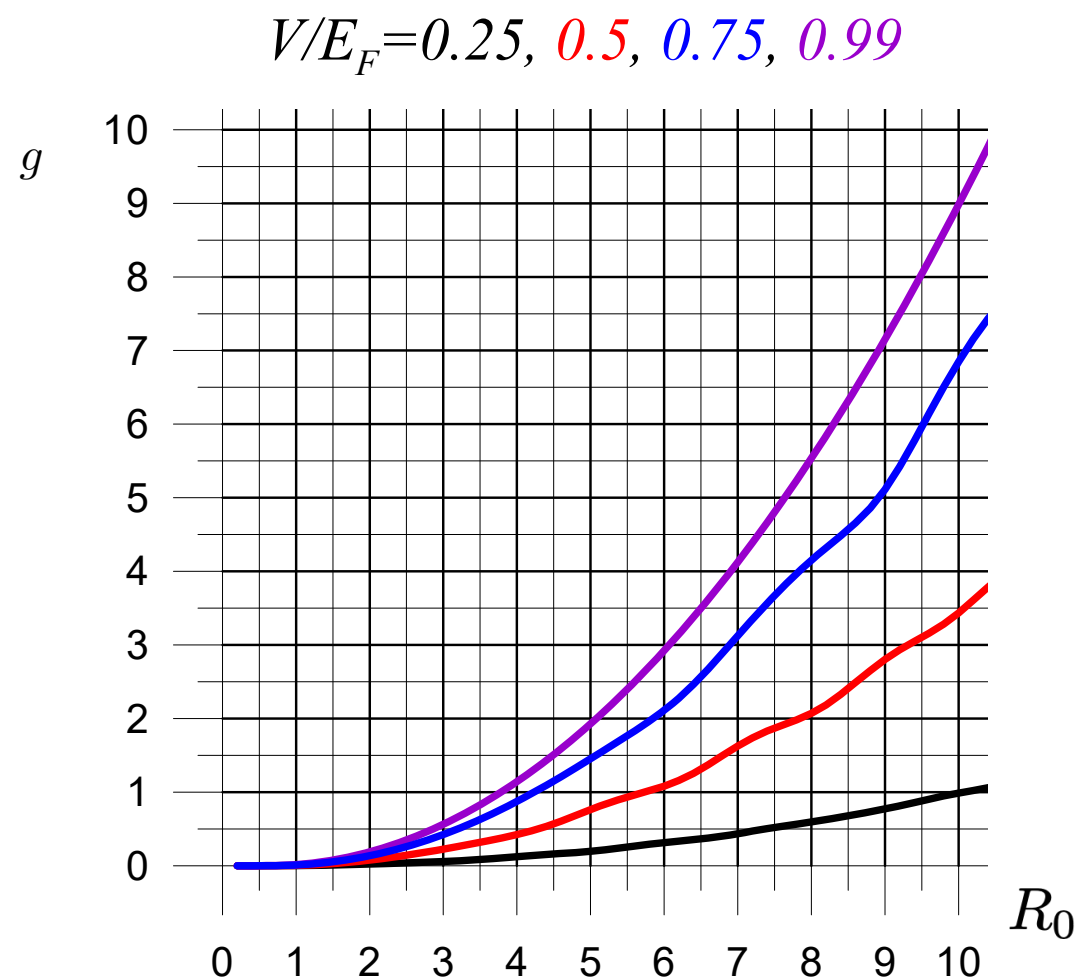
the first bound state is found for (s-wave, $V_0 < 0$): $-mV_0 R_0 = \pi/2$

potential

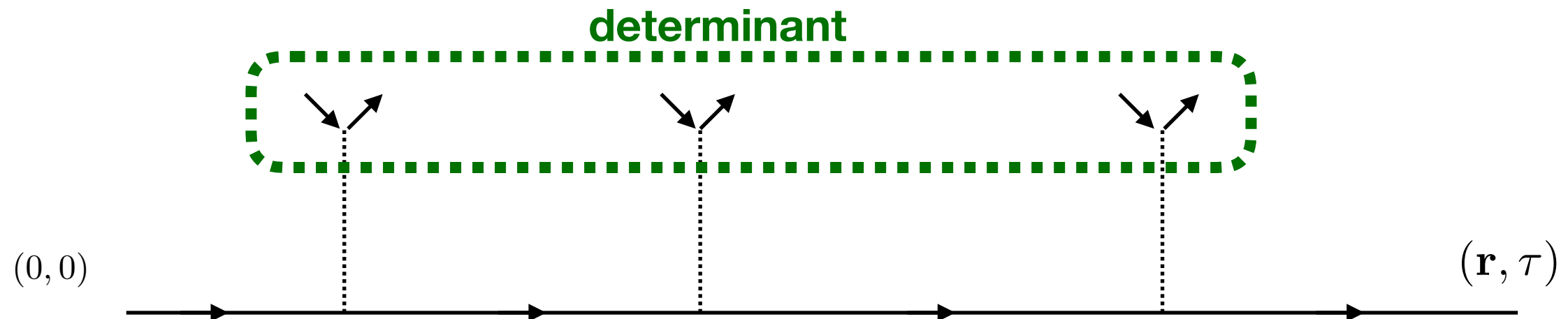
partial wave analysis:

phase shifts:

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell} (2\ell + 1) \sin^2(\delta_{\ell})$$



Green function code at T=0



$$\mathcal{G}(\mathbf{r}, \tau) = \sum_{n=0}^{\infty} (-V_0)^n \prod_{j=1}^{n+1} \mathcal{G}^{\text{imp}}[j, j-1] \det(M_n^{\text{fer}}[1..n, 1..n])$$

weak coupling expansion (cf Rubtsov algorithm)

use of real space - (imaginary) time to get rid of the constraints

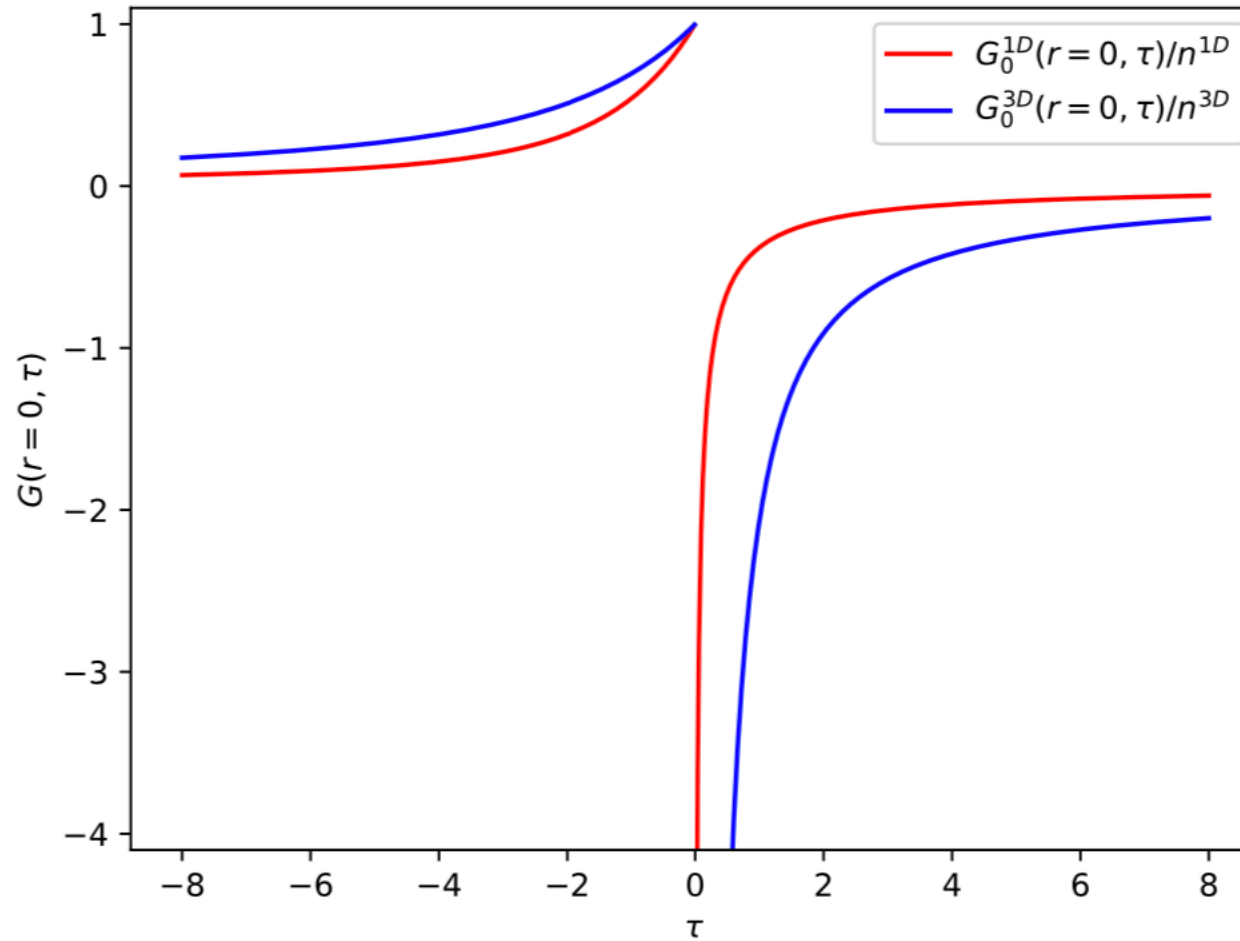
no partition function! normalization is via the 0th order diagram

(not CDet!! because of polaron problem : Feynman expansion ~ path integral)

non-interacting Green functions

$$\begin{aligned}\mathcal{G}_{<}^{1D}(r, \tau < 0) &= \frac{1}{2\pi} \int_{-1}^{+1} dk e^{\left(\sqrt{-\tau}k - \frac{ir}{2\sqrt{-\tau}}\right)^2 - \frac{r^2}{4\tau}} \\ &= \frac{e^{-r^2/4\tau}}{4\sqrt{-\pi\tau}} \left[\operatorname{erfi} \left(\sqrt{-\tau} + \frac{ir}{2\sqrt{-\tau}} \right) + \operatorname{erfi} \left(\sqrt{-\tau} - \frac{ir}{2\sqrt{-\tau}} \right) \right]\end{aligned}$$

$$\begin{aligned}\mathcal{G}_{\text{imp}}(r, \tau) \\ &= -\theta(\tau) \left(\frac{M}{2\pi\tau} \right)^{3/2} e^{-\frac{Mr^2}{2\tau}}\end{aligned}$$



$$\begin{aligned}\mathcal{G}_{<}^{3D}(r, \tau < 0) \\ &= \frac{1}{4\pi\tau} \mathcal{G}_{<}^{1D}(r, \tau) - \frac{e^{-\tau} \sin r}{4\pi^2 r \tau}\end{aligned}$$

FIG. 1: The non-interacting Green function as a function of imaginary time τ at $r = 0$ in 1D (3D) measured with respect to the density $n^{1D} = \frac{1}{\pi}$ ($n^{3D} = \frac{1}{6\pi^2}$). The chemical potential contribution e^τ has been taken into account ($\mu = k_F^2/(2m) = 1$ at $T = 0$).

Green function code at T=0

energy shift:

Green function is exponential in the polaron energy E for large enough times

we can add an energy shift $E_0 < E$ to ensure that the Green function decays exponentially. How far E_0 is detuned from E influences how well we can resolve E

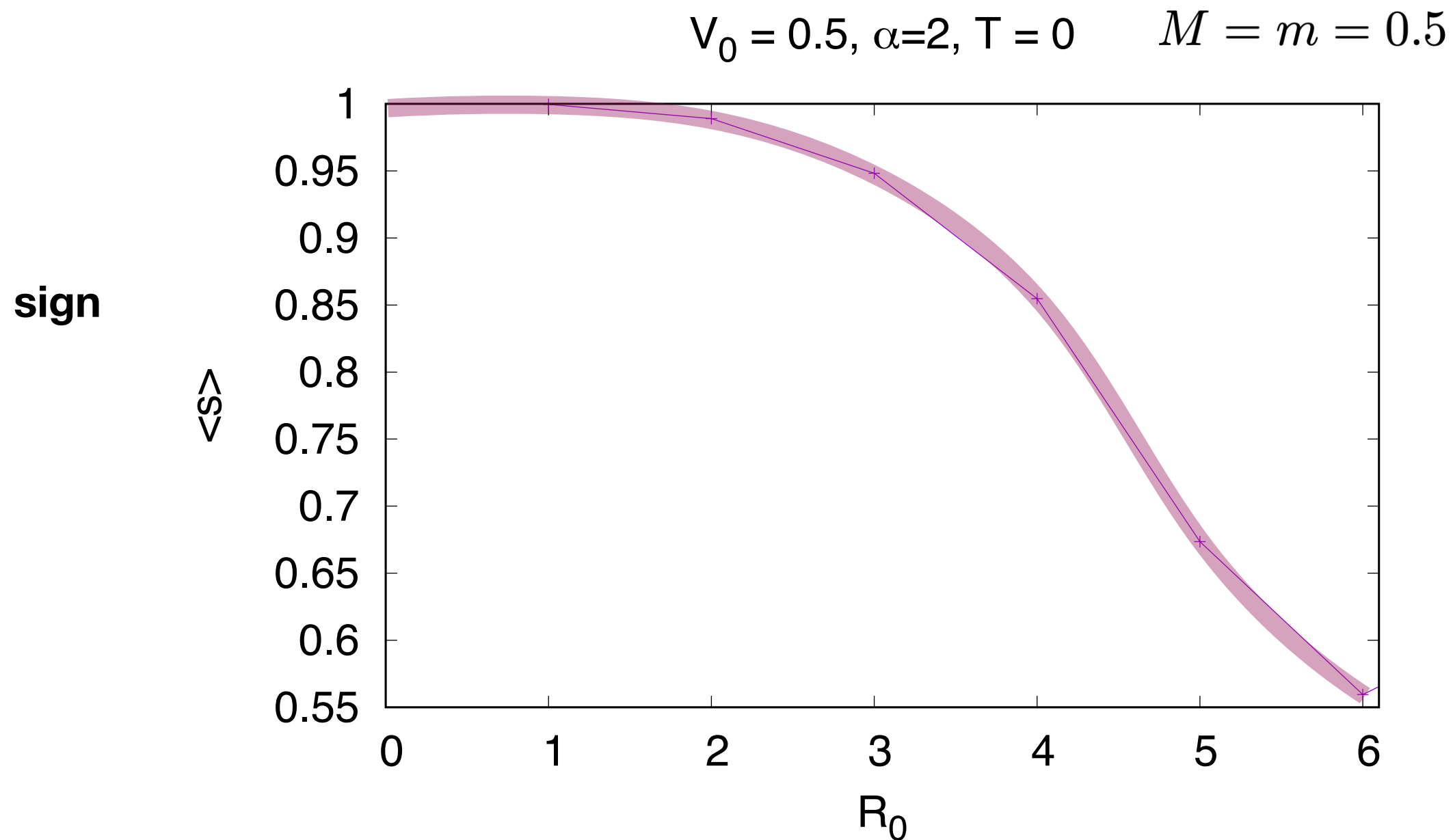
alpha-trick:

For $V_0 > 0$: you can shift the diagonal of the determinant of green functions by $\tilde{\alpha} = \alpha n$

this amounts to a shift of the Green function by $\exp(-\delta E \tau)$

$$\delta E = \tilde{\alpha} \frac{4\pi}{3} V_0 R_0^3$$

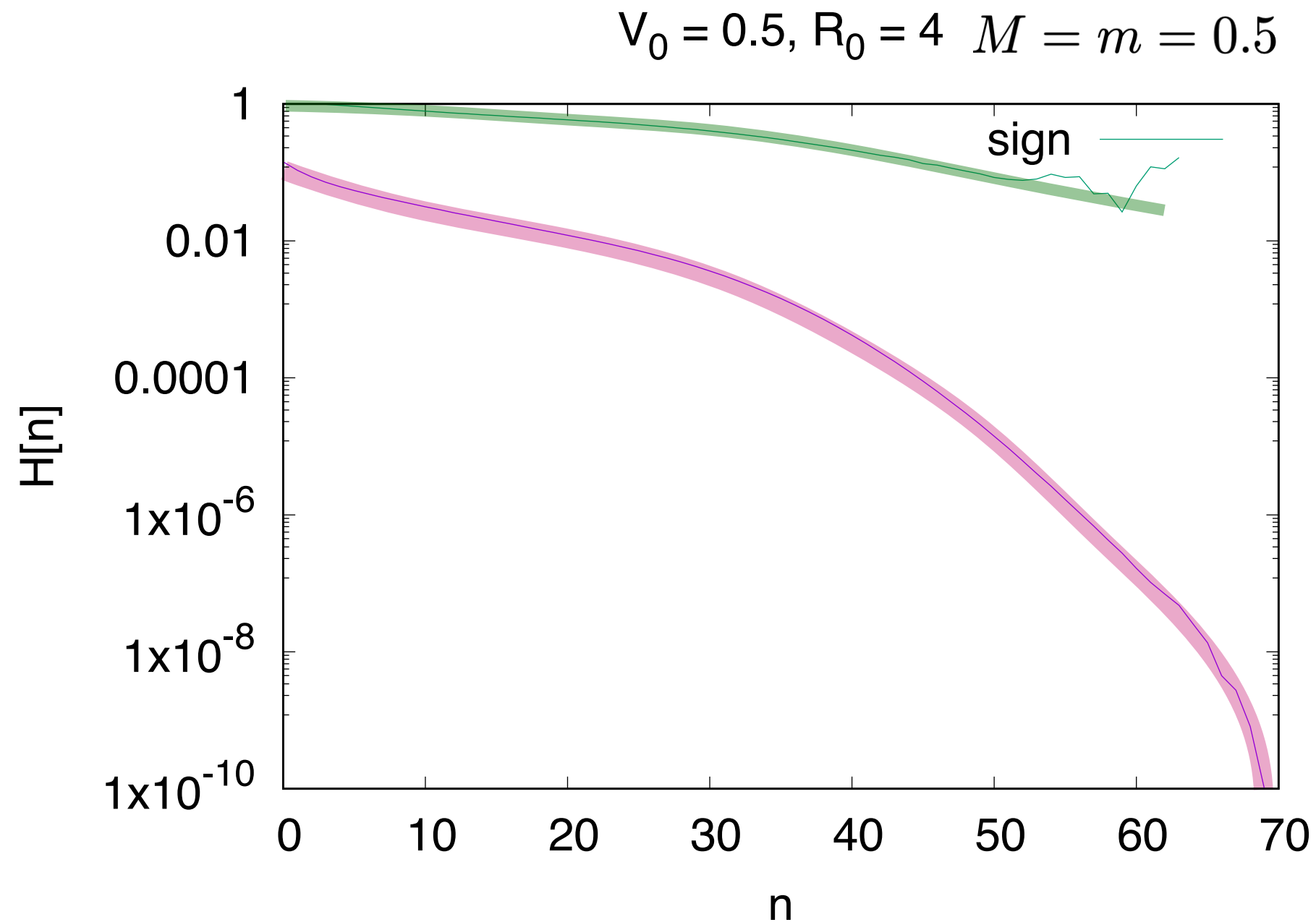
Green function code at T=0



note : single determinant (spin polarized bath)

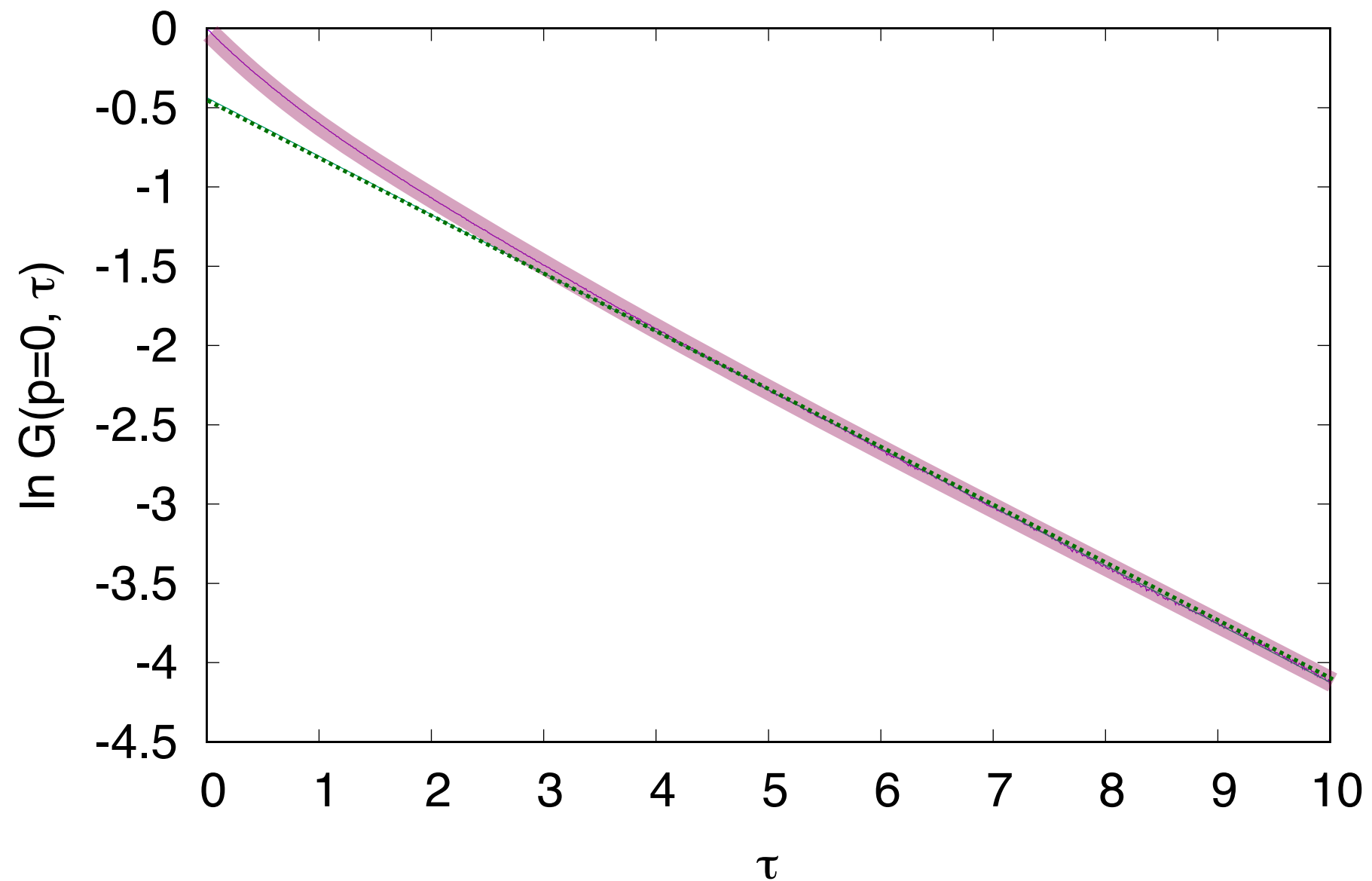
precise evaluation of G_0 is needed

Green function code at T=0

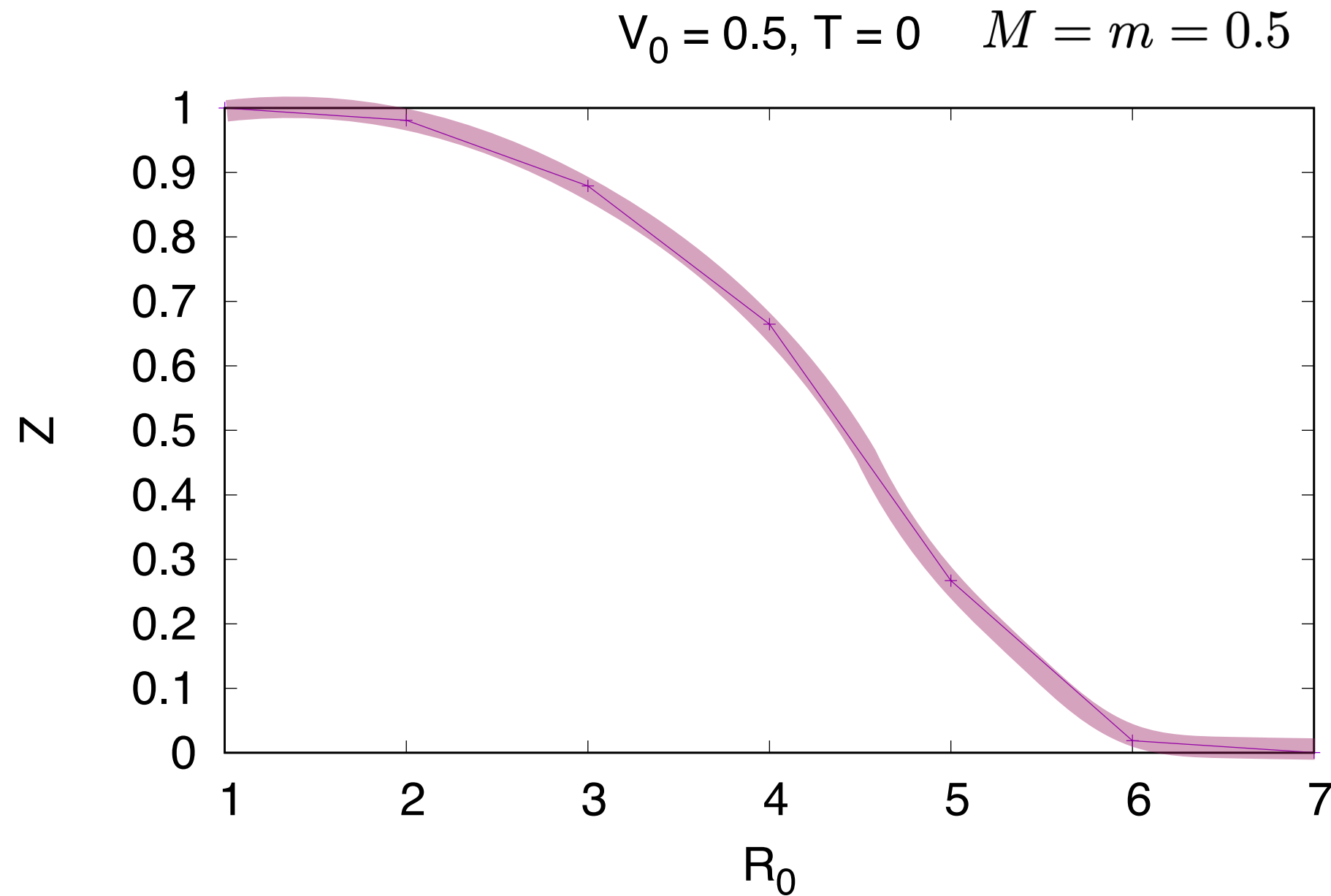


Green function code at T=0

$$V_0 = 0.5, R_0 = 4 \quad M = m = 0.5$$

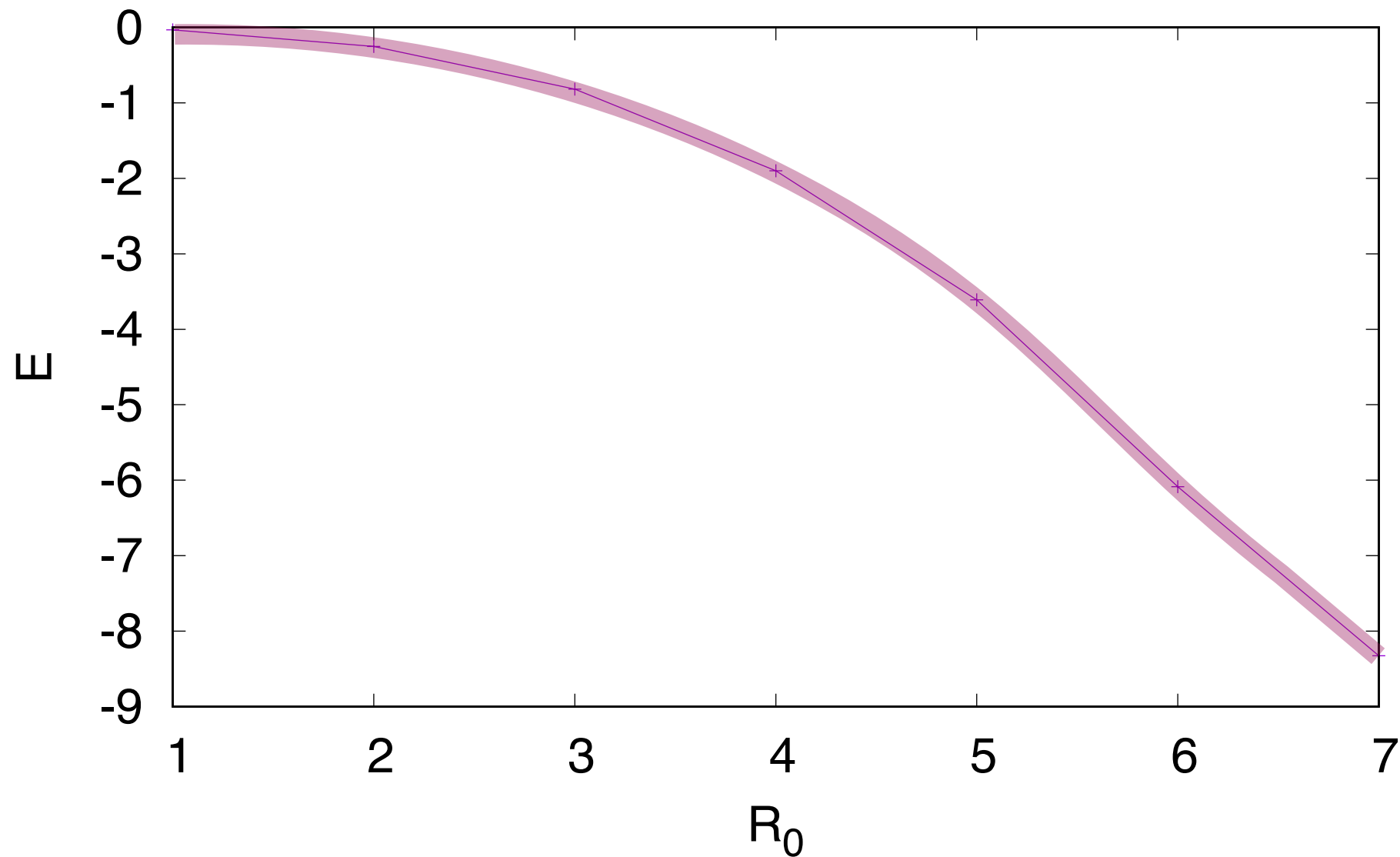


Green function code at T=0



Green function code at T=0

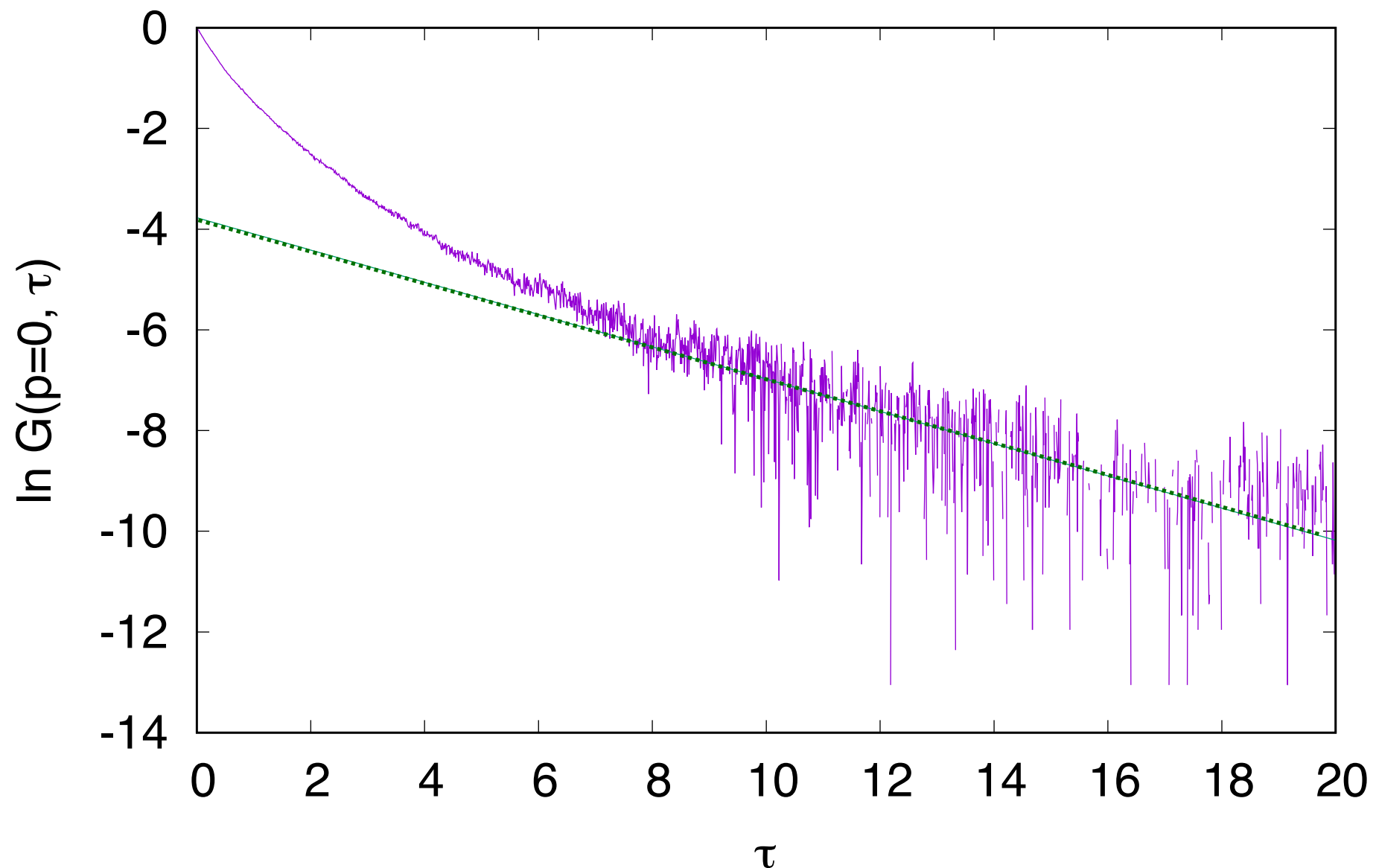
$$V_0 = 0.5, \alpha=2, T=0 \quad M = m = 0.5$$



Green function code at T=0

It is much harder to go to the strong coupling regime:

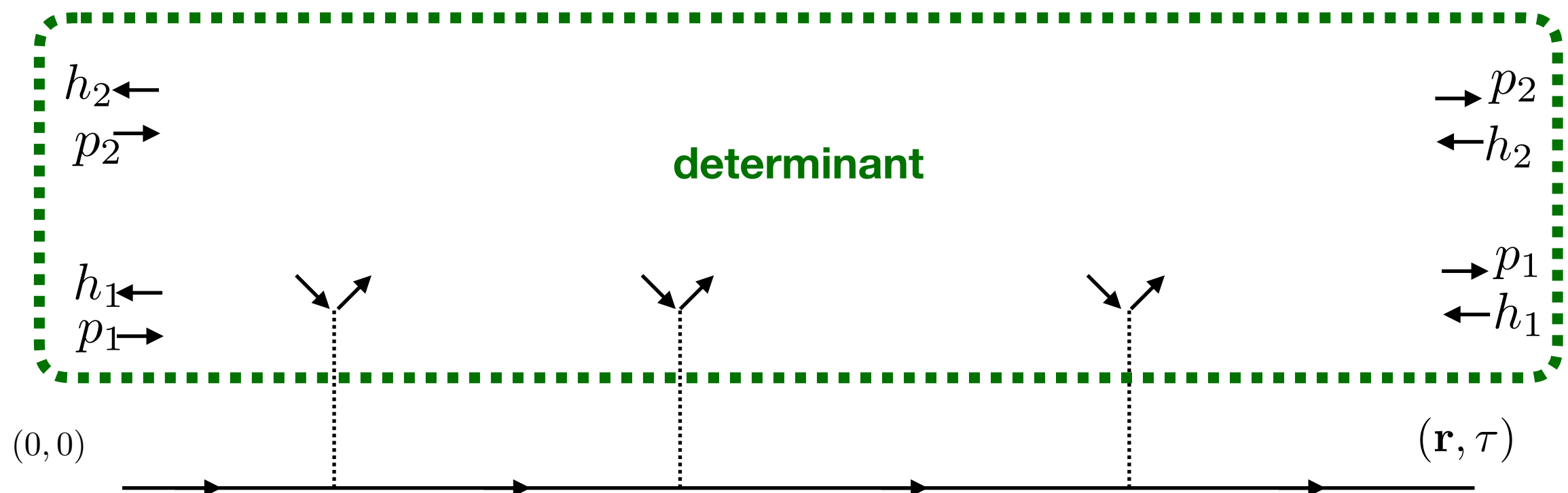
$$V_0 = 0.5, R_0 = 6 \quad M = m = 0.5$$



Green function code at $T=0$

how to go beyond the *problem of low Z factors* ?

elegant solution : dress with conjugate particle hole vertices at the end points
(A.S. Mishchenko, N. V. Prokof'ev, A. Sakamoto, and B. V. Svistunov, arXiv:9910025)



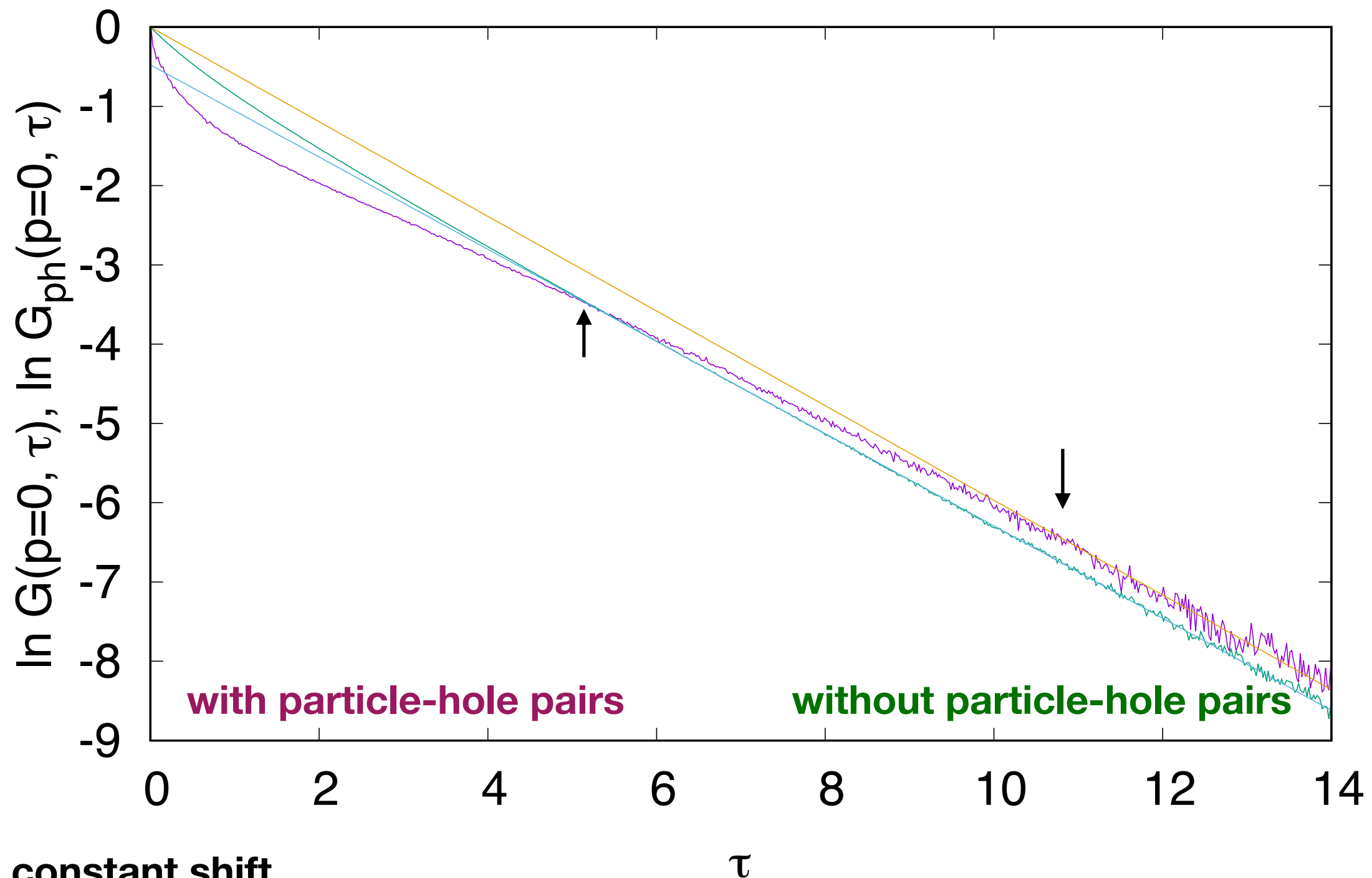
is compatible with the fast update trick; just make sure that you put a 0 for entries that link two external variables

Green function code at T=0

preliminary data

$$V_0 = 1, R_0 = 3$$

$$M = m = 0.5$$

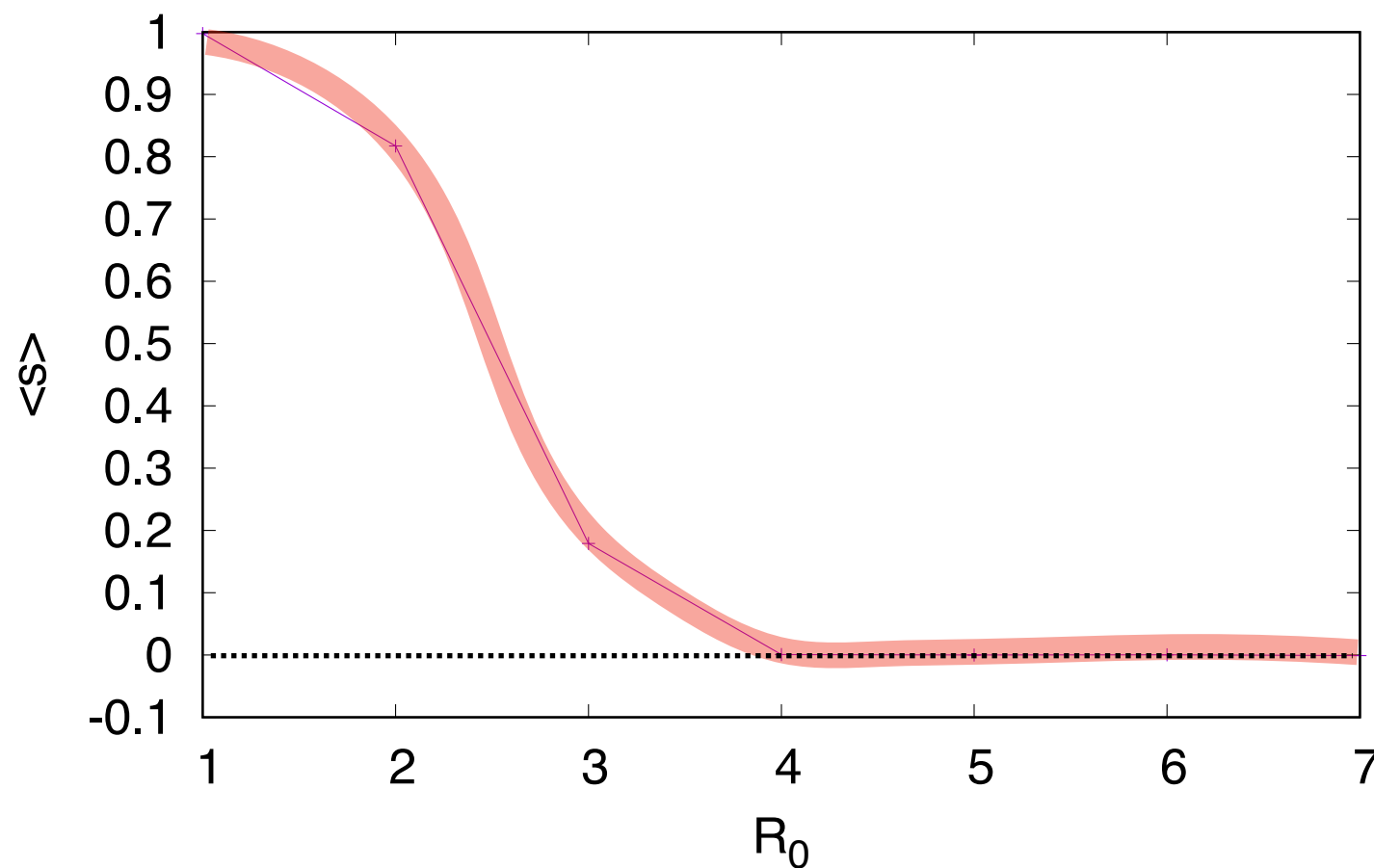


(up to constant shift
terms E_0 and dE)

Green function code at $T=0$

As the noise on the preliminary data suggests, the sign problem is considerably worse

$$V_0 = 1, \alpha = 2 \quad M = m = 0.5$$



expansion order in the number of particle-hole pairs is rather large: centered around 15 for $R_0 = 3$

alternative : flat histogram, reweighting

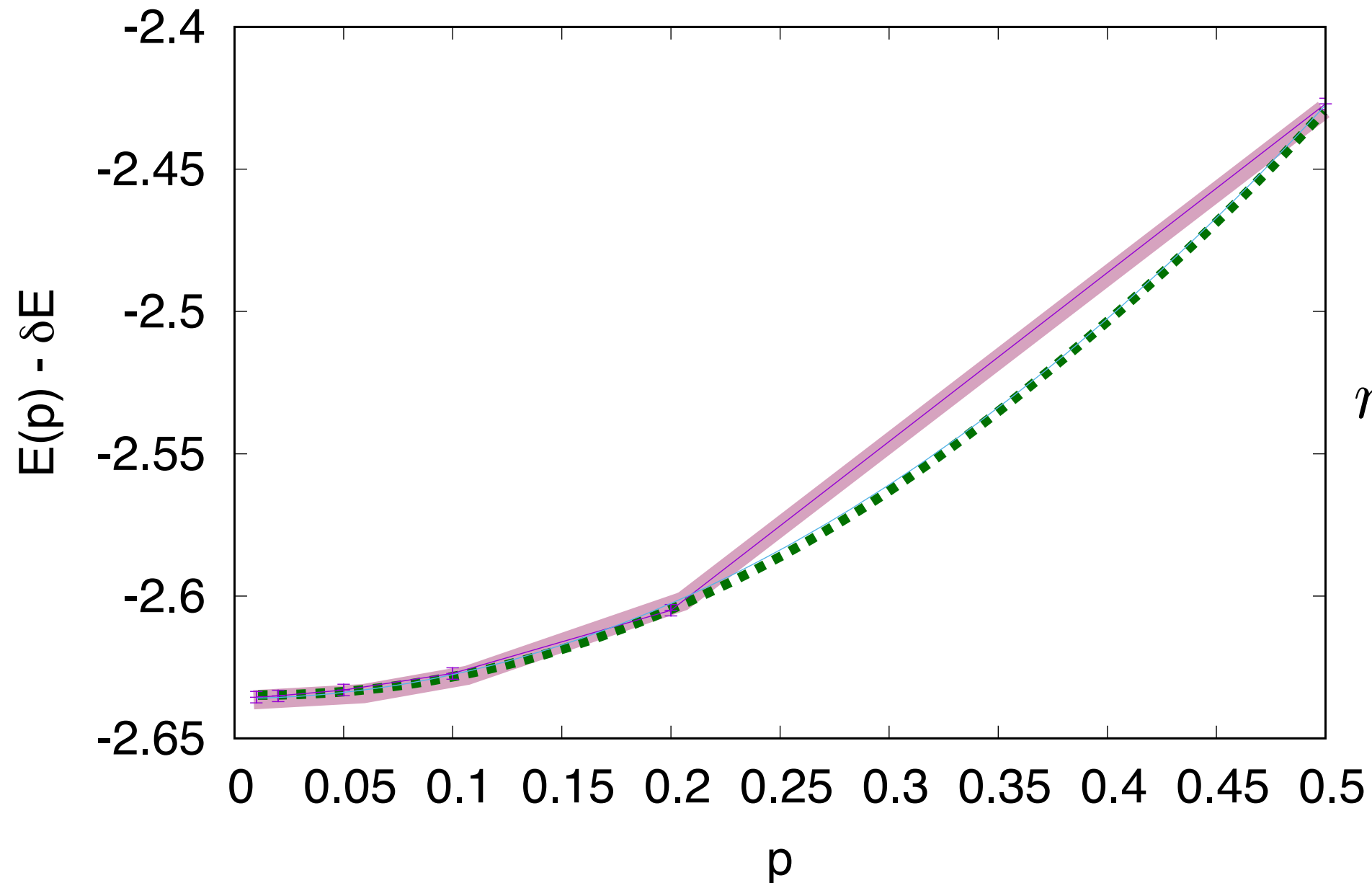
work in progress, currently unsolved



Green function code at T=0

preliminary data
22.7.2019

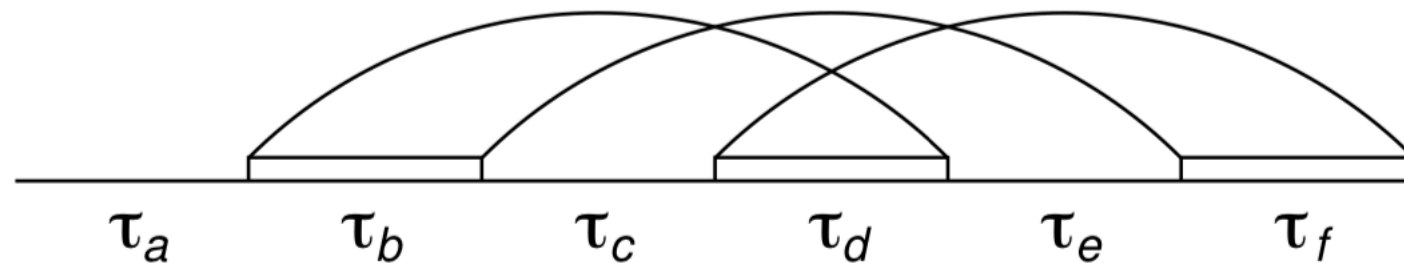
$$V_0 = 0.5, R_0 = 4, \alpha = 2 \quad M = m = 0.5$$



$$m^*/m \approx 1.19(5)$$

extension to Tmatrix code

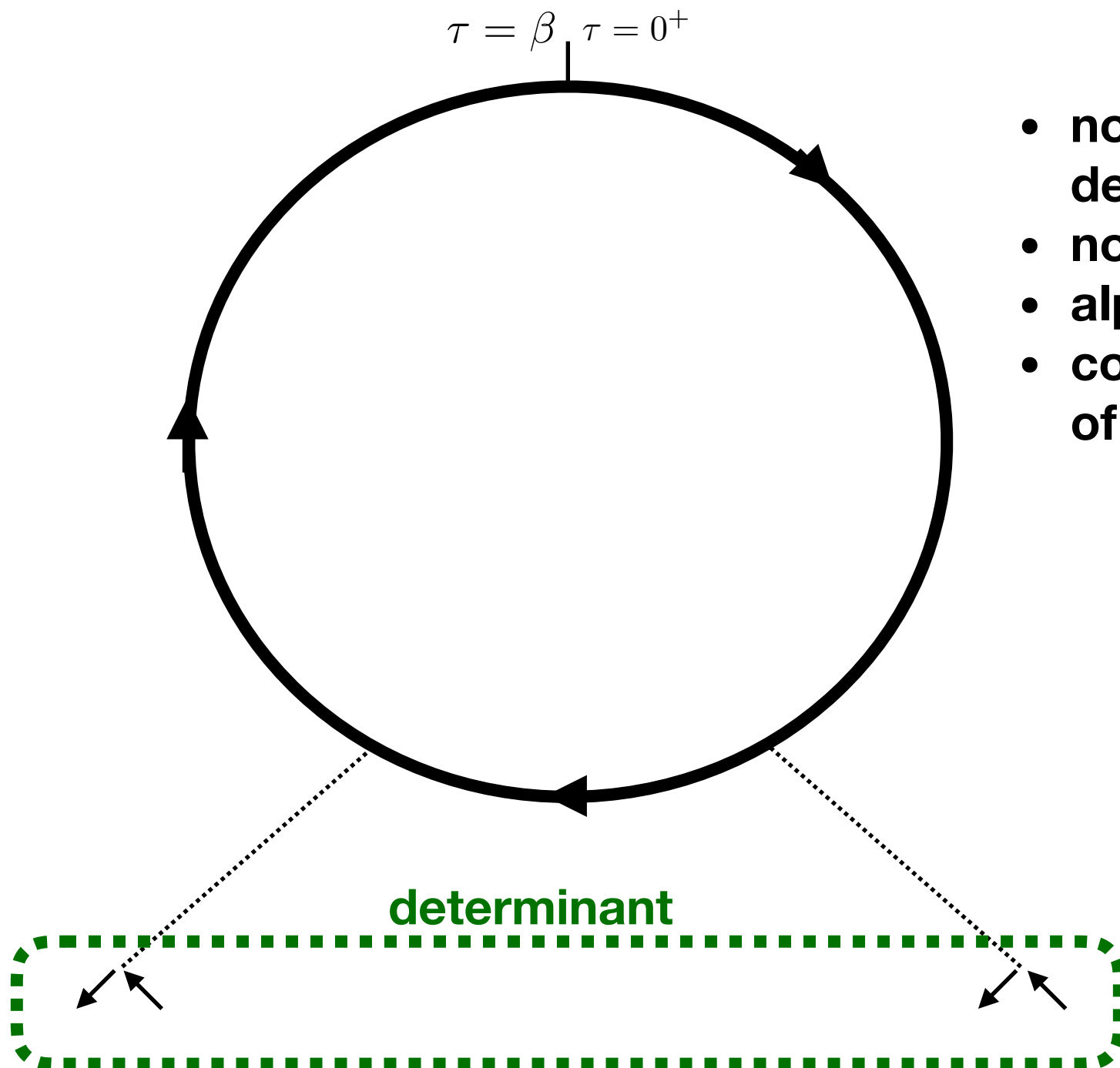
going back to the birth of diagMC : the resonant Fermi polaron problem



straightforward to extend the code to T-matrices

see previous talk by K. Van Houcke

partition function at finite temperature



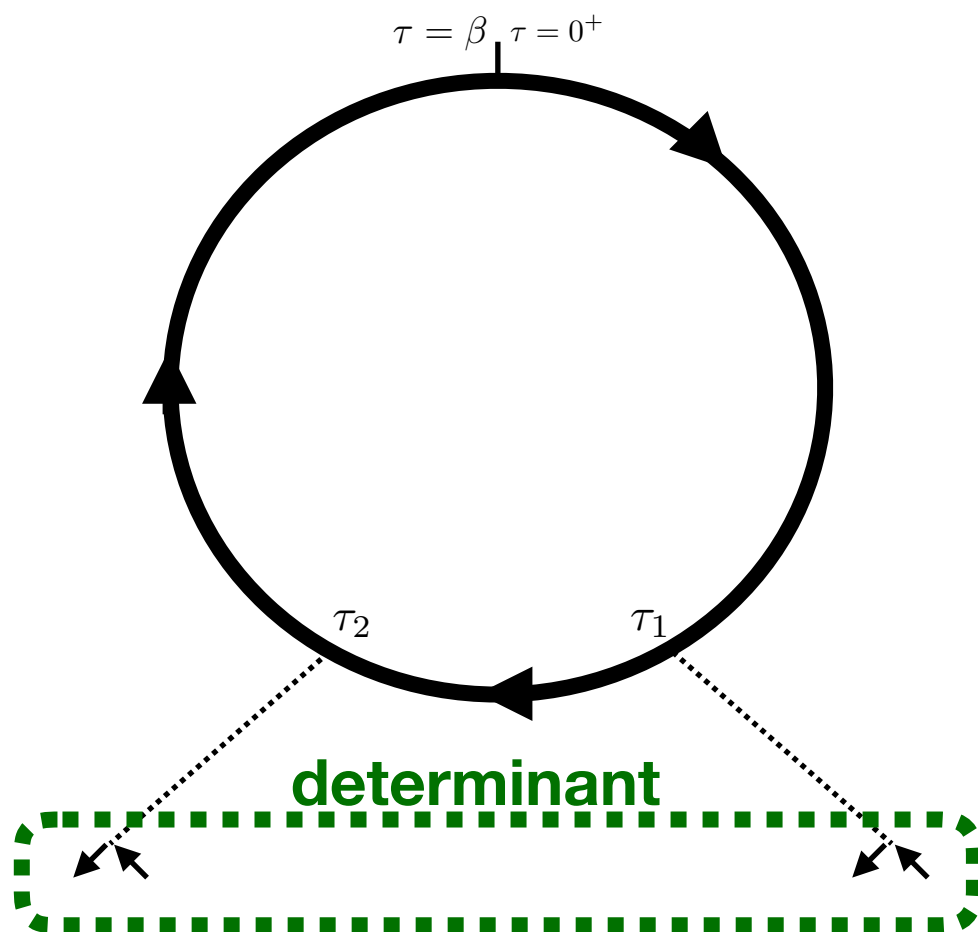
- normalization is not an issue ($1/Z$ in denominator)
- no energy shift trick
- alpha - trick still applicable
- computation of G_0 : interpolation of $dG = G(T) - G(T+0)$

partition function at finite T

estimators for the kinetic energy (impurity) :

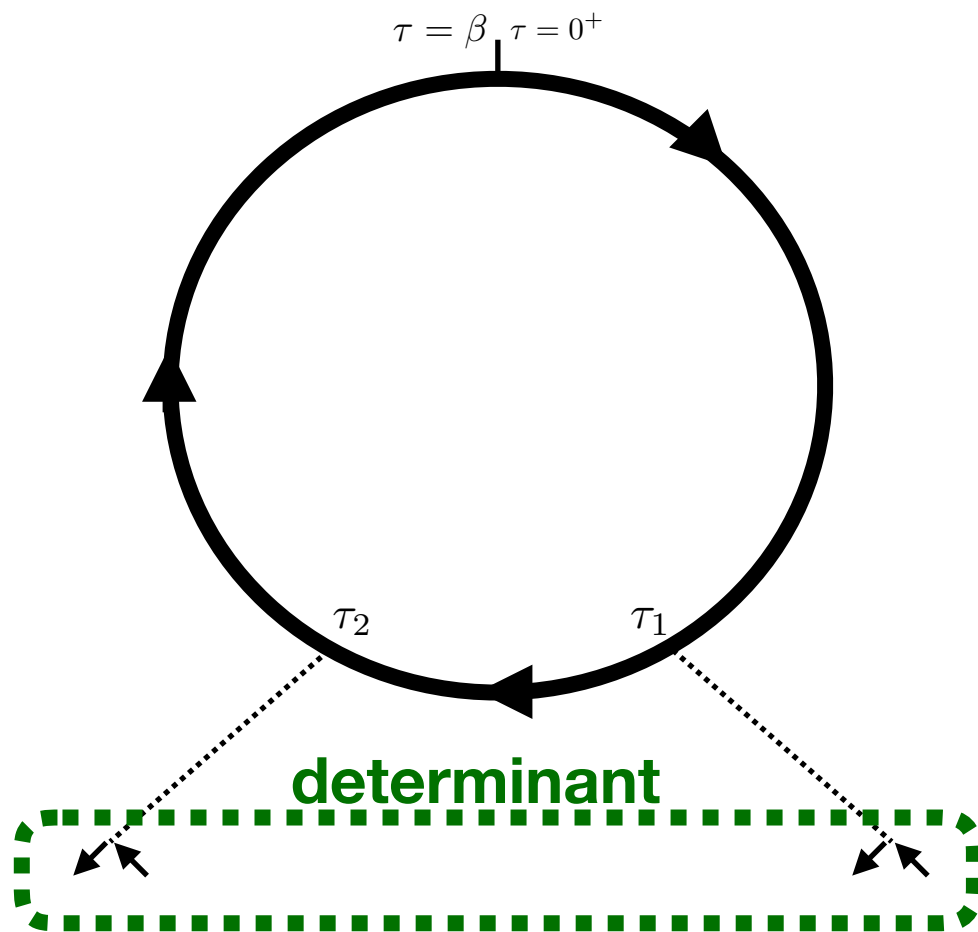
$$\delta\tau_j = \text{mod}(\tau_j - \tau_{j-1}, \beta)$$

$$C_{E_{\text{kin}}} = \frac{1}{\beta} \sum_{j=1}^n m \frac{(\mathbf{r}_j - \mathbf{r}_{j-1})^2}{2\delta\tau_j} - \frac{nd}{2\beta}$$



partition function at finite T

Estimator for the momentum-momentum correlation function in Matsubara space:



$$\delta\tau_j = \text{mod}(\tau_j - \tau_{j-1}, \beta)$$

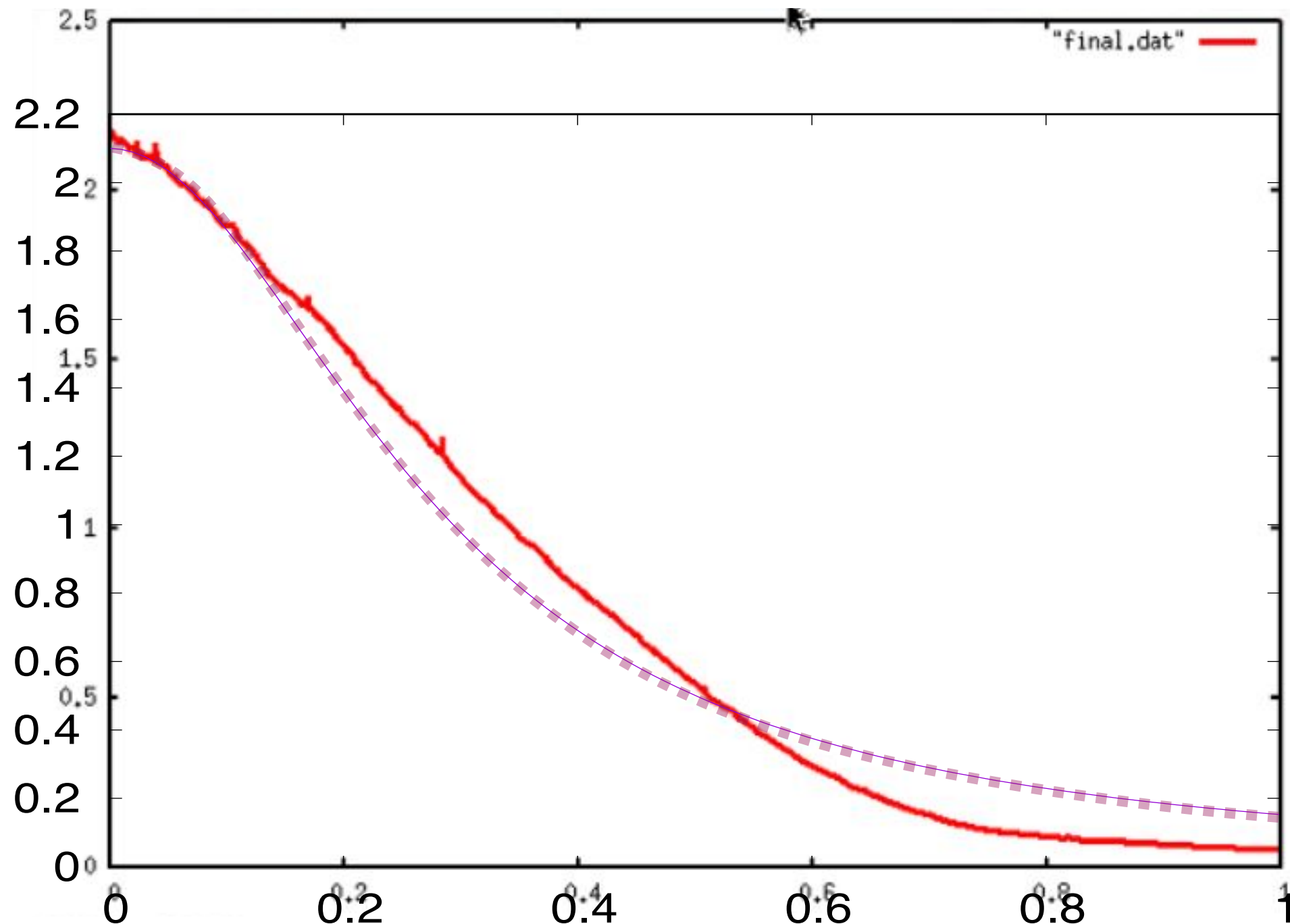
$$F_m(\tau_j, \tau_{j-1}) = \frac{e^{i\omega_m \tau_j} - e^{i\omega_m \tau_{j-1}}}{i\omega_m}$$

$$C_{\text{MC}}(m) = \frac{-1}{3\beta} \left| \sum_j \frac{M(\mathbf{r}_j - \mathbf{r}_{j-1})}{\delta\tau_j} F_m(\tau_j, \tau_{j-1}) \right|^2 + \frac{M}{\beta} \sum_j \frac{|F_m(\tau_j, \tau_{j-1})|^2}{\delta\tau_j}$$

Conductivity

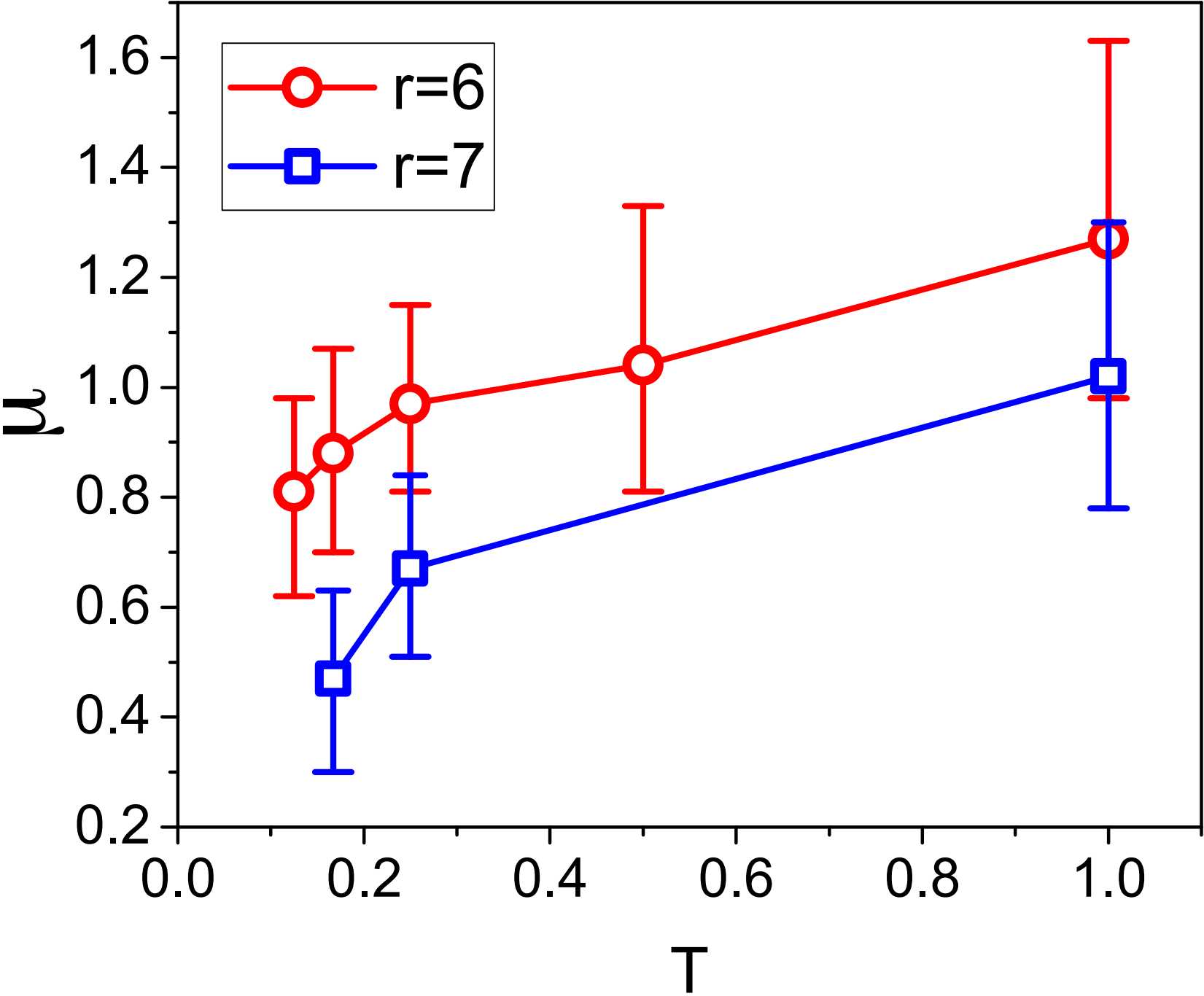
analytic continuation (SOCC -- Andrey Mishchenko)

$$M = m = 0.5 \quad V_0 = 0.5, R_0 = 4$$



preliminary data
22.7.2019

$M = m = 0.5 \quad V_0 = 0.5$



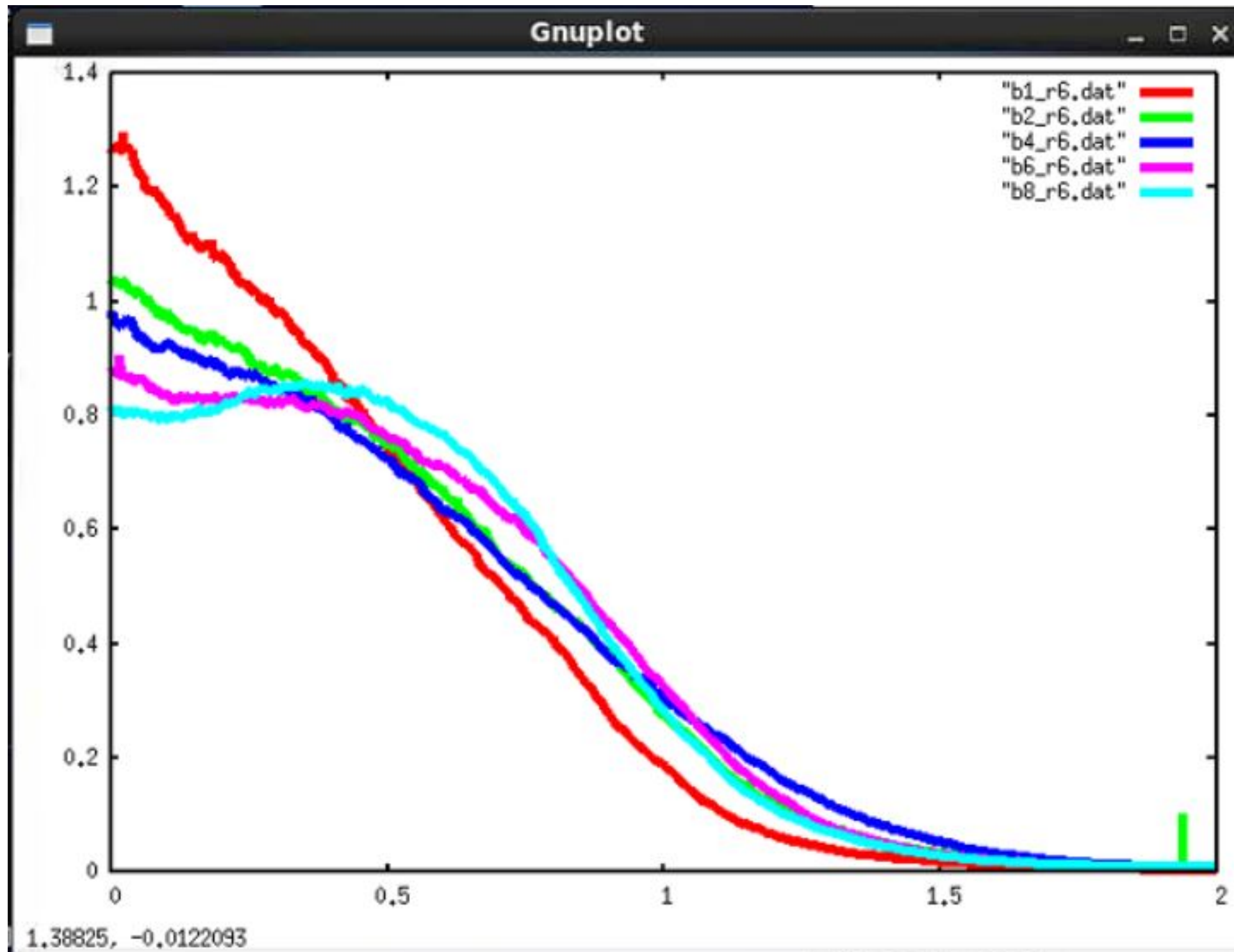
preliminary data

$$M = m = 0.5$$

$$V_0 = 0.5$$

$$R_0 = 6$$

22.7.2019



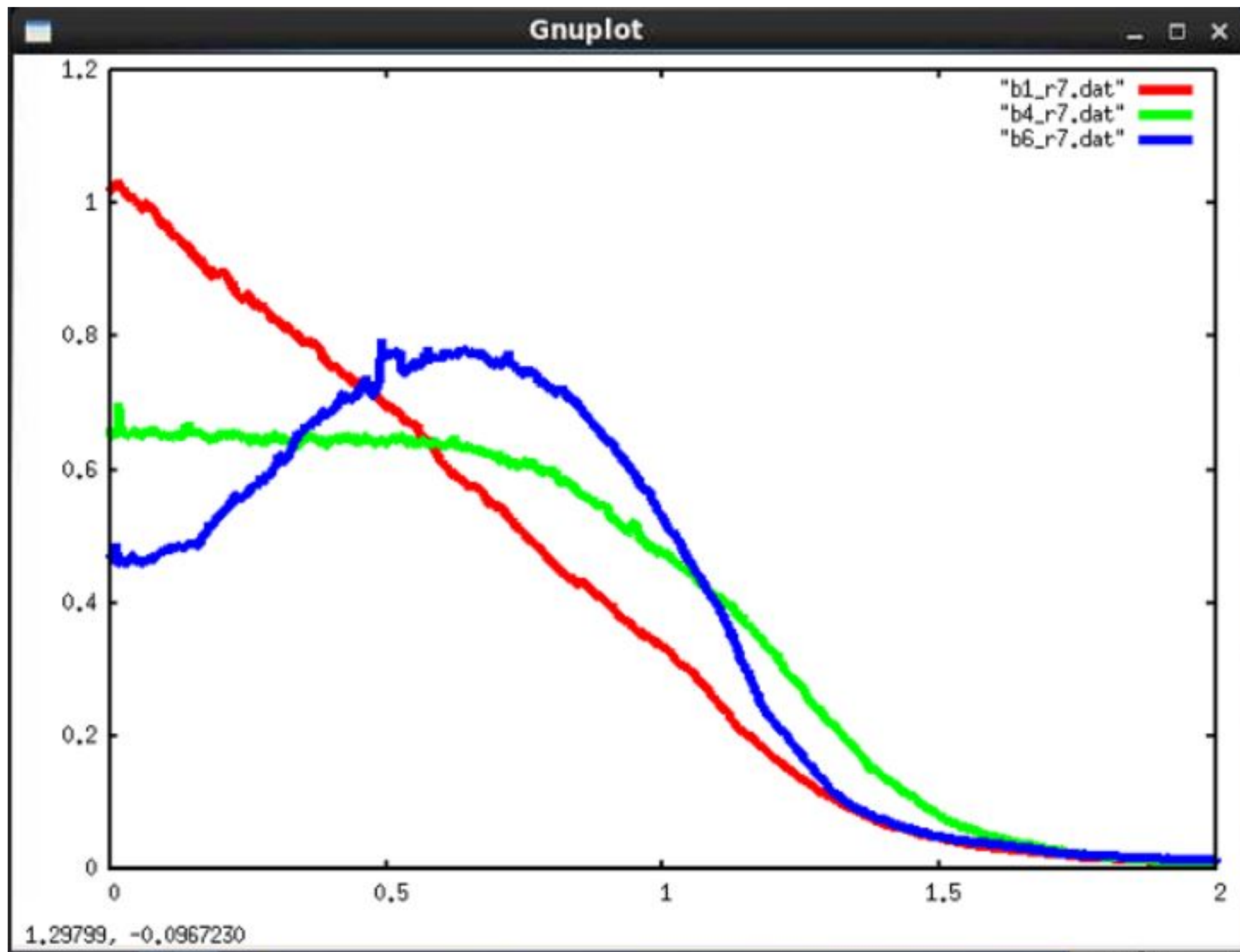
preliminary data

$$M = m = 0.5$$

$$V_0 = 0.5$$

$$R_0 = 7$$

22.7.2019



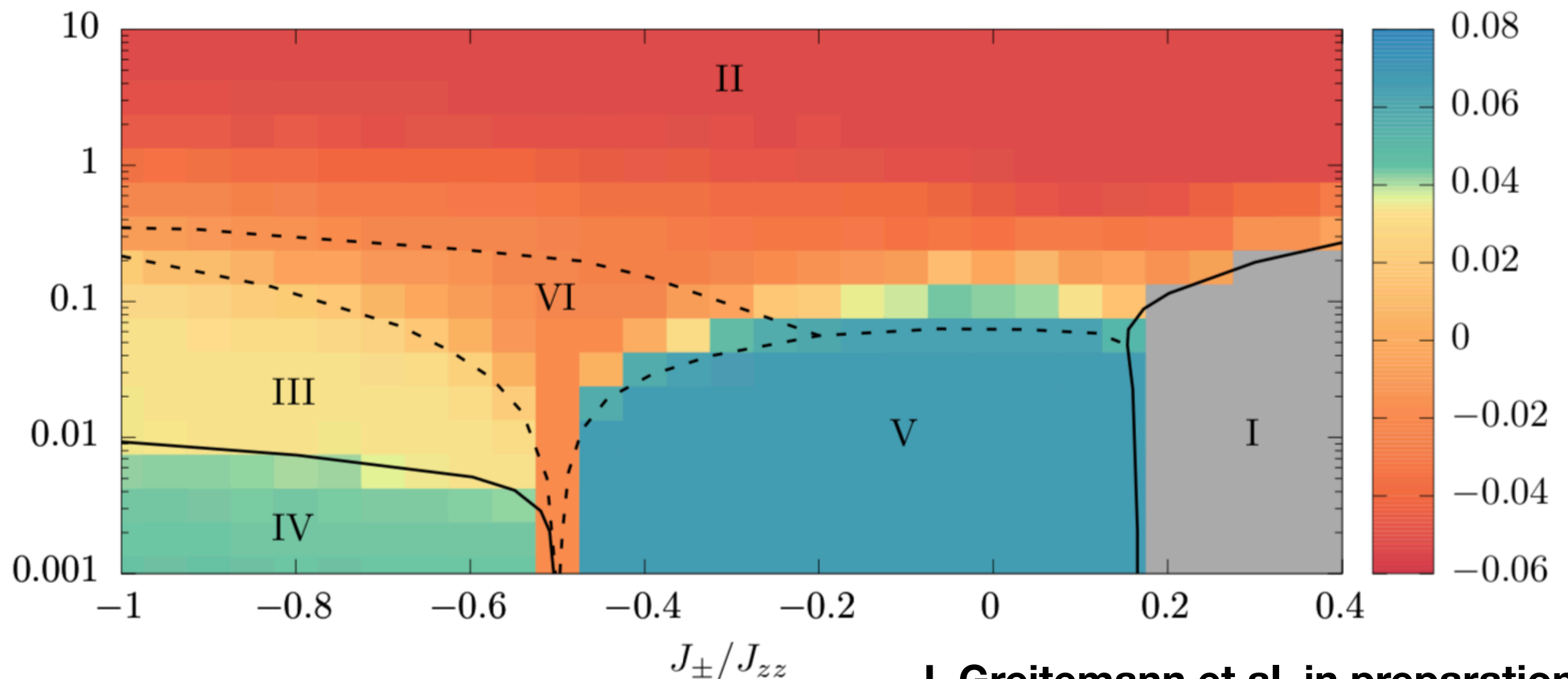
Conclusion

- let the game begin....
- why is the sign so good ... or is it still not good enough
- mobilities in the beyond quasiparticles regime?
- 2D materials : excitons, trions,...
- extension to Keldysh : equilibrium and non-equilibrium (convergence issues)
- extension to continuous space QFT ?-- convergence issues and CDet

Slide for Giuseppe

classical XXZ model on pyrochlore lattice

TK-SVM detection of broken symmetries ("hidden order") as well as learning of local constraints (--> spin liquids)



J. Greitemann et al, in preparation