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"Phase Transitions of a (Super) Quantum Mechanical Matrix Model with a Chemical Potential in terms of partial deconfinement" (arXiv:1707.02898)

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TIFR seminar 2020/1/2, 14:30-15:30

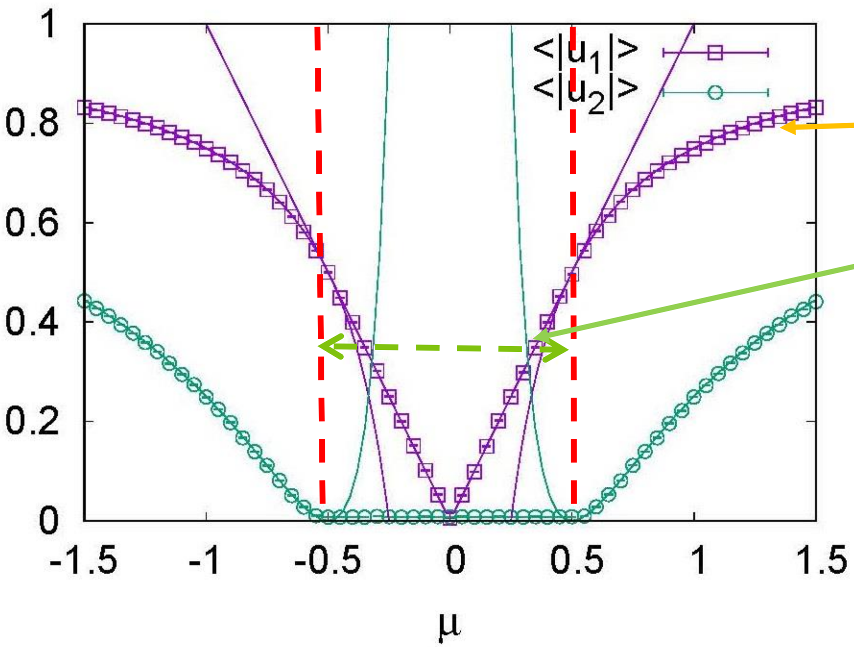
with Pallab Basu (Wits) and Prasant Samantray (IUCAA)

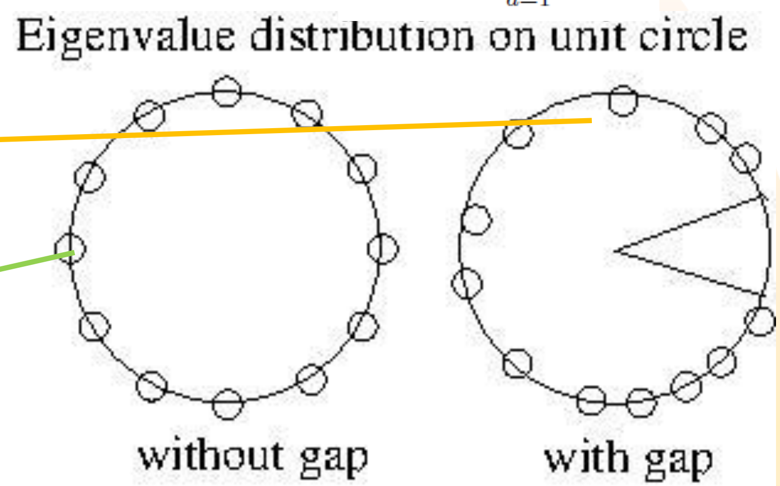
1. Introduction

$$Z_g = \int dU e^{-S_g}, \text{ where } S_g = N\mu(\mathrm{tr}U + \mathrm{tr}U^\dagger).$$

$$U = \mathcal{P}\exp\left(i\int_0^\beta dt A(t)\right).$$

Static diagonal gauge: $A(t) = \frac{1}{\beta}\mathrm{diag}(\alpha_1, \alpha_2, \cdots, \alpha_N),\ (|\alpha_k| < \pi)$ $\quad u_n = \frac{1}{N}\sum_{a=1}^{N} e^{in\alpha_a}.$





$$\langle |u_1| \rangle = \begin{cases} |\mu| & \left(|\mu| \leqq \frac{1}{2}\right) \\ 1 - \frac{1}{4|\mu|} & \left(|\mu| \geqq \frac{1}{2}\right) \end{cases}$$

$d^2\langle|u_1|\rangle/d\mu^2$ is discontinuous at $\mu=1/2$

Gross-Witten-Wadia (GWW) third-order phase transition

[D.J. Gross and E. Witten, Phys. Rev. D21 (1980) 446, S.R. Wadia, Phys. Lett. B93 (1980) 403]

1. Introduction

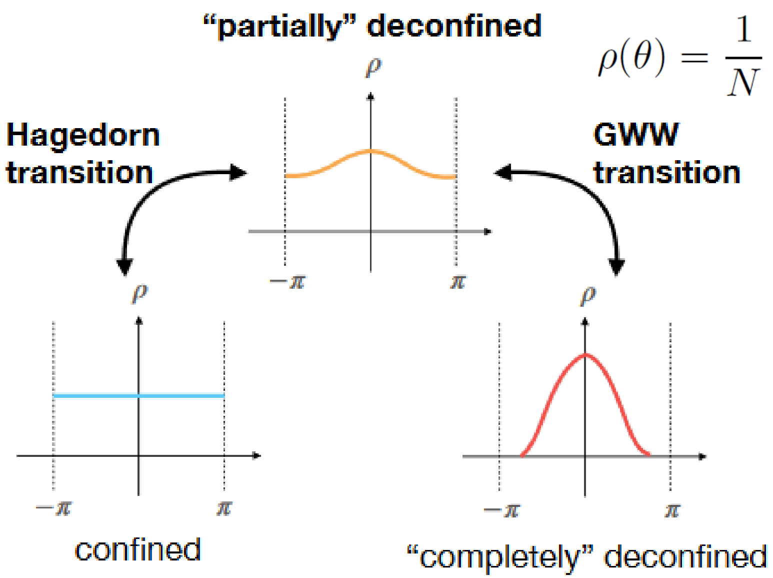
Partial deconfinement

[M. Hanada, G. Ishiki and H. Watanabe, arXiv:1812.05494, 1911.11465]

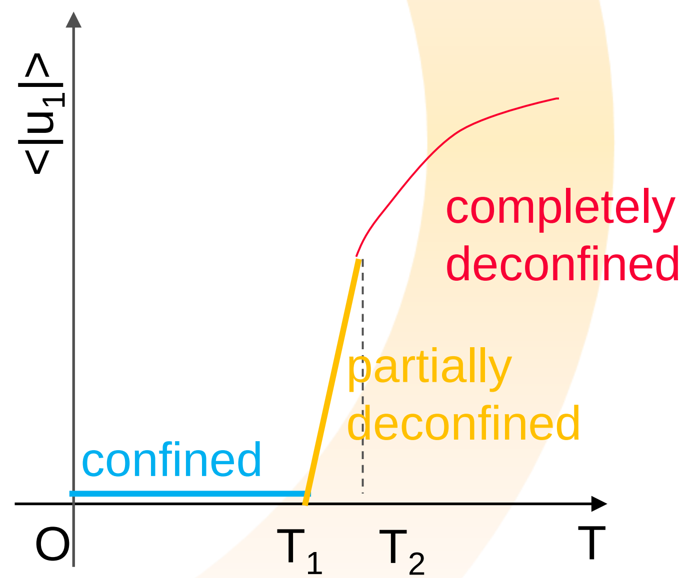
Mixture of M "α_j's " in the deconfinement phase and (N-M) "α_j's " in the confinement phase

$$\rho(\theta) = \frac{N-M}{N} \underbrace{\rho_{\text{confine}}(\theta)}_{=1/2\pi} + \frac{M}{N} \rho_{\text{deconfine}}(\theta)$$

$$\rho(\theta) = \frac{1}{N} \sum_{k=1}^{N} \langle \delta(\theta - \alpha_k) \rangle$$



[Quoted from arXiv:1911.11465]



2. BFSS model

Finite-temperature matrix quantum mechanics with a chemical potential

$S = S_b + S_f + S_g$, where (μ=1,2,….D, β=1/T)

$$S_{\mathrm{b}} = N\int_0^\beta \mathrm{tr}\left\{\frac{1}{2}\sum_{\mu=1}^{D}(D_t X_\mu(t))^2 - \frac{1}{4}\sum_{\mu,\nu=1}^{D}[X_\mu(t),X_\nu(t)]^2\right\}dt$$

$$D_t X_\mu(t) = \partial_t X_\mu(t) - i[A(t), X_\mu(t)]$$

$$S_{\mathrm{f}} = N\int_0^\beta \mathrm{tr}\left\{\sum_{\alpha=1}^{p}\bar{\psi}_\alpha(t)D_t\psi_\alpha(t) - \sum_{\mu=1}^{D}\sum_{\alpha,\eta=1}^{p}\bar{\psi}_\alpha(t)(\Gamma_\mu)_{\alpha\eta}[X_\mu(t),\psi_\eta(t)]\right\}dt$$

$$S_{\mathrm{g}} = N\mu(\mathrm{tr}U + \mathrm{tr}U^\dagger) \qquad U = \mathcal{P}\exp\left(i\int_0^\beta A(t)dt\right)$$

- Bosonic ($S=S_b+S_g$): D=2,3,4,5…
- Fermionic($S=S_b+S_f+S_g$): (D,p)=(3,2),(5,4),(9,16)

(For D=9, the fermion is Majorana-Weyl ($\bar{\Psi}\rightarrow\Psi$)
In the following, we focus on D=3.)

2. BFSS model

$A(t)$, $X_\mu(t)$, $\Psi(t)$: N × N Hermitian $\left(\omega = \frac{2\pi}{\beta}\right)$

Boundary conditions: $A(t+\beta) = A(t), \quad X_\mu(t+\beta) = X_\mu(t) \quad \psi(t+\beta) = -\psi(t)$

Static diagonal gauge:

$$A(t) = \frac{1}{\beta}\mathrm{diag}(\alpha_1, \alpha_2, \cdots, \alpha_N) \qquad -\pi \leqq \alpha_k < \pi$$

⇒ Add the gauge-fixing term $S_{\text{g.f.}} = -\sum_{k,l=1,k\neq l}^{N} \log\left|\sin\frac{\alpha_k - \alpha_l}{2}\right|$

Under this gauge $u_n = \frac{1}{N}\mathrm{tr}U^n = \frac{1}{N}\sum_{k=1}^{N} e^{in\alpha_k}$

Supersymmetry for $S=S_b+S_f$ ($\mu=0$), broken at $\mu\neq0$.

Non-lattice simulation for SUSY case

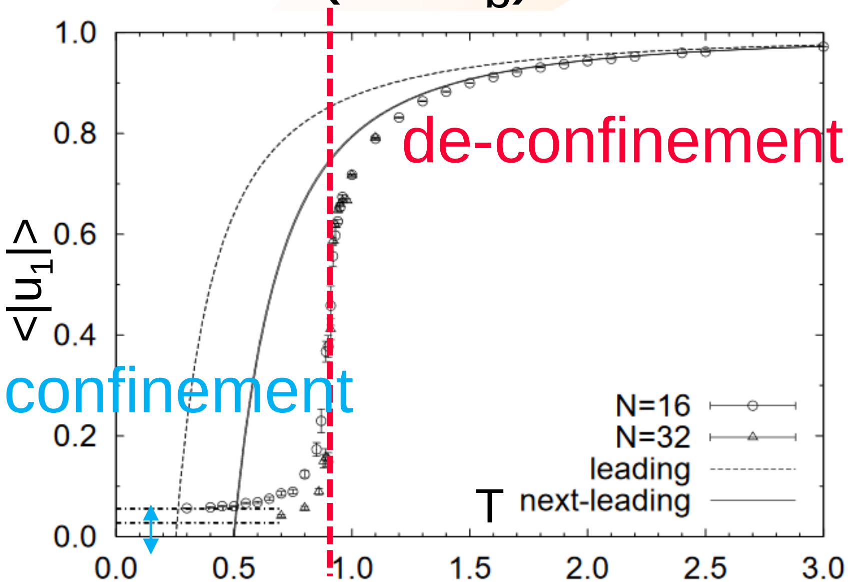
(lattice regularization for the bosonic case)

$$X^{kl}_\mu(t) = \sum_{n=-\Lambda}^{\Lambda} \tilde{X}^{kl}_{\mu,n} e^{i\omega nt}, \quad \psi^{kl}_\alpha(t) = \sum_{r=-\Lambda+\frac{1}{2}}^{\Lambda-\frac{1}{2}} \tilde{\psi}^{kl}_{\alpha,r} e^{i\omega rt}, \quad \bar{\psi}^{kl}_\alpha(t) = \sum_{r=-\Lambda+\frac{1}{2}}^{\Lambda-\frac{1}{2}} \tilde{\bar{\psi}}^{kl}_{\alpha,-r} e^{i\omega rt}.$$

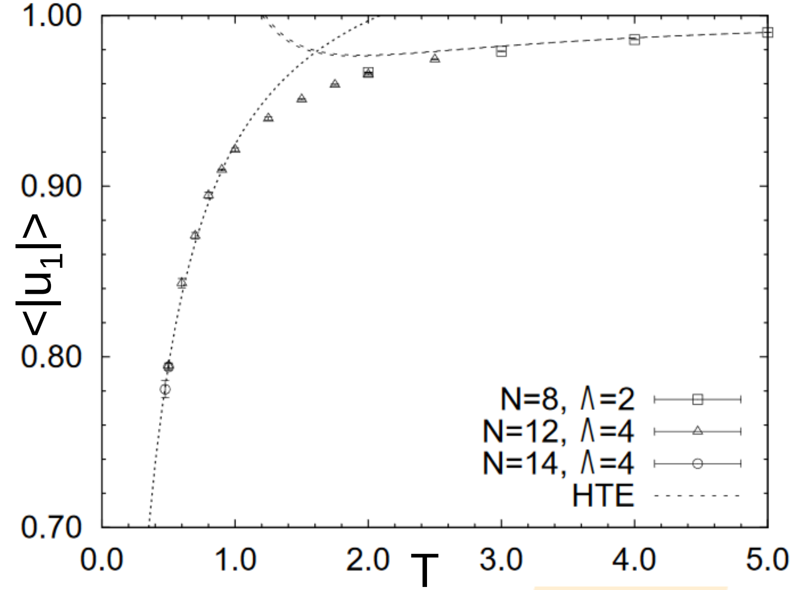
Previous works for μ=0 (without S_g)

Bosonic ($S=S_b$)

SUSY ($S=S_b+S_f$)



[Quoted for D=9 from N. Kawahara, J. Nishimura and S. Takeuchi, arXiv:0706.3517]



[Quoted for D=9 from K.N. Anagnostopoulos, M. Hanada, J. Nishimura and S. Takeuchi, arXiv:0707.4454]

Confinement-deconfinement phase transition at $T=T_{c0}$

$\langle|u_1|\rangle = a_0 \exp(-a_1/T)$

3. Result of the BFSS model

First-order phase transition at D≦20 for bosonic μ=0 ($S=S_b$)

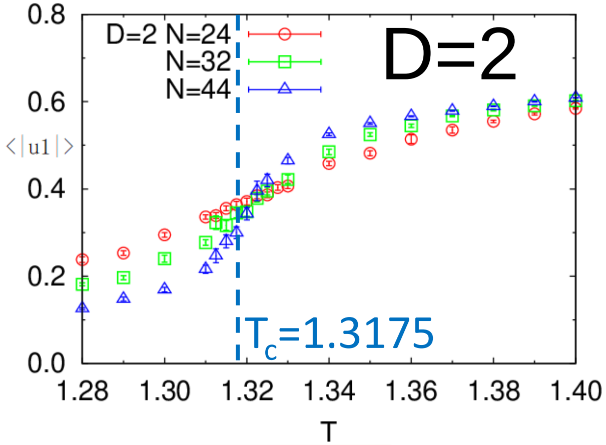
[T. Azuma, T. Morita and S. Takeuchi, arXiv:1403.7764]

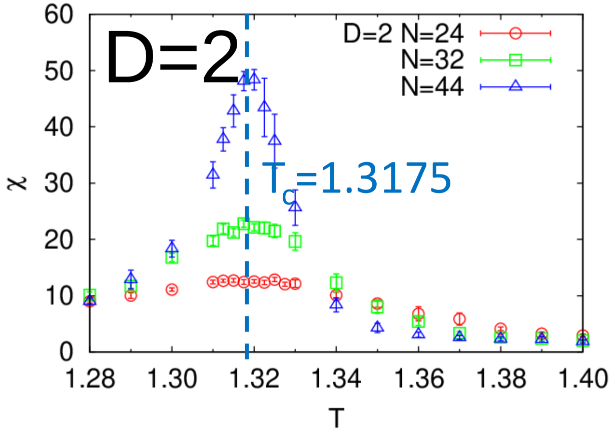
Susceptibility $\chi = N^2\{\langle|u_1|^2\rangle - (\langle|u_1|\rangle)^2\} = \gamma V^p + c\ (V = N^2)$

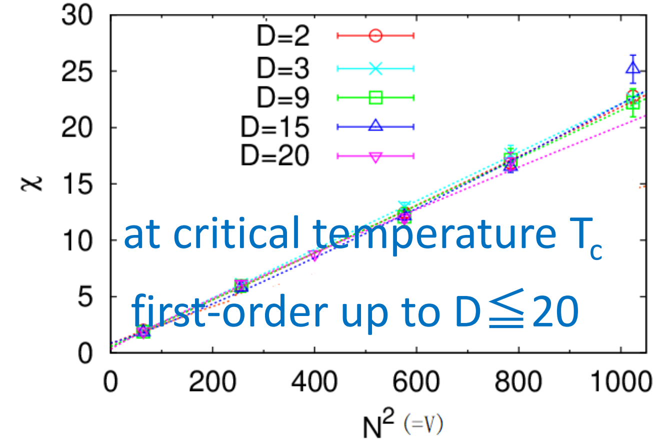
p=1 at critical temperature T_c

⇒ suggests first-order phase transition.

[M. Fukugita, H. Mino, M. Okawa and A. Ukawa, Phys. Rev. Lett.65, 816 (1990)]







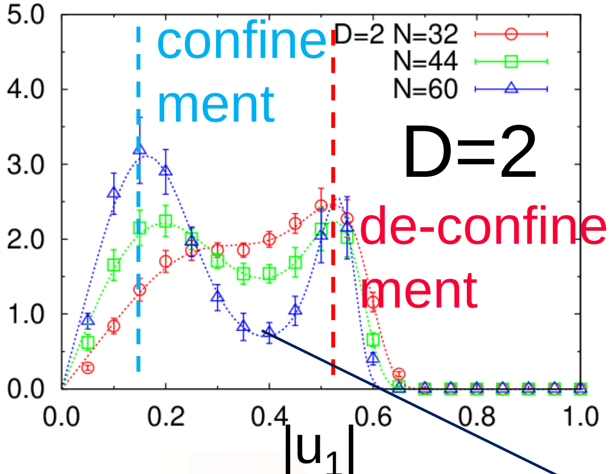
D	2	3	9	15	20
T_c	1.3175	1.0975	0.901	0.884	0.884
p	1.05(3)	1.00(1)	1.01(4)	1.12(14)	0.92(9)

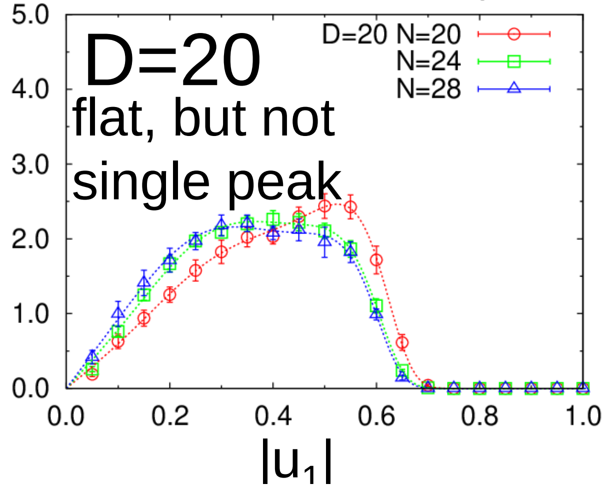
3. Result of the BFSS model

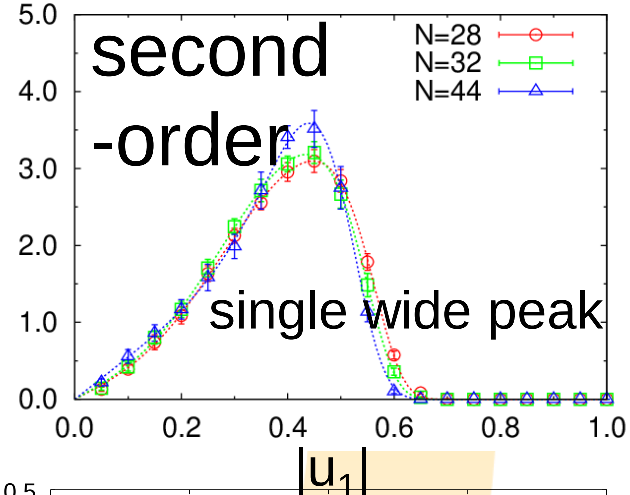
First-order phase transition at D≦20 for bosonic μ=0 ($S=S_b$)

[T. Azuma, T. Morita and S. Takeuchi, arXiv:1403.7764]

Density distribution of $|u_1|$ at $T=T_c$

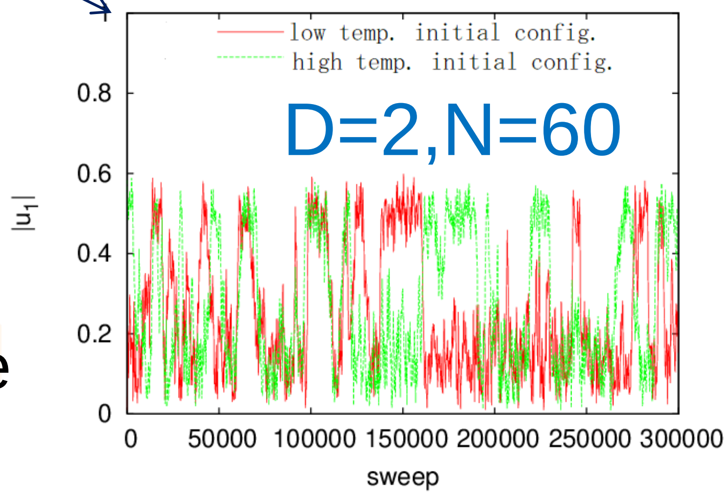


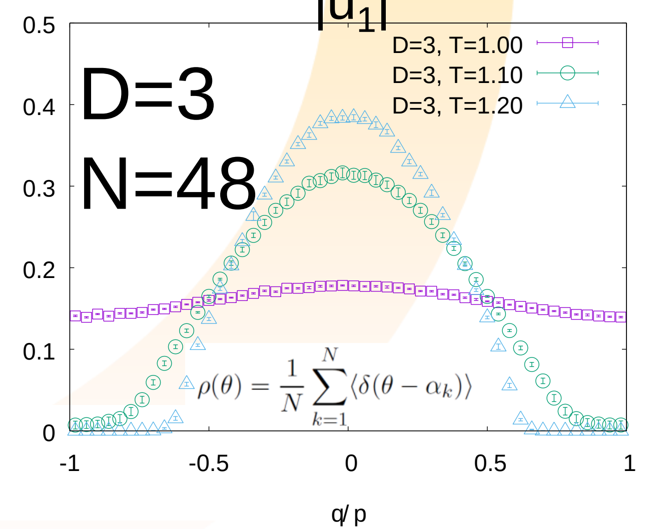




Two peaks⇒ existence of metastable states

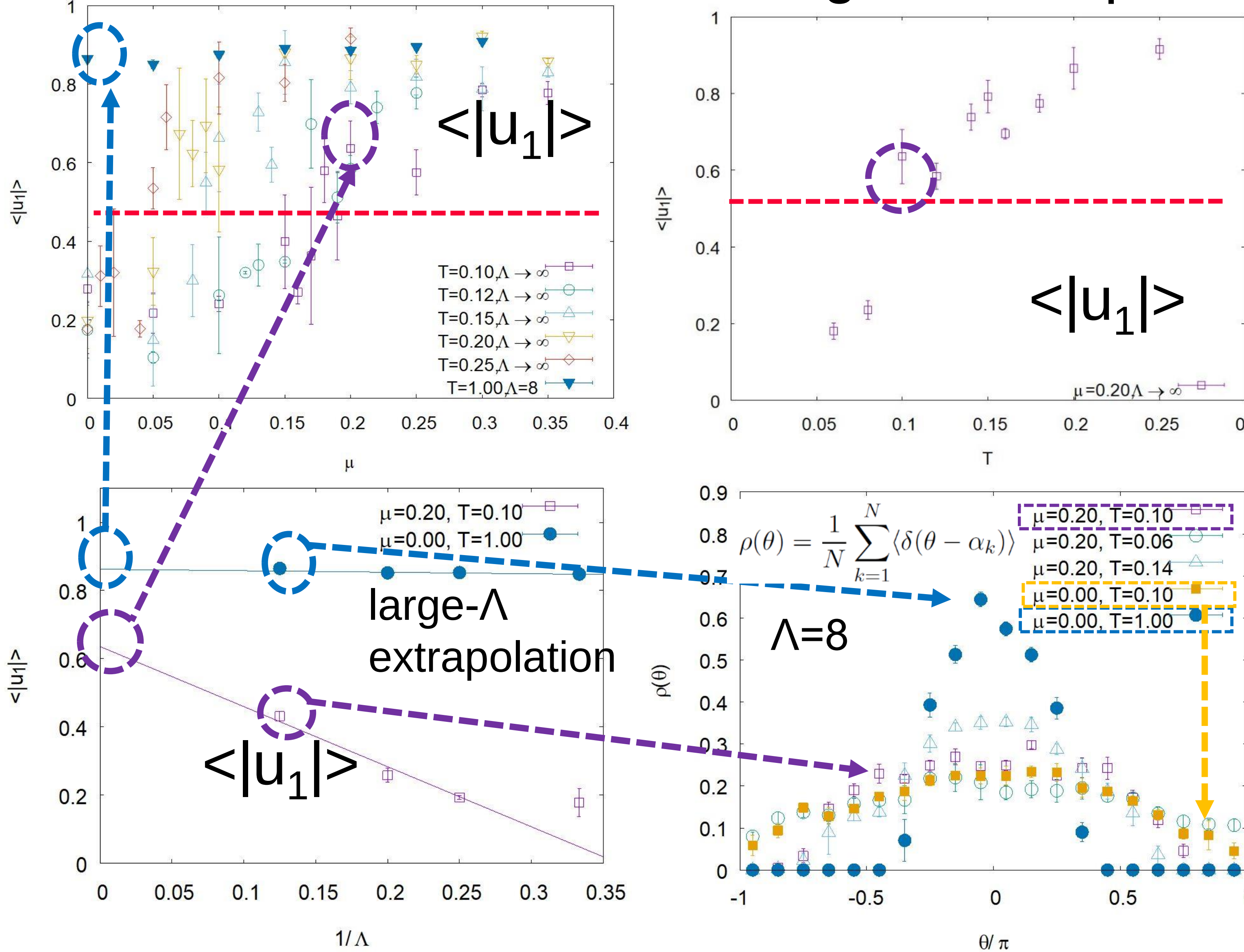
First-order phase transition.





3. Result of the BFSS model

Result of D=3, N=16, after large-Λ extrapolation:

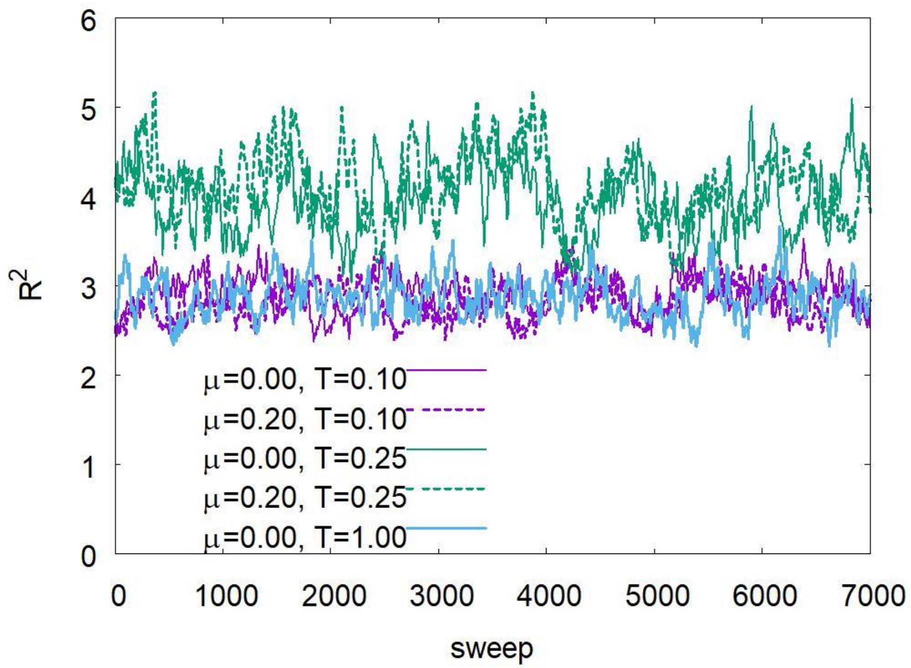


Gapped⇔Ungapped

Possible phase transitions at (μ_c, T_c) where $\langle|u_1|\rangle=0.5$, including μ=0.

3. Result of the BFSS model

Result of D=3, N=16, after large-Λ extrapolation:



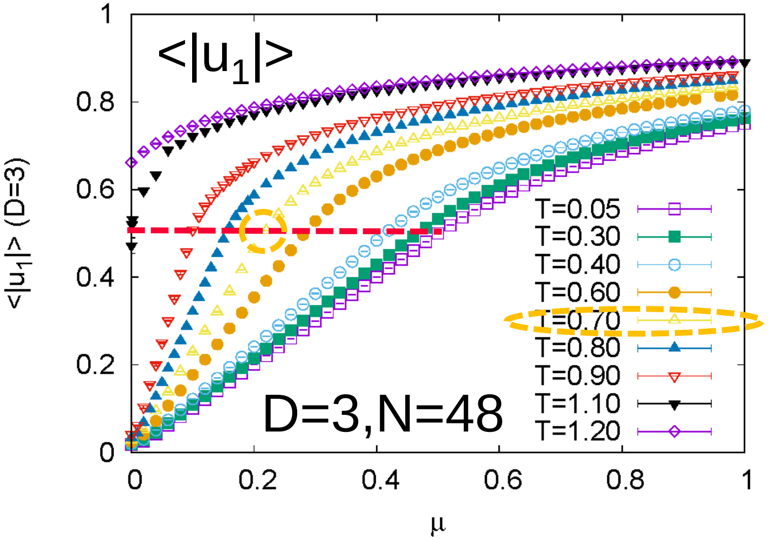
History of $R^2 = \frac{1}{N\beta}\int_0^\beta dt\, \mathrm{tr} X_\mu(t)^2$ at Λ=3

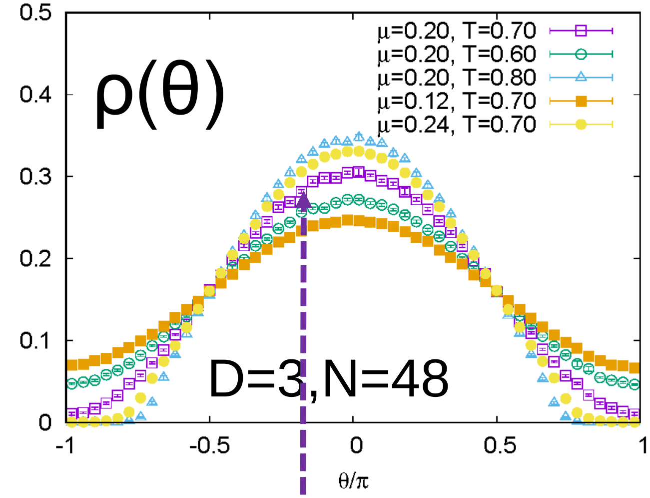
No instability in the typical (μ,T) region.

3. Result of the BFSS model

Bosonic model without fermion $S=S_b+S_g$

[T. Azuma, P. Basu and S.R. Wadia, arXiv:0710.5873]

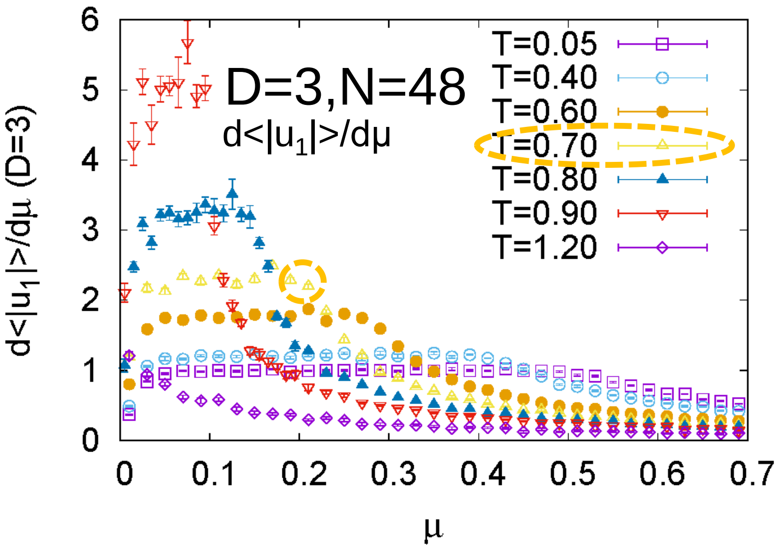


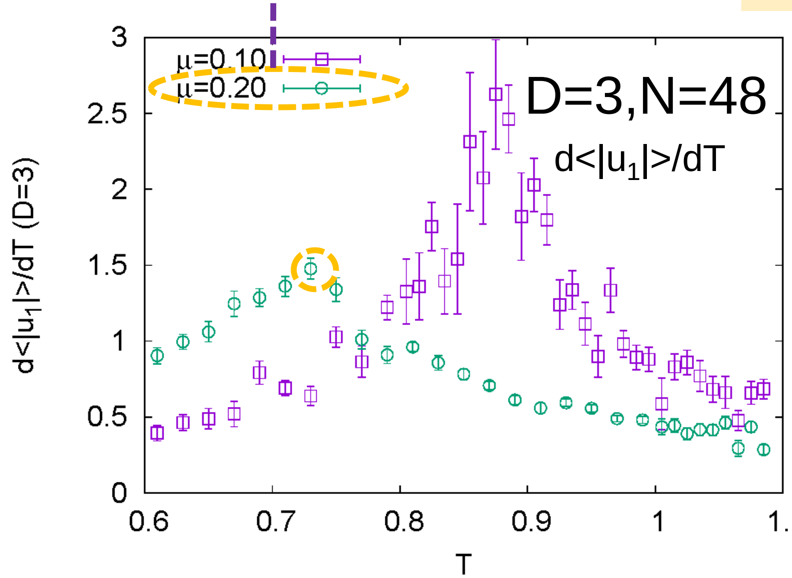


$(\mu_c, T_c) = (0.2, 0.7)$

$$\rho(\theta) = \frac{1}{N}\sum_{k=1}^{N}\langle\delta(\theta-\alpha_k)\rangle$$

develops a gap.





3. Result of the BFSS model

Bosonic model without fermion $S = S_b + S_g$

[T. Azuma, P. Basu and S.R. Wadia, arXiv:0710.5873]

Results of D=3 (D=2,6,9 cases are similar)

Critical points (μ_c, T_c) at $\langle |u_1| \rangle = 1/2$

At (μ_c, T_c), $d\langle |u_{1,2}| \rangle / d\mu$ and $d\langle |u_{1,2}| \rangle / dT$ are not smooth ($d^2\langle |u_{1,2}| \rangle / d\mu^2$ and $d^2\langle |u_{1,2}| \rangle / dT^2$ are discontinuous)

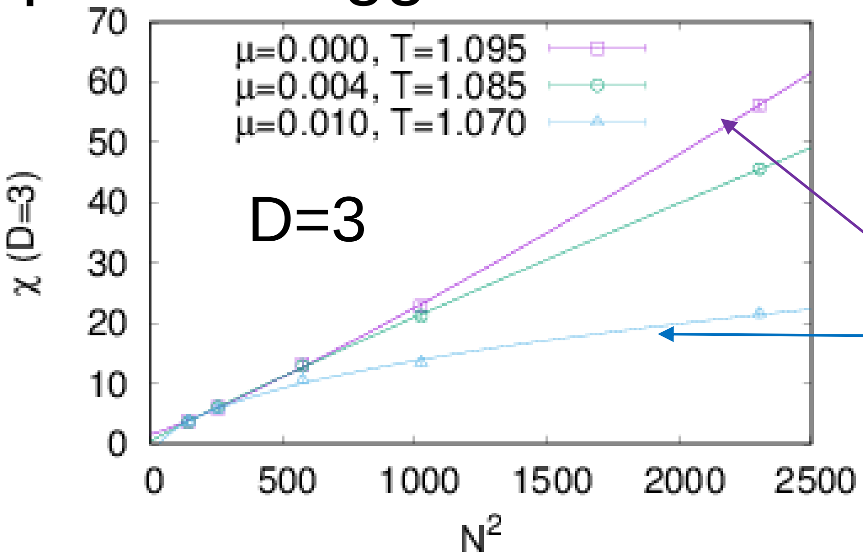
⇒ suggests third-order phase transition.

3. Result of the BFSS model

When μ=0, at the critical point T_{c0}=1.1,
there is a first-order phase transition at small D.
[T. Azuma, T. Morita and S. Takeuchi, arXiv:1403.7764]

$$\chi = N^2\{\langle|u_1|^2\rangle - (\langle|u_1|\rangle)^2\} = \gamma V^p + c \; (V = N^2)$$

p=1 ⇒ suggests first-order phase transition.



μ_c	0.00	0.004	0.01
T_c	1.095	1.085	1.070
p	1.14(4)	0.94(3)	0.42(10)

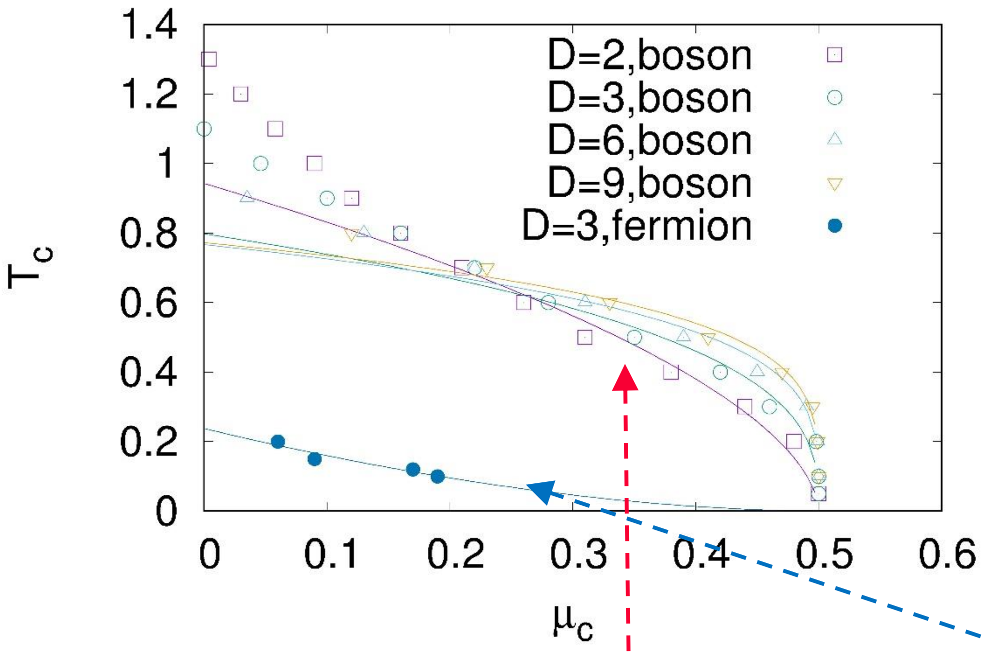
first-order

not first-order

3. Result of the BFSS model

Phase diagram for D=2,3,6,9 (boson) and D=3(fermion) .

Some phase transitions at (μ_c, T_c) where $\langle|u_1|\rangle=0.5$



D=3 SUSY, μ=0:

$\langle|u_1|\rangle = a_0 \exp(-a_1/T)$

$a_0=1.03(1)$, $a_1=0.19(1)$

$\Rightarrow \langle|u_1|\rangle=0.5$ at T=0.28.

[M. Hanada, S. Matsuura, J. Nishimura and D. Robles-Llana, arXiv:1012.2913]

μ=0: $\langle|u_1|\rangle= 0.5$ at $T_c=1.39\times 0.5^{2.30}\simeq 0.28$

Fitting of the critical point by $T_c=a(0.5-\mu_c)^b$.

D	2(boson)	3(boson)	6(boson)	9(boson)	3(fermion)
a	1.36(12)	1.01(15)	0.91(9)	0.90(8)	1.39(72)
b	0.55(6)	0.34(7)	0.25(4)	0.23(4)	2.30(59)

0<b<1: convex upward

b>1: convex downward

4. CLM of the (a,b)-model

Generalization of the Gross-Witten-Wadia (GWW) model

$$S_{\rm g} = N(a{\rm tr}U + b{\rm tr}U^{-1}) \quad V(n) = e^{i(\Delta t)A(t=n(\Delta t))}$$

$$U = \mathscr{P}\exp\left(i\int_0^\beta A(t)dt\right) = V(n_t)V(n_t-1)V(n_t-2)\cdots V(1)$$

U : N×N unitary matrix

a,b are not necessarily the same or real⇒sign problem

Solve this model by Complex Langevin Method (CLM).

Lattice regularization of the temporal direction:

t=0, (Δt), 2(Δt), …, (n_t-1)(Δt), n_t(Δt)=β

Invariant under the gauge transformation

$$A(t) \to g(t)A(t)g^{-1} + ig(t)\partial_t g^{-1}(t) \;\Rightarrow\; V(n) \to g(n+1)V(n)g^{-1}(n)$$

4. CLM of the (a,b)-model

SETSUDAI

Complex Langevin Method (CLM)

⇒Solve the complex version of the Langevin equation.

[Parisi, Phys.Lett. 131B (1983) 393, Klauder, Phys.Rev. A29 (1984) 2036]

The action S(x) is complex for real x.

x(t) is complexified as x⇒z=x+iy

(S(z) is holomorphic by analytic continuation)

$$\dot{z}_k^{(\eta)}(t) = \underbrace{-\frac{\partial S}{\partial z_k(t)}}_{\text{drift term}} + \eta_k(t)$$

- η_μ: real white noise obeying $\exp\left(-\frac{1}{4}\int \eta_k^2(t)dt\right)$

Probability distribution $P(x,y;t) = \left\langle \prod_k \delta(x_k - x_k^{(\eta)}(t))\delta(y_k - y_k^{(\eta)}(t)) \right\rangle_\eta$

$$\langle \cdots \rangle_\eta = \frac{\int \mathscr{D}\eta \cdots \exp\left(-\frac{1}{4}\int \eta_k^2(t)dt\right)}{\int \mathscr{D}\eta \exp\left(-\frac{1}{4}\int \eta_k^2(t)dt\right)} \qquad \langle \eta_k(t_1)\eta_l(t_2)\rangle_\eta = 2\delta_{kl}\delta(t_1 - t_2)$$

4. CLM of the (a,b)-model

P(x,y;t) satisfies $\frac{\partial P}{\partial t} = L^\top P$

When the boundary term vanishes,

$$\int (Lf(x,y))g(x,y)dxdy = \int f(x,y)(L^\top g(x,y))dxdy$$

$$L^\top = \frac{\partial}{\partial x_k}\left\{\mathrm{Re}\left(\frac{\partial S}{\partial z_k}\right) + \frac{\partial}{\partial x_k}\right\} + \frac{\partial}{\partial y_k}\left\{\mathrm{Im}\left(\frac{\partial S}{\partial z_k}\right)\right\}$$

$$L = \left\{-\mathrm{Re}\left(\frac{\partial S}{\partial z_k}\right) + \frac{\partial}{\partial x_k}\right\}\frac{\partial}{\partial x_k} + \left\{-\mathrm{Im}\left(\frac{\partial S}{\partial z_k}\right)\right\}\frac{\partial}{\partial y_k}$$

To justify the CLM, does the following actually hold?

$$\int \underbrace{\mathcal{O}(x+iy)}_{\text{holomorphic}} P(x,y;t)dxdy \stackrel{?}{=} \int \mathcal{O}(x)\rho(x;t)dx$$

$$\frac{\partial \rho(x;t)}{\partial t} = \overbrace{\frac{\partial}{\partial x_k}\left(\frac{\partial S}{\partial x_k} + \frac{\partial}{\partial x_k}\right)}^{=L_0^\top}\rho(x;t) \Rightarrow \rho_{\text{time-indep.}}(x) \propto e^{-S}$$

4. CLM of the (a,b)-model

SETSUDAI

At t=0, we choose $P(x,y;t=0)=\rho(x;t=0)\delta(y)$

Time evolution at t>0: we define an observable O(z;t)

$$\frac{\partial}{\partial t}\mathscr{O}(z;t)=\underbrace{\left(\frac{\partial}{\partial z_k}-\frac{\partial S}{\partial z_k}\right)\frac{\partial}{\partial z_k}}_{=\tilde{L}}\mathscr{O}(z;t) \quad [\text{initial condition } \mathscr{O}(z;t=0)=\mathscr{O}(z)]$$

Setting y=0, $$\frac{\partial}{\partial t}\mathscr{O}(x;t)=\overbrace{\left(\frac{\partial}{\partial x_k}-\frac{\partial S}{\partial x_k}\right)\frac{\partial}{\partial x_k}}^{=L_0}\mathscr{O}(x;t) \quad [\mathscr{O}(x;t=0)=\mathscr{O}(x)]$$

$$\int (L_0 f(x))g(x)dx=\int f(x)(L_0^\top g(x))dx$$

S(z) is holomorphic ⇒ O(z;t) remains holomorphic.

$$Lf(z) = \left\{-\mathrm{Re}\left(\frac{\partial S}{\partial z_k}\right)+\underbrace{\frac{\partial}{\partial x_k}}_{=\partial/\partial z_k}\right\}\underbrace{\frac{\partial f(z)}{\partial x_k}}_{=\partial f(z)/\partial z_k}+\left\{-\mathrm{Im}\left(\frac{\partial S}{\partial z_k}\right)\right\}\underbrace{\frac{\partial f(z)}{\partial y_k}}_{=i\partial f(z)/\partial z_k}$$

f(z)'s holomorphy

$$= \left\{-\left(\frac{\partial S}{\partial z_k}\right)+\frac{\partial}{\partial z_k}\right\}\frac{\partial f(z)}{\partial z_k}=\tilde{L}f(z)$$

Interpolating function $F(t,\tau) = \int dxdy \mathscr{O}(x+iy;\tau) P(x,y;t-\tau)$

$$\frac{\partial F(t,\tau)}{\partial \tau} = \int dxdy \left\{ \frac{\partial \mathscr{O}(x+iy;\tau)}{\partial \tau} P(x,y;t-\tau) + \mathscr{O}(x+iy;\tau) \frac{\partial P(x,y;t-\tau)}{\partial \tau} \right\}$$

$$= \int dxdy (\tilde{L}\mathscr{O}(x+iy;\tau)) P(x,y;t-\tau) - \int dxdy \mathscr{O}(x+iy;\tau) L^{\top} P(x,y;t-\tau)$$

integration by part

$$\overset{\nabla}{=} \int dxdy \overbrace{\{(\tilde{L}-L)\mathscr{O}(x+iy;\tau)\}}^{=0} P(x,y;t-\tau) = 0$$

Similarly, $\frac{\partial}{\partial \tau} \underbrace{\int dx \mathscr{O}(x;\tau)\rho(x;t-\tau)}_{:=G(t,\tau)} \overset{\nabla}{=} 0$ Integration by part w.r.t. real x only.

$$\underbrace{\int \overbrace{\mathscr{O}(x+iy;t=0)}^{=\mathscr{O}(z)} P(x,y;t) dxdy}_{=F(t,0)} \overset{\nabla}{=} \underbrace{\int \overbrace{\mathscr{O}(x+iy;t)}^{=e^{t\tilde{L}}\mathscr{O}(x+iy)} \overbrace{P(x,y;t=0)}^{=\rho(x;t=0)\delta(y)} dxdy}_{=F(t,t)} = \underbrace{\int \mathscr{O}(x;t)\rho(x;t=0)dx}_{=G(t,t)} \overset{\nabla}{=} \underbrace{\int \overbrace{\mathscr{O}(x;t=0)}^{=\mathscr{O}(x)} \rho(x;t) dx}_{=G(t,0)}$$

1. Is the integration by part w.r.t. (x,y) justified?
2. Is $e^{t\tilde{L}}\mathscr{O}(z)$ well-defined at large t? $\frac{\partial \mathscr{O}(z;t)}{\partial t} = \tilde{L}\mathscr{O}(z;t) \Rightarrow \mathscr{O}(z;t) = e^{t\tilde{L}}\mathscr{O}(z)$

4. CLM of the (a,b)-model

1. Integration by part is justified when P(x,y;t) damps rapidly
- in the imaginary direction
- around the singularity of the drift term

[G. Aarts, F.A. James, E. Seiler and O. Stamatescu, arXiv:1101.3270,
K. Nagata, J. Nishimura and S. Shimasaki, arXiv:1508.02377]

2. $$\int dxdy\{e^{\tau\tilde{L}}\mathcal{O}(z)\}P(x,y;t) = \sum_{n=0}^{+\infty}\frac{\tau^n}{n!}\int dxdy\{\tilde{L}^n\mathcal{O}(z)\}P(x,y;t)$$

This series should have a finite convergence radius
⇒Probability of the drift term should fall exponentially.

[K. Nagata, J. Nishimura and S. Shimasaki, arXiv:1606.07627]

Look at the drift term ⇒ Get the drift of CLM!!

4. CLM of the (a,b)-model

Discretized Complex Langevin equation for unitary matrices:
(henceforth, l is the fictitious Langevin time)

$$V(n,l+(\Delta l)) = \exp\left(i \sum_{a=1}^{\mathcal{G}} \lambda_a \left(-(\Delta l) \times \underbrace{v_a(V(n,l))}_{=\frac{d}{d\alpha} S[e^{i\alpha\lambda_a} V(n)]|_{\alpha=0}} + \sqrt{(\Delta l)}\eta_a(n,l) \right) \right) V(n,l) \text{ where}$$

$$\langle \eta_a(n,l)\eta_{a'}(n',l')\rangle = 2\delta_{aa'}\delta_{ll'}\delta_{nn'}, \quad \mathcal{G} = N^2-1 \ (\mathrm{SU}(N))$$

λ^a : basis of SU(N) Lie algebra $\mathrm{tr}(\lambda_a\lambda_b) = \delta_{ab}\ (a,b = 1,2,\cdots,\mathcal{G})$

$$\begin{aligned} v_a(V(n,l)) &= iNa\, \mathrm{tr}(\lambda_a V(n,l)V(n-1,l)\cdots V(1,l)V(n_t,l)\cdots V(n+1,l)) \\ &- iNb\, \mathrm{tr}(\lambda_a V^{-1}(n+1,l)\cdots V^{-1}(n_t,l)V^{-1}(1,l)\cdots V^{-1}(n,l)) \end{aligned}$$

Drift norm $u_A = \sqrt{\frac{1}{N^3 n_t}\sum_{n=1}^{n_t}\sum_{a=1}^{\mathcal{G}} |v_a(V(n,l))|^2}$

4. CLM of the (a,b)-model

SETSUDAI

Excursion problem: V(n) gets too far from unitary

Gauge cooling minimizes the unitary norm

$$\begin{aligned}\mathcal{N}_V &= \sum_{n=1}^{n_t} \mathrm{tr}[V(n)V^\dagger(n) + V^{-1}(n)(V^{-1}(n))^\dagger - 2E] \\ &= \sum_{n=1}^{n_t} \mathrm{tr}\underbrace{[(V^{-1}(n))^\dagger\{E - V(n)^\dagger V(n)\}]}_{=W}\underbrace{[\{E - V(n)V(n)^\dagger\}V^{-1}(n)]}_{=[(V^{-1}(n))^\dagger\{E-V(n)^\dagger V(n)\}]^\dagger = W^\dagger} .\end{aligned}$$

$N_V \geqq 0$ (the equality holds only if V is unitary).

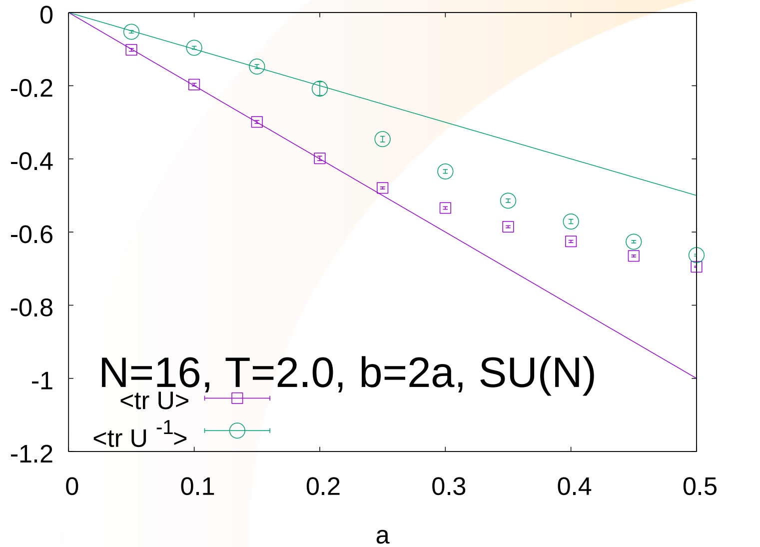
Gauge transformation after each step of discretized Langevin equation (γ_V: real parameter such that N_V is minimized)

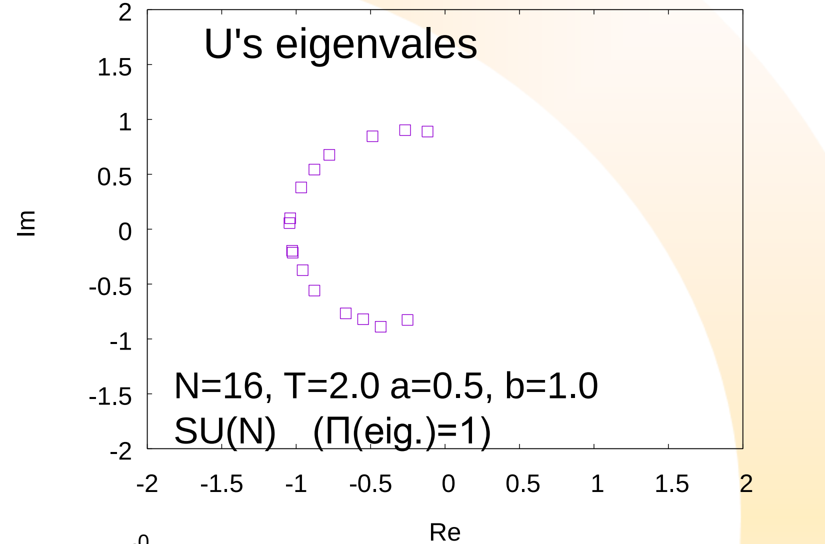
$$V(n) \to e^{\gamma_V H_V(n+1)} V(n) e^{-\gamma_V H_V(n)}$$

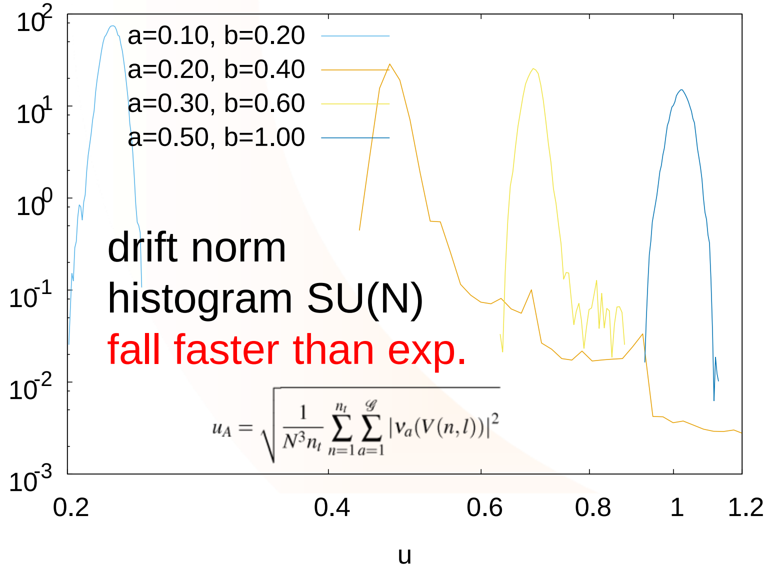
$$H_V(n) = \sum_{a=1}^{\mathscr{G}} \lambda^a \underbrace{\left\{ 2\mathrm{tr}\lambda^a\{-V(n-1)V^\dagger(n-1) + V^\dagger(n)V(n) + (V^{-1}(n-1))^\dagger V^{-1}(n-1) - V^{-1}(n)(V^{-1}(n))^\dagger\} \right\}}_{=G^a(n)} .$$

4. CLM of the (a,b)-model

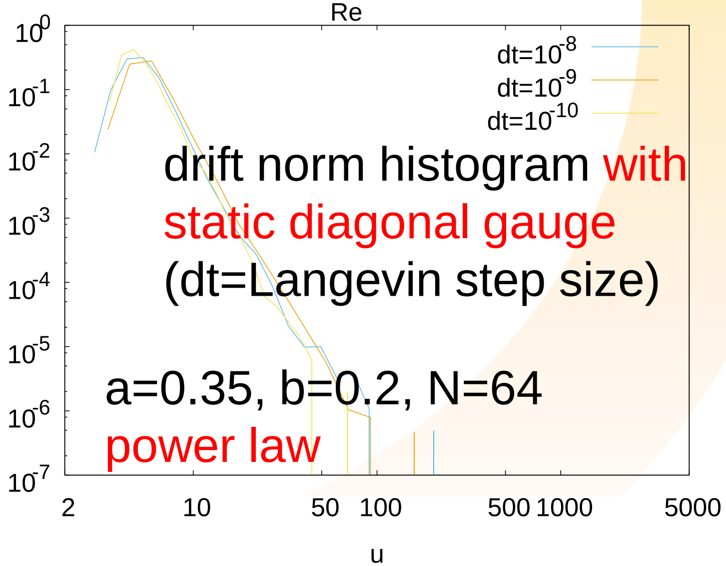
(a,b)-model $S_g = N(a\mathrm{tr}U + b\mathrm{tr}U^{-1})$ $U = \mathscr{P}\exp\left(i\int_0^\beta A(t)dt\right) = V(n_t)V(n_t-1)V(n_t-2)\cdots V(1)$







$$u_A = \sqrt{\frac{1}{N^3 n_t}\sum_{n=1}^{n_t}\sum_{a=1}^{\mathscr{G}}|v_a(V(n,l))|^2}$$



5. Summary

We have studied the matrix quantum mechanics with a chemical potential $S_{\rm g} = N\mu({\rm tr}U + {\rm tr}U^\dagger)$

・bosonic model ⇒ GWW-type third-order phase transition (except for very small μ)

・phase diagram of the bosonic/fermionic model

Future works:

Use of Complex Langevin Method for sign problem:

・Generalization to $S_{\rm g} = N(a{\rm tr}U + b{\rm tr}U^\dagger)$ [P. Basu, K. Jaswin and A. Joseph arXiv:1802.10381]

・supersymmetric quantum mechanics [A. Joseph and A. Kumar, arXiv:1908.04153]

backup: example of the sign problem

Example: Gaussian action [Suri Kagaku2023/1 p14]

$$S(x)=\frac{\beta}{2}(x-i)^2=\underbrace{\frac{\beta}{2}(x^2-1)}_{=\mathrm{Re}S(x)}+i\underbrace{(-\beta x)}_{=\mathrm{Im}S(x)}$$

large β⇒mimics large DOF(β∼V)

V.E.V. w.r.t. ReS

$$\langle x^2\rangle=\frac{\langle e^{-i\mathrm{Im}S(x)}x^2\rangle_{\mathrm{reweighting}}}{\langle e^{-i\mathrm{Im}S(x)}\rangle_{\mathrm{reweighting}}}=\frac{\int e^{-\mathrm{Re}S(x)}e^{-i\mathrm{Im}S(x)}x^2dx\div\int e^{-\mathrm{Re}S(x)}dx}{\int e^{-\mathrm{Re}S(x)}e^{-i\mathrm{Im}S(x)}dx\div\int e^{-\mathrm{Re}S(x)}dx}$$

$$=\Bigg(\underbrace{\int_{-\infty}^{+\infty}x^2e^{i\beta x}e^{\frac{-\beta}{2}(x^2-1)}dx}_{=(\beta^{-1}-1)\sqrt{\frac{2\pi}{\beta}}}\div\underbrace{\int_{-\infty}^{+\infty}e^{\frac{-\beta}{2}(x^2-1)}dx}_{=e^{\beta/2}\sqrt{\frac{2\pi}{\beta}}}\Bigg)\div\Bigg(\underbrace{\int_{-\infty}^{+\infty}e^{i\beta x}e^{\frac{-\beta}{2}(x^2-1)}dx}_{=\sqrt{\frac{2\pi}{\beta}}}\div\underbrace{\int_{-\infty}^{+\infty}e^{\frac{-\beta}{2}(x^2-1)}dx}_{=e^{\beta/2}\sqrt{\frac{2\pi}{\beta}}}\Bigg)$$

highly oscillatory at large β

$$=\frac{(\beta^{-1}-1)e^{-\beta/2}}{e^{-\beta/2}}\overset{\mathrm{numeric}}{\simeq}\frac{(\beta^{-1}-1)e^{-\beta/2}\pm\mathrm{O}(1/\sqrt{N_{\mathrm{config.}}})}{e^{-\beta/2}\pm\mathrm{O}(1/\sqrt{N_{\mathrm{config.}}})}.$$

(Standard deviation of $\bar{X}=\frac{1}{N_{\mathrm{config.}}}\sum_{k=1}^{N_{\mathrm{config.}}}X_k$) $\propto \mathrm{O}\left(\frac{1}{\sqrt{N_{\mathrm{config.}}}}\right)$

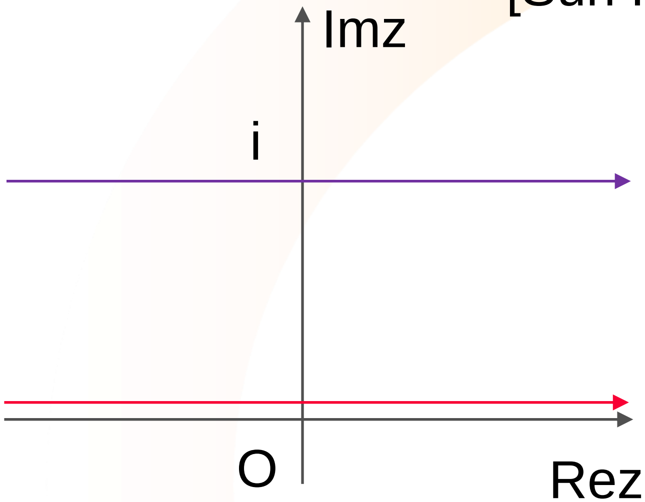
Necessary config.: $N_{\mathrm{config.}}\geq e^{\mathrm{O}(\beta)}$

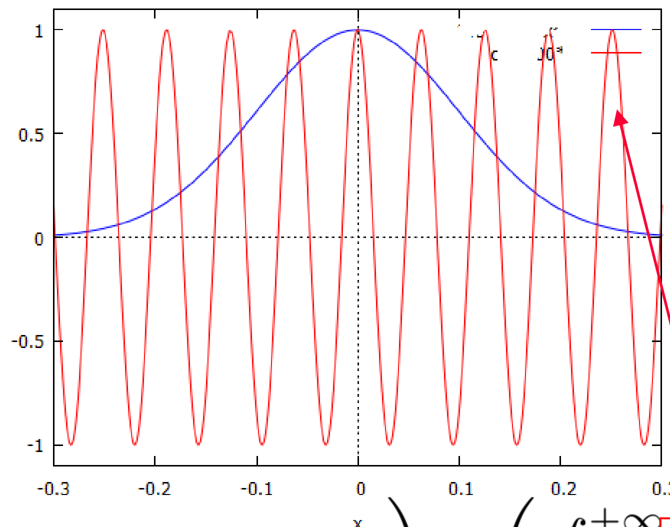
backup: example of the sign problem

Example: Gaussian action

$$S(x) = \frac{\beta}{2}(x-i)^2 = \underbrace{\frac{\beta}{2}(x^2-1)}_{=\mathrm{Re}S(x)} + i\underbrace{(-\beta x)}_{=\mathrm{Im}S(x)}$$

[Suri Kagaku2023/1 p14]





Contour→: $\langle x^2 \rangle = \left(\int_{-\infty}^{+\infty} x^2 e^{i\beta x} e^{\frac{-\beta}{2}(x^2-1)} dx\right) \div \left(\int_{-\infty}^{+\infty} e^{i\beta x} e^{\frac{-\beta}{2}(x^2-1)} dx\right)$

Contour→: x→z=u+i (-∞<u<+∞) No oscillation

$$\langle x^2 \rangle = \left(\int_{-\infty}^{+\infty} (u+i)^2 e^{\frac{-\beta}{2}u^2} du\right) \div \left(\int_{-\infty}^{+\infty} e^{\frac{-\beta}{2}u^2} du\right)$$

Cauchy's theorem⇒both are equivalent

backup: example of CLM

Example [G. Aarts, arXiv:1512.05145]

$$S(x) = \frac{1}{2}\underbrace{(a+ib)}_{=\sigma}x^2, \ (a,b \in \mathbf{R}, \ a>0)$$

S(x) is complex for real x.
Complexify to z=x+iy.

$$S(z) = \frac{1}{2}\sigma z^2 = \frac{1}{2}(a+ib)\overbrace{(x+iy)^2}^{=z^2} = \frac{a(x^2-y^2)}{2} + ibxy, \quad \frac{\partial S}{\partial z} = \sigma z = (a+ib)(x+iy)$$

Complex Langevin equation for this action

$$\dot{x}(t) = -\mathrm{Re}\left(\frac{\partial S}{\partial z}\right) + \eta(t) = (-ax+by) + \eta(t) \quad \dot{y}(t) = -\mathrm{Im}\left(\frac{\partial S}{\partial z}\right) = (-ay-bx)$$

The real white noise satisfies

$$\langle \eta(t_1)\eta(t_2)\rangle = 2\delta(t_1-t_2) \qquad \langle\cdots\rangle = \frac{\int \mathscr{D}\eta \cdots \exp\left(-\frac{1}{4}\int \eta^2(t)dt\right)}{\int \mathscr{D}\eta \exp\left(-\frac{1}{4}\int \eta^2(t)dt\right)}$$

backup: example of CLM

Solution of the Langevin equation

$$x(t) = e^{-at} \underbrace{[x(0)\cos bt + y(0)\sin bt]}_{=A(t)} + \int_0^t \eta(s) e^{-a(t-s)} \cos[b(t-s)]ds$$

$$y(t) = e^{-at}[y(0)\cos bt - x(0)\sin bt] - \int_0^t \eta(s) e^{-a(t-s)} \sin[b(t-s)]ds$$

$$\begin{aligned}\langle x^2 \rangle &= \lim_{t\to+\infty} \langle x^2(t) \rangle = \lim_{t\to+\infty} \Big\{ \underbrace{e^{-2at}A(t)^2}_{\to 0} + 2e^{-at}A(t) \int_0^t \underbrace{\langle \eta(s) \rangle}_{=0} e^{-a(t-s)} \cos[b(t-s)]ds \\ &\quad + \int_0^t \int_0^t \underbrace{\langle \eta(s)\eta(s') \rangle}_{=2\delta(s-s')} e^{-a(2t-s-s')} \cos[b(t-s)]\cos[b(t-s')]dsds' \Big\} \\ &= \lim_{t\to+\infty} \left\{ 2\int_0^t e^{-2a(t-s)} \cos^2[b(t-s)] \right\} ds = \frac{2a^2+b^2}{2a(a^2+b^2)}\end{aligned}$$

Similarly, $\langle y^2 \rangle = \dfrac{b^2}{2a(a^2+b^2)}, \quad \langle xy \rangle = \dfrac{-b}{2(a^2+b^2)}$

This replicates $\langle z^2 \rangle = \langle x^2 \rangle - \langle y^2 \rangle + 2i\langle xy \rangle = \dfrac{a-ib}{a^2+b^2} = \dfrac{1}{\sigma}$

backup: example of CLM

Fokker-Planck equation

$$\frac{\partial P}{\partial t} = L^\top P \quad \text{where} \quad L^\top = \frac{\partial}{\partial x}\left\{\underbrace{\mathrm{Re}\left(\frac{\partial S}{\partial z}\right)}_{=ax-by} + \frac{\partial}{\partial x}\right\} + \frac{\partial}{\partial y}\left\{\underbrace{\mathrm{Im}\left(\frac{\partial S}{\partial z}\right)}_{=ay+bx}\right\}$$

Ansatz for its static solution:

$$P(x,y) = N\exp\left(-\alpha x^2 - \beta y^2 - 2\gamma xy\right) = N\exp\left(-\beta\left(y+\frac{\gamma x}{\beta}\right)^2 - \overbrace{\left(\alpha - \frac{\gamma^2}{\beta}\right)}^{=a(a^2+b^2)/(2a^2+b^2)} x^2\right)$$

$$0 = \partial_t P = L^\top P = [\underbrace{(2a-2\alpha)}_{=0\to a=\alpha} + x^2\underbrace{(4\alpha^2 - 2a\alpha - 2b\gamma)}_{=0\to\gamma=a^2/b} + y^2\underbrace{(4\gamma^2 + 2b\gamma - 2a\beta)}_{=0\to\beta=a(1+2a^2/b^2)} + xy\underbrace{(4(2\alpha-a)\gamma + 2b(\alpha-\beta))}_{=0}]P$$

Using $\frac{\int_{-\infty}^{+\infty} t^2 e^{-At^2}dt}{\int_{-\infty}^{+\infty} e^{-At^2}dt} = \frac{1}{2A} \quad (A>0)$ we have

$$\langle x^2\rangle = \frac{\iint x^2 P(x,y)dxdy}{\iint P(x,y)dxdy} = \frac{1}{2} \div \frac{a(a^2+b^2)}{2a^2+b^2} = \frac{2a^2+b^2}{2a(a^2+b^2)}$$

backup: RHMC

Simulation via Rational Hybrid Monte Carlo (RHMC) algorithm. [Chap 6,7 of B.Ydri, arXiv:1506.02567, for a review]

We exploit the rational approximation

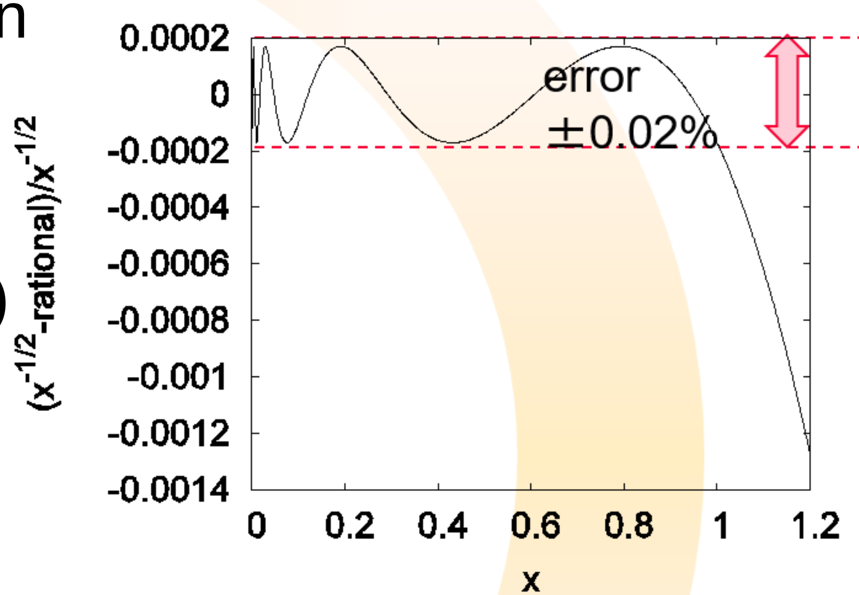
$$x^{-1/2} \simeq a_0 + \sum_{k=1}^{Q} \frac{a_k}{x+b_k}$$

after a proper rescaling.

(typically Q=15⇒valid at $10^{-12}c<x<c$)

a_k, b_k come from Remez algorithm.

[M. A. Clark and A. D. Kennedy, https://github.com/mikeaclark/AlgRemez]



$$S_0 = S_{\rm b} + S_{\rm g} - \log|\det \mathscr{M}|$$

$$|\det \mathscr{M}| = (\det \mathscr{D})^{1/2} \simeq \int dF dF^* \exp\left(-F^* \mathscr{D}^{-1/2} F\right) \simeq \int dF dF^* e^{-S_{\rm PF}}$$

$$S_{\rm PF} = a_0 F^* F + \sum_{k=1}^{Q} a_k F^* (\mathscr{D} + b_k)^{-1} F, \quad (\text{where } \mathscr{D} = \mathscr{M}^\dagger \mathscr{M})$$

F: *bosonic* N_0-dim vector (called *pseudofermion*)

backup: RHMC

Hot spot (most time-consuming part) of RHMC:
⇒Solving $(\mathscr{D}+b_k)\chi_k = F \quad (k=1,2,\cdots,Q)$
by conjugate gradient (CG) method.

Multiplication $\mathscr{M}\chi_k$ ⇒
$\mathscr{M}$ is a very sparse matrix. No need to build $\mathscr{M}$ explicitly.
⇒CPU cost is $O(N^3)$ per CG iteration
The required CG iteration time depends on T.
(while direct calculation of $\mathscr{M}^{-1}$ costs $O(N^6)$.)

Multimass CG solver: [B. Jegerlehner, hep-lat/9612014]
Solve $(\mathscr{D}+b_k)\chi_k = F$ only for the smallest b_k
⇒The rest can be obtained as a byproduct,
which saves O(Q) CPU cost.

backup: RHMC

Conjugate Gradient (CG) method

Iterative algorithm to solve the linear equation Ax=b

(A: symmetric, positive-definite n × n matrix)

Initial config. $\mathbf{x}_0 = 0 \quad \mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0 \quad \mathbf{p}_0 = \mathbf{r}_0$

(for brevity, no preconditioning on x_0 here)

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k \quad \mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k A \mathbf{p}_k \quad \alpha_k = \frac{(r_k, r_k)}{(p_k, Ap_k)}$$

$$\mathbf{p}_{k+1} = \mathbf{r}_{k+1} + \frac{(\mathbf{r}_{k+1}, \mathbf{r}_{k+1})}{(\mathbf{r}_k, \mathbf{r}_k)} \mathbf{p}_k$$

Iterate this until $\sqrt{\frac{(\mathbf{r}_{k+1}, \mathbf{r}_{k+1})}{(\mathbf{r}_0, \mathbf{r}_0)}} < (\text{tolerance}) \simeq 10^{-4}$

The approximate answer of Ax=b is $x = x_{k+1}$.