Grand Canonical Simulations in the IILM

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The Semiclassical Expansion

- In the strong coupling regime, the degrees of freedom appearing in the fundamental lagrangian are not manageable to a perturbative treatment.
- One strategy is then to reparametrize the theory in terms of degrees of freedom that do allow a systematic perturbative expansion, e.g. chiral perturbation theory
- A different approach is to identify non-perturbative field configurations of the fundamental degrees of freedom
- A priori, though, it is plagued by the same shortcomings of normal perturbation theory in that higher order corrections are not under control.
- A posteriori, the method can provide a systematic expansion if the solitonic degrees of freedom dynamically generate a scale at which the coupling is sufficiently small to allow for a systematic perturbative treatment, the semi-classical expansion.

Saturating the path integral

- The rationale is to saturate the partition function with some suitable background configuration.

$$Z[J] = \int [d\phi] \exp(-S[\phi_c + \phi] + J \cdot \phi)$$

- Taking care of zero modes.

$$Z[J] = e^{-S_c} \int_M d^N\xi \sqrt{g} \left(\det \frac{\delta^2 S}{\delta \phi^2} \right)^{-1/2} \exp\left(\frac{1}{2} J \cdot G \cdot J \right)$$

- g is the moduli space metric.
- We are interested in the case where ϕ_c is a superposition of classical solutions.
- g can be approximated within the subspace spaned by the zero modes of the classical solutions.

Quasi Moduli Space approximation

- We assume first that the exact solution has one zero mode, η_1, related to the collective coordinate γ.
- We write the full field, $\phi_c + \phi$, in two equivalent forms

$$\phi_c(\gamma = 0) + \phi = \phi_c(0) + \sum_{n=1}^{\infty} \zeta_n \eta_n(0) = \phi_c(\gamma) + \sum_{n=2}^{\infty} \bar{\zeta}_n \eta_n(\gamma) + O(\gamma^2).$$

- We know that $\eta(0)$ forms a complete basis so we can identify

$$\phi(\{\gamma, \bar{\zeta}\}) = \phi_c(\gamma) - \phi_c(0) + \sum_{n=2}^{\infty} \bar{\zeta}_n \eta_n(\gamma),$$

$$= \sum_{m=1}^{\infty} \left[\left(\phi_c(\gamma) - \phi_c(0) + \sum_{n=2}^{\infty} \bar{\zeta}_n \eta_n(\gamma), \eta_m(0) \right) \right] \eta_m(0).$$

Quasi Moduli Space approximation

- To compute the jacobian for $\{\zeta_n\} \to \{\gamma, \bar{\zeta}_m\}$ we need the following partial derivatives

$$\frac{\partial \zeta_n}{\partial \gamma} = \int \left(\partial_\gamma \phi_c(\gamma) + \sum_{m=2}^{\infty} \bar{\zeta}_m \partial_\gamma \eta_m(\gamma) \right) \eta_n(0),$$

$$\frac{\partial \zeta_n}{\partial \bar{\zeta}_m} = \int \eta_m(\gamma) \eta_n(0),$$

- We really need them at $\gamma = 0$

$$\left.\frac{\partial \zeta_n}{\partial \gamma}\right|_{\gamma=0} = \int \left(\partial_\gamma \phi_c(0) \eta_n(0) - \phi(\bar{\zeta}) \partial_\gamma \eta_n(0) \right),$$

$$\left.\frac{\partial \zeta_n}{\partial \bar{\zeta}_m}\right|_{\gamma=0} = \delta_{mn},$$

Quasi Moduli Space approximation

- To 1-loop order this simplifies to

$$\left.\frac{\partial \zeta_n}{\partial \gamma}\right|_{\gamma=0} = \int \partial_\gamma \phi_c(0)\eta_n(0).$$

- The matrix of derivatives has the following structure

$$\begin{pmatrix} \int \partial_\gamma \phi \eta_1 & 0 & 0 & \cdots \\ \int \partial_\gamma \phi \eta_2 & 1 & 0 & \cdots \\ \int \partial_\gamma \phi \eta_3 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

- The jacobian gives the well known result

$$g = J = \int \partial_\gamma \phi_c \eta_1$$

Quasi Moduli Space approximation

- If the background has more zero modes (to 1-loop order)

$$g_{ab} = \begin{pmatrix} \int \partial_{\gamma_1}\phi\eta_1 & \cdots & \int \partial_{\gamma_N}\phi\eta_1 & 0 & \cdots \\ \int \partial_{\gamma_1}\phi\eta_2 & \cdots & \int \partial_{\gamma_N}\phi\eta_2 & 0 & \cdots \\ \int \partial_{\gamma_1}\phi\eta_3 & \cdots & \int \partial_{\gamma_N}\phi\eta_3 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ \int \partial_{\gamma_1}\phi\eta_N & \cdots & \int \partial_{\gamma_N}\phi\eta_N & 0 & \cdots \\ \vdots & \vdots & \vdots & 1 & 0 \\ \vdots & \vdots & \vdots & 0 & \ddots \end{pmatrix}$$

- We don't know the exact η's.
- Approximate them by the zero modes of the individual classical solutions, $\eta \to O_B \eta$.
- O_B is the matrix that orthonormalizes the set $\{\eta_i\}$.

Quasi Moduli Space approximation

- Coupling the theory to fermions, the low frequency part is again approximated by the individual pseudo-particle zero modes.

$$\begin{aligned} (D+m)_{\text{low}} &= O_F^\dagger \, D \, O_F + m\mathbb{I} \\ D_{ij} &= \langle \xi_i | D | \xi_j \rangle \end{aligned}$$

- ξ_i are the fermionic zero modes of the individual classical solutions.
- O_F is the matrix that orthonormalizes the set $\{\xi_i\}$.

Quasi Moduli Space approximation

- The high frequency fluctuations, presumably orthogonal to the low frequency ones described above, are assumed to factorize.
- Thus, the aim of this method is to describe the low-energy fluctuations by the long wave-length dynamics of some trial classical background.
- Rather similar to the moduli space approximations used in describing (field theory) strings.
- The original field theory is turned into a statistical mechanical system.
- On a practical level, $O_B = O_F = \mathbb{I}$ is assumed in simulations.

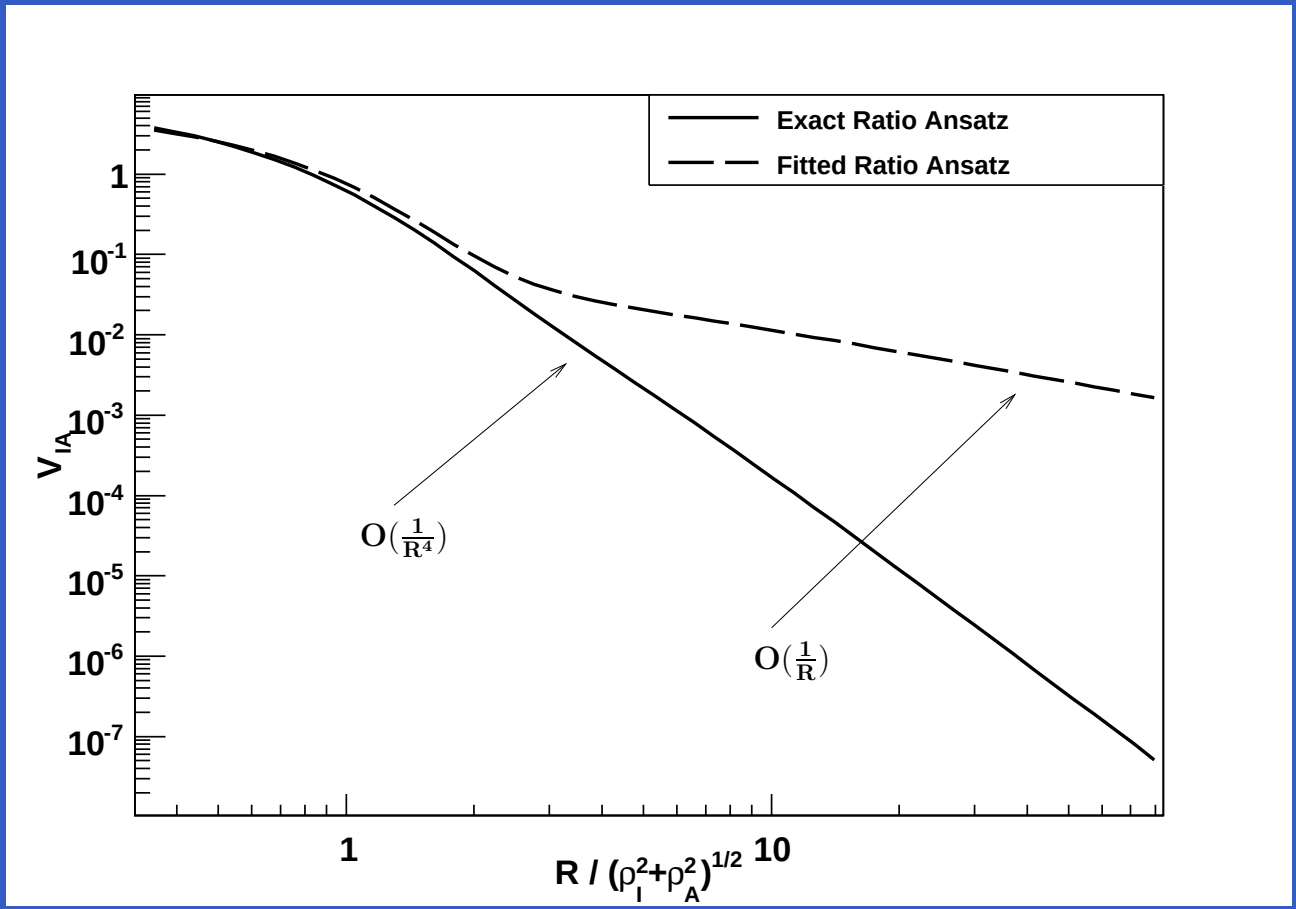
Interacting Instanton Liquid Model

- In QCD, instantons are thought to play an important role in the low-energy regime.
- The IILM is successful in capturing the chiral properties of QCD.
- The partition function used in practice is

$$
\begin{aligned}
Z &= \sum_{N_I N_A} \frac{1}{N_I! N_A!} \int d(\rho) e^{-S_{int}} \prod_f^{N_f} m_f^{|Q|} \det(M_f^2) \\
M_f^2 &= \begin{cases} TT^\dagger + m_f^2 & , Q < 0 \\ T^\dagger T + m_f^2 & , Q > 0 \end{cases} \\
S_{int} &= S[A] - (N_I + N_A) S_0 = \sum_{i<j} S_{ij} \\
A_\mu^a &= -\frac{\bar{\eta}_{\mu\nu}^a \partial_\nu \Pi_1(x, \{x_1, \rho_1\}) + O^{ab} \eta_{\mu\nu}^b \partial_\nu \Pi_2(x, \{x_2, \rho_2\})}{1 + \Pi_1(x, \{x_1, \rho_1\}) + \Pi_2(x, \{x_2, \rho_2\})}
\end{aligned}
$$

Numerical Implementation

- Compute χ_{top} in the IILM and study volume dependence.
- Found that interactions as given in Shuryak et al have unphysical behaviour.



- Also periodicity in T not explicit.

Numerical Implementation

- Split off color degrees of freedom in fieldstrength.

$$F^a_{\mu\nu}F^a_{\mu\nu} = I + (\mathrm{Tr}O^tO + (\bar{\eta}O\eta)_{\mu\nu\mu\nu})J + (\bar{\eta}O\eta)_{\rho\mu\rho\nu}I_{\mu\nu} + (\bar{\eta}O\eta)_{\mu\rho\nu\sigma}I_{\mu\rho\nu\sigma} + (\eta O^tO\eta)_{\mu\rho\nu\sigma}J_{\mu\rho\nu\sigma} + (\bar{\eta}O\eta)_{\alpha\mu\alpha\rho}(\bar{\eta}O\eta)_{\beta\nu\beta\sigma}K_{\mu\rho\nu\sigma}$$

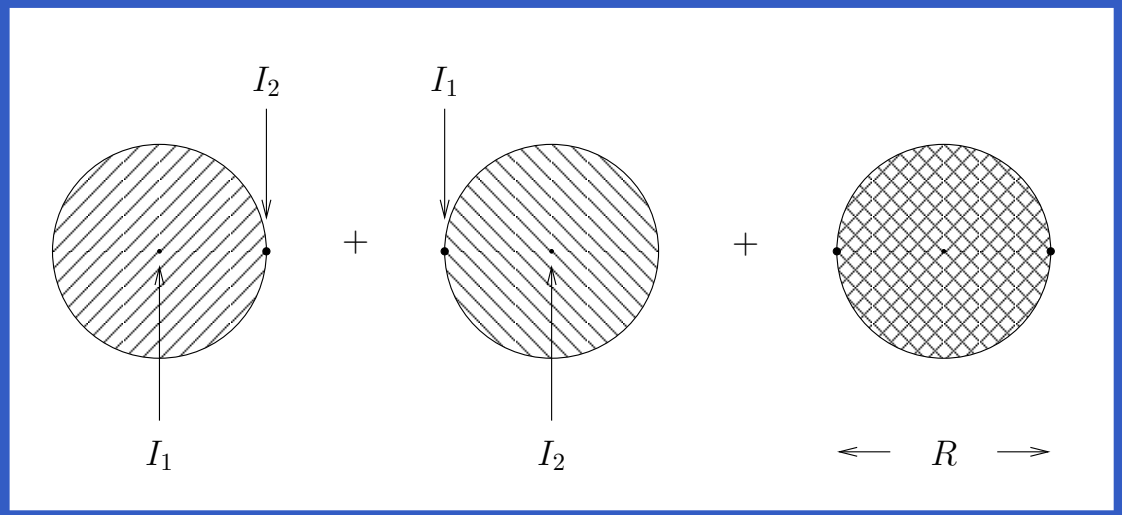
- Similarly for the quark overlaps.

$$T_{IA} = \int d^4x \frac{1}{4\pi^2\rho_I\rho_A}\frac{3}{2}\mathrm{Tr}(U\tau^+_\beta)I_\beta,.$$

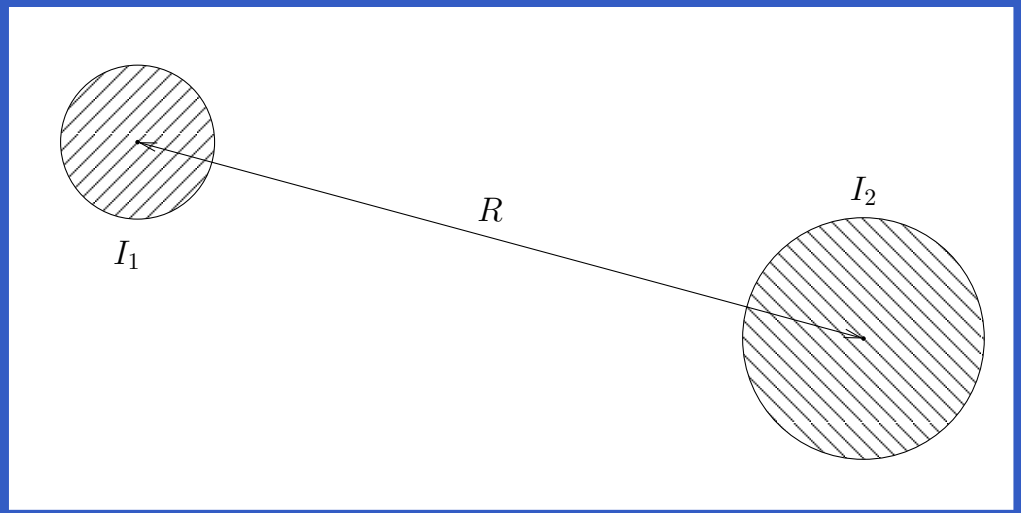
- Use numerical integration to compute interactions.
- Use interpolation and asymptotic matching in simulations.

Numerical Implementation

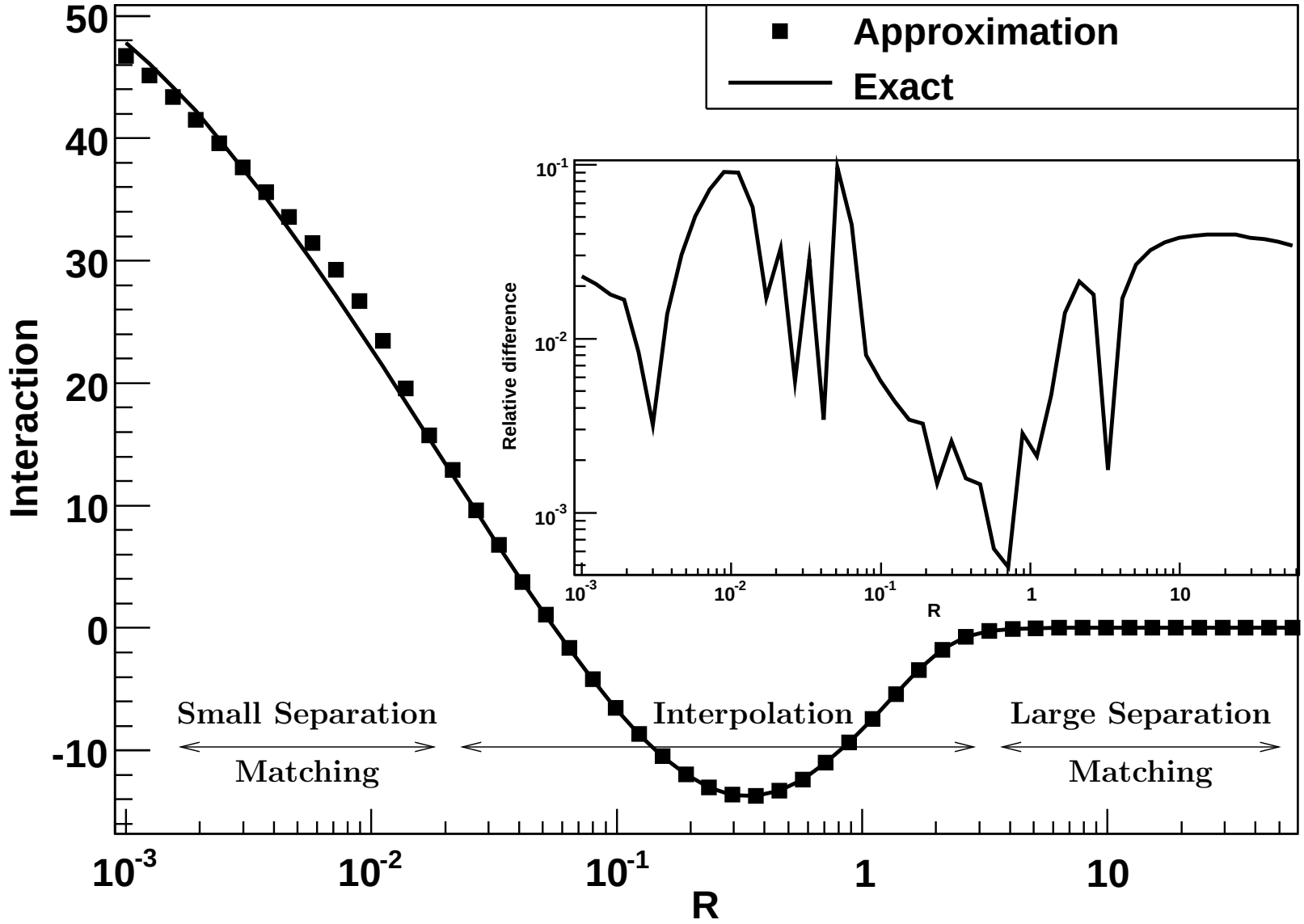
- Small separation asymptotics.



- Large separation asymptotics.



Numerical Implementation



Numerical Implementation

- Interested in thermodynamic limit.
- Want to use 'physical' quark masses.
- Need fairly large ensembles, but complexity is $O(N^3)$.
- Monte Carlo updates can be written as rank 1 modifications.

$$\begin{aligned} T' &= T + \Delta T \\ M'^2 &= M^2 + \Phi\Phi^\dagger - \Psi\Psi^\dagger \end{aligned}$$

- Chlolesky decomposition can be updated in $O(N^2)$.

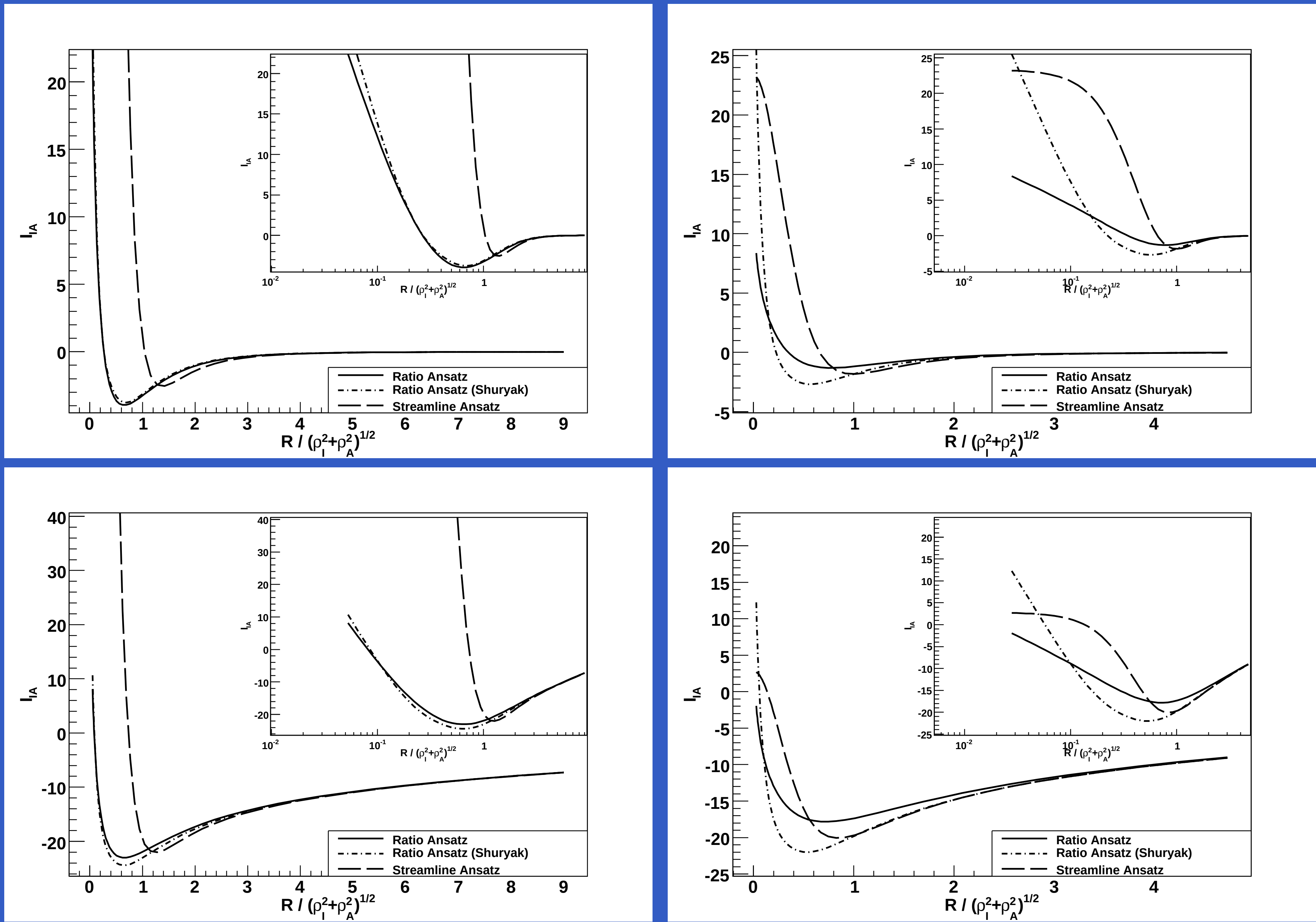
$$M'^2 = L'D'L'^\dagger = M^2 + \alpha z z^\dagger = L(D + \alpha w w^\dagger)L^\dagger$$

- For $N_f = 3$ need $3 \cdot 2 \cdot 2 = 12$ updates. Still for $N = 200$ have a gain of two in speed.

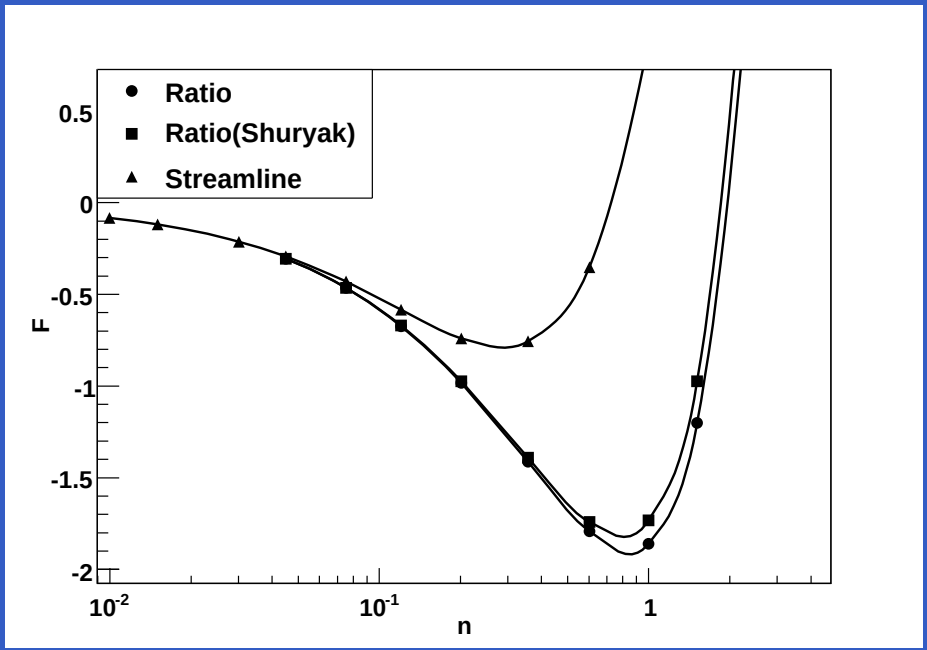
Different Ensembles

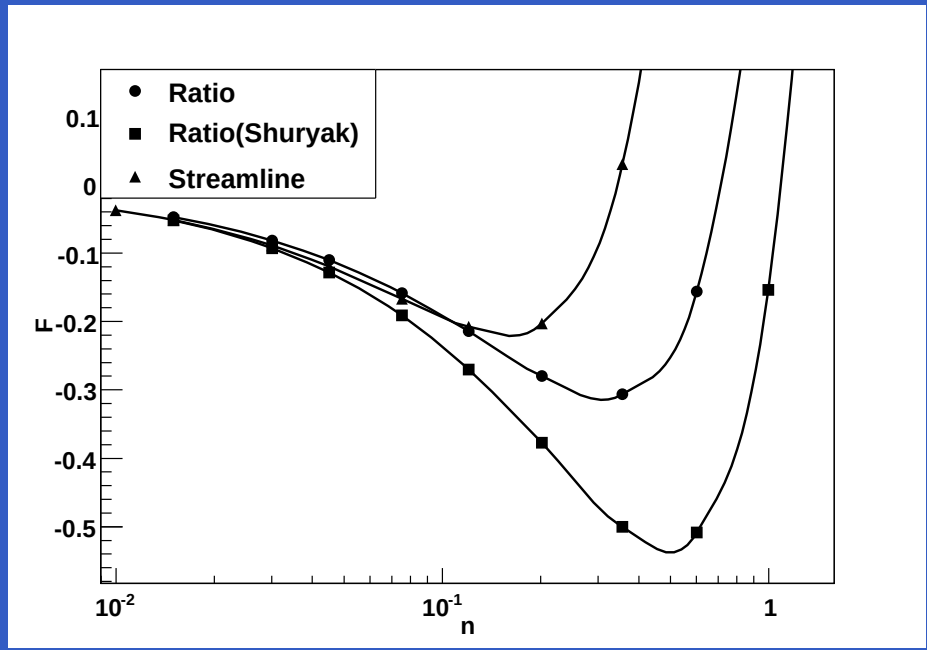
- A precise comparison of the IILM with lattice data in Phys.Rev. D, 2007, 75, 034008 (M. Cristoforetti, P. Faccioli, M. Traini, J. Negele).
- For chiral properties IILM compatible with lattice data if $\mu = 1/\bar{\rho} \approx 600\text{MeV}$.
- Based on the streamline ansatz.
- Can we take over these results for the ratio ansatz?

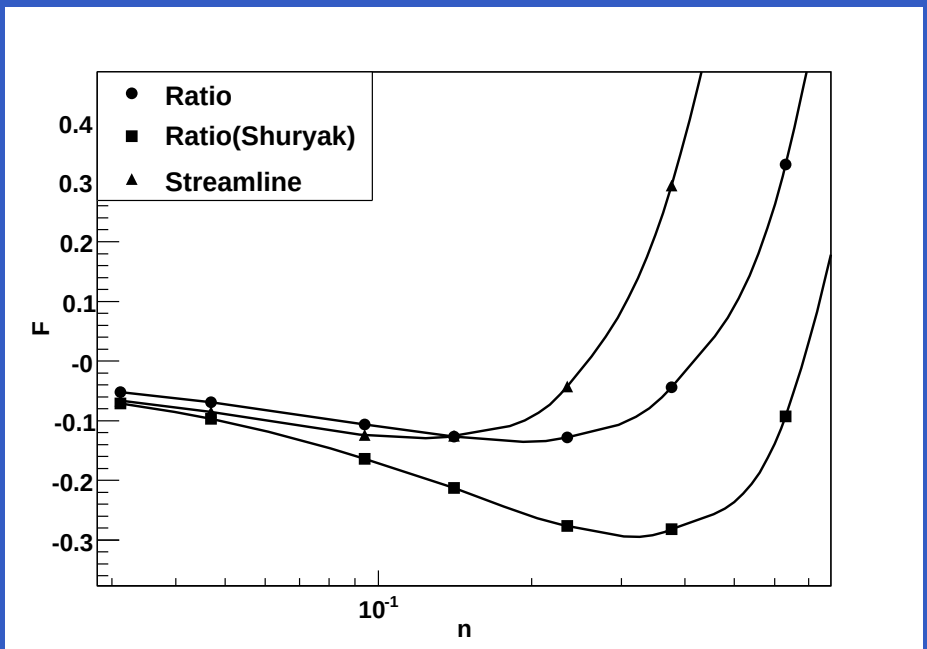
Different Ensembles

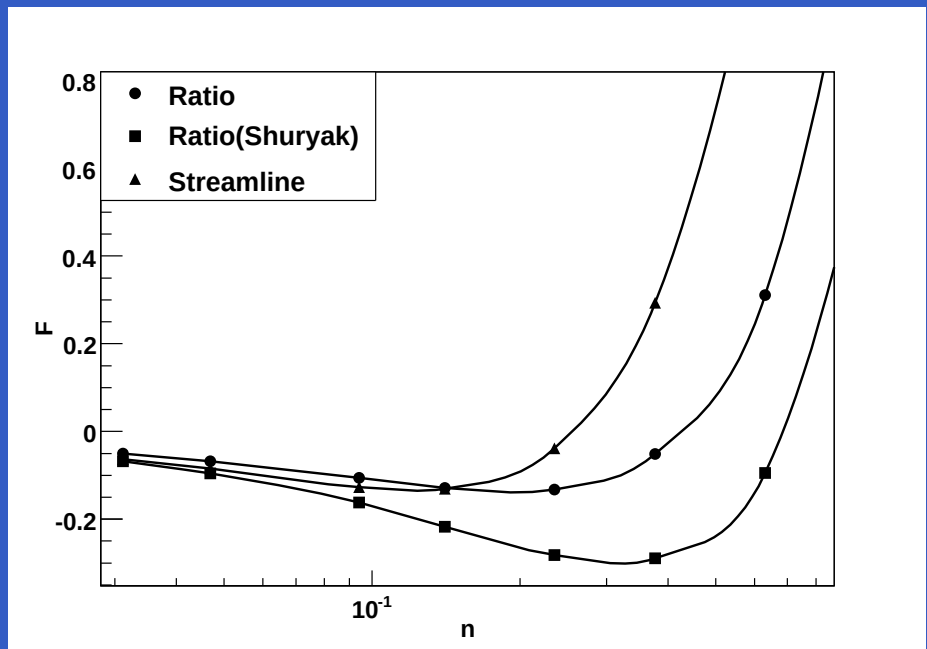


Different Ensembles

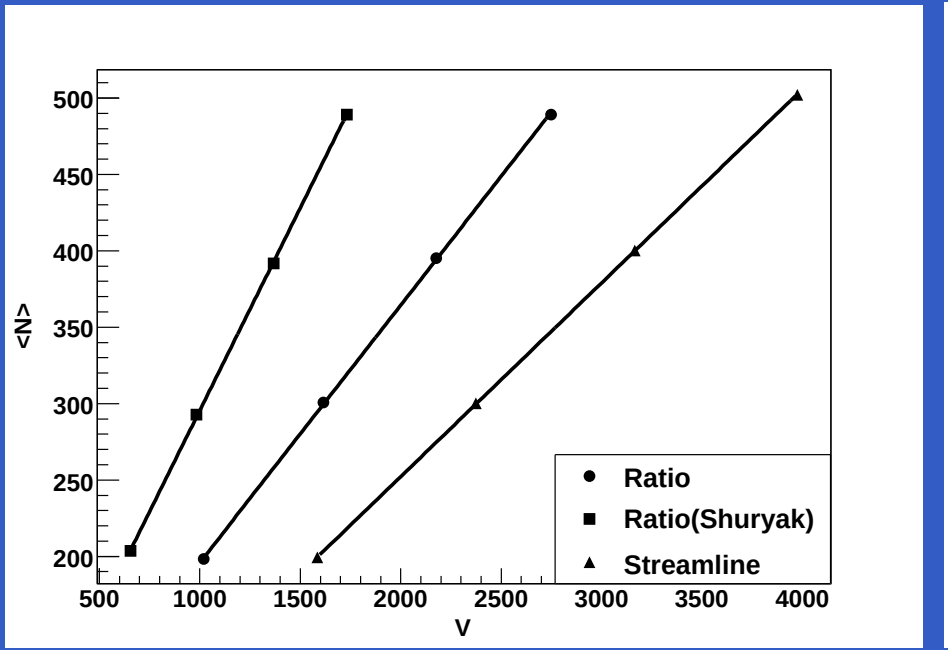


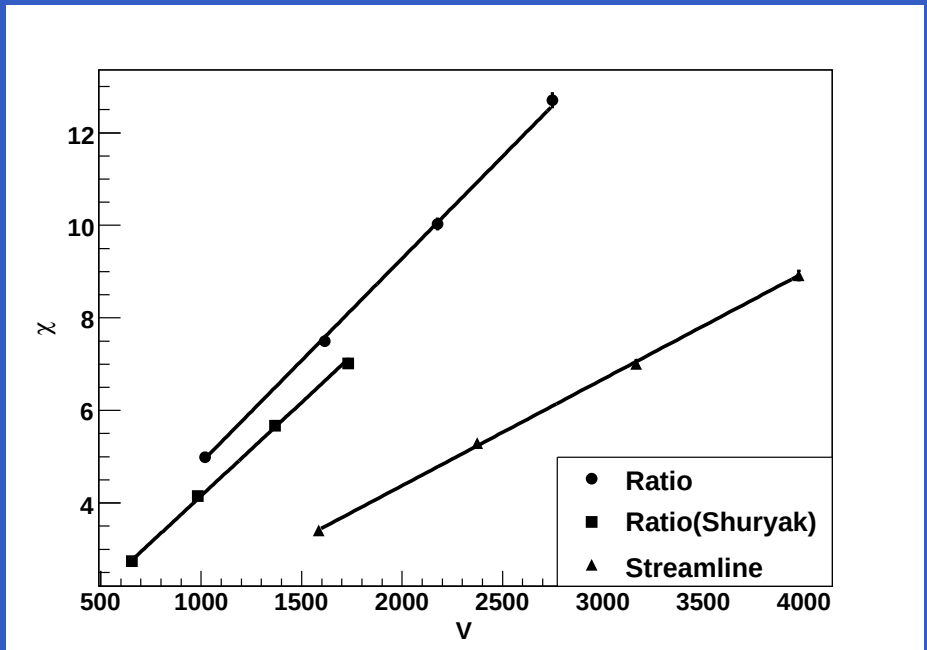


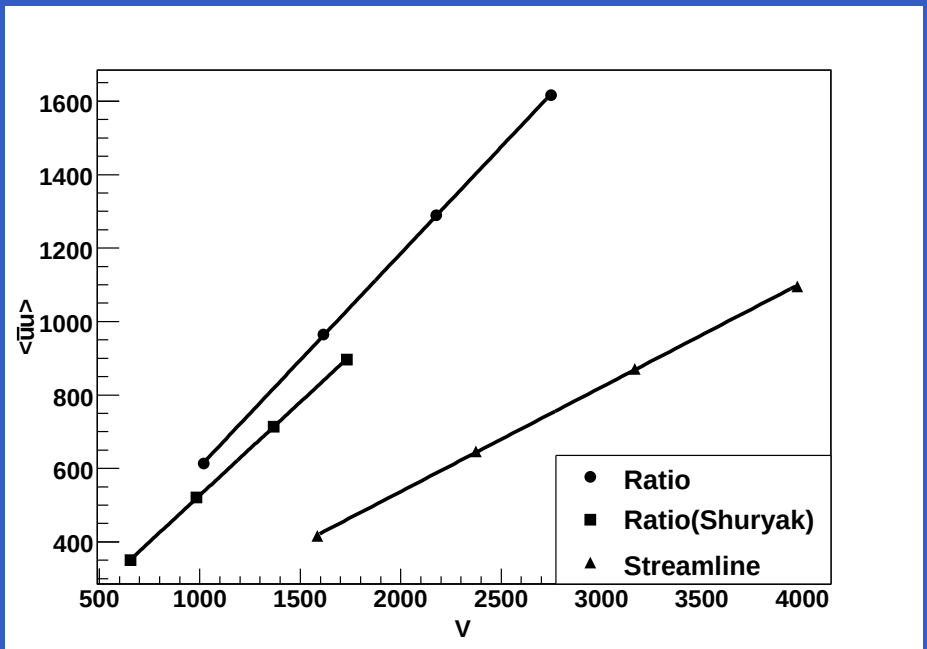


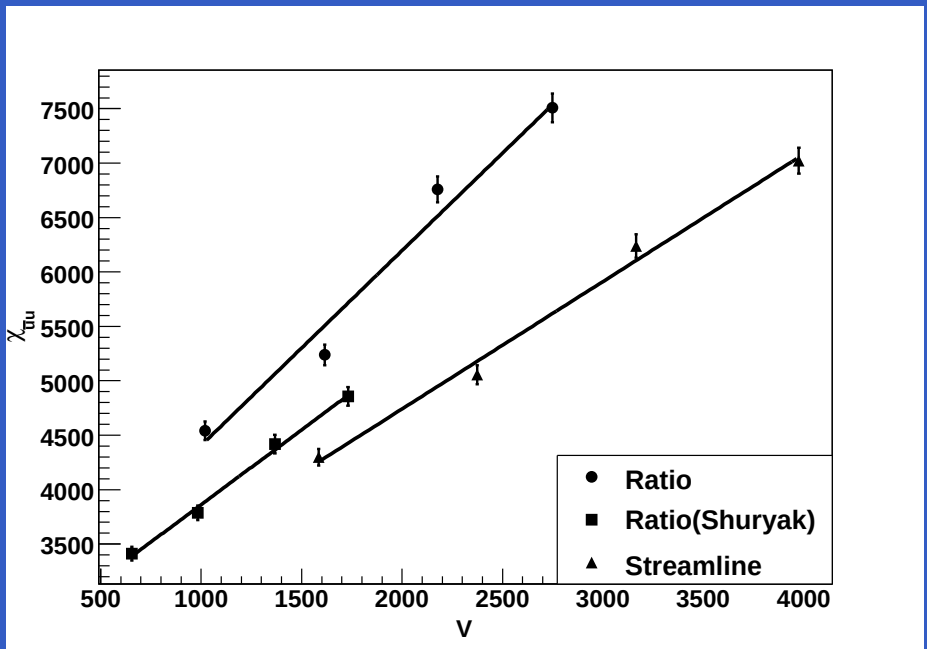


Different Ensembles









Fixing units

- The model has 4 free paremeters: Λ, m_u, m_d and m_s.
- We use chiral perturbation theory results to fix the parameters.

$$\chi = \frac{\langle \bar{q}q \rangle_0}{\frac{1}{m_u} + \frac{1}{m_d} + \frac{1}{m_s}} + O(m^2)$$

- Where χ is infered from grand canonical MC simulations at different volumes.

$$\chi = \lim_{V \to \infty} \frac{\langle (N_l - N_A)^2 \rangle}{V}$$

- We use as input

$$\langle \bar{q}q \rangle_0^{\overline{\text{MS}}}(\mu = 2\text{GeV}) = 250\text{MeV}.$$

Fixing units

- Converting $\overline{\rm MS}$ to PV, we get at 1-loop.

$$\langle\bar{q}q\rangle_0^{\rm PV} = \langle\bar{q}q\rangle_0^{\overline{\rm MS}}(1-\frac{5\alpha_s}{18\pi}) \approx 244{\rm MeV}.$$

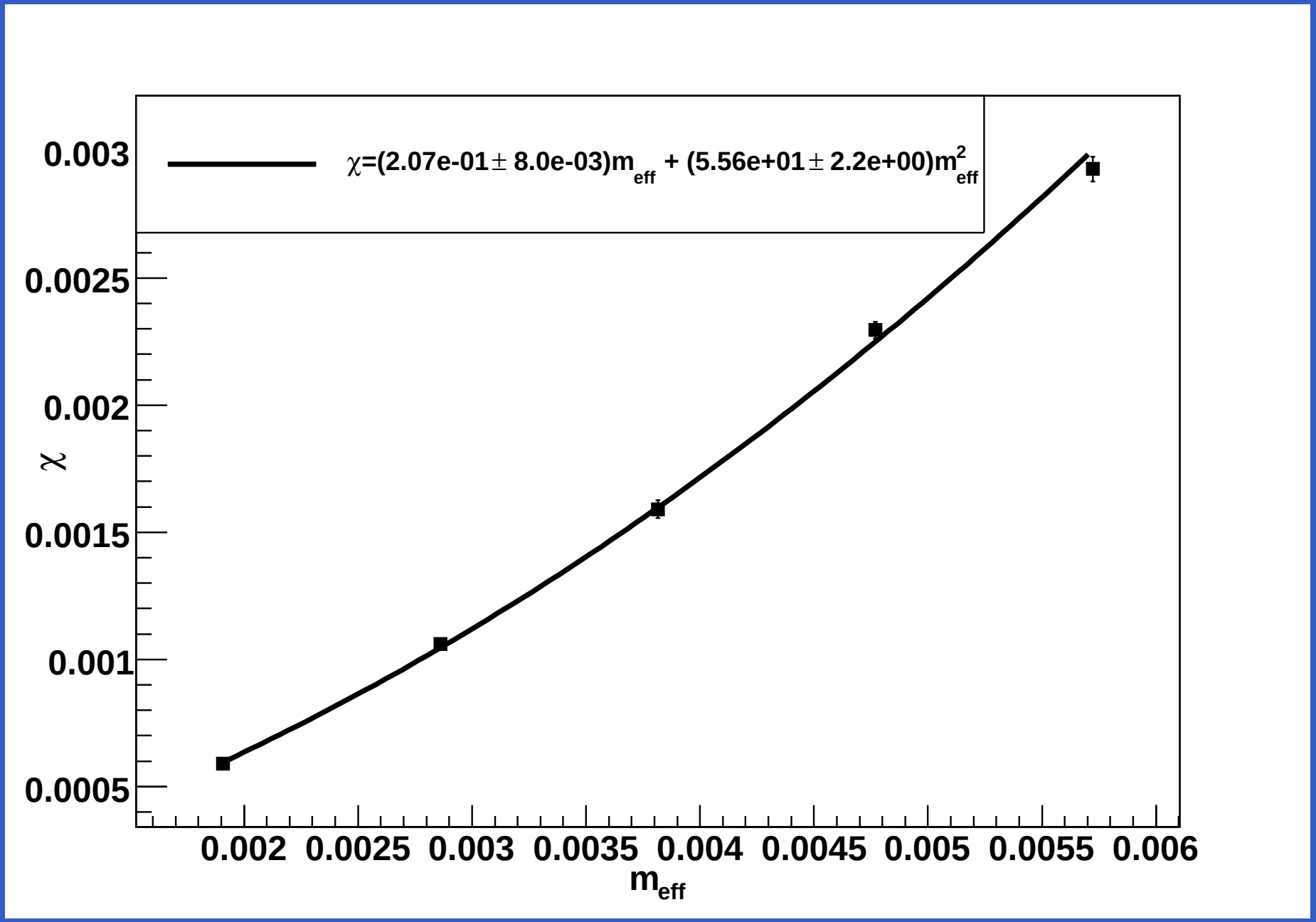
- We run this down to $\mu_\Lambda = \Lambda/\bar{\rho}$ (at 1-loop) and get the self consistency equation

$$\langle\bar{q}q\rangle_0^{\rm PV}(\mu_\Lambda) = \Lambda^3\langle\bar{q}q\rangle_0^{\rm IILM}$$

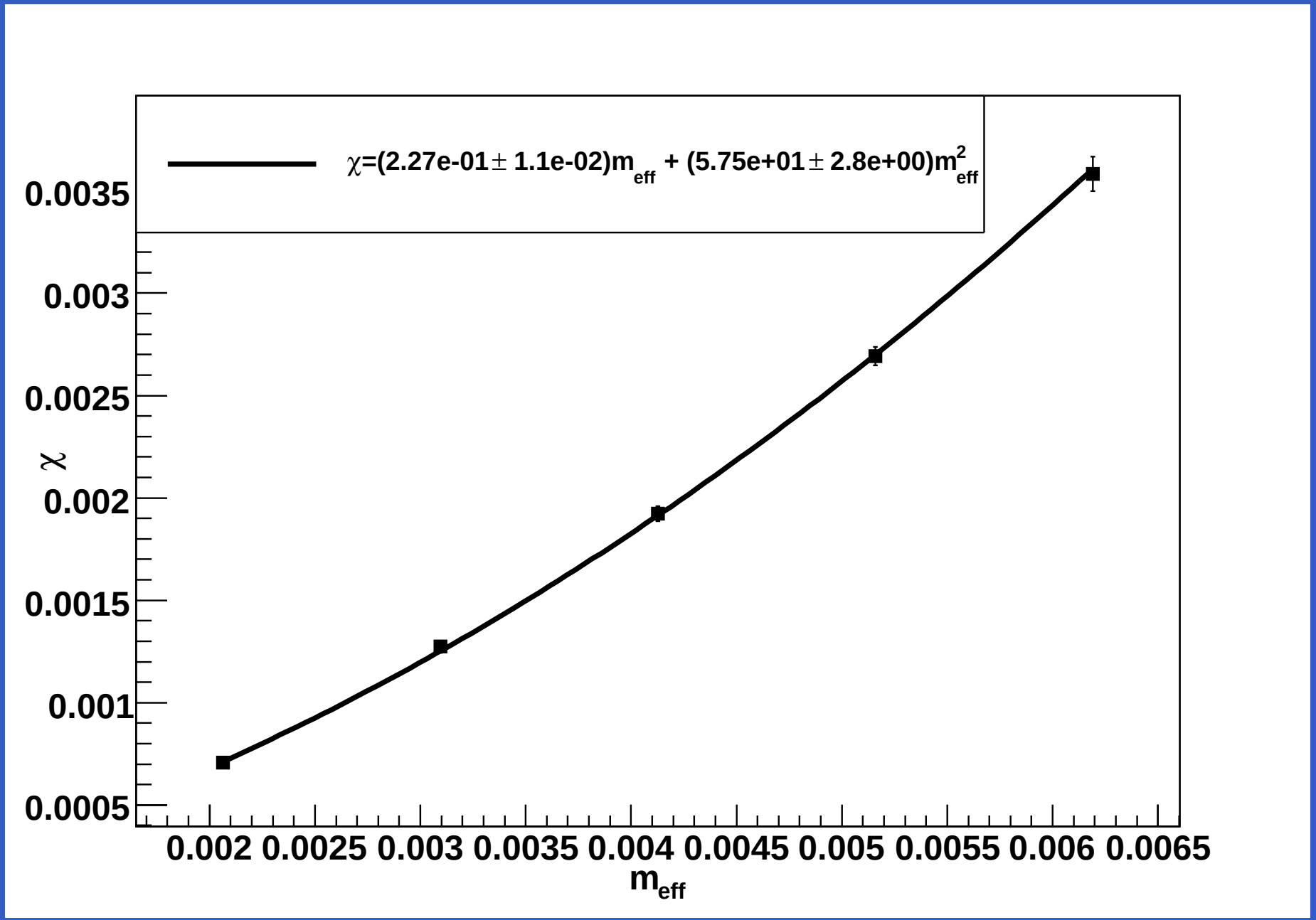
- At $\mu = 2{\rm GeV}$ the 2-loop corrections are already 10%, so that at $\mu = 600{\rm MeV}$ the systematics from higher orders will be substantial..
- We have determined $\langle\bar{q}q\rangle_0^{\rm IILM}$ for two sets of masses, with ratios

$$m^i_{eff} = \begin{cases} 1:1.83:36.7 \\ 1:2.32:45.0 \end{cases}$$

Fixing units



Fixing units



Fixing units

- This gives

$$\Lambda^i = \begin{cases} 401\text{MeV} \\ 389\text{MeV} \end{cases}$$

- The IILM thus generates a scale at

$$\mu^i = \begin{cases} 598(10)\text{MeV} \\ 580(10)\text{MeV} \end{cases}$$

- To fix the quark masses we use again chiral perturbation theory

$$\chi^i = f_\pi^2 m_\pi^2 \frac{z^i}{(1+z^i)^2}$$

- We use $m_\pi \approx 135\text{MeV}$ and $f_\pi \approx 93\text{MeV}$.

Fixing units

- Running up the resulting quark masses to 2GeV and converting back to $\overline{\text{MS}}$ (1-loop)

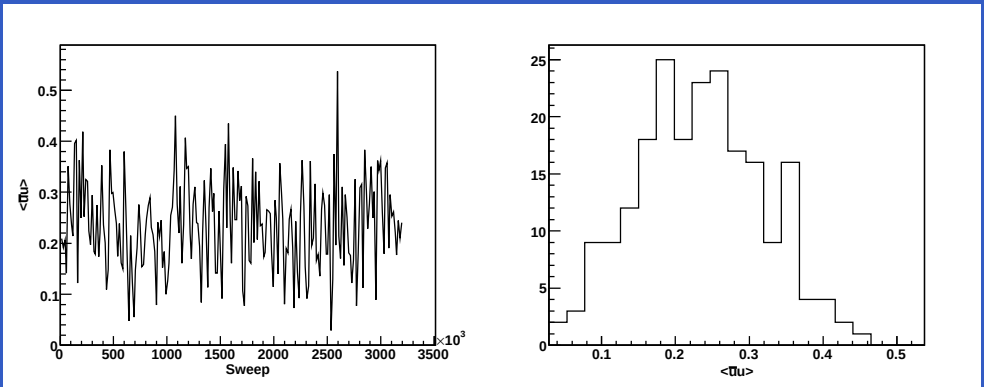
$$m_u = \begin{cases} 1.96\text{MeV} \\ 1.73\text{MeV} \end{cases} \quad m_d = \begin{cases} 3.60\text{MeV} \\ 4.01\text{MeV} \end{cases} \quad m_s = \begin{cases} 72.0\text{MeV} \\ 77.9\text{MeV} \end{cases}$$

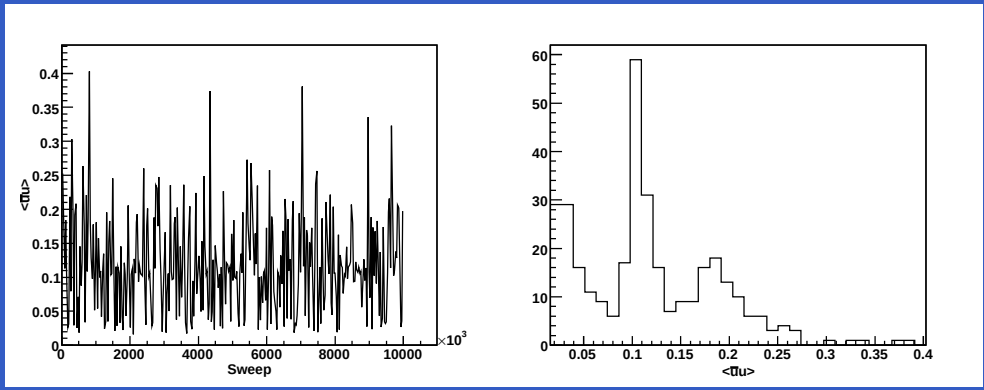
- This is comparable to the usually quoted masses.
- Running up the coupling (2-loop)

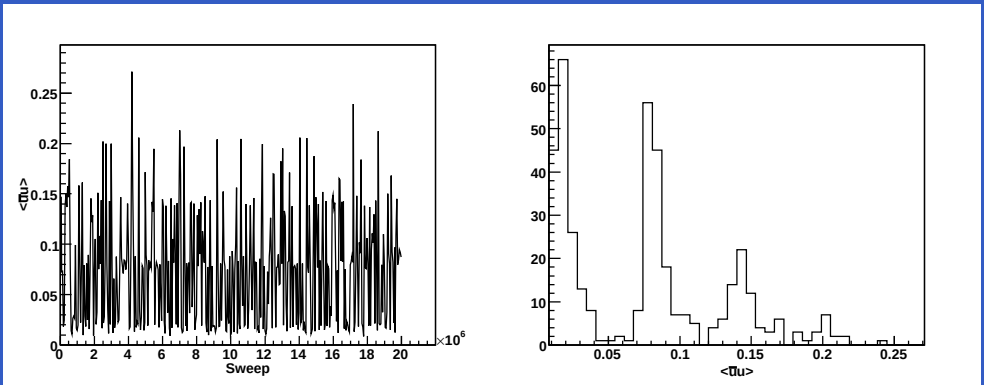
$$\Lambda^{(5)}_{\overline{\text{MS}}} = 320\text{MeV}$$
$$\alpha_s^{\overline{\text{MS}}}(\text{M}_\text{Z}) = 0.125$$

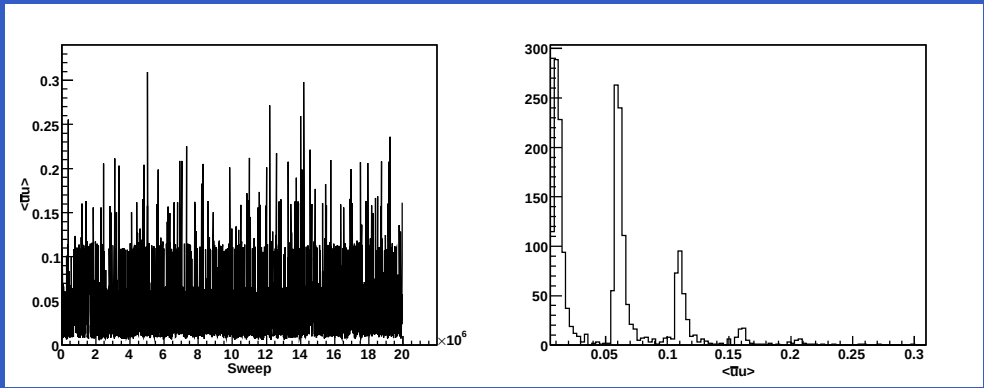
- Encouraging, but given the large uncertainties in using perturbation theory, hard to say how good it really is.

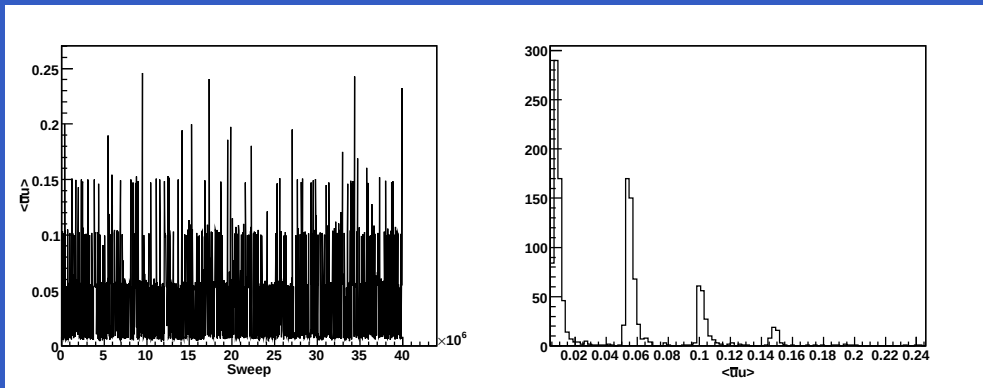
Finite Temperature Quark Condensate





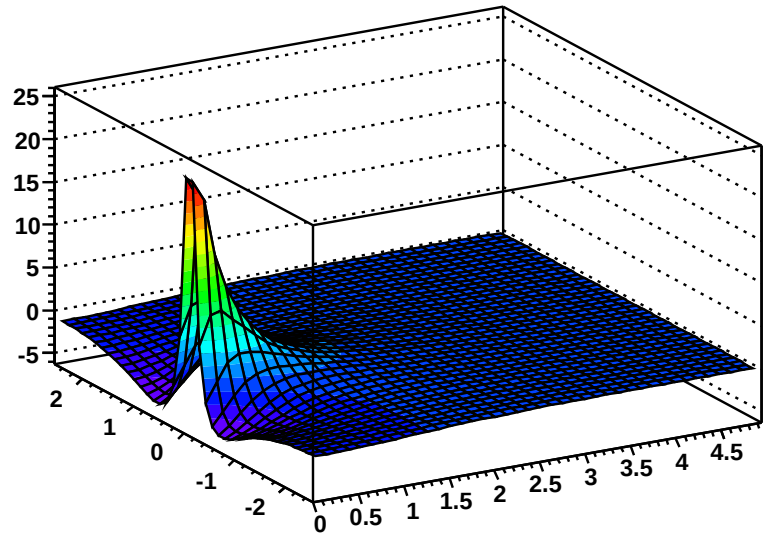




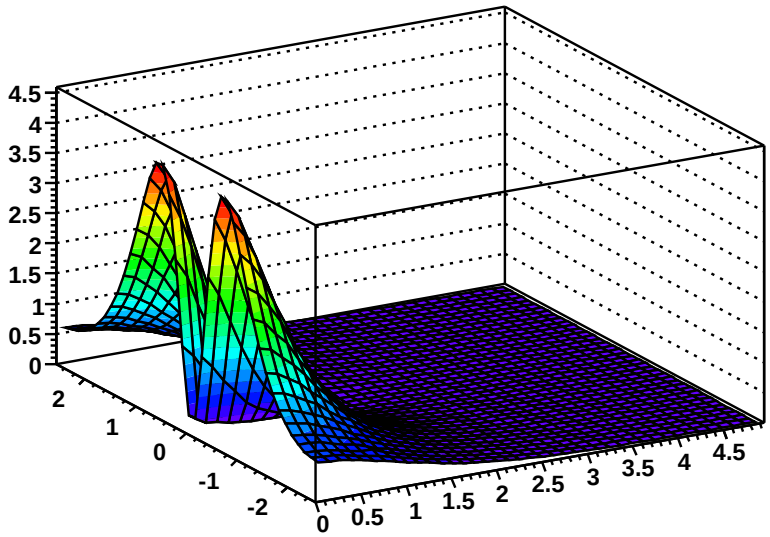


Finite Temperature Interactions

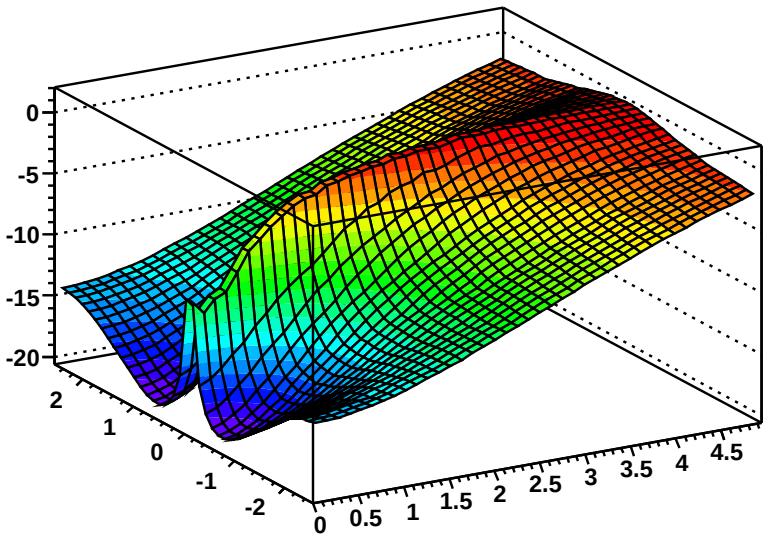
Glue



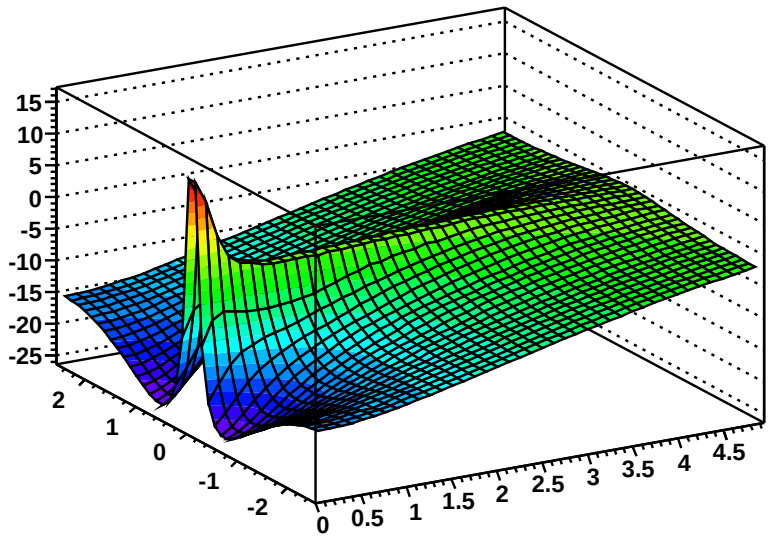
Matter (modulus)



Matter (in exponent)



Interaction



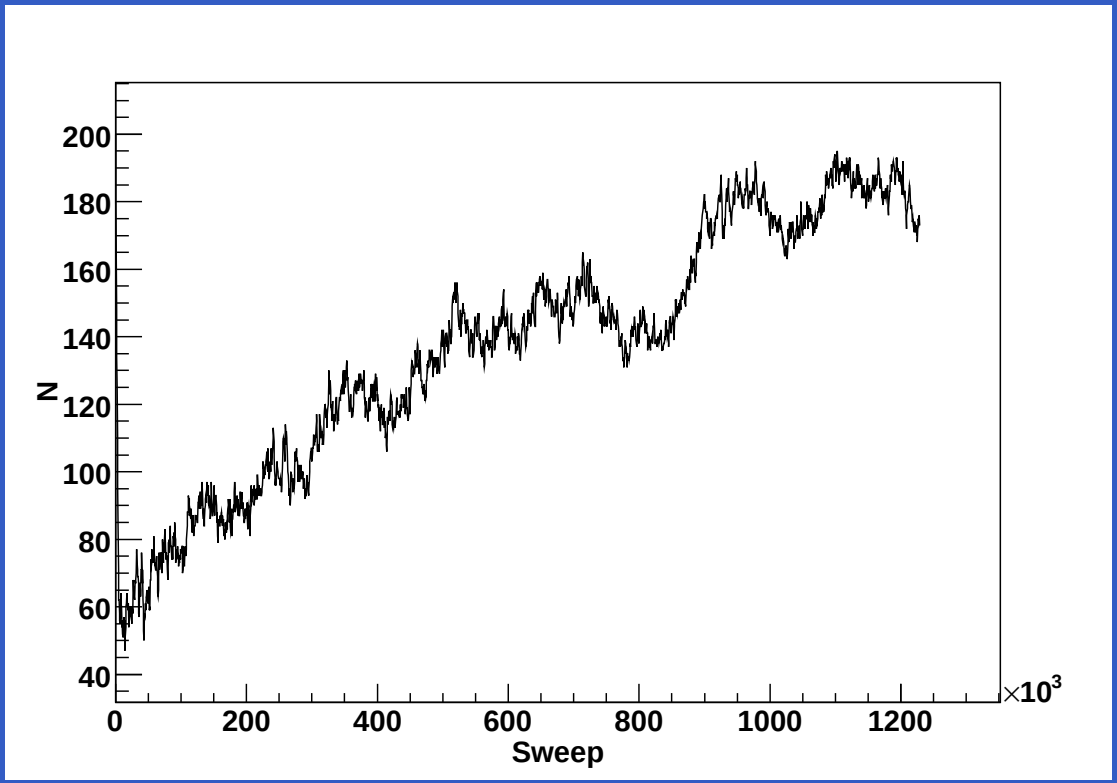
Biased Monte Carlo

- Fermionic interactions are most important, but short ranged.
- Hard to simulate: long autocorrelation times, (practical) non-ergodicity.
- Need importance sampling if

$$V < \Delta V \exp(-H(\Delta V))$$

  where V is the volume of the simulation box and $\Delta V \ll V$ is the small region where the interaction is very strong.
- Well known problem in chemical engineering and computational chemistry: strongly associating fluids.
- Use Biased Monte Carlo techniques.

Biased Monte Carlo



- To ensure ergodicity need moves that
  - preferentially sample the interaction regions, i.e. energy dominated configurations.
  - sweep large portions of phase space, i.e. entropy dominated configurations.

Biased Monte Carlo

- Detailed balance guarantees convergence.

$$P_i^{\mathrm{eq}} P_{ij} = P_j^{\mathrm{eq}} P_{ji}$$

- BMC exploits split into proposal and acceptance probability.

$$P_{ij} = \mathcal{P}_{ij} \mathcal{A}_{ij}$$

- To satisfy detailed balance can use the Metropolis algorithm.

$$\mathcal{A}_{ij} = \min \left[1, \frac{P_j^{\mathrm{eq}}}{P_i^{\mathrm{eq}}} \frac{\mathcal{P}_{ji}}{\mathcal{P}_{ij}} \right]$$

- Apriori complicated geometric problem to place particles into the union of all the interaction regions with uniform probability, say.
- Instead focus on individual interaction regions and sum over all possible routes: Unbonding-Bonding algorithm.

Unbonding-Bonding algorithm

- Basic building blocks.

$$\mathcal{P}^{B}_{(i,j)(i',j)} = \frac{1}{N_l}\frac{1}{N_A}\frac{1}{V_{ij}}$$

$$\mathcal{P}^{U}_{ii'} = \frac{1}{N^{B}_{l}}\frac{1}{V}$$

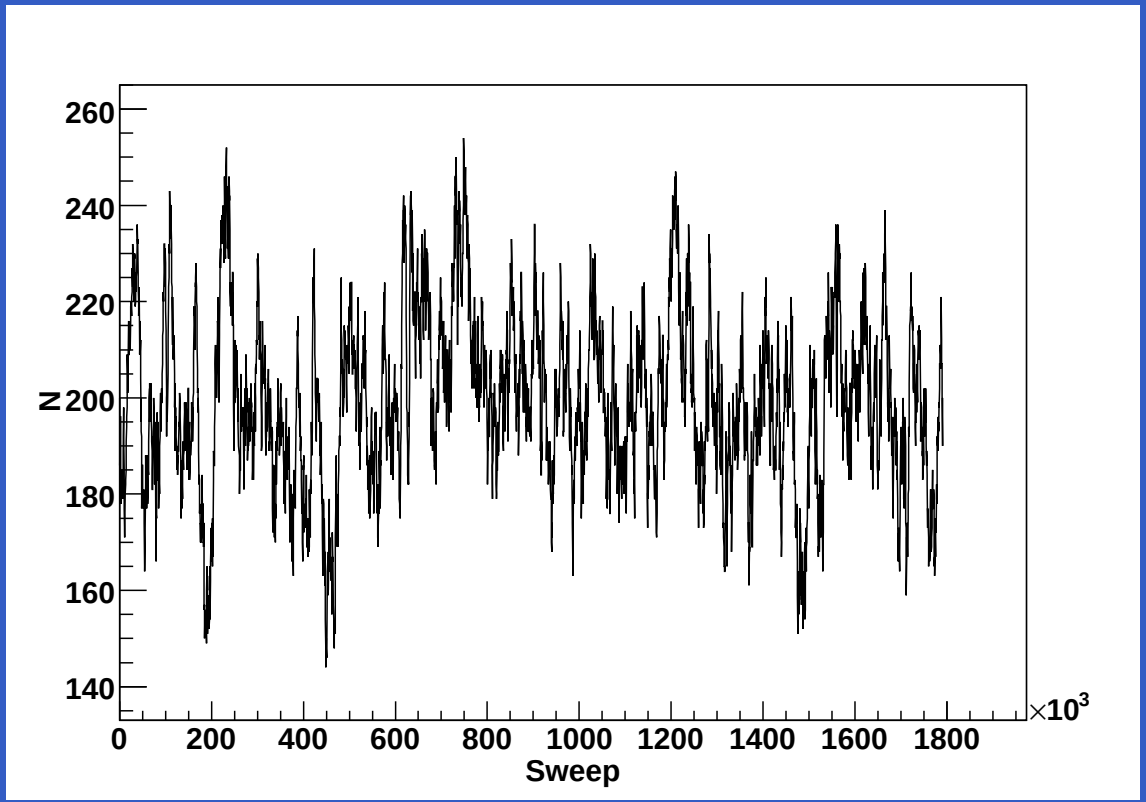
- Summing over all possibilities.

$$\mathcal{P}_{ii'} = \sum_{j}^{N'^{B}_{l}(i)} \mathcal{P}^{B}_{(i,j)(i',j)} + \delta^{B}_{i}\mathcal{P}^{U}_{ii'}$$

$$\mathcal{P}_{i'i} = \sum_{j}^{N^{B}_{l}(i)} \mathcal{P}^{B}_{(i',j)(i,j)} + \delta^{B}_{i'}\mathcal{P}^{U}_{i'i}$$

Biased Monte Carlo

- Based on the UB algorithm, also construct moves to
  - insert/delete particles.
  - insert/delete pairs of oppositely charged instantons.
  - move pairs.



Conclusions

- IILM tries to capture essential features by using instantons as most important degrees of freedom.
- Therefore might be well suited to approximate the topological sector.
- Grand Canonical simulations seem most natural setting.
- The $T = 0$ IILM is believed to describe well the low energy regime of QCD.
- Results are compatible with earlier studies.
- Continuum formulation might be complementary to lattice instanton models.
- Ease to deal with quarks. (determinants)
- Only two-body interactions.
- Need to include new calorons.

Interacting Instanton Liquid Model