The density of states approach at finite chemical potential: a numerical study of the Bose gas.

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Density of states

- The density of states is the volume of phase-space available to the system at given energy

$$\rho(s) = \int [D\phi]\, \delta(s - S[\phi]). \tag{1}$$

- Partition function and observables can be computed using a simple 1-d integral

$$Z(\beta) = \int ds \rho(s) e^{-\beta s}. \tag{2}$$

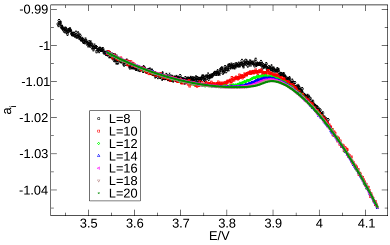
LLR

- Recently proposed algorithm to compute the Density of States in systems with continuum degrees of freedom.[1]
- Based on the simulation of the system in energy intervals.
- Converges to the true log-derivative of the DOS $\frac{d\rho}{ds}$.[2]

[1] Langfeld, Lucini, Rago PhysRevLett.109.111601
[2] Langfeld, Lucini, Pellegrini, Rago in preparation.

LLR

- Very efficient for simulation with metastabilities, e.g. 4d compact U(1).
- First order phase transition $\beta_{C_v}(V) = \beta_{C_v}(\infty) + \sum_{k=1}^{k_{max}} B_k V^{-k}$



L_{min}	k_{max}	$\beta_{C_v}(\infty)$	χ^2_{red}
14	**1**	**1.011125(3)**	**0.91**
12	1	1.011121(3)	2.42
12	**2**	**1.011129(4)**	**0.67**
10	1	1.011116(5)	7.44
10	**2**	**1.011127(3)**	**0.60**
8	1	1.011093(5)	90.26
8	**2**	**1.011126(2)**	**0.62**

Generalised density of states

- At finite chemical potential we have

$$Z = \int [D\phi] \, e^{-\beta S_{Re}[\phi] + i\mu S_{Im}[\phi]} \tag{3}$$

- We can define a generalised density o states

$$P_\beta(s) = \int [D\phi] \, \delta\left(s - S_{Im}[\phi]\right) e^{-\beta S_{Re}[\phi]} \tag{4}$$

- The partition function is the Fourier transform of P

$$Z(\beta, \mu) = \int ds P_\beta(s) e^{i\mu s} \tag{5}$$

Bose gas at finite density.

- LLR was already tested on a Z_3 spin model with complex action, where it seems to work. [3]
- The relativistic Bose gas is a different test since it is known to undergo a second-order phase transition at μ_c and has continuum degrees of freedom.
- Observables are independent from μ below a threshold μ_c.

[3] Gattringer, Torek PLB; Langfeld, Lucini PRL

Bose gas at finite density

- Continuum formulation

$$S[\phi] = \partial_\mu \phi \partial_\mu \phi + (m^2 - \mu^2) \mid \phi \mid^2 + \mu(\phi^* \partial_4 \phi - \phi \partial_4 \phi^*) + \lambda \mid \phi \mid^4 . \quad (6)$$

- On the lattice the chemical potential is introduced as a vector potential

$$\begin{aligned} S[\phi] = \quad & \textstyle\sum_x (2d + m^2) \phi_x^* \phi_x + \lambda (\phi_x^* \phi_x)^2 + \\ & - \textstyle\sum_{\nu=1}^4 \left(\phi_x^* e^{-\mu \delta_{\nu,4}} \phi_{x+\nu} + \phi_{x+\nu}^* e^{\mu \delta_{\nu,4}} \phi_x \right) \end{aligned} \quad (7)$$

Observables

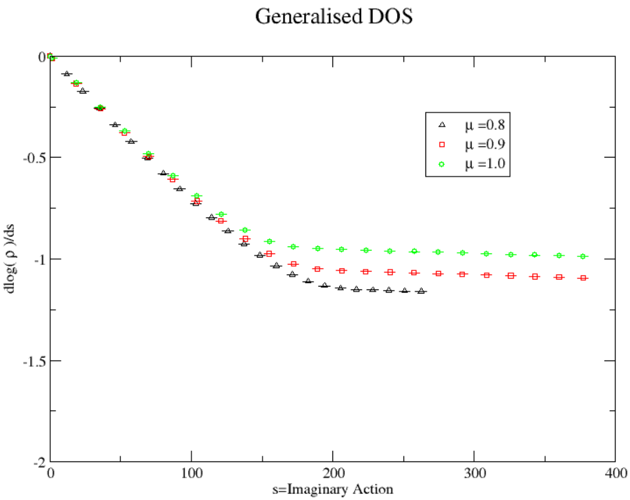
- To quantify the severity of sign problem we are interested in the expectation value of the phase

$$\langle e^{-S_{Im}} \rangle = e^{-V\delta f} \tag{8}$$

- The density of particles is given by

$$\langle n \rangle = \frac{d \log Z}{d\mu} \tag{9}$$

Generalized DOS results



Why not a fft?

- The partition function is given by a fourier transform of the DOS.

$$Z(\beta, \mu) = \int ds e^{i\mu s} P_\beta(s) \tag{10}$$

- P is not known exactly but up to noise coming from the Montecarlo simulation.
- The fourier transform of white noise does not depend on the frequency while $Z(\mu)$ is a fast decaying function. The method breaks at relatively small chemical potential.

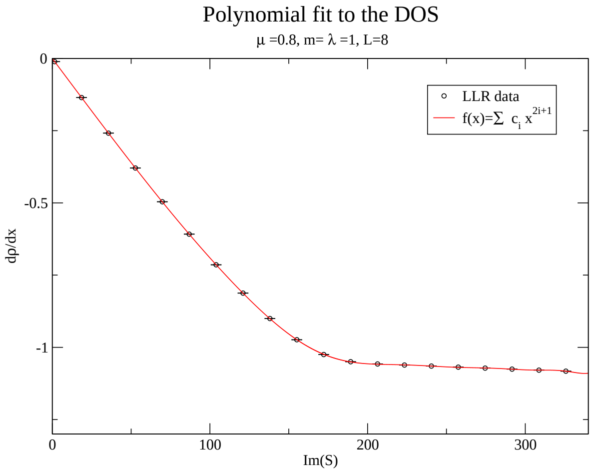
Filtering the noise

- A much better alternative is a fit of the log-derivative of the density of states.

$$P = exp(\sum_i c_i x^{2i}) \tag{11}$$

- The error is now in the coefficients and the fourier transform of every power is a fast decaying function.

Polynomial fit.



Evaluating the fourier transform

- We still need to evaluate the fourier transform of

$$Z = \int exp(\sum_i c_i(\beta, \mu) s^{2i} + i\mu s) ds \tag{12}$$

- Brute-force approach: use numerical integration with multi-precision methods.
- Projection on a base of L^2 with known fourier transform eg. Hermite functions.
- Numerical integration over the Lefschetz Thimble.

Projection on Hermite functions

- $\Psi_n(x) = H_n(x)e^{-\frac{x^2}{2}}$
- $F[\Psi_n(x)] = \lambda_n \Psi_n(x)$
- So that we can project the DOS on this base of functions

$$P(s) \sim \sum_n c_n \Psi_n(s) \tag{13}$$

- We obtain Z as

$$Z(\mu) \sim \sum_n \lambda_n c_n \Psi_n(\mu) \tag{14}$$

Lefschetz Thimble

- Let's consider integrals of the type

$$Z = \int_{-\infty}^{\infty} e^{-S(x)} dx \tag{15}$$

where $S(x)$ is holomorphyc.

- It is possible to deform the integration path in such a way that

$$Z = \sum_k m_k e^{-iS_{Im}(z_k)} \int_{J_k} dz e^{-S_{Re}(z)} \tag{16}$$

where z_k are the fixed point i.e.$\partial_z S = 0$. And J_k are the curves of steepest descent.

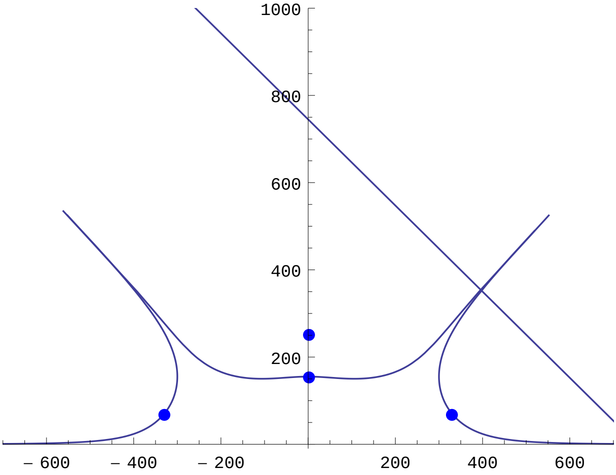
Lefschetz Thimble

- The curves of steepest descent are parametric curves in the complex plane given by the O.D.E.

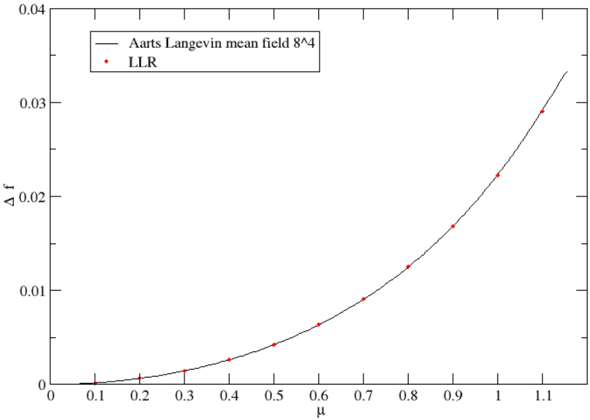
$$\dot{x} = -Re\left\{\partial_z S(z)\right\}, \quad \dot{y} = +Im\left\{\partial_z S(z)\right\} \tag{17}$$

- m_k is the number of intersections between the curves of steepest ascent and the original domain of integration.

Thimbles



Phase factor



Conclusions

- We presented an application of the LLR algorithm to a system with a severe sign problem.
- We believe that with this method we can extract meaningful observable at finite density, at least if the shape of the DOS is regular enough.
- Further studies and development are still needed to decide whether is useful also for more realistic cases.