Reducing the Sign Problem using Line Integrals

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Motivation

- Reduce the sign problem
- Some systems can be well approximated by expanding around the stable points
- Does not want to calculate the determinant or products of non-sparse matrices
- Does not require analytic continuation
- Sample along regions of importance
- Attempted solution:
  - Change sampling from a point to a line
- Many possible lines:
  - Follow lines where the imaginary part of the action is changing, such that oscillations will cancel out

Overview

- The path of the lines
- Sampling lines with equal probability
- The line Integral
- Cutoff on integral region
- Implementation
  - Usage example: 1D Quantum mechanical Anharmonic oscillator with x^4 potential
- https://arxiv.org/pdf/2205.02257.pdf

The path of the lines

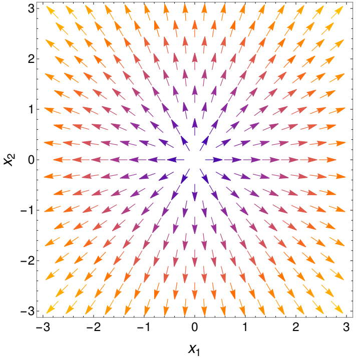
- Will focus on systems that can be written as

$$\langle O \rangle = \int d^N x \exp(-E(x)) \frac{O(x)}{\langle 1 \rangle}, \quad E \in \mathbb{C} \tag{1}$$

- Want to sample lines from which oscillations will cancel
- Solution: Follow the direction in which the imaginary part of the Energy or action E (depending on the system of interest) changes

$$\frac{\partial E_{im}(x)}{\partial x_j} \equiv F_j(x)$$
$$\frac{dx_j}{d\tau} = F_j(x)$$

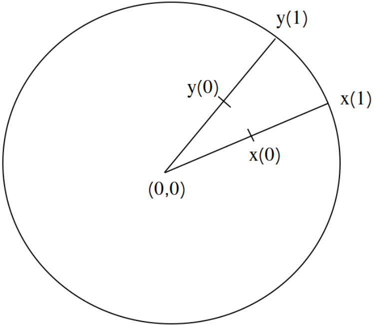
- Example on the right: $E = i(x_1^2 + x_2^2)$



Sampling lines with equal probability

- We need to make sure that every point is counted the same amount of times
- Include volume factor V_{rel} for how often a point is counted, compared to start position of line

- Example: $E = i(x_1^2 + x_2^2)$
- 2 Slightly different starting points $x(0)$ and $y(0)$
- At later time (1) the points are further separated
- Need to count contribution to line integral as $\left|\frac{x(1)}{x(0)}\right|$
- Similar to radial coordinates



Change in volume factor

- We look at the change of the unit vectors v under a infinitesimal change with the force

$$
\begin{aligned}
\left[dx_i(x+\epsilon_2 v) - dx_i(x)\right]/\epsilon_2 &= \\
\epsilon\left[F_i(x+\epsilon_2 v) - F_i(x)\right]/\epsilon_2 &= \epsilon \frac{\partial^2 E_{im}(x)}{\partial x_i \partial x_j} v_j + O(\epsilon_2) \\
\frac{V_{rel}(\tau+\epsilon)}{V_{rel}(\tau)} = \det\left[I_{ij} + \epsilon \frac{\partial^2 E_{im}(x(\tau))}{\partial x_i \partial x_j}\right] &= 1 + \epsilon \sum_{j=1}^{N} \frac{\partial^2 E_{im}(x(\tau))}{\partial^2 x_j} \\
&\quad + O(\epsilon^2)
\end{aligned} \tag{2}
$$

- The change of the volume factor is therefore proportional to the size of the lattice

$$
\frac{d \log(V_{rel}(\tau))}{d\tau} = \sum_{j=1}^{N} \frac{\partial^2 E_{im}(x(\tau))}{\partial^2 x_j} \tag{3}
$$

The line integral

- Collecting everything into an integral gives us

$$
\begin{aligned}
I_O(x_0) &= \int_{-\infty}^{\infty} O(x(s)) \exp\left[-E(x(s))\right] V_{rel}(s) ds \quad (4) \\
&= \int_{-\infty}^{\infty} O(x(\tau)) \exp\left[-E(x(\tau)) + \sum_{j=1}^{N} \int_0^{\tau} \frac{\partial^2 E_{im}(x(\tau'))}{\partial^2 x_j} d\tau'\right] |F(x_0)| d\tau
\end{aligned}
$$

- $x(\tau)$ is obtained by following the defined path in both positive and negative τ
- s is the distance traveled along the line

$$\frac{ds}{d\tau} = |F(x(\tau))| \quad (5)$$

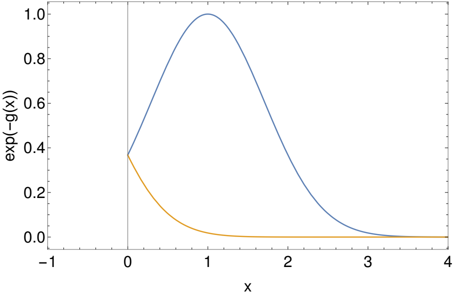
Cutoff the line integral

- We do not want to sample all the way out to infinity
- Cutoff integral with small trick

$$\int_{-\infty}^{\infty} \exp(-E(x))dx = \text{constant} \cdot \int_{-\infty}^{\infty} \exp(-\mathrm{E}(\mathrm{x}) - \mathrm{g}(\mathrm{s}))\mathrm{dxds} \quad (6)$$

$$= \text{constant} \cdot \int_{-\infty}^{\infty} \exp(-\mathrm{E}(\mathrm{x}+\mathrm{s}) - \mathrm{g}(\mathrm{s}))\mathrm{dxds} \quad (7)$$

- Example with $g(s) = s^2$, starting at $x = 1$
- In case a stable point is hit, direction of integration should be reversed, but s should keep increasing



Implementation

- The entire procedure can be implemented as a set of differential equations

$$F_j(x) = \frac{\partial E_{im}}{\partial x_j} = \frac{dx_j}{d\tau} \tag{8}$$

$$\frac{ds}{d\tau} = \sqrt{\sum_{j=1}^{N} F_j(x)^2} \tag{9}$$

$$\frac{dJ}{d\tau} = \sum_{j=1}^{N} \frac{\partial^2 E_{im}}{\partial^2 x_j} \tag{10}$$

$$\frac{dI_O}{d\tau} = O(x(\tau))e^{-E(x(\tau))-g(s)+J}|F(x_0)| \tag{11}$$

$$I_O = I_O(\tau = \infty) - I_O(\tau = -\infty) \tag{12}$$

- We have defined $J = \log(V_{rel}(\tau))$
- $|F(x_0)|$ can be absorbed into the initial conditions of J
- We will use $g(s) = (s/\sigma)^2$

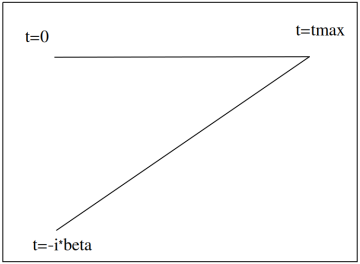
Example: 1d anharmonic oscillator

- As an example of its usage we calculate the correlator for

$$< O > \; = \; Tr(e^{-\beta H} x e^{-itH} x e^{itH}) / Tr(e^{-\beta H}) \quad (13)$$

$$H \; = \; \frac{p^2}{2} + \frac{x^2}{2} + \frac{\lambda x^4}{4!} \quad (14)$$

- We will look at the strongly coupled case $\lambda = 24$
- $\beta = 1.0$
- Compare with solution from discretizing x



Approach

- The force and double derivative becomes

$$
\begin{aligned}
\langle O \rangle &= \int d^N x \exp\left(\sum_{j=1}^{N} i[\frac{(x_j - x_{j+1})^2}{2a_j} - \frac{(a_j + a_{j-1})}{2}(\frac{x_j^2}{2} + \frac{\lambda x_j^4}{4!})] \right) \frac{O(x)}{\langle 1 \rangle} \\
E &= -\sum_{j=1}^{N} i[\frac{(x_j - x_{j+1})^2}{2a_j} - \frac{(a_j + a_{j-1})}{2}(\frac{x_j^2}{2} + \frac{\lambda x_j^4}{4!})] \\
\frac{\partial E_{im}}{\partial x_j} &= -Im\left(i[\frac{(x_j - x_{j+1})}{a_j} + \frac{(x_j - x_{j-1})}{a_{j-1}} - \frac{(a_j + a_{j-1})}{2}(x_j + \frac{\lambda x_j^3}{3!})] \right) \\
\frac{\partial^2 E_{im}}{\partial^2 x_j} &= -Im\left(i[\frac{1}{a_j} + \frac{1}{a_{j-1}} - \frac{(a_j + a_{j-1})}{2}(1 + \frac{\lambda x_j^2}{2})] \right)
\end{aligned}
$$

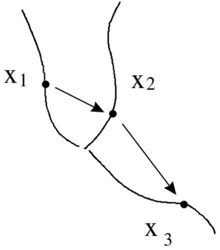
Importance Sampling

$$\langle O \rangle = \frac{\int d^N x I_O(x)}{\int d^N x I_1(x)} = \frac{\int d^N x |I_1(x)| \times I_O(x)/|I_1(x)|}{\int d^N x |I_1(x)| \times I_1(x)/|I_1(x)|} \quad (15)$$

- We will sample on the start position of the line using the metropolis algorithm

$$\langle O \rangle = \frac{\sum_j I_O(x_j)/|I_1(x_j)|}{\sum_j I_1(x_j)/|I_1(x_j)|}$$

$$O = x(0)x(t)$$

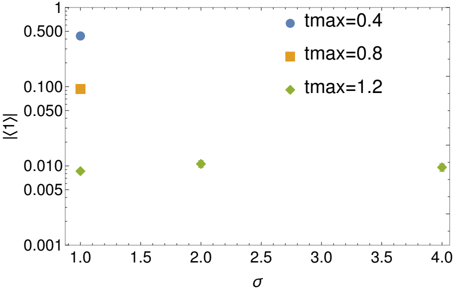


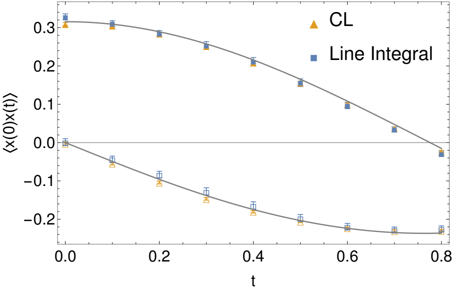
- The subscript O indicates the observable included in the line integral and j indicates the j'th measurement
- We define the average phase $\langle 1 \rangle$ as

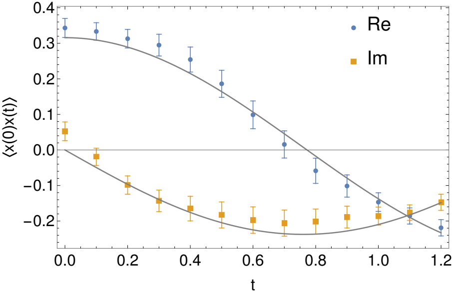
$$\langle 1 \rangle = \sum_j I_1(x_j)/|I_1(x_j)| \quad (16)$$

Correlator

- $\langle x(0)x(t)\rangle$
- Correlator is possible up around $t = 1.2$
- Average sign becomes too small afterwards

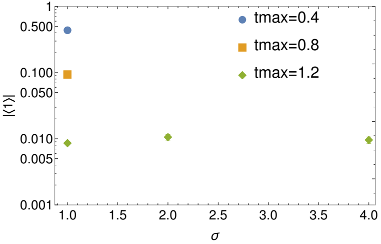






Summary

- We have defined a set of line integrals whose sum adds up to the original integral
- The lines are defined such that oscillations cancels out
- The lines can be implemented using standard ordinary differential equations



- Shown example of strongly coupled anharmonic oscilator
- Cost due to average sign and other hidden cost like precision limits us currently to $t_{max} = 1.2$
- Still room for optimization