Problem Set 8 Solution

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1 Problem 1

1.1

We consider $J(q,t)$ as a function describing the instant fraction of particles passing point q at a given time. Specifically, $J(q_B,t)$ describes the leaving probability density at q_B, as we regard q_B as an absorption state. Thus ϕ_B is the total probability left from q_B across time, which is the splitting probability. $p(q,0)$ shows the initial case where the starting point is q_0 or not, yet $p(q_A,t)$ and $p(q_B,t)$ only show that both q_A and q_B are absorbing states.

1.2

$$\int_0^\infty dt\frac{dp}{dt} = -\int_0^\infty dt\frac{\partial J(q,t)}{\partial t}$$
$$p(q,\infty) - p(q,0) = -\int_0^\infty dt\frac{\partial J(q,t)}{\partial t}$$
$$p(q,\infty) - \delta(q-q_0) = -\int_0^\infty dt\frac{\partial J(q,t)}{\partial t}$$
$$\delta(q-q_0) = \int_0^\infty dt\frac{\partial J(q,t)}{\partial t}$$

as in infinite amount of time all probability density is extinct due to non-zero probability of edge cases.

1.3

$$\int_q^{q_B} \delta(q-q_0) = \int_0^\infty dt\int_q^{q_B} dx\frac{\partial J(x,t)}{\partial x}$$
$$\Theta(q_0,q) = \phi_B(q_0) - \int_0^\infty dtJ(q,t)$$

Splitting probability occurs.

1.4

$$\int_{q_A}^{q_B} dq\Theta(q_0, q) = \int_{q_A}^{q_0} dq e^{\beta w(q)}$$

$\int_0^\infty dtJ(q,t)$ is zero when integrated after multiplied by Boltzmann factor, since the Boltzmann factor cancels from the definition of J in (2), and thus the integration of such an odd function becomes zero, and the only thing left is $\phi_B \int_{q_A}^{q_B} dq e^{\beta w(q)}$, and thus

$$\phi_B = \int_{q_A}^{q_0} dq e^{\beta w(q)} / \int_{q_A}^{q_B} dq e^{\beta w(q)}$$

1.5

Plug in the error function, we finalize the result to be

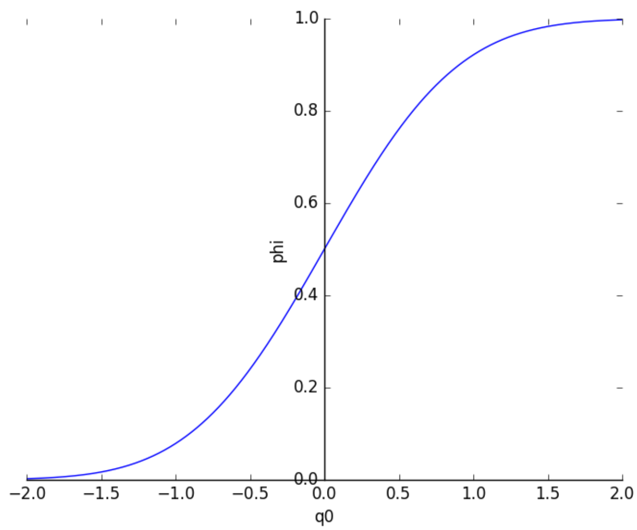
$$1 - \frac{1}{2} erfc(-\sqrt{\frac{1}{2}\beta m\omega} q_0)$$

as erfc($-\infty$) is simply 2.

1.6

In this graph below, we discover the crossover region (between 0.1 and 0.9) to be $[-\frac{1}{\sqrt{\frac{1}{2}m\omega^2/k_BT}}, \frac{1}{\sqrt{\frac{1}{2}m\omega^2/k_BT}}]$. Such crossover region should be within a k_BT of the peak of barrier.

function.png limmer lab/error function.png



2 Problem 2

2.1

Notice the definition of R,

$$\gamma(q(t+\Delta t)-q(t))/\Delta t = -\frac{dw}{dq}+\eta$$

$$q(t+\Delta t) = q(t) - \frac{1}{\gamma}\frac{dw}{dq}\Delta t + R$$

2.2

$$< R^2 >=< \gamma^{-1}\int_t^{t+\Delta t} dt'\gamma^{-1}\int_t^{t+\Delta t} dt''\eta(t')\eta(t'') >$$

$$= \gamma^{-2}\int_t^{t+\Delta t}\int_t^{t+\Delta t} dt'dt'' < \eta(t')\eta(t'') >$$

$$= \gamma^{-1}\int_t^{t+\Delta t}\int_t^{t+\Delta t} dt'dt'' 2k_BT\delta(t'-t'')$$

$$= 2k_BT\Delta t/\gamma$$

$$= 2D\Delta t$$

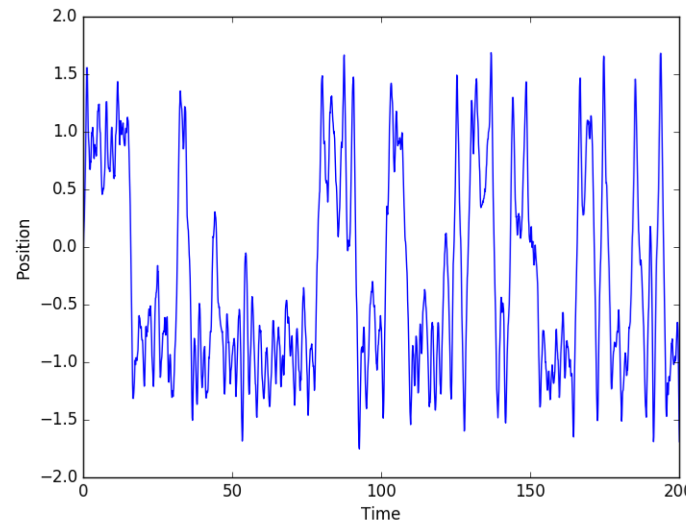
2.3

In this case, from $\gamma\dot{q} = -\frac{dw}{dq}+\eta = \overline{F}+\eta$, we integrate left side to get

$$q(t)-q(0) = \eta^{-1}\overline{F}t + \eta^{-1}\int_0^t dt'\eta(t')$$

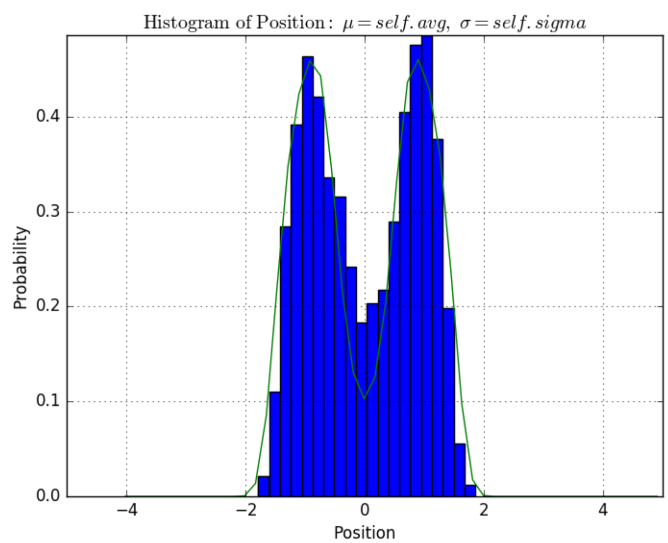
Since $\beta = \frac{1}{k_BT}$ and $D = \frac{1}{\beta\gamma}$, $< q(t)-q(0) > /t = \gamma^{-1}\overline{F} = \beta D\overline{F}$ as the average of η is 0 overall.

2.4



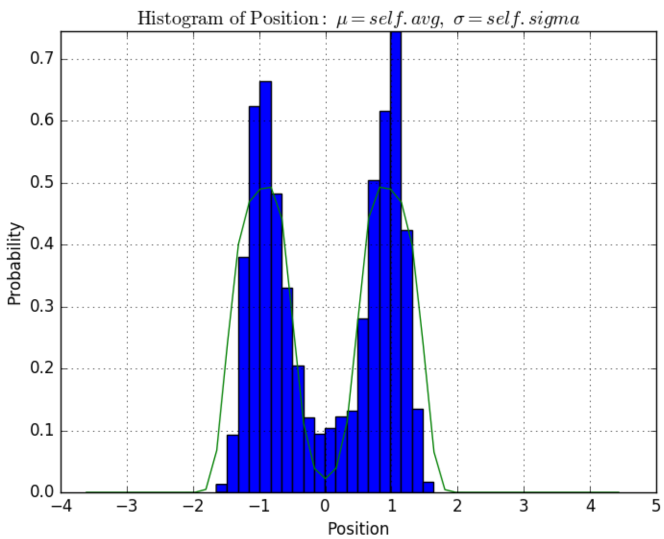
Simulation shows 10000 repeats with $\Delta t = 0.001$

2.5

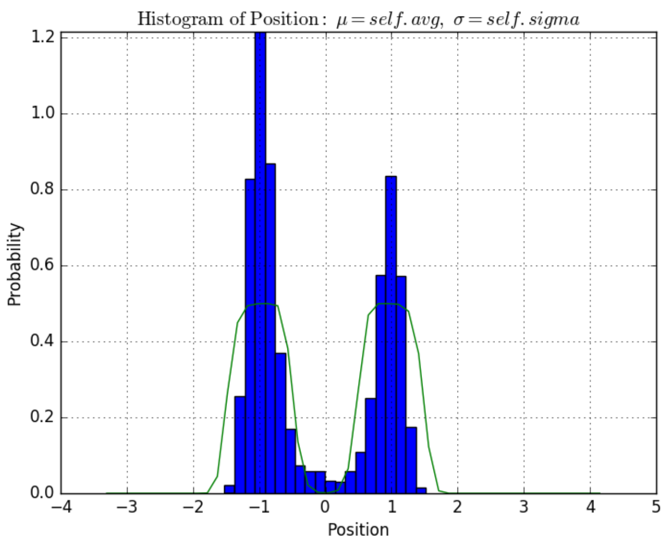


Histogram of q from the data above

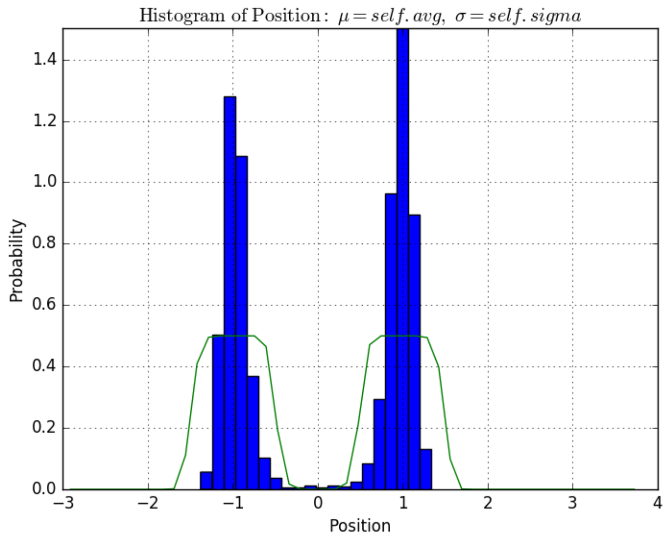
2.6



$k_B T = 0.2$



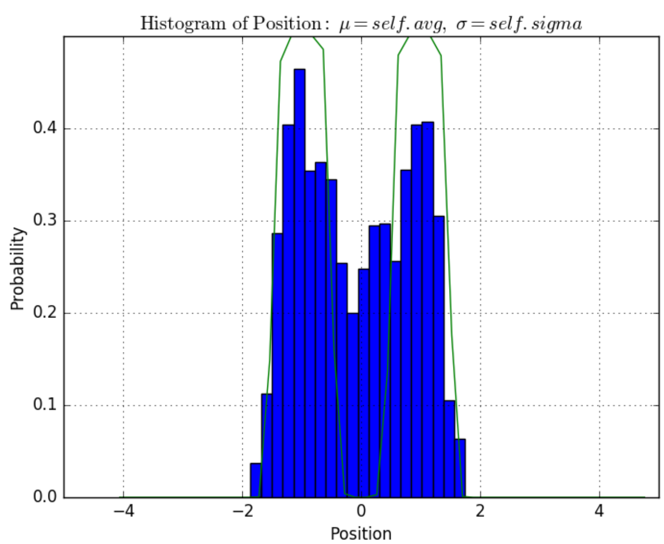
$k_B T = 0.1$



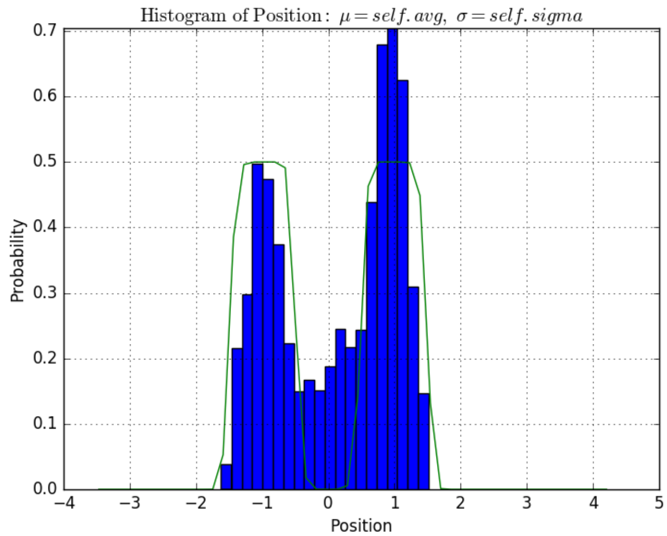
$k_B T = 0.05$

The middle barrow increases with smaller $k_B T$ and the peak height becomes sharper. I expect coherency of Boltzmann distribution and Langevin, and the algorithm sounds inaccurate for the Boltzmann distribution. Similar situation applies in next question, which the error should increase with increasing Δt.

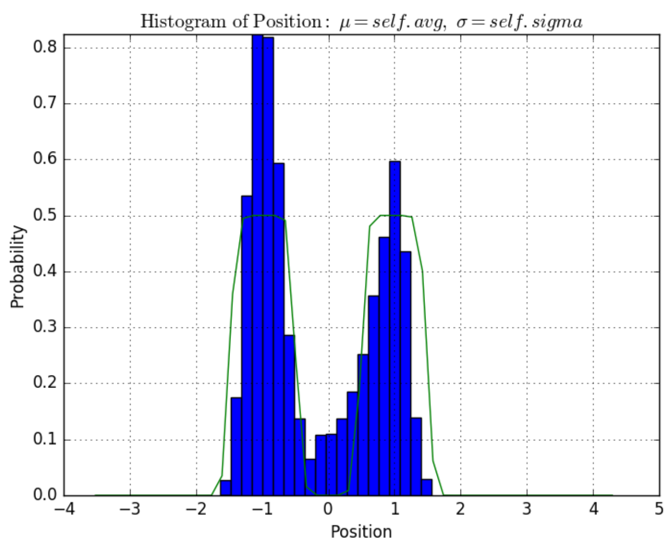
2.7



$\Delta t = 0.01$



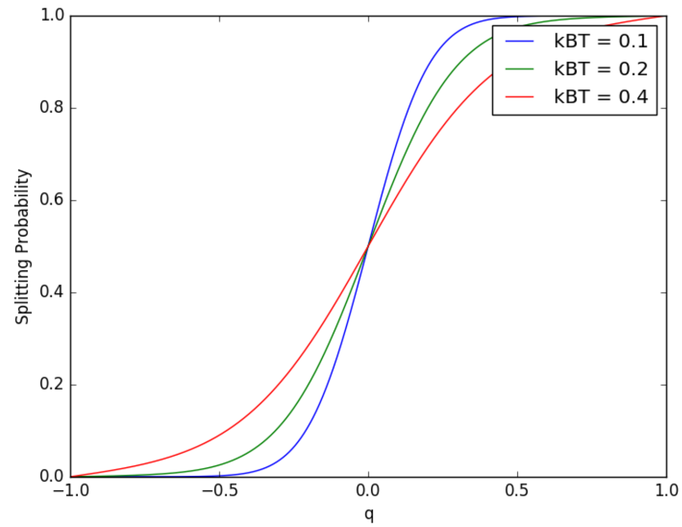
$\Delta t = 0.02$



$\Delta t = 0.03$

3 Problem 3

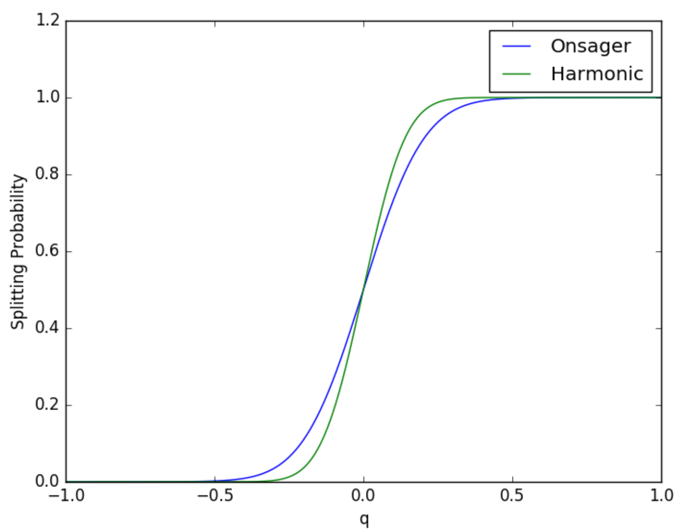
3.1



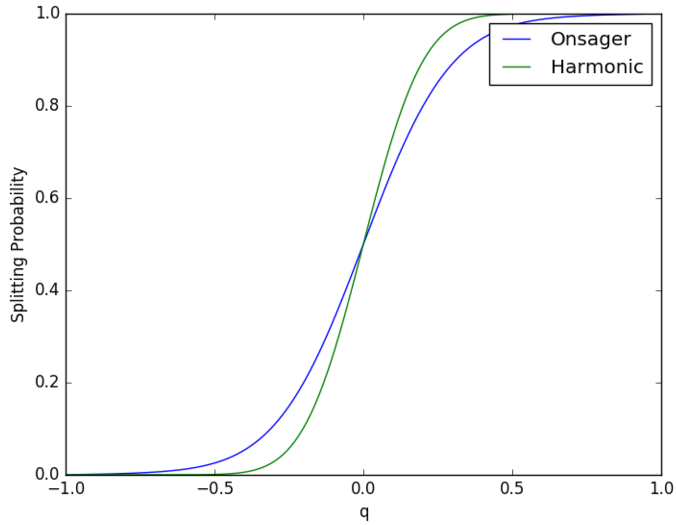
Splitting probability as a function of q_0:

3.2

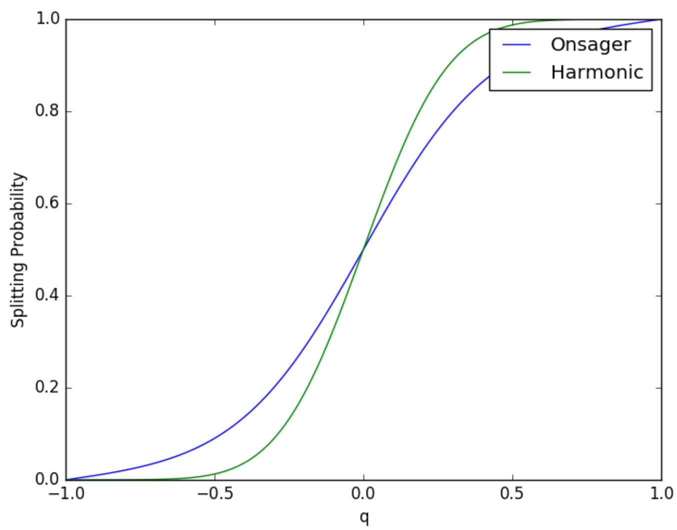
Comparison between Onsager and Harmonic Oscillator.



$k_B T = 0.1$


Onsager
Harmonic
Splitting Probability
q
1.0
0.8
0.6
0.4
0.2
0.0
−1.0
−0.5
0.0
0.5
1.0

$k_BT = 0.2$


Onsager
Harmonic
Splitting Probability
q
1.0
0.8
0.6
0.4
0.2
0.0
−1.0
−0.5
0.0
0.5
1.0

$k_BT = 0.4$