

Complex Langevin Dynamics in 3D XY Model

(Project Report)



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Abstract

In this project, we have investigated the three-dimensional XY model at finite chemical potential with the help of complex Langevin dynamics. The field configurations of the model were updated using complex Langevin evolution in the simulation time. We have computed the expectation values of the action density for different temperature and chemical potential values. The simulations were performed on a cubic lattice with volume 8^3 .

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Contents

1	Introduction	5
2	Complex Langevin Dynamics	5
2.1	Langevin Equations	5
2.2	Justification of the Complex Langevin Method	6
3	Complex Langevin Dynamics and the 3D XY Model	7
3.1	The Action of the Model	7
3.2	The Drift Terms	10
3.3	Discretized Langevin Equations	12
3.4	Adaptive Step Size	12
4	Simulation Results	13
5	Conclusions	17

1 Introduction

Theories having finite chemical potential or correspondingly complex action S have complex probability weight

$$p(\phi) \sim e^{-S(\phi)} = |e^{-S}|(\cos \theta + i \sin \theta), \quad (1.1)$$

which can be negative or positive, and thus importance sampling cannot be used. This situation makes it difficult for the use of the numerical nonperturbative treatment based on Monte Carlo. This problem known as the *sign problem*. New formulations have been used to evade the sign problem and one of such formulations is the *complex Langevin method*. In the complex Langevin method, when the action is complex, field configurations become complexified and they evolve according to the Langevin equations to reach an equilibrium value.

2 Complex Langevin Dynamics

2.1 Langevin Equations

In the complex Langevin method, if the field configuration is ϕ , then it evolves according to the equation given as

$$\frac{\partial \phi_x(t)}{\partial t} = -\frac{\delta S[\phi_x]}{\delta \phi_x} + \eta_x(t), \quad (2.1)$$

where η is a noise term and t is a fictitious time or the Langevin time.

Now when the action S becomes complex, the field ϕ is also complexified

$$\phi \rightarrow \phi^R + i\phi^I. \quad (2.2)$$

Now putting this in Eq. (2.1), we can get the following Langevin equations

$$\frac{\partial \phi_x^R(t)}{\partial t} = K_x^R + \sqrt{N_R} \eta_x^R(t), \quad K_x^R = -\operatorname{Re} \frac{\delta S[\phi_x]}{\delta \phi_x} \bigg|_{\phi_x \rightarrow \phi_x^R + i\phi_x^I} \quad (2.3)$$

and

$$\frac{\partial \phi_x^I(t)}{\partial t} = K_x^I + \sqrt{N_I} \eta_x^I(t), \quad K_x^I = -\operatorname{Im} \frac{\delta S[\phi_x]}{\delta \phi_x} \bigg|_{\phi_x \rightarrow \phi_x^R + i\phi_x^I}, \quad (2.4)$$

where the noise term follows the mathematical relations

$$N_R - N_I = 1, \quad (2.5)$$

$$\langle \eta_x^R(t) \rangle = \langle \eta_x^I(t) \rangle = \langle \eta_x^R(t) \eta_{x'}^I(t') \rangle = 0, \quad (2.6)$$

and

$$\langle \eta_x^R(t) \eta_{x'}^R(t') \rangle = \langle \eta_x^I(t) \eta_{x'}^I(t') \rangle = 2\delta_{xx'}\delta(t - t'). \quad (2.7)$$

In other words, the noise has mean 0 and standard deviation 2 (Gaussian noise). Now we take only the real noise into account and ignore the complex noise because it is shown that in the case of a complex noise, complex Langevin does not converge to the correct result.

2.2 Justification of the Complex Langevin Method

Let the configuration space be \mathcal{M} . Upon complexifying the fields, the space becomes $\mathcal{M}_{\mathcal{C}}$. Then $P[\phi^R, \phi^I, t]$ will be the probability density on $\mathcal{M}_{\mathcal{C}}$, which evolves according to the Fokker-Planck equation

$$\frac{\partial P[\phi^R, \phi^I, t]}{\partial t} = L^T P[\phi^R, \phi^I, t], \quad (2.8)$$

where L^T is the Fokker-Planck operator given by

$$L^T = \frac{\partial}{\partial \phi^R} \left[N_R \frac{\partial}{\partial \phi^R} - K^R \right] + \frac{\partial}{\partial \phi^I} \left[N_I \frac{\partial}{\partial \phi^I} - K^I \right]. \quad (2.9)$$

Now we can consider the complex probability density ρ in \mathcal{M} as well, which evolves according to the Fokker-Planck equation

$$\frac{\partial \rho[\phi, t]}{\partial t} = L_0^T \rho[\phi, t], \quad (2.10)$$

where L_0^T is the complex Fokker-Planck operator

$$L_0^T = \frac{\partial}{\partial \phi} \left[\frac{\partial}{\partial \phi} + \frac{\partial S}{\partial \phi} \right]. \quad (2.11)$$

Equation (2.11) has a stationary solution $\rho[\phi] \sim e^{-S}$.

Now looking at observables, in the case of the probability density $P[\phi^R, \phi^I, t]$, the expectation value of an observable O is given by

$$\langle O \rangle_{P(t)} = \frac{\int P[\phi^R, \phi^I, t] O[\phi^R + i\phi^I] d\phi^R d\phi^I}{\int P[\phi^R, \phi^I, t] d\phi^R d\phi^I} \quad (2.12)$$

and for the complex probability density ρ , the expectation value of an observable O is given by

$$\langle O \rangle_{\rho(t)} = \frac{\int \rho[\phi, t] O[\phi] d\phi}{\int \rho[\phi, t] d\phi}. \quad (2.13)$$

Now, for holomorphic observables with at most having exponential growth, under certain assumptions, it can be shown that

$$\langle O \rangle_{P(t)} = \langle O \rangle_{\rho(t)} \quad (2.14)$$

given the initial condition that

$$\langle O \rangle_{P(0)} = \langle O \rangle_{\rho(0)}. \quad (2.15)$$

In the limit of $t \rightarrow \infty$, the dependence on initial condition will disappear. Thus, in the infinite Langevin time limit, the noise averages of the observables become equal to quantum expectation values irrespective of the initial configuration. Thus, the applicability of the complex Langevin method is justified.

3 Complex Langevin Dynamics and the 3D XY Model

3.1 The Action of the Model

In the 3D XY model, the action at non-zero chemical potential is given by

$$\begin{aligned} S = & -\beta \sum_{x,y,z} \left[\cos(\phi_{x,y,z} - \phi_{x+1,y,z}) + \cos(\phi_{x,y,z} - \phi_{x,y+1,z}) \right. \\ & \left. + \cos(\phi_{x,y,z} - \phi_{x,y,z+1} - i\mu) \right], \end{aligned} \quad (3.1)$$

where (x, y, z) represents a lattice point at the position vector and $\phi_{x,y,z}$ lies in $(0, 2\pi)$.

The theory is defined for lattices of size $\Omega = N_T N_S^2$ where z direction is the temporal direction and x and y directions are spatial. Note the presence of chemical potential only in temporal direction. The theory undergoes a transition at vanishing chemical potential at critical value of $\beta_c = 0.45421$. When $\beta > \beta_c$, the phase is called ordered phase and when $\beta < \beta_c$, the phase is called disordered phase.

Now, by taking the field configurations to be complex, we get

$$\begin{aligned}
S = -\beta \sum_{x,y,z} & \left[\cos(\phi_{x,y,z}^R - \phi_{x+1,y,z}^R + i[\phi_{x,y,z}^I - \phi_{x+1,y,z}^I]) \right. \\
& + \cos(\phi_{x,y,z}^R - \phi_{x,y+1,z}^R + i[\phi_{x,y,z}^I - \phi_{x,y+1,z}^I]) \\
& \left. + \cos(\phi_{x,y,z}^R - \phi_{x,y,z+1}^R + i[\phi_{x,y,z}^I - \phi_{x,y,z+1}^I - \mu]) \right]. \quad (3.2)
\end{aligned}$$

As $\cos(A + iB) = \cos(A) \cosh(B) - \sin(A) \sinh(B)$, and by writing $S = S^R + iS^I$ we have

$$\begin{aligned}
S^R = -\beta \sum_{x,y,z} & \left[\cos(\phi_{x,y,z}^R - \phi_{x+1,y,z}^R) \cosh(\phi_{x,y,z}^I - \phi_{x+1,y,z}^I) \right. \\
& + \cos(\phi_{x,y,z}^R - \phi_{x,y+1,z}^R) \cosh(\phi_{x,y,z}^I - \phi_{x,y+1,z}^I) \\
& \left. + \cos(\phi_{x,y,z}^R - \phi_{x,y,z+1}^R) \cosh(\phi_{x,y,z}^I - \phi_{x,y,z+1}^I - \mu) \right]. \quad (3.3)
\end{aligned}$$

The code to compute the real part of the action is given below.

```

function S_r = realpartofaction(Phi_old_r, Phi_old_I, u, b,n)
    S_r = 0;
    for x = 1:n
        for y = 1:n
            for z = 1:n
                S_r = S_r + (-b) * ((cos(Phi_old_r(x,y,z) - Phi_old_r(modul((x + 1),n),y,z))) * (cosh(Phi_old_I(x,y,z) - Phi_old_I(modul((x + 1),n),y,z)))));
                S_r = S_r + (-b) * ((cos(Phi_old_r(x,y,z) - Phi_old_r(x,modul((y + 1),n),z))) * (cosh(Phi_old_I(x,y,z) - Phi_old_I(x,modul((y+1),n),z)))));
                S_r = S_r + (-b) * ((cos(Phi_old_r(x,y,z) - Phi_old_r(x,y,modul((z + 1),n)))) * (cosh(Phi_old_I(x,y,z) - Phi_old_I(x,y,modul((z + 1),n)) - u)))));
            end
        end
    end

function modss = modul(x,y)
    if mod(x,y) == 0
        modss = y;
    else
        modss = mod(x,y);
    end
end

```


We have the imaginary part of the action

$$S^I = -\beta \sum_{x,y,z} \left[\sin(\phi_{x,y,z}^R - \phi_{x+1,y,z}^R) \sinh(\phi_{x,y,z}^I - \phi_{x+1,y,z}^I) \right. \\ \left. + \sin(\phi_{x,y,z}^R - \phi_{x,y+1,z}^R) \sinh(\phi_{x,y,z}^I - \phi_{x,y+1,z}^I) \right. \\ \left. + \sin(\phi_{x,y,z}^R - \phi_{x,y,z+1}^R) \sinh(\phi_{x,y,z}^I - \phi_{x,y,z+1}^I - \mu) \right]. \quad (3.4)$$

When the equilibrium is reached, expectation value of the imaginary part of action, i.e., S^I tends to 0 and thus, only the real part accounts for the expectation value of the action.

The code to compute the imaginary part of the action is given below.

```
function S_I = imagpartofaction(Phi_old_r, Phi_old_I, u, b, n)
    S_I = 0;
    for x = 1:n
        for y = 1:n
            for z = 1:n
                S_I = S_I + (b) * ((sin(Phi_old_r(x,y,z) - Phi_old_r(modul((x + 1), n), y, z))) * (sinh(Phi_old_I(x,y,z) - Phi_old_I(modul((x + 1), n), y, z)))));
                S_I = S_I + (b) * ((sin(Phi_old_r(x,y,z) - Phi_old_r(x, modul((y + 1), n), z))) * (sinh(Phi_old_I(x,y,z) - Phi_old_I(x, modul((y+1), n), z)))));
                S_I = S_I + (b) * ((sin(Phi_old_r(x,y,z) - Phi_old_r(x,y, modul((z + 1), n)))) * (sinh(Phi_old_I(x,y,z) - Phi_old_I(x,y, modul((z + 1), n)) - u)))));
            end
        end
    end
end
```

Now, if chemical potential is of form $\mu = i\mu_I$, then the action becomes real and hence, real Langevin can be used in this case. We have

$$S_{\text{imag}} = -\beta \sum_{x,y,z} \left[\cos(\phi_{x,y,z} - \phi_{x+1,y,z}) + \cos(\phi_{x,y,z} - \phi_{x,y+1,z}) \right. \\ \left. + \cos(\phi_{x,y,z} - \phi_{x,y,z+1} + \mu_I) \right]. \quad (3.5)$$

The code to compute the real part of the action is given below.

```
function S_r = reallangevinaction(Phi_old_r, u, b, n)
    S_r = 0;
    for x = 1:n
        for y = 1:n
            for z = 1:n
                S_r = S_r + (-b) * (cos(Phi_old_r(x,y,z) - Phi_old_r(modul((x + 1), n), y, z)));
            end
        end
    end
end
```

```

        S_r = S_r + (-b) * (cos(Phi_old_r(x,y,z) - Phi_old_r(x,modul((y +
        1),n),z)));
        S_r = S_r + (-b) * (cos(Phi_old_r(x,y,z) - Phi_old_r(x,y,modul((z
        + 1),n)) + u));
    end
end
end
end

```

3.2 The Drift Terms

Now differentiating Eq. (3.1) with respect to $\phi_{x,y,z}$

$$\begin{aligned}
 \frac{\partial S}{\partial \phi_{x,y,z}} = & +\beta \left[\sin(\phi_{x,y,z} - \phi_{x+1,y,z}) + \sin(\phi_{x,y,z} - \phi_{x,y+1,z}) \right. \\
 & + \sin(\phi_{x,y,z} - \phi_{x,y,z+1} - i\mu) + \sin(\phi_{x,y,z} - \phi_{x-1,y,z}) \\
 & \left. + \sin(\phi_{x,y,z} - \phi_{x,y-1,z}) + \sin(\phi_{x,y,z} - \phi_{x,y,z-1} + i\mu) \right]. \quad (3.6)
 \end{aligned}$$

Now, by complexifying and using $\sin(A + iB) = \sin(A) \cosh(B) + i \cos(A) \sinh(B)$ we get

$$\begin{aligned}
 K_{x,y,z}^R = & -\text{Re} \frac{\partial S}{\partial \phi_{x,y,z}} \\
 = & -\beta \left[\sin(\phi_{x,y,z}^R - \phi_{x+1,y,z}^R) \cosh(\phi_{x,y,z}^I - \phi_{x+1,y,z}^I) \right. \\
 & + \sin(\phi_{x,y,z}^R - \phi_{x-1,y,z}^R) \cosh(\phi_{x,y,z}^I - \phi_{x-1,y,z}^I) \\
 & + \sin(\phi_{x,y,z}^R - \phi_{x,y+1,z}^R) \cosh(\phi_{x,y,z}^I - \phi_{x,y+1,z}^I) \\
 & + \sin(\phi_{x,y,z}^R - \phi_{x,y-1,z}^R) \cosh(\phi_{x,y,z}^I - \phi_{x,y-1,z}^I) \\
 & + \sin(\phi_{x,y,z}^R - \phi_{x,y,z+1}^R) \cosh(\phi_{x,y,z}^I - \phi_{x,y,z+1}^I - \mu) \\
 & \left. + \sin(\phi_{x,y,z}^R - \phi_{x,y,z-1}^R) \cosh(\phi_{x,y,z}^I - \phi_{x,y,z-1}^I + \mu) \right]. \quad (3.7)
 \end{aligned}$$

The real part of the gradient of the action is computed using the following code segment.

```

function gradSr = complexgradientreal(Phi_old_r,Phi_old_I,u,b,n)
%Initial configurations as Phi_old_r and Phi_old_I, chemical potential as u, beta
as b
%Making an array of size n*n*n with all entries as 0
gradSr = zeros(n,n,n);

for x = 1:n
    for y = 1:n

```

```

    for z = 1:n
        aax = (sin(Phi_old_r(x,y,z) - Phi_old_r(modul((x + 1),n),y,z))) *
            (cosh(Phi_old_I(x,y,z) - Phi_old_I(modul((x + 1),n),y,z)));
        bbx = (sin(Phi_old_r(x,y,z) - Phi_old_r(modul((x - 1),n),y,z))) *
            (cosh(Phi_old_I(x,y,z) - Phi_old_I(modul((x - 1),n),y,z)));

        aay = (sin(Phi_old_r(x,y,z) - Phi_old_r(x,modul((y + 1),n),z))) *
            (cosh(Phi_old_I(x,y,z) - Phi_old_I(x,modul((y + 1),n),z)));
        bby = (sin(Phi_old_r(x,y,z) - Phi_old_r(x,modul((y - 1),n),z))) *
            (cosh(Phi_old_I(x,y,z) - Phi_old_I(x,modul((y - 1),n),z)));

        aaz = (sin(Phi_old_r(x,y,z) - Phi_old_r(x,y,modul((z + 1),n)))) *
            (cosh(Phi_old_I(x,y,z) - (u) - Phi_old_I(x,y,modul((z + 1),n))));
        bbz = (sin(Phi_old_r(x,y,z) - Phi_old_r(x,y,modul((z - 1),n)))) *
            (cosh(Phi_old_I(x,y,z) + (u) - Phi_old_I(x,y,modul((z - 1),n))));

        gradSr(x,y,z) = (-b) * (aax + bbx + aay + bby + aaz + bbz);
    end
end
end
end

```

We have the imaginary part of the gradient

$$\begin{aligned}
 K_{x,y,z}^I &= -\text{Im} \frac{\partial S}{\partial \phi_{x,y,z}} \\
 &= -\beta \left[\cos(\phi_{x,y,z}^R - \phi_{x+1,y,z}^R) \sinh(\phi_{x,y,z}^I - \phi_{x+1,y,z}^I) \right. \\
 &\quad + \cos(\phi_{x,y,z}^R - \phi_{x-1,y,z}^R) \sinh(\phi_{x,y,z}^I - \phi_{x-1,y,z}^I) \\
 &\quad + \cos(\phi_{x,y,z}^R - \phi_{x,y+1,z}^R) \sinh(\phi_{x,y,z}^I - \phi_{x,y+1,z}^I) \\
 &\quad + \cos(\phi_{x,y,z}^R - \phi_{x,y-1,z}^R) \sinh(\phi_{x,y,z}^I - \phi_{x,y-1,z}^I) \\
 &\quad + \cos(\phi_{x,y,z}^R - \phi_{x,y,z+1}^R) \sinh(\phi_{x,y,z}^I - \phi_{x,y,z+1}^I - \mu) \\
 &\quad \left. + \cos(\phi_{x,y,z}^R - \phi_{x,y,z-1}^R) \sinh(\phi_{x,y,z}^I - \phi_{x,y,z-1}^I + \mu) \right]. \quad (3.8)
 \end{aligned}$$

The imaginary part of the gradient of the action is computed using the following code segment.

```

function gradSi = complexgradientimag(Phi_old_r,Phi_old_I,u,b,n)
%Initial configurations as Phi_old_r and Phi_old_I, chemical potential as u, beta
as b
%Making an array of size n*n*n with all entries as 0
gradSi = zeros(n,n,n);

    for x = 1:n
        for y = 1:n
            for z = 1:n
                ccx = (cos(Phi_old_r(x,y,z) - Phi_old_r(modul((x + 1),n),y,z))) *
                    (sinh(Phi_old_I(x,y,z) - Phi_old_I(modul((x + 1),n),y,z))));
            end
        end
    end
end

```

```

        ddx = (cos(Phi_old_r(x,y,z) - Phi_old_r(modul((x - 1),n),y,z))) *
              (sinh(Phi_old_I(x,y,z) - Phi_old_I(modul((x - 1),n),y,z))));

        ccy = (cos(Phi_old_r(x,y,z) - Phi_old_r(x,modul((y + 1),n),z))) *
              (sinh(Phi_old_I(x,y,z) - Phi_old_I(x,modul((y + 1),n),z))));
        ddy = (cos(Phi_old_r(x,y,z) - Phi_old_r(x,modul((y - 1),n),z))) *
              (sinh(Phi_old_I(x,y,z) - Phi_old_I(x,modul((y - 1),n),z))));

        ccz = (cos(Phi_old_r(x,y,z) - Phi_old_r(x,y,modul((z + 1),n)))) *
              (sinh(Phi_old_I(x,y,z) - Phi_old_I(x,y,modul((z + 1),n)) - u));
        ddz = (cos(Phi_old_r(x,y,z) - Phi_old_r(x,y,modul((z - 1),n)))) *
              (sinh(Phi_old_I(x,y,z) - Phi_old_I(x,y,modul((z - 1),n)) + u));

        gradSi(x,y,z) = (-b) * (ccx + ddx + ccy + ddy + ccz + ddz);

    end
end
end
end

```

3.3 Discretized Langevin Equations

Integrating the Langevin equations by discretizing Langevin time as $t = n\epsilon_n$, we get

$$\phi_{x,y,z}^R(n+1) = \phi_{x,y,z}^R(n) + \epsilon_n K_{x,y,z}^R + \sqrt{\epsilon_n} \eta_{x,y,z}, \quad (3.9)$$

$$\phi_{x,y,z}^I(n+1) = \phi_{x,y,z}^I(n) + \epsilon_n K_{x,y,z}^I. \quad (3.10)$$

The code segment implementing this is given below.

```

function Phi_new_r = complexlangevinreal(Phi_old_r, gradSr, epsilon, eta, n)
    Phi_new_r = zeros(n,n,n);
    Phi_new_r = Phi_old_r + (epsilon * gradSr) + power(epsilon,0.5) * eta;
end

function Phi_new_I = complexlangevinimag(Phi_old_I, gradSi, epsilon, n)
    Phi_new_I = zeros(n,n,n);
    Phi_new_I = Phi_old_I + (epsilon * gradSi);
end

```

Note that, only real noise is used and this real noise is different for each lattice point.

3.4 Adaptive Step Size

Equations (3.7) and (3.8) clearly do not have upper bounds and thus problems like runaways (field configurations going to infinity) can occur. In order to avoid this problem, adaptive step size is introduced, which is computed at each time step as

$$\epsilon_n = \min \left\{ \epsilon, \epsilon \frac{\langle K^{\max} \rangle}{K_n^{\max}} \right\}, \quad (3.11)$$

where

$$K_n^{\max} = \max_{x,y,z} |K_{x,y,z}^R + iK_{x,y,z}^I|. \quad (3.12)$$

Here ϵ is targeted step size and $\langle K^{\max} \rangle$ is expected value of K^{\max} .

```
function epsilon1 = adaptivestepsize(avgKmax, Kmax , targetedstepsize)
    epsilon1 = 0;
    if Kmax > avgKmax
        epsilon1 = targetedstepsize * (avgKmax/Kmax);
    else
        epsilon1 = targetedstepsize;
    end
end
```

4 Simulation Results

In Fig. 1 we show the Langevin time history of the real part of the action density for various β values for the case $\mu^2 = 0$.

In Fig. 2 we show the Langevin time history of the imaginary part of the action density for various β values for the case $\mu^2 = 0$.

In Fig. 3 we show the expectation value of the action density against the square of the chemical potential for different β values.

5 Conclusions

Complex Langevin method seems to work well for large β values while it fails to produce correct results for small β values ($\beta < 0.5$), which can be seen by the disagreement between the real Langevin and complex Langevin for the expectation values of the action density at $\mu^2 = 0$.

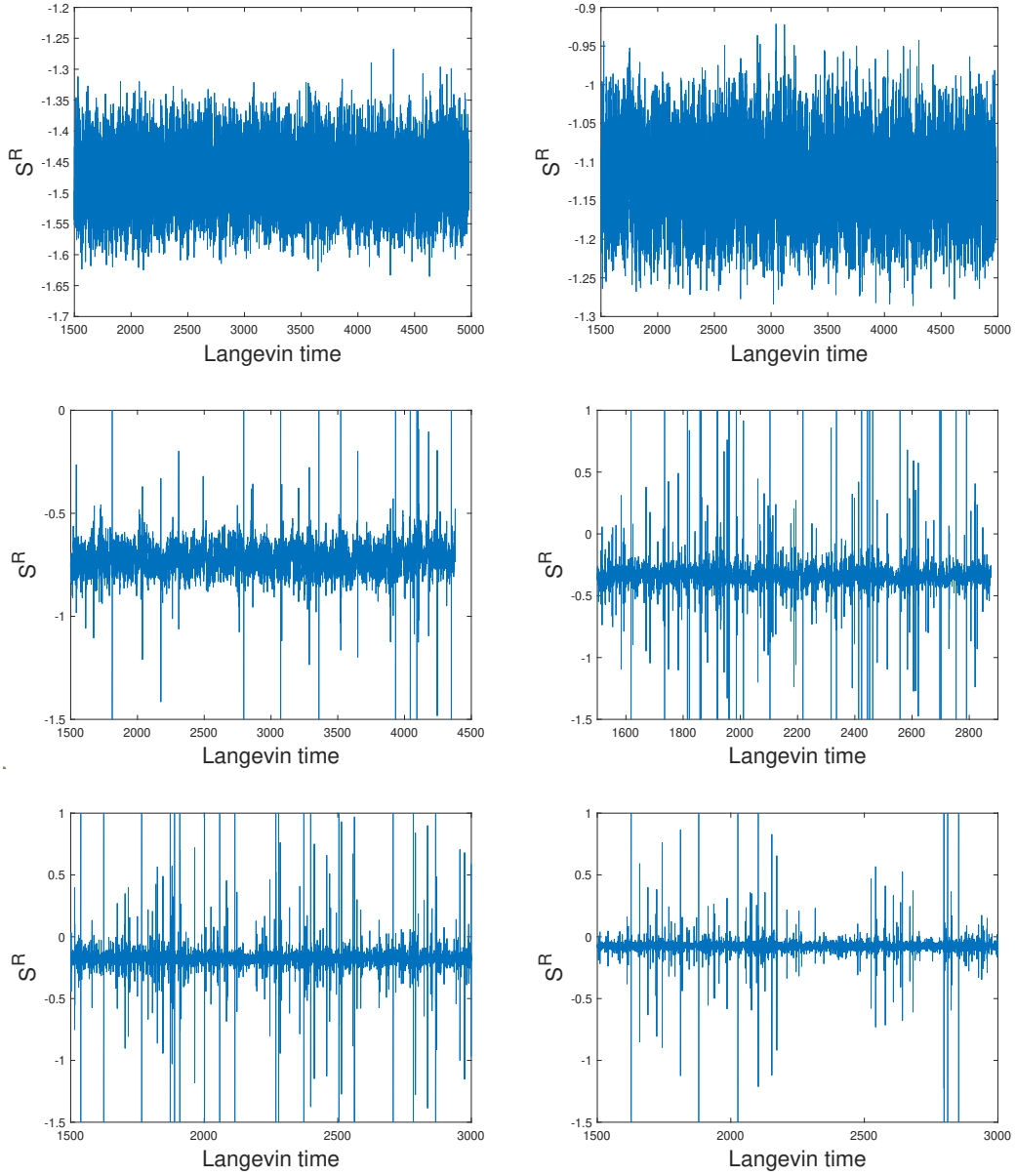


Figure 1: Real part of the action density is plotted against the Langevin time after equilibrium is reached. Simulations are performed at $\mu^2 = 0$. (a) $\beta = 0.7$ (top left) (b) $\beta = 0.6$ (top right) (c) $\beta = 0.5$ (middle left) (d) $\beta = 0.4$ (middle right) (e) $\beta = 0.3$ (bottom left) (f) $\beta = 0.2$ (bottom right).

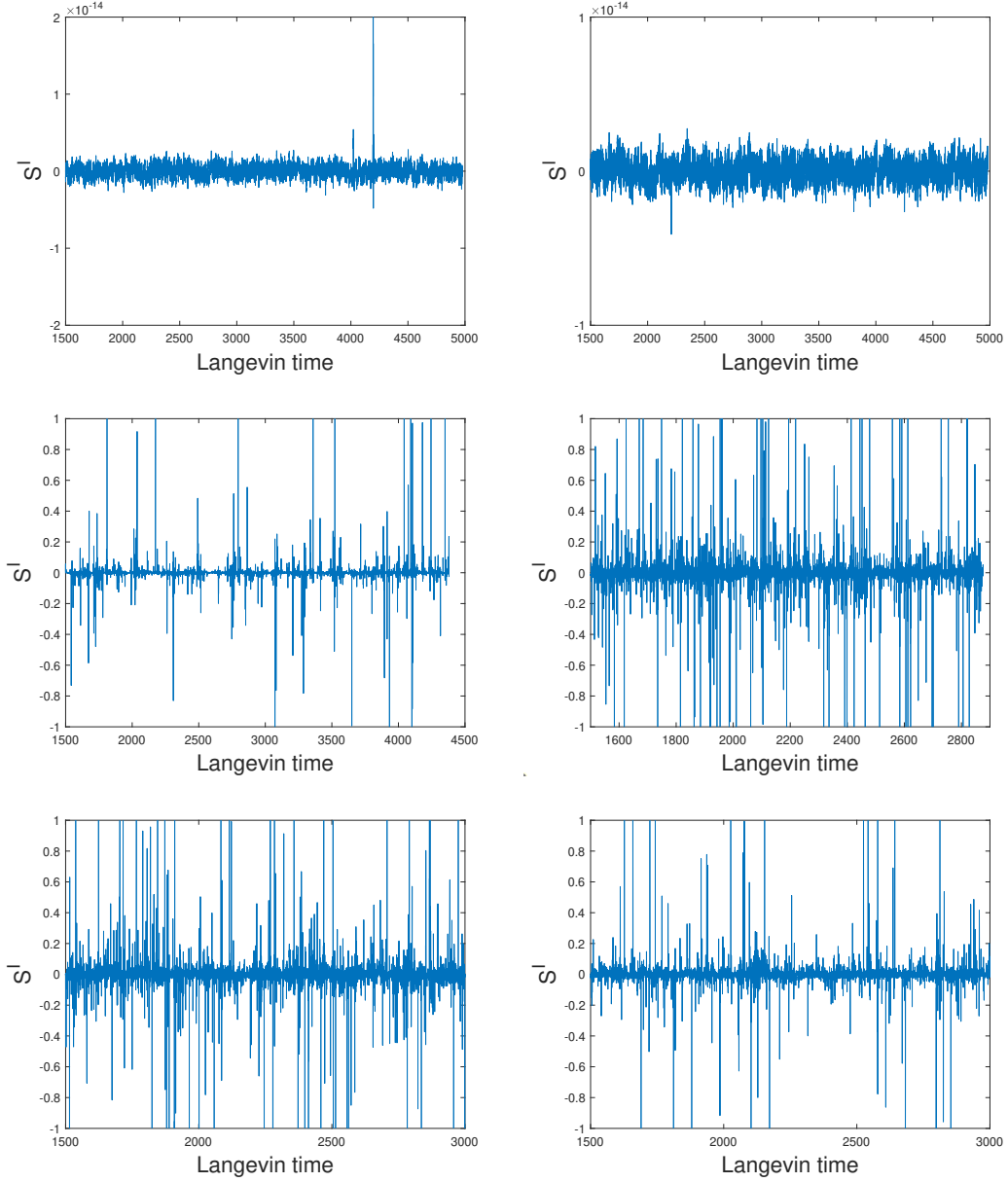


Figure 2: Imaginary part of the action density is plotted against the Langevin time after equilibrium is reached. Simulations are performed at $\mu^2 = 0$. (a) $\beta = 0.7$ (top left) (b) $\beta = 0.6$ (top right) (c) $\beta = 0.5$ (middle left) (d) $\beta = 0.4$ (middle right) (e) $\beta = 0.3$ (bottom left) (f) $\beta = 0.2$ (bottom right).

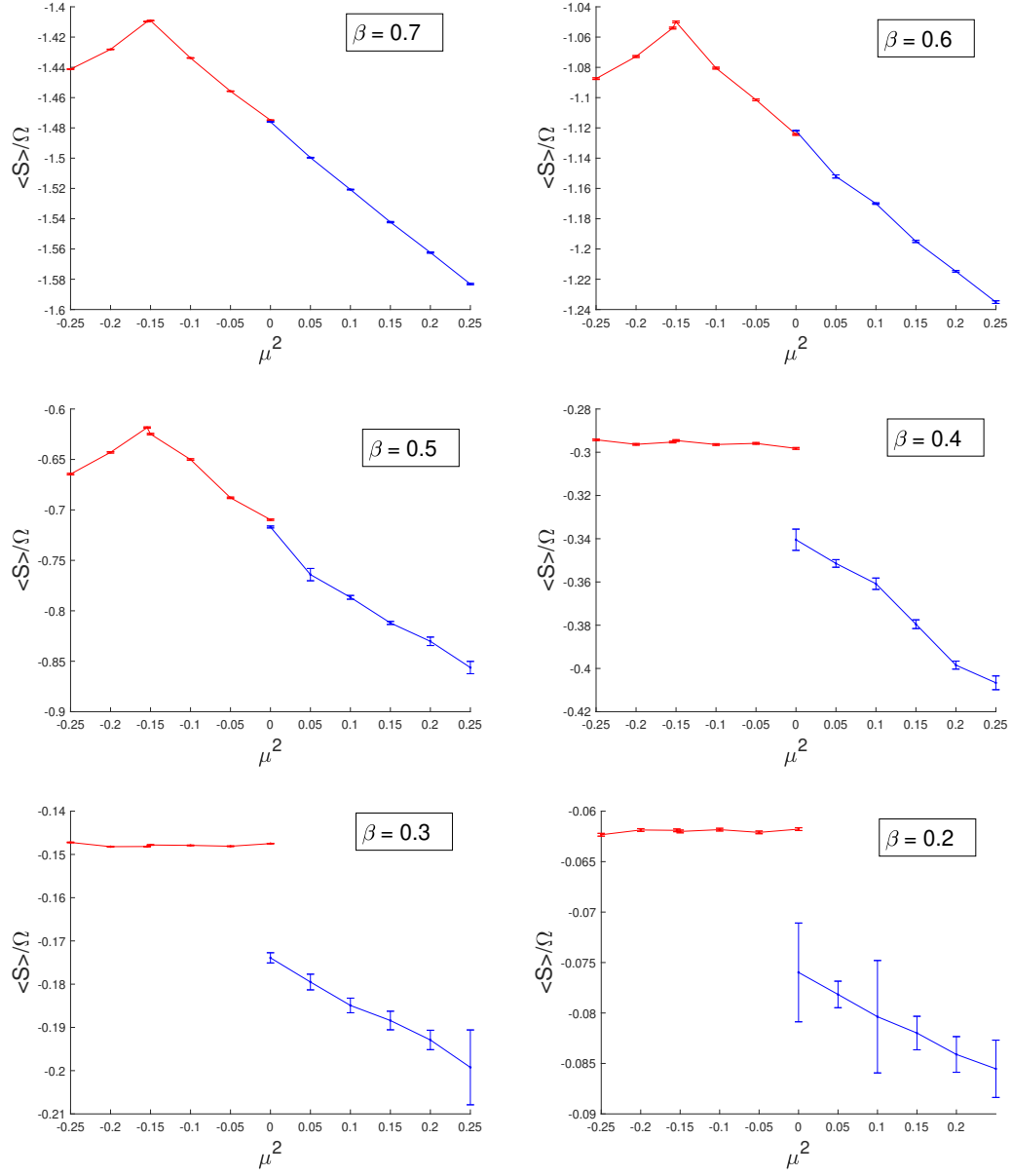


Figure 3: The expectation value of the action density is plotted against the square of the chemical potential for different β values.

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