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On the modification of the lattice action

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Abstract. We show the importance of the quadratic term in the lattice action for Monte Carlo simulations. The effects of this action modification are analysed through the calculations of some simple non-relativistic quantum systems.

Feynman introduced the path integral formulation of quantum mechanics in 1948 [1]. Since that time path integrals have been used in many areas of physics. In an imaginary time formulation, Feynman's path integral reveals a connection between classical statistical mechanics and quantum theory. In particular, in this formulation, the quantum propagator is mathematically equivalent to a statistical partition function. This analogy is the basis for a wide application of Monte Carlo techniques in simulation of different quantum systems. The simulation is actually the numerical evaluation of path integrals. Although it seems that the main results have been achieved in lattice gauge field theories, it is very interesting to also test these ideas in simpler models, such as one-dimensional Schrödinger systems, as was shown by Creutz and Freedman [2]. The main reason for this interest is the desire for a better understanding of the workings of the Monte Carlo method.

In this paper we communicate a result about the importance of the quadratic term in the lattice action for non-relativistic quantum systems, when the partition function is calculated by using the Monte Carlo method. Under specific conditions, this modification significantly reduces the dimension of the lattice considered or, equivalently, the dimensions of computed integrals. We show that the quadratic term in the lattice action is important when the potential is a steep function in the lattice spacing units. However, this rapid change should take place in the domain where the position probability for the moving particle is appreciable. Also , this modification is invariant under the transformations which are symmetries of the Feynman path integral procedure.

We start by a series expansion of the transition amplitude for a short time period ε

$$K(x, x'; \varepsilon) = \delta(x'-x) - i\varepsilon\langle x'|H|x\rangle + \tfrac{1}{2}(-i\varepsilon)^2\langle x'|H^2|x\rangle + \dots \tag{1}$$

where for the one-dimensional system we assume

$$\langle x'|H|x\rangle = \int \frac{dp}{2\pi}[\tfrac{1}{2}p^2 + \tfrac{1}{2}(V(x') + V(x))]\exp[ip(x'-x)] \tag{2}$$

and

$$\langle x'|H^2|x\rangle = \int \frac{dp}{2\pi}[\tfrac{1}{4}p^4 + \tfrac{1}{2}(V(x') + V(x))^2p^2 + V(x')V(x)]\exp[ip(x'-x)]. \tag{3}$$

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By inserting (2) and (3) in the transition amplitude given by (1), we obtain an expansion which includes the quadratic term in ε:

$$K(x, x'; \varepsilon) = \int \frac{dp}{2\pi} \{1 - i\varepsilon[\tfrac{1}{2}p^2 + \tfrac{1}{2}(V(x') + V(x))] + \tfrac{1}{2}(-i\varepsilon)^2[\tfrac{1}{4}p^4 + \tfrac{1}{2}(V(x') + V(x))^2 p^2 + V(x')V(x)] + \dots\} \exp[ip(x' - x)]. \tag{4}$$

On the other hand, one can formally express the transition amplitude by the action modification through the ε^2 term in the form

$$K(x, x'; \varepsilon) = \int \frac{dp}{2\pi} \exp\{ip(x' - x) - i\varepsilon[\tfrac{1}{2}p^2 + \tfrac{1}{2}(V(x') + V(x)) + i\varepsilon Q]\}. \tag{5}$$

Comparison of (4) and (5) gives the following expression for the modification Q:

$$Q = \tfrac{1}{2}[\tfrac{1}{2}(V(x') - V(x))]^2. \tag{6}$$

Now, in the Euclidean (imaginary time) version of the discrete time lattice, the transition amplitude given by (5) with Q defined by (6) becomes

$$F(x', t' | x, t) = \int (Dx) \exp(-S) \tag{7}$$

where

$$S = S_0 + S_2. \tag{7a}$$

The standard action S_0 is

$$S_0 = a \sum_j \{\tfrac{1}{2}m[(x_j - x_{j-1})/a]^2 + \tfrac{1}{2}(V(x_j) + V(x_{j-1}))\} \tag{8}$$

and the modification term S_2, which is formally quadratic in the lattice spacing a, is

$$S_2 = \tfrac{1}{2}a^2 \sum_j [\tfrac{1}{2}(V(x_j) - V(x_{j-1}))]^2. \tag{9}$$

Here we have introduced the standard notation for a discrete lattice:

$$t_{j+1} - t_j = a/i$$
$$x(t_j) = x_j \tag{10}$$
$$t' - t = N\varepsilon$$

and $j = 0, \dots, N$.

In the naive $a \to 0$ limit, the action S simply becomes S_0. Also, the modification term S_2 is negligible if

$$\frac{a[\tfrac{1}{2}(V(x_j) - V(x_{j-1}))]^2}{m[(x_j - x_{j-1})/a]^2 + V(x_j) + V(x_{j-1})} \ll 1. \tag{11}$$

By using the fact that $\langle (x_j - x_{j-1})^2 \rangle = a/m$ in the $a \to 0$ limit, we can recast the condition (11) in the form

$$\frac{a^3 |(d/dx)V(x)|^2}{4m|1 + 2aV(x)|} \ll 1. \tag{12a}$$

The generalisation of the condition (12*a*) for the three-dimensional case is

$$\frac{a^3|\text{grad } V(r)|^2}{4m|3+2aV(r)|} \ll 1. \tag{12b}$$

It is interesting to notice the invariance of the condition (12*a*) under the scaling transformations

$$\begin{aligned} x' &= \lambda x \qquad & V'(x') &= gV(x) \\ m' &= m/g\lambda^2 \qquad & a' &= a/g \end{aligned} \tag{13}$$

where λ and γ are arbitrary parameters. It is very easy to check that the ground-state energy E shows the scaling law under the transformations given by (13), namely

$$E' = gE.$$

As a demonstration of the effects of the modified action in practical Monte Carlo simulations we present some results for the ground states of the Coulomb and exponential potentials. Our approach is based on the Metropolis procedure described by Creutz and Freedman [2] which we extend to our complete three-dimensional calculations.

For the Coulomb potential $V = -c/r$, with the parameters $c = 1$, $a = 0.15$, $N = 500$ and particle mass $m = 2$, the condition (12*b*) is not satisfied in the interval $(0, \frac{1}{3}r_B)$, where r_B is the Bohr radius. Consequently, for the lattice dimension $N \approx 10^3$ and the respective a, the equilibrium in the simulation is not reached by using the action S_0. It is reached by using the modified action S. In this equilibrium we performed calculations by using the action S_0 again. Figure 1 shows the ground-state probability densities. The crosses represent the average over 340 iterations, and the circles over the last 140 iterations, after the equilibrium has been reached. The full curve represents the exact result. Significant discrepancies are seen between this simulation and exact results, especially in the small-r region. In figure 2 the ground-state energy is plotted as a function of the number of iterations, after the equilibrium has been reached. The exact result is $E = -1$. In figure 3 the ground-state probability densities are presented after 300 iterations in equilibrium by using the modified action S. In Figure 4 the ground-state energy is plotted as a function of the number of iterations in equilibrium.

For the exponential potential $V = -B\exp(-r/d)$ one can choose the parameters B and d, so that the condition (12*b*) is satisfied or not.

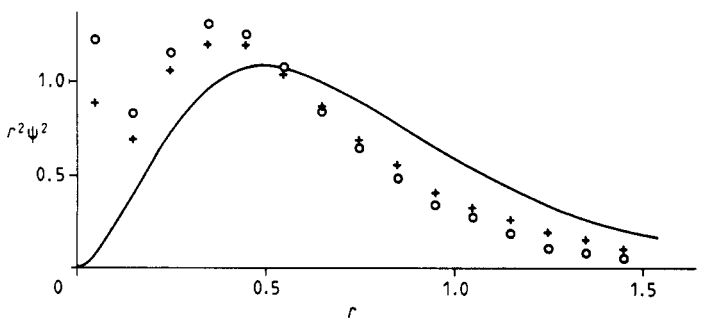

Figure 1. The ground-state probability densities for the Coulomb potential. The radial coordinate r is expressed in $\hbar = 1$ units. The full curve is the exact result. The crosses represent the average over 340 iterations in simulation with the action S_0. The circles are the average over the last 140 iterations in the same simulation.

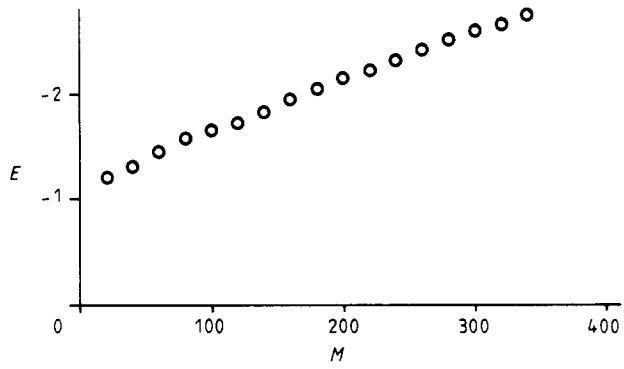

Figure 2. The ground-state energy for the Coulomb potential as a function of the number of iterations in simulation with the action S_0.

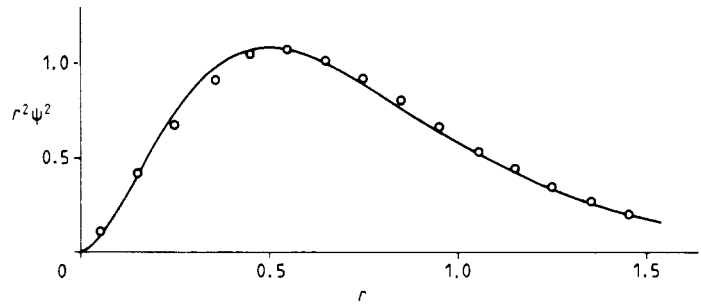

Figure 3. The ground-state probability densities for the Coulomb potential. The full curve is the exact result. The circles represent the average over 300 iterations with the action S.

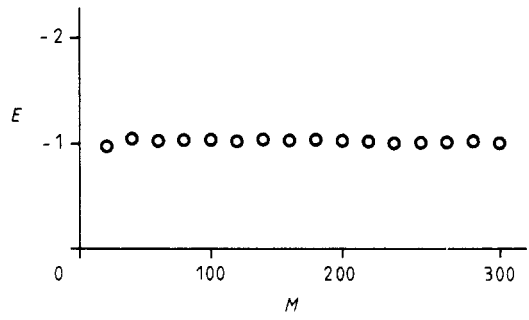

Figure 4. The ground-state energy for the Coulomb potential as a function of the number of iterations in simulation with the action S.

For the choice $B = -3.972$ and $d = 1$, the condition (12b) is satisfied for the parameters $a = 0.1$, $N = 200$, assuming the particle mass $m = 1$. The exact ground-state energy is $E = -0.5$. Under these conditions, our simulation yields $E = -0.520 \pm 0.01$ by using the action S_0 after 400 iterations in equilibrium. The respective ground-state probability densities are presented in figure 5.

For the choice $B = -29.365$ and $d = 0.25$, and other parameters from the preceding example, the condition (12b) is not satisfied in the interval $(0, \frac{2}{3}r_M)$ where r_M is the

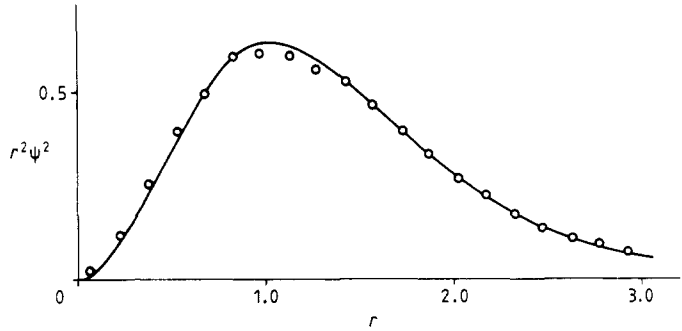

Figure 5. The ground-state probability densities for the exponential potential with $B = -3.972$ and $d = 1$. The full curve is the exact result. The circles represent the result of simulation with the action S_0.

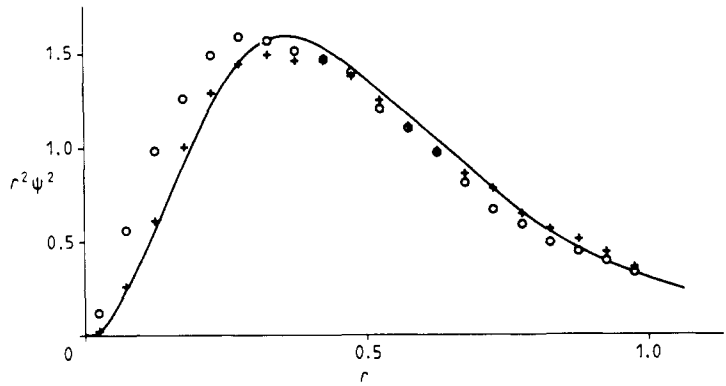

Figure 6. The ground-state probability densities for the exponential potential with $B = -29.365$ and $d = 0.25$. The full curve is the exact result. The circles represent the result of simulation with the action S_0. The crosses are the result of simulation with the action S.

probability distribution maximum. By using the action S_0 in the simulation we obtain $E = -2.95 \pm 0.05$, while the exact energy is $E = -2$. Under the same conditions, the simulation with the action S gives $E = -2.08 \pm 0.05$. Figure 6 shows the respective ground-state probability densities.

To conclude, in this paper we have derived the quadratic term in the lattice action for non-relativistic quantum systems and show the criterion of its importance, when the partition function is calculated by using the Monte Carlo method. The above numerical examples illustrate and support our analysis.

References

[1] Feynman R P 1948 *Rev. Mod. Phys.* **20** 367
[2] Creutz M and Freedman B 1981 *Ann. Phys., NY* **132** 427