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Accelerated Dynamics in HMC Simulations of Lattice Field Theory

MPhys Project Report

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Abstract

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Personal statement

Acknowledgments

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2 Background

2.1 Quantum Mechanics

In quantum mechanics we are often interested in calculating the path integral:

$$\langle x_b, t_b | x_a, t_a \rangle = \int \mathcal{D}x\,(t) \exp\left(\frac{i}{\hbar} S_M\left[x\,(t)\right]\right). \tag{1}$$

$\langle x_b, t_b | x_a, t_a \rangle$ is the transition amplitude for a particle in position eigenstate (in the Heisenberg picture) $|x_a, t_a\rangle$ to move to position eigenstate $|x_b, t_b\rangle$; this gives us the probability amplitude of a particle at x_a at time t_a to move to position x_b at time t_b. The term on the right of equation 1 is known as the "Fenyman path integral". The measure $\int \mathcal{D}x\,(t)$ is an integral over all paths between x_a and x_b. $S_M\left[x\,(t)\right]$ is the Minkowski action of a particle on the path $x\,(t)$ and is defined by:

$$S_M\left[x\,(t)\right] = \int_{t_a}^{t_b} dt \left[\frac{1}{2} m \left(\frac{dx}{dt}\right)^2 - V(x)\right], \tag{2}$$

where $x\,(t_a) = x_a$ and $x\,(t_b) = x_b$ are the boundary conditions.

Due to the oscillating integrand in equation 1, it is not clear the integral will converge, and the integral measure needs to be defined before we proceed. In order to do this we follow the steps in [?] to get equation 1 into a form we can work with.

The first step is to discretise time as in figure 1. Then for each time site on the lattice t_i we have a position $x_i = x\,(t_i)\,\forall i \in [0, N]$. In our notation for the labelling of the position eigenstates in equation 1 we also have $x_b = x_N = x\,(t_N)$ and $x_a = x_0 = x\,(t_0)$ in order to match with figure 1. ϵ is the spacing between lattice sites and so $\epsilon = \frac{t_b - t_a}{N} = t_{i+1} - t_i$ and for $k \in [0, N]\,, t_k = t_a + k\epsilon$. In order to discretise the action in equation 2 we approximate the derivative by a forward difference and the integral as a Rieman sum, taking the lattice spacing as our small parameter:

SHOULD I DO WICK TRANSFORMATION FIRST?

CHECK INDEXING IS CORRECT

$$S_M\left\{x_i\right\} = \sum_{i=0}^{N-1} \epsilon \left[\frac{1}{2} m \left(\frac{x_{i+1} - x_i}{\epsilon}\right)^2 - V\left(x_i\right)\right]. \tag{3}$$

Since $\forall i \in [1, N-1]\,, -\infty < x_i < \infty$ we may define the measure in equation 1 as:

WHY IS THIS TRUE? CRUETZ-

$$\int_{x_a}^{x_b} \mathcal{D}x = \lim_{N\to\infty} A_N \prod_{n=1}^{N-1} \int_{-\infty}^{\infty} dx_n, \tag{4}$$

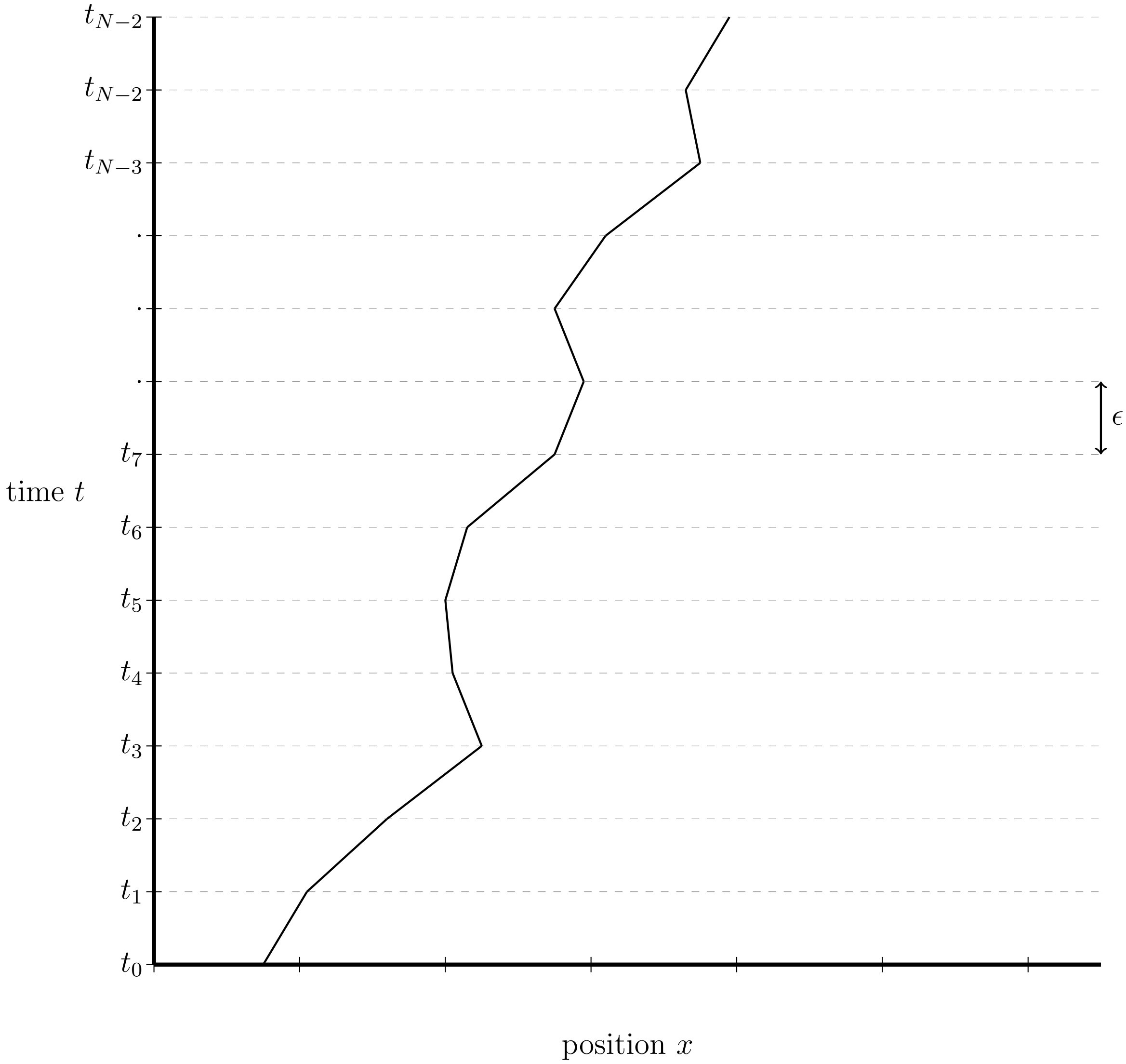

Figure 1. Discretising time into a lattice of spacing ϵ. Diagram taken and redrawn from [**?**]
.

where $A_N = (\nu(\epsilon))^N$ and $\nu(\epsilon)$ is a normalisation factor on each discrete interval. So that for our discrete time lattice, the path integral is given by:

$$\langle x_b, t_b | x_a, t_a \rangle \sim \int_{-\infty}^{+\infty} \prod_{i=1}^{N-1} dx_i \exp\left(\frac{i}{\hbar} S_M \{x_i\}\right). \tag{5}$$

In the limit that $N \to \infty$ (or equivelantly $\epsilon \to 0$) we recover equation 1 from equation 47 exactly.

In order to work with the discrete path integral in equation 47 we have one final step. We make a "Wick rotation" into imaginary time; this is done via the substitution:

SHOULD THE INDEXES ON THE PRODUCT BE FROM ZERO TO N?

$$t = i\tau. \tag{6}$$

Applying this to the discretized theory developed above by defining $a = i\epsilon$, we now have a lattice in imaginary time, of lattice spacing a, substituting a into equation 3:

$$S_M \{x_i\} = \sum_{i=0}^{N-1} \epsilon \left[\frac{1}{2} m \left(\frac{x_{i+1} - x_i}{\epsilon}\right)^2 + V(x_i)\right] = i S_E \{x_i\}. \tag{7}$$

The quantity $S_E \{x_i\}$ is the discretized "Euclidean" action; it has this name because the effect of the Wick transformation is that it turns the Mikowski metric ds_M on the coordinates (x, y, z, t) into the Euclidean metric ds_E on the coordinates (x, y, z, τ) and visa-versa:

$$ds_M^2 = -dt^2 + dx^2 + dy^2 + dz^2 = d\tau^2 + dx^2 + dy^2 + dz^2 = ds_E^2. \tag{8}$$

This is a very useful result since upon substitution into the discrete path integral in equation 47 we find:

$$\langle x_b, t_b | x_a, t_a \rangle \sim \int_{-\infty}^{+\infty} \prod_{i=1}^{N-1} dx_i \exp\left(-\frac{1}{\hbar} S_E \{x_i\}\right). \tag{9}$$

This is known as the discrete euclidean path integral and it far better defined since the integrand is now exponentially suppressed. We are now able to make a connection to statistical mechanics that enables us to compute the values we want in later sections. We have the standard result from statistical physics that for a system with $N-1$ degrees of freedom labelled by x_i for $i \in [0, N-1]$ then the partition function is given by:

$$Z \sim \int_{-\infty}^{+\infty} \prod_{i=1}^{N-1} dx_i \exp\left(-\beta H(x_i)\right), \tag{10}$$

with $\beta = \frac{1}{k_B T}$ where T is the system temperature and k_B is the Boltzman constant. Comparing equation 9 to equation 10 we can see that the discretized Euclidean path integral is a partition function on a system with $N-1$ degrees of freedom, provided that we take:

$$S(\{x_i\}) = H(\{x_i\}), \tag{11}$$

and in units where $k_B = 1$:

$$\hbar = T. \tag{12}$$

We then have a Boltzmann factor given by $\exp\left(-\frac{1}{\hbar}S\{x_i\}\right)$. So in summary we now have a classical interpretation of our quantum calculation of the path integral. Our lattice is essentially a one dimensional crystal of size $N-1$ at temperature T with a continuous variable x_i at each crystal site, and its Hamiltonian is given by $S(\{x_i\})$.

It is interesting to note that in quantum mechanics, due to the uncertainty principle $\sigma_x \sigma_p \geq \frac{\hbar}{2}$, $\hbar$ provides a measure of quantum fluctuations in our system. As $\hbar \to 0$ we recover classical physics and in this limit the only path in the path integral that contriubtes to the transition amplitude is the classical one. On the other hand, in statistical mechanics T provides a measure of statistical fluctations in our system, and in the limit that $T \to 0$ these fluctations go to zero. Hence taking the limit that $\hbar \to 0$ and $T \to 0$ we see statistical mechanics on a (real) crystal lattice is equivelant quantum mechanics in imaginary time.

From now on we will use Z to refer to the RHS of equation 9.

3 Methods

4 Results and Discussion

4.1 Quantum Harmonic Oscillator

4.2 Quantum Anharmonic Oscillator

5 Conclusion

Appendices

Note — Appendices are provided for completeness only and any content included in them will be disregarded for the purposes of assessment.

A Derivation of the discrete path integral for quantum harmonic oscillator

Here we follow the derivation given in [?] for the exact result of the path integral for discrete theory and a particle of mass $m = 1$. Since in [?] the derivation has several typographical mistakes and jumps in the algebra that make it difficult to follow for the reader, we have choosen to reproduce it with corrections and alterations.

For a quantum harmonic oscillator of mass $m = 1$, the discrete Euclidean path integral is given in equation 9 as:

FIX IN-DEX-ING

$$Z = \int_{-\infty}^{+\infty} \prod_{i=1}^{N-1} dx_i \exp\left(- \sum_{j=0}^{N-1} a \left[\frac{1}{2} \left(\frac{x_{j+1} - x_j}{a} \right)^2 + \frac{1}{2} \mu^2 x_j^2 \right] \right). \tag{13}$$

We begin by defining an operator T such that its matrix elements in the Schrodinger picture are given by:

$$\langle x' | \hat{T} | x \rangle = \exp\left(-\frac{1}{2a} (x' - x)^2 - \frac{\mu^2 a}{4} \left(x^2 + x'^2 \right) \right). \tag{14}$$

Then we can use the completeness relation that:

$$\hat{1} = \int_{-\infty}^{\infty} |x\rangle \langle x| \,. \tag{15}$$

By inserting $N - 1$ copies of this relation into the expression (one inbetween each pair of $\hat{T}$s):

$$Tr\left(\hat{T}^N \right), \tag{16}$$

and using the defintion of the matrix elements in equation 14, we recover the path integral in equation 13, that is:

$$Z =\sim Tr\left(\hat{T}^N \right). \tag{17}$$

Here we take the trace over the physical Hilbert space, so that for any operator $\hat{A}$ in the Schrodinger eigenbasis, the trace is:

$$Tr\left(\hat{A} \right) = \int_{-\infty}^{\infty} dx \langle x| \hat{A} |x\rangle \,, \tag{18}$$

which is of course basis independent.

The next step is to make the ansatz that:

$$\hat{T} = \int_{-\infty}^{\infty} d\omega e^{\frac{-\mu^2 a}{4}\hat{x}^2} e^{-i\hat{p}\omega} e^{-1\frac{1}{2a}\omega^2} e^{\frac{-\mu^2 a}{4}\hat{x}^2}, \tag{19}$$

then, using that canonical momentum generates translations on position, that is:

$$e^{-i\hat{p}\Delta} |x\rangle = |x + \Delta\rangle \tag{20}$$

which can easily be shown by Fourier transforming the position eigen basis into momentum space, acting with the momentum operator in the exponential then Fourier transforming back into position space; we can calculate the matrix element $\langle x'| T |x\rangle$ and recover equation 14. We observe that the integral over ω in equation 19 is Gaussian; we may use the standard result:

$$\int_{-\infty}^{+\infty} dx e^{-\alpha x^2 + i\beta x} = \sqrt{\frac{\pi}{\alpha}} e^{-\frac{\beta^2}{4a}}, \tag{21}$$

this result follows from completing the square on x, analytically continuing the integral over x into the complex plane and creating a rectangular contour in the lower half plane, then applying residue theory, it is valid provided $\alpha \in \mathbb{R}_{>0}$ and $\beta \in \mathbb{R}$. Applying the identity in equation 21 to equation 19 gives:

$$\hat{T} = \sqrt{2\pi a} e^{-\frac{-\mu^2 a}{4}\hat{x}^2} e^{-\frac{a}{2}\hat{p}^2} e^{-\frac{\mu^2 a}{4}\hat{x}^2}. \tag{22}$$

Notice at this stage in our derivation we could apply the Baker-Cambell-Hausdorff formula to combine the exponentials; dropping $\mathcal{O}\left(a^2\right)$ would then give the harmonic oscillator Hamiltonian exponentiated. Since this system is exactly solvable in the discrete case, we will avoid doing this and keep all terms.

The canconical commutation relation of quantum mechanics gives:

$$[\hat{x}, \hat{p}] = i\hbar, \tag{23}$$

which can be along with the identities that for operators $\hat{A}$ and $\hat{B}$:

$$\left[\hat{A}, \hat{B}^n\right] = n\hat{B}^{n-1}\left[\hat{A}, \hat{B}\right] \tag{24}$$

and

$$\left[\hat{A}^n, \hat{B}\right] = n\hat{A}^{n-1}\left[\hat{A}, \hat{B}\right], \tag{25}$$

if $\left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right] = \left[\hat{B}, \left[\hat{A}, \hat{B}\right]\right] = 0$, to show that:

$$FILL \tag{26}$$

and

$$FILL. \tag{27}$$

Using identities FILL and FILL we can easily show that:

$$\hat{x}\hat{T} = \hat{T}\left[\left(1 + \frac{a^2\mu^2}{2}\right)\hat{x} - ia\hat{p}\right], \tag{28}$$

and

$$\hat{p}\hat{T} = \hat{T}\left[\left(1+\frac{a^2\mu^2}{2}\right)\hat{p} + ia\mu^2\left(1+\frac{a^2\mu^2}{4}\right)\hat{x}\right]. \tag{29}$$

Iterating equations and a second time gives:

$$\left[\hat{p}^2 + \mu^2\left(1+\frac{a^2\mu^2}{4}\right)\hat{x^2}, \hat{T}\right] = 0. \tag{30}$$

Defining a new angular frequency parameter ω by:

$$\omega^2 = \mu^2\left(1+\frac{a^2\mu^2}{4}\right), \tag{31}$$

then from equation 30 we have that $\hat{T}$ commutes with the simple harmonic oscillator Hamiltonian:

$$\hat{H} = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\omega^2\hat{x}^2. \tag{32}$$

Since $\hat{H}$ and $\hat{T}$ commute we know $\hat{T}$ is diagonalized by the eigenstates of $\hat{H}$.

The Hamiltonian is in the form of a harmonic oscillator with angular frequency ω, therefore we may define the corresponding ladder operators:

$$\hat{a}^\dagger = \frac{1}{\sqrt{\omega}}\left(\hat{p} + i\omega\hat{x}\right) \tag{33}$$

and

$$\hat{a} = \frac{1}{\sqrt{\omega}}\left(\hat{p} - i\omega\hat{x}\right) \tag{34}$$

which allows us to write:

$$\hat{H} = \left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\omega \tag{35}$$

The eigenstates of $\hat{H}$ satisfy the standard relations:

$$\hat{a}\left|0\right\rangle = 0, \tag{36}$$

$$\left(\hat{a}^\dagger\right)^n\left|0\right\rangle = \left|n\right\rangle, \tag{37}$$

and

$$\left\langle n|n\right\rangle = n!. \tag{38}$$

Using the identities of equations A and A we can show that:

$$\hat{a}\hat{T} = \hat{T}\hat{a}\left(1+\frac{a^2\mu^2}{2} - a\mu\left(1+\frac{a^2\mu^2}{4}\right)^{\frac{1}{2}}\right). \tag{39}$$

Since the eigenstates of $\hat{H}$ given as $\left|n\right\rangle$ diagonalise $\hat{T}$, for λ_i the eigenvalues of $\hat{T}$:

$$\hat{T}\left|n\right\rangle = \lambda_n\left|n\right\rangle. \tag{40}$$

We can then use that $\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle$ and equation 39 to show the ratio:

$$\frac{\lambda_n}{\lambda_{n-1}} = 1 + \frac{a^2\mu^2}{2} - a\mu\left(1 + \frac{a^2\mu^2}{4}\right)^{\frac{1}{2}} := R \tag{41}$$

We may therefore conclude that : FIND OUT WHY THIS IS TRUE

$$\hat{T} = \sqrt{2\pi a}KR^{\frac{\hat{H}}{\omega}}, \tag{42}$$

for some normalisation constant K. We may then calculate K by first taking the trace of $\hat{T}$ over the energy eigenbasis $|n\rangle$:

$$\frac{1}{\sqrt{2\pi a}}Tr\left(\hat{T}\right) = K\sum_{n=0}^{n=\infty} R^{n+\frac{1}{2}} = \frac{K}{a\mu}, \tag{43}$$

where we have used that $\hat{H}\,|n\rangle = E_n\,|n\rangle = \left(n+\frac{1}{2}\right)\omega$ for the harmonic oscillator in units where $\hbar = 1$, and in order to compute the sum we have used that $|R| < 1$. The trace over the energy eigen basis is given by:

$$Tr\left(\hat{A}\right) = \sum_{n=0}^{N} \langle n|\,\hat{A}\,|n\rangle \tag{44}$$

We then take the trace of $\hat{T}$ over the position eigenbasis according to equation 18:

$$\frac{1}{\sqrt{2\pi a}}Tr\left(\hat{T}\right) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp e^{\frac{-\mu^2 a x^2}{2}} e^{-\frac{ap^2}{2}} = \frac{1}{\mu a}, \tag{45}$$

where this time in order to take the trace of $\hat{T}$ we have taken the trace of equation 22 and Fourier transformed the $|x\rangle$ in the expression into momentum space. Since the trace of an operator is a basis independent quantity we may compare equations 43 and 45 which gives $K = 1$ so that:

$$T = \sqrt{2\pi a}R^{\frac{\hat{H}}{\omega}}. \tag{46}$$

We may now explicitly compute the trace expression for the discrete path integral given in equation 16 using the result for $\hat{T}$ in equation 46. We again take the trace over the energy eigenstates and use the fact that $|R| < 1$ to compute the resulting sum, this gives:

$$Z = (2\pi a R)^{\frac{N}{2}} \frac{1}{1-R^N}. \tag{47}$$

This is the exact expression for the discrete path integral of a quantun harmonic oscillator of mass $m = 1$, angular frequency μ on an imagainary time lattice of $N-1$ sites with lattice spacing a.

The correlation functions are given by: FIND OUT WHY THIS IS TRUE

$$\langle x_i x_{i+j}\rangle = \frac{1}{Z}Tr\left(\hat{x}\hat{T}^j\hat{x}\hat{T}^{N-j}\right) = \frac{1}{2\omega\left(1-R^n\right)}\left(R^j + R^{N-j}\right). \tag{48}$$

Taking $j = 0$, equation 48 becomes:

$$\langle x^2 \rangle = \frac{1}{2\mu \left(1 + \frac{a^2\mu^2}{4}\right)^{\frac{1}{2}}} \left(\frac{1 + R^N}{1 - R^N}\right). \tag{49}$$

We have shown in above that the discrete theory for the harmonic oscillator leads to a quantum system with the Hamiltonian given in equation 32. This is the Hamiltonian of a quantum harmonic oscillator of angular frequency ω rather than μ and hence we employ the standard result from quantum theory that for a a quantum harmonic oscillator of angular frequency ω the ground state wave function is given by:

CHECK THIS LOGIC IS CORRECT

$$\psi(x) = \left(\frac{\omega}{\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{1}{2}\omega x^2\right) \tag{50}$$