Lattice Quantum Mechanics for Novices

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In this paper we explore the application of discrete path integral as a non-perturbative approach in quantum mechanics. We will start by introducing the formulation and using it to find energy levels in a quartic potential, followed by a brief qualitative discussion on how the method is generalized to investigate phenomena in non-perturbative field theories such as quark confinement in QCD.

I. INTRODUCTION

Lattice field theory was first introduced by K.G. Wilson in 1974 as an attempt to understand quark confinement [1]. The approach has undergone immense development in recent years thanks to the increasing availability of the high level of computing power that is required for lattice calculations. Nowadays most personal computers and laptops are powerful enough for small to medium scale lattice calculations.

The lattice method is important as it complements perturbation theory where the latter fails. The most prominent example of a non-perturbative theory is quantum chromodynamics where perturbative approaches completely break down in the low energy regime due to the large coupling constant. In such regime lattice field theory is the only tool that we have for making predictions. Its importance will continue to rise in the future as computing power becomes cheaper.

Although the main arena of the lattice method is really in QCD and other gauge theories that are much more complicated than ordinary quantum mechanics, the basic idea is fairly simple and can be well illustrated through consideration of simple quantum mechanical systems. In this paper we will concern ourselves with the energy levels of a one-dimensional quartic potential, and how they can be obtained through the lattice method. In the final section we will briefly describe how the method generalizes in QCD, but details beyond the scope of this paper are left for interested readers to pursue on their own.

II. BASIC FORMALISM

We will begin by drawing connections between quantum mechanics and statistical physics and show how we can calculate energy levels of our system using ensemble averages. We set $\hbar = 1$ throughout this paper.

A. Eucildean Path Integral

Consider a one-dimensional system described by some potential function $V(x)$. A particle in the system can be described using the states $|x, t\rangle \equiv e^{i\hat{H}t} |x\rangle$[1] where $\hat{H}$ is the Hamiltonian of the system. The propagator is given by the path integral

$$\langle x_f | e^{-i\hat{H}(t_f - t_i)} | x_i \rangle = \int \mathcal{D}x(t) e^{iS[x(t)]} \quad (1)$$

where $S[x(t)]$ denotes the action along the path $x(t)$ and $\mathcal{D}x(t)$ is some measure corresponding to integrating over all paths. It is important to note that the exponent on the left is an operator (q-number) while the exponent on the right is an ordinary number (c-number). The path integral bridges the two types of quantities. We can think of this loosely as the path integral converting c-numbers into q-numbers, so what enters into the integrand of the path integral will come out as (some matrix element of) operators.

Unfortunately the path integral is ill-defined mathematically[2]. We will regularize it in two steps, through which we will be able to draw connection from quantum to statistical physics. First we discretize time such that the integral becomes an ordinary multiple integral over positions at each time steps. In other words, we replace the continuous time dimension t by a discrete lattice t_n, $n = 0, 1, 2, ..., N$, where $t_n = t_i + na$ and a is the lattice spacing. As a result the path becomes discretized

$$x(t) \rightarrow \{x_n = x(t_n)\} \quad (2)$$

$$\int \mathcal{D}x(t) \rightarrow A \int_{-\infty}^{\infty} dx_1 dx_2 ... dx_{N-1} \quad (3)$$

$$S \rightarrow \sum_{n=0}^{N} \left[\frac{1}{2a} m(x_{n+1} - x_n)^2 - aV(x_n) \right] \quad (4)$$

Note that here we do not integrate over initial and final positions because they are held fixed. For simplicity we choose to use the periodic boundary condition,

$$x_0 = x_N \quad (5)$$

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[1] By $|x, t\rangle$ of course we do not mean an eigenstate of position and time, which we know does not exist. We should think of it as the time-displaced position basis in the Heisenberg picture, i.e. given by $\langle x, t | \psi \rangle = \langle x | \psi(t) \rangle$. It is also useful to note that $\langle x_2, t_2 | \hat{O}(t) | x_1, t_1 \rangle = \langle x_2 | e^{-\hat{H}(t_2 - t)} \hat{O} e^{-\hat{H}(t - t_1)} | x_1 \rangle$. Everything on the left hand side is in Heisenberg picture and everything on the right hand side is in Schrödinger picture.

[2] The measure is infinite-dimensional (which is banned in mathematics) and with an oscillatory integrand of modulus one.

The prefactor A in front of the integral is not important for our calculations.

Next we perform a procedure called the Wick rotation[3] which is a change of variable that replaces the imaginary time $\tau = it$ by real time t. Under such rotation we have

$$L = \frac{1}{2}m\dot{x}^2 - V \rightarrow \frac{1}{2}m(i\dot{x})^2 - V = -H \qquad (6)$$

and thus arriving at our final form:

$$\langle x_0| e^{-\hat{H}(t_f - t_i)} |x_0\rangle = \int \mathcal{D}x(t)e^{-S[x(t)]} \qquad (7)$$

where the action is now given by

$$S = \sum_{n=0}^{N} \left[\frac{1}{2a}m(x_{n+1} - x_n)^2 + aV(x_n) \right] \qquad (8)$$

Note the difference in sign due to the Wick rotation.

B. Ensemble Average

Now let the end position x_0 vary instead of being fixed and define (while still keeping our periodic boundary condition)

$$\langle O \rangle = \frac{\int \mathcal{D}x(t)O[x]e^{-S[x]}}{\int \mathcal{D}x(t)e^{-S[x(t)]}} \qquad (9)$$

where the integration is over x_0 as well and O, which we will call the observable, denotes an arbitrary functional of x, or more precisely, a function of $x_0, x_1, ..., x_{N-1}$.

This strongly resembles the definition of an ensemble average in statistical physics, and indeed we can think of e^{-S} as the Boltzmann factor that is proportional to the probability of the particle following the given path. If we can generate random paths $\{X_j(t)\}$ according to this Boltzmann distribution, then the ensemble average is simply given by

$$\langle O \rangle = \frac{\sum\limits_{j} O[X_j]}{N_{path}} \qquad (10)$$

where N_{path} is the number of paths in our set of samples. In the following section, we will give a method for generating such a set of random paths that respects the Boltzmann distribution. Then we will return to discuss the choice of O and show how we can express the energy in terms of ensemble average.

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[3] It is in fact the other way round. The Euclidean, discretized path integral provides us with a well-defined mathematical object of which the usual path integral can be viewed as an analytical continuation. Thus to be mathematically correct we should define the path integral as the Wick rotation of the discrete Euclidean path integral under continuum limit. But here we are not doing it entirely for mathematical reasons, we can think of it as a trick to cast quantum mechanics into statistical physics.

III. IMPLEMENTATION

A. Metropolis algorithm

To generate random paths with the correct distribution we can use a procedure called the Metropolis algorithm [2, 3], which goes as follows:

1. Start with the previous path, if there is no previous path then start with an arbitrary path, e.g. $x_n = 0$ for all n which is called a cold start.

2. For each lattice site $n(= 0, 1, ..., N-1)$:

   (a) Update the position x_n by $x_n \rightarrow x_n + \epsilon r$ where r is a random number from -1 to 1.

   (b) Calculate the difference in S before and after the update.

   (c) If $\Delta S < 0$ (favorable), then the new position is kept.

   (d) If $\Delta S > 0$ (unfavorable), then pick a random number r' from 0 to 1. If $r' < e^{-\Delta S}$ then the new position is kept, otherwise restore the original position.

3. Add the path into our collection and repeat from step 1 to get a new path.

It can be seen that algorithm tries to drive the path towards lower energy configurations (2c), which are more probable and thus contain the most important contributions, while also reproducing random fluctuations modulated by the Boltzmann factor (2d). Hence it is intuitive that the algorithm should reproduce qualitatively the correct distribution. A rigorous proof that this indeed gives the correct distribution can be found in [2].

There are several important technicalities concerning the algorithm. Firstly it is important to discard the first N_{therm} paths generated because they are too far from the equilibrium path as we are starting cold. This is called *thermalization*. The choice of N_{therm} will general differ for different systems as well as different kind measurements on the same system.

It is also important that we discard some number (N_{cor}) of paths in between each path that we keep, which is called *decorrelation*. This is because each path given by the update is inevitably statistically correlated to the previous path. Therefore we need to "space out" the paths we keep to ensure randomness. There is no general rule for the choice of N_{cor}, but anything from 15-50 is typical.

It is also important to keep track of the acceptance rate, i.e. the percentage frequency of new position being accepted. This depends mainly on ϵ. An ϵ that is too small results in slow or inadequate exploration of the configuration space while it being too large results in constant rejection of new updates. Usually we want to choose ϵ such that it gives an acceptance rate around 60-80%.

In general all the parameters has to be determined by trial and error. It is useful to generate plots that show how the path and the quantity we want to measure evolve with each update in order to pick the right parameters.

B. Measurements

1. Ground state energy

We shall proceed our derivation using continuous time, which corresponds to taking the limit $a \to 0$ in the lattice formulation. We calculate the ground state energy of the system by considering the following observable

$$O = H(t) = \frac{1}{2}m(\dot{x}(t))^2 + V(x(t)) \qquad (11)$$

which is simply the total energy of the particle at time t_n. Combining equations 7 and 9 we have (note that x_0 is being integrated over in equation 9 but not in 7)

$$
\begin{aligned}
\langle H(t) \rangle &= \frac{\int dx_0 \, \langle x_0 | e^{-\hat{H}(t_f-t)} \hat{H} e^{-\hat{H}(t-t_i)} | x_0 \rangle}{\int dx_0 \, \langle x_0 | e^{-\hat{H}(t_f-t_i)} | x_0 \rangle} \quad (12) \\
&= \frac{\sum_k \int dx_0 | \langle x_0 | E_k \rangle |^2 e^{-E_k(t_f-t_i)} E_k}{\sum_k \int dx_0 | \langle x_0 | E_k \rangle |^2 e^{-E_k(t_f-t_i)}} \quad (13) \\
&= \frac{\sum_k e^{-E_k(t_f-t_i)} E_k}{\sum_k e^{-E_k(t_f-t_i)}} \quad (14)
\end{aligned}
$$

where we used $\hat{H}(t) = e^{\hat{H}t}\hat{H}e^{-\hat{H}t}$ for the first equality[4]. The second equality follows by inserting a resolution of unity by energy eigenbases with eigenvalues E_k, and the third equality follows from the fact that the energy eigenstates are normalized.

If we write $T = t_f - t_i$ and take the limit $T \to \infty$, then higher energy terms will be suppressed by the exponential prefactors and only the ground state energy term survives, hence

$$\langle H(t) \rangle = \frac{e^{-E_0 T} E_0}{e^{-E_0 T}} = E_0 \qquad (15)$$

We have just established the important result that, under the limits $a \to 0$ (small lattice spacing) and $T \to \infty$ (large lattice size), the ensemble average of energy at time t gives us the ground state energy! It is important to note that the result is independent of t so in additional to averaging over different paths, we also average over t when we calculate the ensemble average to gain better statistics.

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[4] The path integral converts $H(t)$ (c-number) into the corresponding operator $\hat{H}(t)$ (do not confuse the bracket with multiplication!), and we are bringing the Hamiltonian in the Heisenberg picture into the Schrödinger picture. See also footnote 1.

Now in order to calculate the ensemble average on the lattice, we need a discrete version of equation 11. Naively we may choose to use

$$H(t_n) = \frac{1}{2}m\left(\frac{x_{n+1} - x_n}{a}\right)^2 + V(x_n) \qquad (16)$$

but this will not work as the average of the first term will diverge as $a \to 0$. The easiest way to see this is perhaps to note that the action (equation 8), which is convergent in the small spacing limit, has a term of the form $\Delta x^2/a$, so the term $\Delta x^2/a^2$ will diverge as $1/a$. In other words the physically important paths in the path integral formulation are non-differentiable [5]. Therefore the derivative is ill-defined in the continuum limit.

The remedy is to use an expression that is local in time given by the virial theorem:

$$\langle \frac{1}{2}mv^2 \rangle = \frac{1}{2}\langle xV'(x) \rangle \qquad (17)$$

thus we can instead use

$$H(t_n) = \frac{1}{2}x_n V'(x_n) + V(x_n) \qquad (18)$$

to extract the ground state energy [2].

2. Ground state wavefunction

The square of the wavefunction can be obtained in a straight-forward manner. We can obtain the probability of finding the particle within some interval $(x', x' + \delta x)$ by simply counting how many times the position falls within this interval throughout the set of paths. A rigorous proof that this procedure indeed gives the correct result can be found in [2]. The wavefunction for the ground state can be obtained by the relation

$$P(x' < x < x' + \delta x) = |\psi(x')|^2 \, \delta x \qquad (19)$$

Note that this only gives us the amplitude but not the phase. For some simple cases (e.g. ground state of quartic potential) the phase is not important so we can simply take the positive square root. In general, however, we cannot completely determine the wavefunction due to this phase ambiguity.

3. First excited state energy

The energy of the first excited state can be obtained by considering the observable called the two-point correlator defined as

$$
\begin{aligned}
\langle x(t_2)x(t_1) \rangle &= \frac{\sum_k e^{-E_k T} \langle E_k | \hat{x} e^{-(\hat{H}-E_k)t} \hat{x} | E_k \rangle}{\sum_k e^{-E_k T}} \quad (20) \\
&= \langle E_0 | \hat{x} e^{-(\hat{H}-E_0)t} \hat{x} | E_0 \rangle \quad (T \to \infty) \quad (21)
\end{aligned}
$$

where $t = t_2 - t_1$, and we have taken the limit $T \to \infty$ in the last equality. The derivation is very similar to that of equation 14 so the details have been skipped. To further simplify this expression, let us take a closer look at the state $|\psi\rangle = \hat{x} |E_0\rangle$. This state has an odd parity because the operator $\hat{x}$ changes sign under parity transformation, thus we can expand ψ using odd bases:

$$|\psi\rangle = \sum_{k \ odd} c_k |E_k\rangle \tag{22}$$

and thus

$$\langle x(t_2)x(t_1)\rangle = \langle\psi| e^{-(\hat{H}-E_0)t} |\psi\rangle \tag{23}$$

$$= \sum_{k \ odd} |c_k|^2 e^{-(E_k-E_0)t} \tag{24}$$

$$= |c_1|^2 e^{-(E_1-E_0)t} \quad (t \to \infty) \tag{25}$$

Therefore under the limits $a \to 0$ and $T, t \to \infty$, the two-point correlator is related to the energy difference between the ground state and the first excited state. Specifically, the energy difference is the log-derivative of the correlator. Returning to the lattice formulation, if we denote the two-point correlator on the lattice by $G(n) = \langle x(t_i + na)x(t_i)\rangle$, we then have, under the same limits,

$$\ln\left(\frac{G(n)}{G(n+1)}\right) = a(E_1 - E_0) \quad \text{(for n large)} \tag{26}$$

$$E_1 = E_0 + \frac{1}{a}\ln\left(\frac{G(n)}{G(n+1)}\right) \tag{27}$$

which gives us the energy of the first excited state.

It is perhaps interesting to point out that in the above derivation the only important thing is to use an observable with odd parity, not necessarily $\hat{x}$. For example the correlator $\langle x^3(t_2)x^3(t_1)\rangle$ will work just as well.

4. Higher excited states

Finding energies of higher excited states is much more involved and generally not discussed in introductory materials. Below are some methods that can be used to study higher excited states. Interested readers are referred to [6].

1. Curve fitting:
   The correlator actually contains information of all odd states. Therefore, once we have determined E_1 we can perform a functional fit of the form in equation (24) to extract the next odd energy level. We can repeat this process to get to higher and higher energies. For even states we may use an even correlator (e.g. with x^2) and go through the same process.

2. Variational method:
   Instead of using a single correlator, we can instead consider a matrix of correlators with different overlaps onto the energy eigenbases. The eigenvalue of the matrix will produce energy differences of higher energy states [6].

3. Supersymmetry:
   From the ground state wavefunction we can construct the supersymmetric partner potential to our original potential. The ground state of the partner system will then be the first excited state of the original system [4]. In additional to energy, this method also allows one to find the (square of) wavefunction of the first excited state.

IV. EXAMPLE: QUARTIC POTENTIAL

The results for a particle with $m = 1$ in a potential $V(x) = x^4$ is summarised in this section. The code that was used to generate these results is in the appendix. We used $N_{lattice} = 5000$, $a = 0.1$, $N_{therm} = 500$, $N_{cor} = 100$, and $\epsilon = 0.2$. The acceptance rate was 82%.

The evolution of the ground state energy at each update, without any thermalization or decorrelation is shown in figure 1. The same plot with both thermalization and decorrelation is shown in figure 2. The final measured value for ground state energy is $E_0 = 0.665 \pm 0.0028$[5]. The energy of the first excited state is measured using the ratio of correlators at the end of the lattice (putting $n = N_{lattice}$ in equation 27). The measured value is $E_1 = 2.393 \pm 0.0028$. These values can be compared to values that appeared in, for example, [8].

The wavefunction of the ground state (which we chose to be positive and real) is plotted in figure 3.

V. LATTICE QCD

We will end with a short discussion on how this method generalizes for more complicated problems, in particular to gauge theories such as QCD. For detailed discussion, the reader is referred to [3] and [7]

A. Link variable

We note that throughout our discussion in previous sections the only dimension that is being discretized is time. The lattice we were using is just one dimensional and we were assigning a continuous number x at each

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[5] The error here is the sampling error. The systematic error due to discretization depends on how fast the discrete path integral converges to the continuum limit, which is too technical to be discussed here. In short the systematic error decays exponentially as N grows so it is almost certainly overwhelmed by the sampling error.
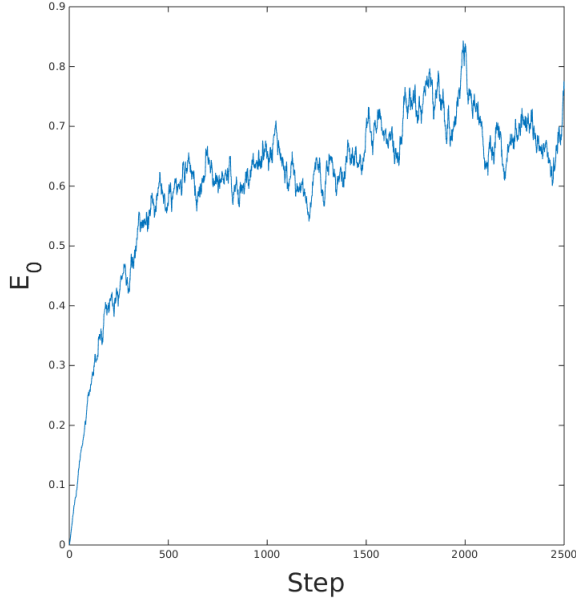
FIG. 1: Evolution of ground state energy through Metropolis updates. From the graph we can see how the initial measurements of ground state energy deviate significantly from the average measurement, which demonstrates the need for thermalization. Informed by the graph we can choose $N_{therm} \approx 500$.
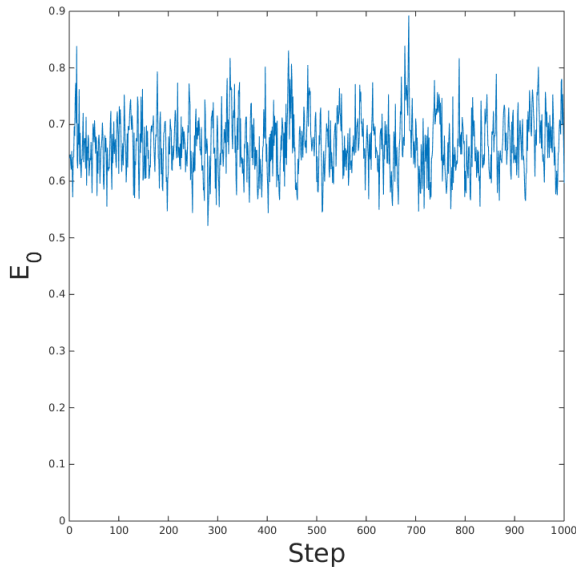

FIG. 2: Evolution of ground state energy with thermalization and decorrelation. We can see the thermalization removed the unwanted starting paths. A lot of local correlations are also removed, giving us a much more random series.
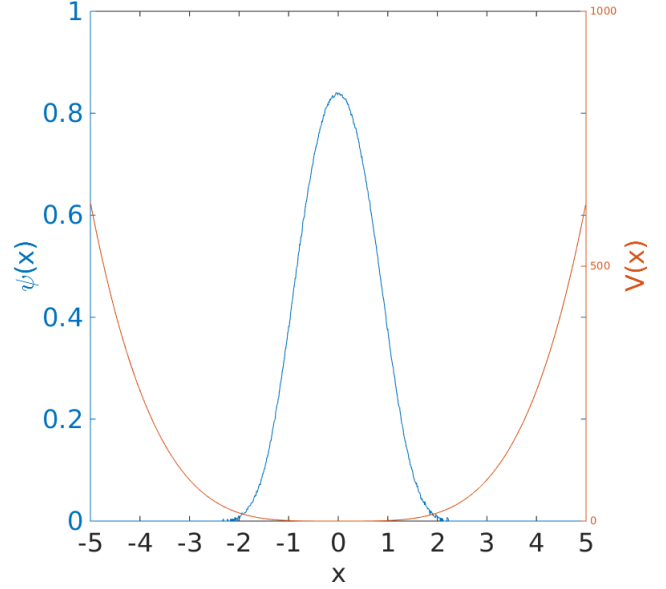

FIG. 3: The wavefunction of the ground state of the quartic potential. The result obtained from lattice method is the same from that obtained by numerically solving the Schrödinger equation [9].

lattice site. For higher dimensional systems our lattice does not change except that we assign more variables (x, y, z, ...) at each site. The only discrete dimension is time in lattice quantum mechanics. This reflects the fact that time is special in quantum mechanics as it is a parameter unlike positions which are really operators.

In quantum field theory this is no longer true. Space and time are treated on equal footing as parameters. Therefore to do lattice field theory we need to use a multi-dimensional lattice on spacetime.

It is natural then to think that we should assign a continuous value at each lattice site that represents the value of the field at that point of spacetime. For gauge theories, however, this is not how it is done. We keep track of continuous values that live on the edges between two sites rather than on the sites themselves. The reason for this is to preserve the gauge invariance of the theory which will lead to much convenience. These variables are called the "link" variables and can be thought of as parallel transports of the gauge field. For QCD these link variables are SU(3) matrices.

B. Wilson loop and quark confinement

Once we introduced link variables it is easy to generalize the action S. Since the action is gauge invariant, it only depends on quantities that are gauge invariant. Therefore we can put our link variables into a closed loop which is manifestly gauge invariant. These loops are called Wilson loops and the 1 by 1 Wilson loops,
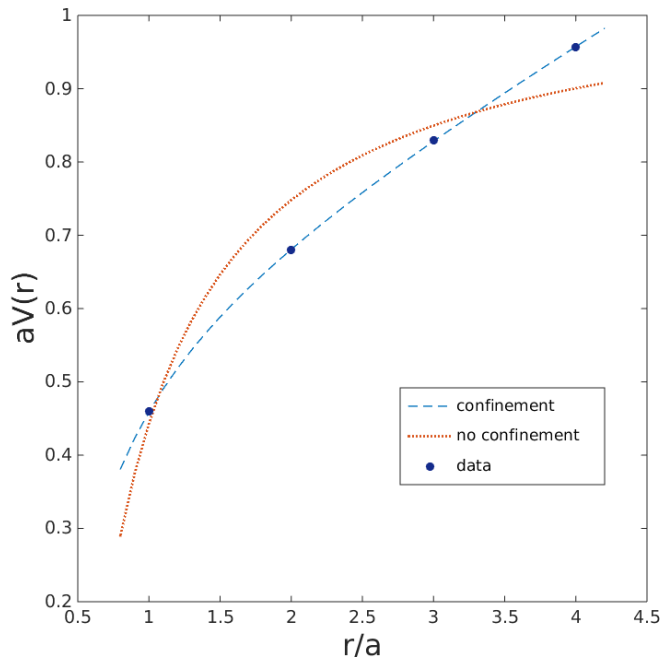
FIG. 4: Graph showing the static quark potential calculated using the lattice method. The potential is fitted by $V_{QCD}(r) = \sigma r - b/r + c$ and $V_{Coulomb}(r) = -d/r + e$. The linear term corresponds to quark confinement. We see that the result from lattice calculation clearly exhibits quark confinement.

called "plaquettes", reproduce the gauge action under the continuum limit.

These loops are not only useful as means to calculate the action, which is an important step in the Metropolis algorithm. They also perform similar role as the correlator and allows us to extract useful information such as the potential due to static gluon field. This potential describes the attraction between a quark (color charge) and an anti-quark (anti-color charge) just as the static electric potential describes the attraction between a positive and negative charge. A plot of the static quark potential is reproduced in figure 4. We can see that the potential

contains a linear term which gives rise to the important phenomenon of quark confinement. This is a nice example which demonstrates the great power of the lattice method, which is not merely a tool for calculation but also a source of new physical insights.

VI. CONCLUSION

The lattice method is a very elegant approach which draws upon the striking assemblance between quantum mechanics and statistical physics. The resulting formalism is non-perturbative and therefore do not suffer from limitations of perturbation theories. Through our example of a 1D particle in a quartic potential, we see that the basic idea of the method is in fact quite simple and easy to implement.

We also see during our short excursion into lattice QCD that the lattice method is more than a tool for numerical calculation. In many occasions, it is also a source of new physical insights, revealing and illuminating various novel phenomena such as quark confinement, monopoles, phase structures of gauge theories, static properties of glueballs and hadrons, etc.

The field of lattice theories is still relatively new and there are yet a lot of open questions and unsolved problems. For example, it is still not completely clear how one can simulate all the real-time dynamics instead of just extracting static quantities like we did in this paper. Once various theoretical and technical issues have been resolved, we will eventually be able to calculate *ab initio* dynamical quantities such as cross-sections of nuclear reactions, which will lead to great implications for many other fields such as nuclear physics, astrophysics and cosmology. We hope that the paper will serve as a starting point for the reader to delve deeper into this vast and exciting field.

Acknowledgments

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Appendix A:
Code for 1D Lattice Simulation

The code below is written in C and relies on the GNU Scientific Library (`http://www.gnu.org/software/gsl/`) for random number generation.

```
/* ========================================
 * Code for 8.06 Term Paper (Spring 2015)
 *
 * Author : To Chin Yu (ytc@mit.edu)
 * Purpose: 1D lattice simulation
 * V(x) = alpha*x^2 + lambda*x^4
 * ========================================
 */
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#define sq(x) pow((x),2.0)
#define cb(x) pow((x),3.0)
#define qd(x) pow((x),4.0)

// GSL Random Number Generator (https://www.gnu.org/software/gsl/)
#include <gsl/gsl_rng.h>
const gsl_rng_type * T; gsl_rng * r;

// Parameters
#define N_lat    5000   // Lattice size
#define a        0.1    // Lattice spacing
#define N_therm  500    // Thermalization
#define N_meas   1000   // Number of configuration to measure
#define N_skip   100    // Decorrelation
#define alpha    0      // Strength of potential (harmonic)
#define lambda   1      // Strength of potential (anharmonic)
#define epsilon  0.2    // Size of fluctuation
// for wavefunction
#define N_bin 1000      // Number of bins for x
#define dx 0.01
#define x_range 5.0     // x in [-range, range]

// Globals
double x[N_lat];        // Lattice
int acc, tot;           // Acceptance rate = acc/tot
double E0;              // Ground state energy
double C[N_lat];        // Correlator
double psi[N_bin];      // Wavefunction

// Output Files
FILE *fE0, *fCorRatio, *fpsi;

// Prototypes
void setup();
void cleanup();
void update();

int main(void){
  setup();

  // Thermalize
  for(int n=0;n<N_therm;n++){ update(); }

  // Do updates and measurements
  for(int n=0;n<N_meas;n++){
    // Decorrelate
    for(int m=0;m<N_skip;m++){ update(); }
    // Measurements:
    // 1. E0
    E0=0;
    for(int i=0;i<N_lat;i++){
      E0 += ( 2*x[i]*lambda*cb(x[i]) + lambda*qd(x[i]) )/N_lat;
    }
    fprintf(fE0,"%f\n", E0);
    // 2. Correlator
    for(int i=0;i<N_lat;i++){
      for(int T=0;T<N_lat;T++){
        C[T] += x[i]*x[(i+T)%N_lat] / (N_lat*N_meas);
      }
    }
    // 3. Wavefunction
    for(int i=0;i<N_lat;i++){
      if(abs(x[i])<x_range){
        psi[(int)floor((x[i]+x_range)/dx)]+=1;
      }
```

```
    }
  }
  // Write correlator ratio
  for(int T=0;T<N_lat;T++){
    fprintf(fCorRatio,"%f \n", C[T]/C[(T+1)%N_lat]); // for large T, this gives a(E1-E0)
  }
  // Write wavefunction
  for(int i=0;i<N_bin;i++){
    fprintf(fpsi,"%f %f\n", i*dx-x_range, sqrt(psi[i]/(dx*N_meas*N_lat)));
  }

  printf("Acceptance rate: %f \n", (double)acc/tot);

  cleanup();
  return 0;
}

// Calculate difference in action
double dS(int i, double x_old){
  return (x[i]*(x[i]-x[(i+1)%N_lat]-x[(i-1+N_lat)%N_lat])/a
          + alpha*a*sq(x[i]) + lambda*a*qd(x[i]))
         - (x_old*(x_old-x[(i+1)%N_lat]-x[(i-1+N_lat)%N_lat])/a
              + alpha*a*sq(x_old) + lambda*a*qd(x_old));
}
// Metropolis update
void update(){
  double x_old;
  double d; // Difference in action
  for(int i=0;i<N_lat;i++){
    x_old=x[i];
    x[i]=x[i] + epsilon * (gsl_rng_uniform(r)-0.5)*2;
    acc++; tot++;
    d=dS(i,x_old);
    if(d>0){
      if(exp(-d)<gsl_rng_uniform(r)){ x[i]=x_old; acc--; } // Revert to old value
    }
  }
}

void setup(){
  // Cold start
  for(int i=0;i<N_lat;i++){ x[i]=0; C[i]=0; }

  // Initialize variables
  acc = 0;
  tot = 0;
  E0 = 0;
  for(int i=0;i<N_bin;i++){ psi[i]=0; }

  // Create Files
  fE0=fopen("E0.txt", "w+");
  fCorRatio=fopen("CorRatio.txt", "w+");
  fpsi=fopen("psi.txt", "w+");

  // Setup random environment
  gsl_rng_env_setup();
  T = gsl_rng_mt19937;
  r = gsl_rng_alloc (T);
}

void cleanup(){
  gsl_rng_free (r);

  // Close Files
  fclose(fE0);
  fclose(fCorRatio);
  fclose(fpsi);
}
```