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Lattice QCD SUPA course report

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Abstract. This is a report on the homework assignment for Christine Davies' graduate Lattice QCD course taught under the SUPA banner (http://my.supa.ac.uk/course/view.php?id=36). I present a study of calculations of the first excited energy level of the one-dimensional quantum harmonic oscillator using numerical path integrals performed using a custom C library that allows the calculation of energy levels for arbitrary potentials in one-dimensional quantum mechanics.

Contents

1 Introduction

Due to the mathematical complexity of quantum theories it is generally difficult or impossible to solve problems in these exactly by analytical means except in a small family of special cases. One solution to this dilemma is to give up the hope of finding exact solutions and instead use perturbation theory to some order in some suitably small parameter to approximate solutions with more-or-less controlled and understood errors due to the neglected higher order corrections. In the context of the quantum field theories used in high-energy physics this solution is adopted almost universally through the Feynman diagram formalism which chooses the couplings between different fields as the expansion parameters.

This way of performing calculations breaks down for Quantum Chromodynamics (QCD) at low energy scales. The beta function which determines the running of the strong coupling $g_s(\mu^2)$ is given by:

$$\mu^2 \frac{d\alpha_S}{d\mu^2} = \beta(\alpha_S) = -(b_0\alpha_S^2 + b_1\alpha_S^3 + b_2\alpha_S^4 + ...) \tag{1.1}$$

Here b_n are numerical constants which can be calculated perturbatively and are known to four-loop order, and $\alpha_S = \frac{g_s^2}{4\pi}$. Crucially the leading coefficient b_0 is positive for $N_f \leq 16$ where N_f is the number of active flavours. This means the coupling will decrease as we go higher in energy scale but increase with decreasing scales, eventually diverging completely within the perturbative scheme. This suggests we can't rely on the Feynman diagram formalism for making low energy predictions with the theory. In high-energy physics this problem is typically solved by using phenomenological models such as parton showers and fragmentation functions which are tuned to data and matched on to perturbative calculations performed at some higher (perturbative) scale. To truly test the theory in the low energy regime we should compare experimental data to predictions made from first principle calculations however, and tuned phenomenological models can not provide these.

The most successful approach to dealing with this problem is lattice QCD, which uses the path integral formulation of quantum mechanics and a discretised spacetime grid to make physical predictions with first principle calculations using very limited experimental input in a well-defined way. In this report I will present results obtained with a custom C library based on the outline given in [1] for solving problems in a one-dimensional quantum mechanics toy model using this approach, and study the solutions obtained to make statistical error estimations and understand various features of these which also will be reflected in realistic lattice QCD results. The following section is largely reproduced from [1] but is included for completeness.

2 Path integrals and the quantum harmonic oscillator

The path integral formulation of quantum mechanics states we can calculate the (quantum mechanical) transition amplitude from x_a to x_b in time T using the classical action L through a path integral:

$$U(x_a, x_b, T) = \int \mathcal{D}x(t) e^{i\int_0^T dt L} \tag{2.1}$$

Here $x(t)$ are path configurations with begin at x_a and end at x_b. By Wick-rotating to Euclidean time we turn the oscillating exponential into an exponentially decaying one (and change signs in the lagrangian accordingly):

$$U(x_a, x_b, T) = \int \mathcal{D}x(t) e^{-\int_0^T dt L} \tag{2.2}$$

We can now hope to be able to perform quantum mechanical calculations numerically after discretising the paths either by performing the integration explicitly, or by averaging over some randomly generated paths $x_i(t)$ with a probability density P:

$$P(x_i(t)) \propto e^{-\int_0^T dt L} \tag{2.3}$$

These two options can be compared by referring to the simple situation of trying to integrate d-dimensional functions numerically: explicit evaluation using for example the trapezoidal rule is faster and more precise for low dimensional problems but in higher dimensions the error scaling will completely favour the Monte Carlo technique as the error always scales as $1/\sqrt{N}$ (where N is the number of Monte Carlo integration points or randomised paths in our case) while the explicit techniques will have an error that scales to some power in d. For realistic quantum field theory calculations the number of degrees of freedom will approach infinity, and therefore we clearly need to use the random path approach for such calculations.

Going back to extracting observables, to calculate the ground state energy we can study 2.2 with $x_a = x_b = x$ in the hamiltonian formulation of quantum mechanics:

$$\begin{aligned} U(x, x, T) &= \langle x | e^{-\hat{H}T} | x \rangle \\ &= \sum_n \langle x | e^{-\hat{H}T} | E_n \rangle \langle E_n | x \rangle \\ &= \sum_n \langle x | E_n \rangle e^{-E_n T} \langle E_n | x \rangle \end{aligned}$$

$$\Rightarrow \lim_{T\to\infty} U(x,x,T) = e^{-E_0 T}|\langle x|E_0\rangle|^2$$
$$\Rightarrow \int dx \lim_{T\to\infty} U(x,x,T) = e^{-E_0 T} \tag{2.4}$$

Hence if we are able to calculate 2.2 at large T we can extract the ground state energy. In quantum field theories we are typically interested in excited states however. To study excited states using path integrals we have to introduce intermediate operators into the propagation of the ground state. Consider:

$$\langle 0|x(t_2)x(t_1)|0\rangle = \frac{\int \mathcal{D}x(t)x(t_2)x(t_1)e^{-\int_0^T dtL}}{\int \mathcal{D}x(t)e^{-\int_0^T dtL}} \tag{2.5}$$

Unlike before here we integrate over all initial and final points of the paths as well as the intermediate steps. In hamiltonian quantum mechanics the numerator can be simplified through the following steps:

$$\begin{aligned}
&\int dx\ \langle x|e^{-\hat{H}(t_f-t_2)}\hat{x}e^{-\hat{H}(t_2-t_1)}\hat{x}e^{-\hat{H}(t_1-t_i)}|x\rangle \\
&= \int dx \sum_{n,m}\langle x|e^{-\hat{H}(t_f-t_2)}|E_n\rangle\langle E_n|\hat{x}e^{-\hat{H}(t_2-t_1)}\hat{x}e^{-\hat{H}(t_1-t_i)}|E_m\rangle\langle E_m|x\rangle \\
&= \delta_{nm}\sum_{n,m} e^{-E_n(t_f-t_2)}\langle E_n|\hat{x}e^{-\hat{H}(t_2-t_1)}\hat{x}|E_m\rangle e^{-E_m(t_1-t_i)}
\end{aligned}$$

Where the δ function comes from integrating over the (orthogonal) states. Using $t = t_2 - t_1$ and again putting in $t_i = 0$, $t_f = T$ we can rewrite this as:

$$\langle 0|x(t_2)x(t_1)|0\rangle = \frac{\sum_n e^{-E_n T}\langle E_n|\hat{x}e^{-(\hat{H}-E_n)t}\hat{x}|E_n\rangle}{\sum_n e^{-E_n T}}$$
$$\Rightarrow \lim_{T\to\infty}\langle 0|x(t_2)x(t_1)|0\rangle = \langle E_0|\hat{x}e^{-(\hat{H}-E_0)t}\hat{x}|E_0\rangle \tag{2.6}$$

$\langle E_0|\hat{x}|E_0\rangle = 0$ since $\hat{x}$ switches parity when it acts on a state, so sandwiching in a complete set of energy eigenstates once again we get the first non-zero contribution from $|E_1\rangle$. Then if we take t to be large but still $\ll T$, this contribution will dominate and:

$$\lim_{T\to\infty}\langle 0|x(t_2)x(t_1)|0\rangle \overset{t\,\text{large}}{\to} |\langle E_0|\hat{x}|E_1\rangle|^2 e^{-(E_1-E_0)t} \tag{2.7}$$

This allows us to extract the first excitation level from a numerical path integral calculation. Notice that the size of $|\langle E_0|\hat{x}|E_1\rangle|^2$ compared to $|\langle E_0|\hat{x}|E_n\rangle|^2$ will determine how quickly this convergence happens, which means an appropriate choice of operator $\hat{O}$ will allow us to extract the first excited state for lower values of t, or could alternatively allow us to extract information about higher excited states if we managed to suppress $|\langle E_0|\hat{O}|E_1\rangle|^2$ as well as $|\langle E_0|\hat{O}|E_0\rangle|^2$.

The harmonic oscillator has the following classical lagrangian (after a Wick-rotation):

$$L = \frac{p^2}{2m} + \frac{m}{2}\omega^2 x^2 \tag{2.8}$$

To perform numerical path integrals we need to discretise the classical action S to allow it to be calculated in the context of the discretised paths $x_i(t)$ we want to use. We can make a first order finite difference approximation to find the contribution from a short time period a between t_i and $t_i + a$ as:

$$\delta S = \int_{t_i}^{t_i+a} dtL \approx a\left(\frac{m}{2}\left(\frac{x_{i+a}-x_i}{a}\right)^2 + \frac{1}{2}\left(\frac{m}{2}\omega^2 x_{i+a}^2 + \frac{m}{2}\omega^2 x_i^2\right)\right) \tag{2.9}$$

This is of course a local expression which means we can easily calculate the contribution to the action from one part of the path x_i[1] as:

$$S^{1^{st}}(x_i) = \frac{mx_i}{a}\left(x_i - x_{i+a} - x_{i-a}\right) + \frac{ma\omega^2 x_i^2}{2} \tag{2.10}$$

By going through a bit more algebra we can make a higher order finite difference approximation which changes this to:

$$S^{2^{nd}}(x_i) = \frac{mx_i}{a}\left(\frac{5}{4}x_i - \frac{4}{3}(x_{i+a} + x_{i-a}) + \frac{1}{12}(x_{i+2a} + x_{i-2a})\right) + \frac{ma\omega^2 x_i^2}{2} \tag{2.11}$$

I will sometimes refer to $S_i^{2^{nd}}$ as the improved action.

We are now ready to use $S_i^{1^{st}}$ and $S_i^{2^{nd}}$ to generate ensembles of paths with the correct probability density 2.3. This can be achieved using the Metropolis algorithm, which proceeds by deciding on a constant ϵ and looping over all x_i, updating each point as follows:

1. Cache the old x_i and $S = S(x_i)$
2. Add a generated random number $\xi \in (-\epsilon, \epsilon)$ to x_i so $x'_i = x_i + \xi$
3. Calculate $S' = S(x'_i)$ and generate a random number $\eta \in (0, 1)$
4. If $S' - S > 0$ and $\exp(S - S') < \eta$, reverse the change in x_i to the cached value

By applying the Metropolis algorithm to our path many times and storing the resulting paths we can generate a large ensemble of paths with the correct probability distribution, allowing us to average out path integrals and access the value of for example 2.5.

3 Estimating statistical errors

Generating several path ensembles to estimate the statistical error on the calculated observables would be incredibly expensive so in presenting results I will make use of the so-called bootstrap method for estimating errors. Instead of generating several ensembles I will randomly chose among the calculated values for my chosen observable and calculate a new average based on these. By repeating this procedure several times and assuming the full path ensemble has the correct probability distribution among the paths, I will get a decent estimate of the variance of the calculated result.

[1] Note I use the subscript to refer to the time coordinate here, as opposed to as a label for a particular path configuration as above.

Of course the original observable is generally processed in some way to retrieve the information we want to obtain, for example I will be plotting:

$$\frac{\log\left(G(t)/G(t+a)\right)}{a} \approx E_1 - E_0, \qquad G(t) = \langle 0|x(t_2)x(t_1)|0\rangle, \qquad t = t_2 - t_1 \tag{3.1}$$

This means the error on $G(t)$ also needs to be propagated correctly through the calculation to get the final uncertainty on the excited energy level. The error that is ultimately presented is one standard deviation calculated by this method.

4 Results

4.1 Calculation of the first excited energy level

Solving the quantum harmonic oscillator defined by the classical action 2.8 analytically we get energy levels $E_n = \omega(\frac{1}{2}+n)$[2] so we would like to confirm that using the path integral Monte Carlo approach to calculate $E_1 - E_0$ we get ω. This is shown in figure 1. Clearly the path integral calculation works very well for $\omega = 1$ and is still decent for $\omega = 2$ but is not reliable for $\omega = 4$ for the coarse discretisation shown in the plot on the left. This can be understood as a failure of our calculation to model very quickly changing paths, which will become more important as we increase ω. Indeed, using a finer discretisation as done in the plot on the right completely solves this problem and also improves the results for the other values of w.

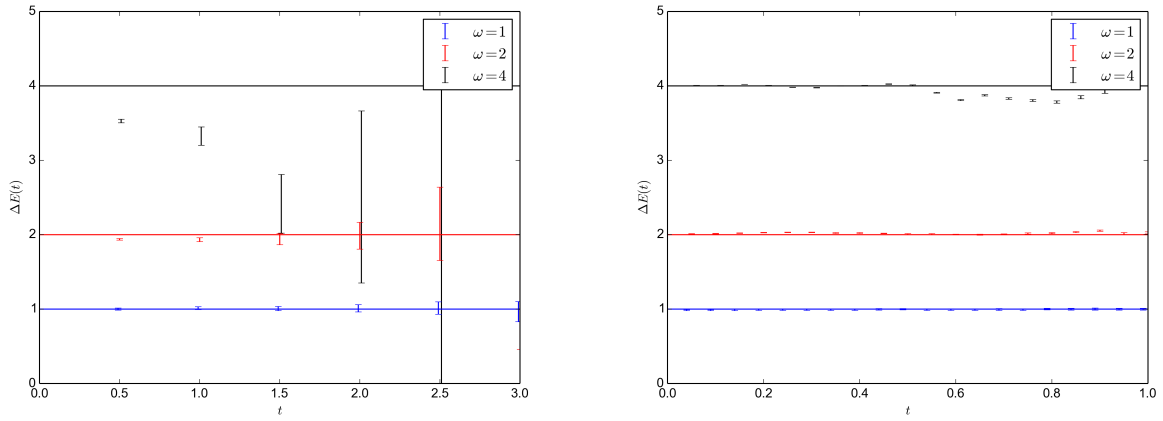

Figure 1: Results for $\Delta E = E_1 - E_0$ when varying ω with $T = 10$, $a = 1/2$ (left), $a = 1/20$ (right), $N = 10^4$, $\epsilon = 1.4$ as a function of time, using the unimproved action 2.10. Due to the appropriate choice of operator the results converge to the asymptotic value very quickly. The horizontal lines of corresponding colour show the exact result.

4.2 Using the improved action

We can attempt to make up for the errors due to the coarse discretisaton on the left hand in figure 1 by using the improved action 2.11 which has errors that are two orders higher in a. Results for the same setup with the improved and unimproved action are presented on the left in figure 2. The improved action takes longer to approach the asymptotic value (and does so from below) but is more accurate for higher t.

[2]Note we have been working with $\hbar = 1$ from the beginning.

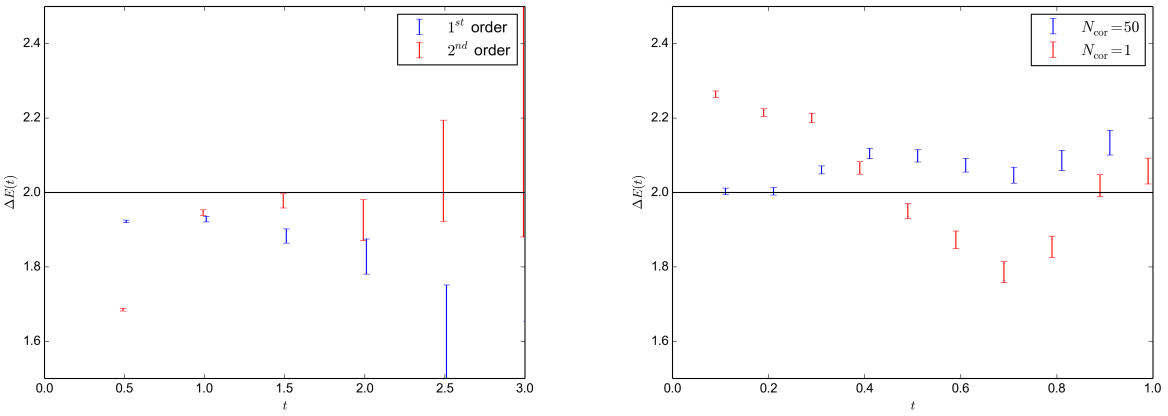

Figure 2: Left: Results for $\Delta E = E_1 - E_0$ for the 1^{st} (2.10) and 2^{nd} (2.11) order finite difference actions with $\omega = 2$, $T = 10$, $a = 1/2$, $N = 10^6$, $\epsilon = 1.4$ as a function of time. The horizontal line shows the exact result.
Right: Results for $\Delta E = E_1 - E_0$ for $N_{\text{cor}} = 1$ and 50 with the unimproved action, $\omega = 2$, $T = 10$, $a = 1/10$, $N = 10^3$, $\epsilon = 1.4$ as a function of time. The horizontal line shows the exact result.

4.3 Failing to thermalise and using correlated paths

The previous results have all been calculated with $N_{\text{cor}} = 50$, where this is the number of updates of the path that are performed before a new one is stored, and the path initially is thermalised by updating the path $5 \times N_{\text{cor}}$ times before storing the first one. The right plot in figure 2 shows the result using this default value of N_{cor} and $N_{\text{cor}} = 1$ for a relatively low value of $N = 10^3$, which will force the high correlation between the paths and low thermalisation of the initial path to bias the calculation which then fails to produce the correct result.

5 C library

The results in the previous section were obtained using a custom C library which can be obtained from (https://github.com/karlnordstrom/LatticeCode). In theory it supports arbitrary potentials in one-dimensional quantum mechanics and any operator $\hat{O}$, although in practice the user has to implement these as functions passed to the relevant parts of the code as functional pointers. It is designed to be relatively fast, allowing calculations with $N = 10^5$, $N_{\text{cor}} = 50$, $T = 10$, $a = 1/10$ with errors calculated through 100 bootstrap sets in less than a second on a modern CPU. It makes use of Makoto Matsumoto's Mersenne Twister [2] MT64 (http://www.math.sci.hiroshima-u.ac.jp/~m-mat/MT/emt64.html) to generate pseudorandom numbers.

6 Conclusion

I have presented a study of numerical path integral results in the context of the first excited energy level of the quantum harmonic oscillator, where we conveniently know the exact solution. I have shown how a coarse discretisation makes it impossible to make predictions for high frequencies since we fail to model irregular paths, how using an improved action can correct some of the error in

using a coarse discretisation, and the importance of thermalising and removing correlations between paths.

References

[1] G. Lepage, *Lattice QCD for novices*, hep-lat/0506036.

[2] M. Matsumoto and T. Nishimura, *Mersenne twister: A 623-dimensionally equidistributed uniform pseudo-random number generator*, *ACM Trans. Model. Comput. Simul.* **8** (Jan., 1998) 3–30.