Abstract

Systems of ultra-cold gases in light-induced periodic potentials, often called optical lattices, are of great experimental and theoretical interest, and have been since the first experimental realisation of Bose-Einstein condensation in 1995. This is largely due to the parallels between the behaviour of bosons on optical lattices and condensed matter systems, where electrons can be modelled as moving on a lattice generated by the periodic array of atom cores. This project investigates the time evolution of a system of bosons prepared in a far-from-equilibrium state on a one-dimensional or two-dimensional optical lattice. The key question of interest is whether the system relaxes to some sort of equilibrium state or if it exhibits exact and regular revival to the initial state.

Introduction

The question of how, and under what conditions, closed quantum systems approach thermal equilibrium is an old question that forms the basis of a large and active field of research. Thermalisation is well understood in the context of classical mechanics, where it emerges from the chaotic dynamics of sufficiently unconstrained systems. However, the time evolution of quantum systems is strictly linear, and hence they do not exhibit chaotic dynamics. Nonetheless, there are a number of closed quantum systems in which thermalisation is observed, in the sense that the systems relax to states in which the values of macroscopic quantities are stationary, universal with respect to widely differing initial conditions, and predictable using statistical mechanics [**?**].

This project investigates the time evolution of a variety of different systems composed of noninteracting and interacting bosons on one-dimensional and two-dimensional optical lattices that are prepared in far-from-equilibrium states. These systems are investigated analytically where possible, and with numerical methods for larger and more complicated systems where an analytic approach is not tractable.

We focus primarily on gaining a strong understanding of smaller systems of few lattice sites and bosons, as these can be solved exactly.

1 Experiments with optical lattices

This project considers the thermalisation behaviour of systems of bosons on optical lattices. One of the main factors that make these systems interesting to work with are the deep similarities between the Hamiltonians of systems that can be generated using bosons on an optical lattices and those of electrons moving on a lattice potential produced by a periodic array of atom cores. We can simulate these condensed matter systems with ultracold atoms by using optical lattices to generate the periodic potential.

An optical lattice is produced by overlapping multiple laser beams and making use of the interference pattern. The alternating bright and dark areas of the interference pattern act as a periodic potential on the atoms through the optical dipole force [**?**]. By superimposing different combinations of laser beams at particular frequencies and amplitudes, any lattice geometry that can be constructed via Fourier synthesis can, in principle, be produced [**?**]. This fine degree of control over the lattice parameters, in conjunction with the ability to tune the strength of interparticle interactions by manipulating Feshbach resonances [**?**], makes ultracold bosons on optical lattices an excellent arena in which to explore various model Hamiltonians for condensed matter systems and quantum optics.

As we are dealing with large numbers of indistinguishable bosons, we will exclusively use the second quantised representation, which is much more succint as it makes no reference to unique identities of individual particles. For a discussion of the mathematics of second quantisation, see **??**.

In this formalism, the Hamiltonian that describes our system is

2 First quantised representation

This dissertation will deal exclusively with bosons on optical lattices, and not investigate cases involving fermions. There are a number of different contributions to the Hamiltonian for bosons on optical lattices, and these contributions can be seen to have analogues in condensed matter systems. The individual bosons will have kinetic energy, and the potential created by the lattice also contributes to how the system evolves in time, so it must feature in the Hamiltonian. The bosons may be interacting, and there may also be an external potential imposed that can vary in strength from site to site.

With regards to the interparticle interactions, we consider repulsive scattering interactions. We will consider systems that are dilute, in the sense that the average spacing between bosons is much greater than the effective range of the interparticle interactions. This makes it reasonable to consider only two-particle scattering events and neglect the rare higher order collisions, provided we keep the strength of the interparticle interactions small. Even when reduced to its two-body form, $U(x, x')$, the form of the interatomic scattering potential has short range terms that can be difficult to deal with. We can replace this object with a mathematically more convenient effective potential, corresponding to contact interaction, with the same scattering cross-section at low energy. Because the ultracold bosons have such low energy, s-wave scattering dominates, and the interparticle interaction potential can be expressed simply in terms of

the s-wave scattering length, a_s, as

$$U_{\text{eff}} = \frac{2\pi\hbar^2 a_s}{m} \sum_{i,j} \delta(x_i - x_j). \tag{1}$$

For simplicity, we will introduce the notation $U_0 = \frac{4\pi\hbar^2 a_s}{m}$. Having made these simplifications, we can construct a first quantised Hamiltonian for a one-dimensional system of interacting bosons on an optical lattice, in the presence of an external potential V_{ext}

$$\hat{h} = \sum_i -\frac{\hbar^2}{2m}\partial_{x_i}^2 + \sum_i V_{\text{lattice}}(R_i) + V_{\text{ext}}(x) + \frac{U_0}{2}\sum_{i,j}\delta(x_i - x_j). \tag{2}$$

Similar Hamiltonians are frequently used to describe systems of electrons on atomic lattices. To promote conciseness, we introduce the abbreviations

$$\hat{h}_1 = \sum_i -\frac{\hbar^2}{2m}\partial_{x_i}^2 + \sum_i V_{\text{lattice}}(R_i), \quad \hat{h}_{\text{ext}} = V_{\text{ext}}(x), \quad \hat{h}_{\text{int}} = \frac{U_0}{2}\sum_{i,j}\delta(x_i - x_j)$$

so that $\hat{h} = \hat{h}_1 + \hat{h}_{\text{ext}} + \hat{h}_{\text{int}}$.

3 The Bose-Hubbard model

The Hamiltonian for a weakly interacting BEC in a one-dimensional optical lattice and subject to harmonic trapping potential is given by the sum of $\hat{H}_1$, $\hat{H}_{\text{ext}}$ and $\hat{H}_{\text{int}}$:

$$\hat{H}_{\text{1D}} = J\sum_i (\hat{a}_i^\dagger \hat{a}_{i+1} + \text{h.c.}) + \frac{U_0}{2}\sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i + \sum_i \epsilon_i \hat{a}_j^\dagger \hat{a}_j, \tag{3}$$

and is known as the Bose-Hubbard Hamiltonian. The ϵ_i's refer to on-site energies at each lattice site due to the harmonic trap, and the middle term gives an interaction energy when there is more than one particle on a particular site. This project will look at scenarios where there is no external harmonic potential which produces different on-site energies for different sites (the uniform lattice potential remains, so J is still defined as before). In the absence of this external potential, the Hamiltonian in one dimension reduces to

$$\hat{H}_{1D} = J\sum_i (\hat{a}_i^\dagger \hat{a}_{i+1} + \text{h.c.}) + \frac{U_0}{2}\sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i.$$

This project aims to explore the dynamics of both this one-dimensional system and the two-dimensional version where we couple multiple chains of lattice sites together. The system Hamiltonian in two dimensions is

$$\hat{H}_{2D} = \left(J\sum_{i,j} \hat{a}_{i,j+1}^\dagger \hat{a}_{i,j} + J'\sum_{i,j} \hat{a}_{i,j}^\dagger \hat{a}_{i+1,j} \right) + \text{h.c.} + \frac{U_0}{2}\sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i, \tag{4}$$

where the i index denotes which chain is being referred to and the j index denotes how far along the chain a site is. J' is another hopping parameter, in this case characterising the hopping between sites on different chains.

Figure 1: The blue circles here represent lattice sites and the crosses denote individual bosons. Hopping between any two neighbouring sites on the same chain is characterised by J, whereas hopping between chains is characterised by J'. A three by three lattice is shown here, but the system can be extended to arbitrary size.

We are interested in the time evolution of these systems as it relates to their thermal behaviour.

4 Thermalisation

4.1 Overview

Thermalisation refers to a relaxation of a system to states where the values of macroscopic quantities are stationary, universal with respect to widely differing initial conditions, and predictable using statistical mechanics [**?**]. We observe thermalisation in a wide variety of classical systems, and there are strong theoretical reasons for anticipating this thermalisation. However, many of these reasons don't apply when considering quantum systems. The question of which, if any, quantum systems exhibit thermalisation and how the thermal states can be characterised is of considerable theoretical and experimental interest.

4.2 Classical systems

To see why thermalisation is common and even expected in many classical systems, we need to understand the property of ergodicity and the impact of chaotic dynamics on it. If you start an isolated system in a particular configuration corresponding to a particular point in phase space, it can move through that phase space along the constant-energy manifold. A system is ergodic if the long-term time average of any single phase space trajectory is equivalent to an ensemble average.

Aside from a few rare examples that are usually emphasised in physics textbooks, the equations of motion for most classical systems do not have simple analytic solutions [**?**]. This means that we usually need to resort to numerical methods to determine the evolution of these systems in time by solving nonlinear partial differential equations. It is a well known fact about such systems that they display an extreme sensitivity to the initial conditions, such that the uncertainties or errors in the initial conditions can grow exponentially as the system evolves in time, not merely as a result of numerical approximations made but as an intrinsic property of the system. Our inability to know the initial conditions of a real system with infinite precision presents an notoriously challenging obstacle to long term predictions of these nonlinear systems, such as the weather.

The nonlinearities present in chaotic systems drive them in seemingly irregular motion. This allows the system to quickly and essentially uniformly explore the constant-energy manifold irrespective of the initial conditions. This promotes ergodicity, and thereby provides justification for the fundamental assumption of statistical mechanics - all accessible microstates are equiprobable.

This combination of factors is what leads us to expect our classical systems to thermalise.

4.3 Quantum systems

The time evolution of quantum mechanical systems is governed by the Schrödinger equation, which is linear. This implies that the key ingredient in producing dynamical chaos in classical systems, namely, the presence of nonlinear equations of motion, is absent from quantum systems.

Without nonlinearities promoting exploration the phase space, it is not obvious how one would justify applying the assumption of ergodicity to quantum systems. Hence, it is unclear if, or when, we should expect quantum systems to thermalise, or what statistical ensemble we could use to characterise the relaxed states. One possible source of theoretical predictions is the Eigenstate Thermalisation Hypothesis, (ETH) proposed independently by Deutsch [**?**] and Srednicki [**?**]. If the necessary conditions hold for the ETH to be applied (it does not hold for particular classes of Hamiltonians with "atypical" eigenstates, such as those of integrable systems), then ity implies that the expectation values of observables as well as their fluctuations in isolated quantum systems far from equilibrium relax to (nearly) time-independent results that can be described using traditional statistical mechanics ensembles [**?**]. Making predictions about our system using the ETH would require considerable use of Random Matrix Theory, which is beyond the scope of this dissertation but could form the basis of future work.

5 Integrable systems

There are a number of classical, isolated systems that do not display thermalisation. The main difference between these systems and those which approach thermal equilibrium is the extent to which they are constrained relative to the number of degrees of freedom that they possess. This observation is formalised in the notion of integrability. A system is said to be integrable if it has half as many independent integrals of motion (which are conserved) as it has degrees of freedom [**?**]. An integral of motion for a Hamiltonian is a smooth function I defined on an open subset of the phase space such that $\dot{I} = 0$ on solutions. So $I(x(t)) =$ constant, where $x(t)$ is the solution of the equations of motion for a particular initial condition. If $x_1(t)$ and $x_2(t)$ are solutions for different initial conditions, then in most cases $I(x_1(t)) \neq I(x_2(t))$. Integrability is a useful property, though it is quite rare.

Theoretically, we can find exact solutions for the equations of motion for a system if it is integrable, otherwise we cannot. In classical mechanics, the idea of integrability is well-understood and neatly defined. The situation in quantum mechanics is much more challenging. One reason for this is that the Heisenberg uncertainty principle prevents us from applying the idea of points in phase space with particular trajectories. However, a commonly used definition of quantum integrability requires the presence of a large number of local operators (more precisely, linear combinations of these operators) that commute with the Hamiltonian and each other and thus provide a set of conserved quantities. With respect to the systems that we are dealing with, it has been shown that a one-dimensional lattice chain of non-interacting bosons is an integrable system (according to the previously mentioned definition of quantum integrability) [**?**].

This is particularly interesting in light of the fact that the ETH is not satisfied for integrable systems. This may lead us to expect that we will not observe thermalisation in noninteracting one-dimensional systems, as it has recently been shown that the ETH must be satisfied for thermalisation to occur [**?**] on the level of the eigenstates. Nonetheless, it has been argued [**?**] that the existence of those conserved quantities does not preclude the thermalization of physical observables.

The conserved quantities constrain the time evolution in such a way that not all of the constant-energy manifold is accessible. However, the system may still explore the reduced phase space ergodically. This idea has inspired the use of a generalised Gibbs ensemble (GGE), which includes a linear combination of the conserved quantities in the partition function, to predict the mean values of physical observables in whatever sort of equilibrium state that the integrable system relaxes into [**?**].

6 Experimental studies

6.1 A quantum Newton's cradle

Kinoshita et. al. investigated [**?**] the thermalisation of an out-of-equilibrium one-dimensional Bose gas, which is a nearly-integrable system. They started with several thousand arrays of one-dimensional Bose gases, each containing from 40 to 250 ^{87}Rb atoms. The atoms were trapped by combining a blue-detuned two-dimensional optical lattice, which provides tight transverse confinement, with a red-detuned crossed dipole trap providing weak axial trapping. In order to create the non-equilibrium momentum distributions, they then pulsed on a 3.2 THz detuned one-dimensional lattice, which depleted the zero momentum state and put the atoms in a superposition momentum state of $\pm 2\hbar k$. The two parts of the wavefunction then oscillated out of phase with each other, colliding with each other twice every full cycle and either reflecting off each other elastically or transmitting straight through like a "ghostly" Newton's cradle (see figure **??**).

Figure 2: Sketches at various times of two out of equilibrium clouds of atoms in a one-dimensional anharmonic trap. At time $t = 0$ the atoms are put into a momentum superposition with $2\hbar k$ to the right and $2\hbar k$ to the left. The two parts of the wave function oscillate out of phase with each other with a period τ. Each atom collides with the opposite momentum group twice every full cycle, for instance, at $t = 0$ and $t = \frac{\tau}{2}$. Figure is from reference [**?**].

The weak anharmonicity of the trap caused the atoms to gradually dephase. However, as can be seen from figure **??**, the momentum distribution after dephasing was not Gaussian (as one would expect for a thermalised state), and did not noticeably tend toward this Gaussian equilibrium distribution, even after thousands of collisions.

Figure 3: The blue and green curves in the above figure are projections from models that take into account loss and heating. The red line is the actual distribution observed. The dashed line is a Gaussian with the same number of atoms and r.m.s. width as the actual distribution.

To the extent that the actual distribution in figure **??** conforms to the projected distribution rather than to the Gaussian, the atoms have not thermalised. This absence of thermalisation extended from the Tonks–Girardeau regime, which has very strong repulsive interactions between bosons so only pairwise collisions can occur, to the intermediate coupling regime, where there can be three- (or more) body collisions. This study represents a significant experimental breakthrough on the question of the time evolution of out-of-equilibrium one-dimensional Bose gases.

6.2 Relaxation in an Integrable Many-Body Quantum System

Inspired by the "A Quantum Newton's Cradle" study, investigations were made into a completely integrable many-body quantum system, and the authors demonstrated strong agreement between their numerical data and the predictions generated using the generalised Gibbs ensemble. In this study the authors, Rigol et. al [**?**], started with a Hamiltonian for hard-core bosons with no interactions on a one-dimensional lattice with L lattice sites and periodic boundary conditions .

$$\hat{H} = -J \sum_{i=1}^{L} (\hat{a}_i^\dagger \hat{a}_{i+1} + \text{h.c.}) \tag{5}$$

They then mapped their bosonic system to a free fermionic one using a Jordan-Wigner transformation:

$$\hat{H} = -J \sum_{i=1}^{L} (\hat{c}_i^\dagger \hat{c}_{i+1} + \text{h.c.}) \tag{6}$$

Here $\hat{c}_i^\dagger$ and $\hat{c}_{i+1}$ are fermionic creation and annihilation operators. The integrals of motion were the fermionic quasi-momentum distribution operators, and the system thus must be integrable because there are as many of these operators as they had lattice sites. They have numerically investigated the time evolution of this system and found it to undergo relaxation to an equilibrium state. The quasi-momentum distribution of this equilibrium state was shown to have excellent agreement (see figure **??**) with the predictions of a generalised Gibbs ensemble, in which the partition function is extended to include all of the integrals of motion.

Figure 4: Equilibrium (quasi-)momentum distribution after relaxation in comparison with the predictions of the grand-canonical and of the fully constrained thermodynamic ensembles. The prediction of the fully constrained ensemble is virtually indistinct from the results of the dynamical simulation. Image taken from [**?**].

They further showed that their generalised equilibrium state carries more memory of the initial conditions than the usual thermodynamic one, which is consistent with their system not satisfying the ETH because it is integrable.

7 System size and analyticity

Whilst the main focus of this project is on smaller lattices with few particles, it is of interest to investigate larger system sizes (necessarily by approximate methods) to see how much of the qualitative behaviour of the small systems is preserved in the larger ones.

7.1 Dimensionality of many-body systems

We can decompose any time evolved state $|\psi(t)\rangle$ of our system in terms of its state at $t = 0$, $|\psi(0)\rangle$, and the energy eigenvectors $|E_n\rangle$ (see section **??** for details):

$$|\psi(t)\rangle = \sum_j e^{iE_j t} |E_j\rangle \langle E_j|\psi(0)\rangle. \tag{7}$$

Calculating $|\psi(t)\rangle$ from the above formula requires that we diagonalise the Hamiltonian and find its energy eigenvectors and eigenvalues. This is easy for small systems, in particular those that have only a single particle on them. This method has the significant advantage of being "analytic", at least up to the precision of the values stored for the eigenvalues and eigenvectors. All instances of $|\psi(t)\rangle$ are calculated from the initial state $|\psi(0)\rangle$, so the value we calculate for $|\psi(t)\rangle$ is independent of the time-step between each instance of $|\psi(t)\rangle$ that we calculate. This has the further advantage that in a numerical algorithm we need not concern ourselves with drifting of the norm. However, as the number of lattice sites and particles in the system increases, the time required to apply this method increases dramatically. This is because the dimensionality $\mathcal{D}$ of the system grows according to

$$\mathcal{D} = \frac{(N + P - 1)!}{P!(N - 1)!}, \tag{8}$$

where N is the number of lattice sites and P is the number of particles on the lattice. Unsurprisingly, this is the same as the number of possible pure number states (since these form an orthonormal basis), and so the formula deduced is just the formula for the number of ways to arrange P objects into N containers that is familiar from elementary statistical mechanics. The Hamiltonian can be represented in the basis of energy eigenvalues as a $\mathcal{D} \times \mathcal{D}$ square matrix. However diagonalising this matrix, determining its energy eigenvalues and then evolving the system according to equation (**??**) quickly becomes impractical for systems with large numbers of particles and lattice sites.

8 Results

9 Revival

In a subset of the integrable systems considered, we observed regular instances in which the system would return to the state in which it was initially prepared (it "revives"). To see why we might expect to see revival in some cases, consider the initial state of the system $|\psi(0)\rangle$, which evolves in time according to

$$|\psi(t)\rangle = e^{i\hat{H}t} |\psi(0)\rangle \,, \tag{9}$$

where –for sake of brevity and transparency– the constant $\hbar^{-1}$ has been incorporated into the time scale. Now noting that we can use the completeness relation for the energy eigenstates to expand the initial state in the energy basis

one obtains

$$\begin{aligned}|\psi(t)\rangle &= e^{i\hat{H}t}\sum_j |E_j\rangle\langle E_j|\psi(0)\rangle \\ &= \sum_j e^{i\hat{H}t}|E_j\rangle\langle E_j|\psi(0)\rangle \\ &= \sum_j e^{iE_jt}|E_j\rangle\langle E_j|\psi(0)\rangle \\ &= \sum_j c_j e^{iE_jt}|E_j\rangle . \end{aligned} \tag{10}$$

From here it can be seen that the only time dependence appears in the complex exponentials, each of which is 2π-periodic. If we can find some common time t^* such that $E_j t^* = 2\pi k_j$, where $k_j \in \mathbb{Z}$ for all j, we will recover the initial state exactly, i.e., $|\psi(t^*)\rangle = |\psi(0)\rangle$. The next section describes the conditions necessary for the existence of the revival time.

9.1 Exact revival

We observe an exact and regular revival in precisely the cases in which the eigenvalues are mutually rational, i.e., they are either all rational, or are all rational when divided by the same irrational number.

Definition (Mutually rational set)**.** *We say that a set of eigenvalues are mutually rational if they are all rational when divided by a common real number.*

For example, the set of hypothetical eigenvalues $\{0, \sqrt{2}, 2\sqrt{2}, \frac{3\sqrt{2}}{10}\}$ is mutually rational, whereas $\{0, \sqrt{2}, \sqrt{3}\}$ is not. In the case of mutually rational eigenvalues, we can write $E_j = \frac{p_j}{q_j}$, where p_j, $q_j \in \mathbb{Z}$. The revival time is then given by

$$t^* = \frac{2\pi Q_{\mathrm{LCM}}}{P_{\mathrm{HCF}}}, \tag{11}$$

where Q_{LCM} is the lowest common multiple of $\{q_j\}$ and P_{HCF} is the highest common factor of the $\{p_j\}$.

We are yet to find any systems with nonzero interparticle interaction that have mutually rational eigenvalues. In one dimension, the only systems that we have found that meet the criterion of mutually irrational eigenvalues are those with fewer than 4 lattice sites. In two dimensions, the only systems that exhibit revival have three or fewer chains and three or fewer lattice sites on each chain (see section **??**).

To demonstrate this exact revival, consider a one-dimensional lattice with three sites with a single boson and hopping constant J. The Hamiltonian for this system is

$$\hat{H}_{3\times1} = \begin{pmatrix} 0 & -J & 0 \\ -J & 0 & -J \\ 0 & -J & 0 \end{pmatrix}. \tag{12}$$

Diagonalising this matrix yields the eigenvalues $\{-\sqrt{2}J, 0, \sqrt{2}J\}$. These are mutually rational (if we divide them all by $\sqrt{2}J$ they are all rational). If we rescale the energies by $\sqrt{2}J$ by absorbing that factor into the time scale, then we

get eigenvalues $\{-1, 0, 1\}$. We can see from the graph of the simulation below that this matches up with a return to the initial state at times that are multiples of 2π.

Figure 5: Revival for a system with 3 lattice sites and a single boson.

The reason that there appear to be several revivals that our method "misses" is that states with different phases in the coefficients of the eigenvectors can also produce $\langle n_1 \rangle = 1$, whereas the revival time that is calculated in our method corresponds to exact revival of the initial wave function and not $\langle n_1 \rangle \sim \|\psi(t)\|^2$.

9.2 Approximate revival

The range of systems for which the eigenvalues are mutually rational is a small one. All systems which have nonzero interparticle interactions have mutually irrational eigenvalues. One of the most interesting results so far is that even in the one-dimensional single particle case, if there are more than three lattice sites, the eigenvalues will be irrational. We can demonstrate this by considering a single chain of five sites with one boson. The Hamiltonian for this system is

$$\hat{H}_{5\times 1} = \begin{pmatrix} 0 & -J & 0 & 0 & 0 \\ -J & 0 & -J & 0 & 0 \\ 0 & -J & 0 & -J & 0 \\ 0 & 0 & -J & 0 & -J \\ 0 & 0 & 0 & -J & 0 \end{pmatrix}. \tag{13}$$

The eigenvalues of this system are $\{-\sqrt{3}J, -J, 0, J, \sqrt{3}J\}$. These are clearly not mutually rational, so we cannot find an exact revival time for this system, despite the fact that it is fully integrable [**?**].

Note that the eigenvalues of a system with 4 lattice sites are also mutually irrational as they are

$$\frac{J}{2}\left\{-1-\sqrt{5}, 1+\sqrt{5}, 1-\sqrt{5}, -1+\sqrt{5}\right\}$$

but those for a system of 5 lattice sites are more convenient to work with.

Running a simulation of this system of 5 lattice sites where we start a single boson off on the first site, we find that the probability of finding the boson on the first site never quite reaches unity again.

Figure 6: Absence of exact revival for a system with 5 lattice sites and a single boson.

Judging the figure above by eye, it may appear that we have exact revival, but this is not actually the case. If we look at how long it takes for the system to get within ϵ of its initial state (i.e. $\||\psi(t)\rangle - |\psi(0)\rangle\| < \epsilon$) we get the graph below. Note that t^* denotes the time at which the system got within a particular value of ϵ of the initial state the first time after $t = 0$.

Figure 7: Recurrence times for varying values of ϵ.

While we see that the system does appear to get arbitrarily close to revival, but it can take arbitrarily long to do so. This result can be explained in terms of the Poincaré recurrence theorem.

9.3 The Poincaré Recurrence Theorem

In 1890, Henri Poincaré proved [**?**, **?**] the following theorem for classical mechanics:

> Any phase-space configuration (q, p) of a system enclosed in a finite volume will be repeated as accurately as one wishes after a finite (be it possibly very long) interval of time.

This theorem was extended to quantum systems in 1956 by P. Bocchieri and A. Loinger [**?**], where they gave a slightly different form:

Theorem (Quantum recurrence)**.** *Let us consider a system with discrete energy eigenvalues E_n; if $\Psi(t_0)$ is its state vector in the Schrödinger picture at the time t_0 and ϵ is any positive number, at least one time t^* will exist such that the norm $\|\Psi(t^*) - \Psi(t_0)\|$ of the vector $\Psi(t^*) - \Psi(t_0)$ is smaller than ϵ.*

Proof. The proof presented by Bocchieri and Loinger shows the theorem to be true for an infinite-dimensional system. In this dissertation, we investigate only finite-dimensional systems, and a simpler version of the proof can be constructed. We first show that there is a time t^* at which $\| |\psi(t^*)\rangle - |\psi(t_0)\rangle \|^2 < 2\epsilon'$ for any $\epsilon' > 0$ and then extend this to $\| |\psi(t^*)\rangle - |\psi(t_0)\rangle \| < \epsilon$. Note that in the following we will introduce the notation $\tau = t^* - t_0$ and $\alpha^2(t^*) = \| |\psi(t^*)\rangle - |\psi(t_0)\rangle \|^2$.

Let us establish an upper bound for $\alpha(t^*)$. Since α^2 is the square of the norm, we can write it as a scalar product of $|\psi(t^*)\rangle - |\psi(t_0)\rangle$ with itself, and also expand each wavefunctions in the basis of energy eigenfunctions.

$$\begin{aligned}
\alpha^2(t^*) &= \left(\langle\psi(t^*)| - \langle\psi(t_0)|\right)\left(|\psi(t^*)\rangle - |\psi(t_0)\rangle\right) \\
&= 2 - \langle\psi(t^*)|\psi(t_0)\rangle - \langle\psi(t_0)|\psi(t^*)\rangle \\
&= 2 - \sum_{j,n=1}^{\mathcal{D}} c_n^* c_j e^{iE_n t^*} e^{-iE_j t_0} \langle E_n|E_j\rangle - \sum_{j,n=1}^{\mathcal{D}} c_j^* c_n e^{iE_j t_0} e^{-iE_n t^*} \langle E_j|E_n\rangle.
\end{aligned}$$

Since the energy eigenfunctions are orthonormal, $\langle E_j|E_n\rangle = \delta_{ij}$, the right hand side simplifies to

$$\alpha^2(t^*) = 2 - \sum_{n=1}^{\mathcal{D}} |c_n|^2 e^{iE_n(t^*-t_0)} - \sum_{n=1}^{\mathcal{D}} |c_n|^2 e^{-iE_n(t^*-t_0)}.$$

Furthermore due to the totality of the energy basis the ℓ_2 norm of the expansion coefficients is unity, i.e., $\sum_{n=1}^{\mathcal{D}} |c_n|^2 = 1$, thus

$$\alpha^2(t^*) = 2\sum_{n=1}^{\mathcal{D}} |c_n|^2 \left(1 - \cos(E_n\tau)\right) \leq 2\sum_{n=1}^{\mathcal{D}} \big(1 - \cos(E_n\tau)\big).$$

It is sufficient to show that there is a τ such that $\sum_{n=1}^{\mathcal{D}} \left(1 - \cos\left(E_n\tau\right)\right) < \epsilon'$. This is actually a standard result in the theory of almost-periodic functions [**?**].

Evidently, if we know that there exists a time t^* such that

$$\sum_{n=1}^{\mathcal{D}} (1 - \cos(E_n \tau)) < \epsilon', \tag{14}$$

then at this same time $\alpha^2(t^*) < 2\epsilon'$, which implies

$$\alpha(t^*) = \| |\psi(t^*)\rangle - |\psi(t_0)\rangle \| < \sqrt{2\epsilon'}.$$

Taking $\epsilon = \sqrt{2\epsilon'}$ shows that $\| |\psi(t^*)\rangle - |\psi(t_0)\rangle \|$ is guaranteed be arbitrarily small at some arbitrarily large time t^*. ■

9.4 Large one-dimensional systems

To determine the mutual rationality or mutual irrationality of the eigenvalues for an arbitrarily large one-dimensional system with a single particle, we look to a recent result about the eigenvalues of tridiagonal matrices proven by W. Yueh [**?**]. A tridiagonal matrix has the form

$$A_{N\times N} = \begin{pmatrix} b & c & 0 & 0 & \dots & 0 \\ a & b & c & 0 & \dots & 0 \\ 0 & a & b & c & \dots & 0 \\ 0 & 0 & a & b & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & c \\ 0 & 0 & 0 & 0 & a & b \end{pmatrix}. \tag{15}$$

It was shown that the eigenvalues of $A_{N\times N}$ are given by

$$\lambda_k = -b + 2\sqrt{ac}\cos\left(\frac{k\pi}{N+1}\right), \tag{16}$$

where $k = 1, 2, \dots, N$. The Hamiltonian of any one-dimensional system with N sites and a single particle has exactly this form, namely

$$\hat{H}_N = \begin{pmatrix} 0 & -J & 0 & 0 & \dots & 0 \\ -J & 0 & -J & 0 & \dots & 0 \\ 0 & -J & 0 & -J & \dots & 0 \\ 0 & 0 & -J & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & -J \\ 0 & 0 & 0 & 0 & -J & 0 \end{pmatrix}, \tag{17}$$

and consequently has eigenvalues ($k = 1, 2, \dots, N$)

$$E_k = 2J\cos\left(\frac{k\pi}{N+1}\right). \tag{18}$$

Including multiplicities one expects N eigenvalues for $\hat{H}_N$. The number of k values in (**??**) is indeed N. Taking into account that $\cos(\cdot)$ is a strictly monotonically decreasing function in $(0, \pi)$ we can conclude that the system has no degenerate energy eigenvalues.

The set of energy eigenvalues is particularly interesting when combined with Niven's theorem [**?**].

Theorem (Niven's theorem)**.** *If θ is rational in degrees, say $\theta = 2\pi r$ for some rational number r, then the only rational values of the trigonometric functions of θ are as follows:* $\sin(\theta)$, $\cos(\theta) = 0, \pm\frac{1}{2}, \pm 1$*;* $\sec(\theta)$, $\csc(\theta) = \pm 1, \pm 2$*; and* $\tan(\theta)$, $\cot(\theta) = 0, \pm 1$.

In other words, this theorem tells us that if x is rational *in degrees*, then the only possible rational values of $\cos(x)$ are $0, \pm\frac{1}{2}$ and ± 1. Note in our case that $\frac{k\pi}{N+1} \neq 0, \pi$ for $k = 1, 2, \ldots, N$, so $\cos(\frac{k\pi}{N+1}) \neq \pm 1$ and we are left with 3 rational options.

When we are evaluating in degrees, equation (**??**) becomes

$$E_k = 2J \cos\left(\frac{180k}{N+1}\right). \tag{19}$$

The argument of cosine here is clearly rational since N and k are integers. Hence we know that for a system with non-degenerate eigenvalues, there can be at most three eigenvalues, $\{0, \pm\frac{J}{2}\}$, that are rational. So $\mathcal{D} \leq 3$ for a system with all eigenvalues rational (the lattice must have at most 3 sites). We must have at least $(N-3)$ irrational eigenvalues for any larger system size.

The spectrum of a one-dimensional system with N sites and a single particle has proven to be (**??**). It is apparent that E_k is a strictly monotonically decreasing function as k increases because $\cos(x)$ is strictly monotonically decreasing on the interval $x \in (0, \pi)$ and $0 < \frac{k\pi}{N+1} < \pi$ for $k = 1, \ldots, N$. Thus, $E_{k_2} < E_{k_1}$ whenever $k_1 < k_2$. We have shown –invoking Niven's theorem– that for all $N > 3$ the values of the cosine function are irrational. However, this result on its own does not guarantee the violation of recurrence, as the latter notion requires the energy eigenvalues to be *mutually* irrational. We thus have to prove that there is no such case when all eigenvalues are the multiples of the same irrational number.

Below we answer the question: is there a *rational* γ such that $E_{k_1} = \gamma E_{k_2}$ for $k_1 \neq k_2$?

Theorem (Mutual Rationality Recurrence Theorem)**.** *Consider the sequence of energy eigenvalues*

$$E_k = \cos\left(\frac{k\pi}{N+1}\right) \qquad k = 1, 2, \ldots N$$

where $N > 3$. There are no pair of integers, k_1 and k_2, and rational number γ such the equality $E_{k_1} = \gamma E_{k_2}$ is satisfied.

Proof. First we notice that if the equality $E_{k_1} = \gamma E_{k_2}$ is satisfied for a particular triplet (k_1, k_2, γ) with a rational γ, then swapping the indices and taking the reciprocal of γ also leads to a satisfactory triplet, $(k_2, k_1, \frac{1}{\gamma})$. Thus the rationality of γ does not depend on whether k_1 is bigger than k_2 or the other way around.

Without restricting generality we may assume that $k_1 < k_2$. Therefore $E_{k_1} > E_{k_2}$ and consequently $|\gamma| > 1$. Let us substitute the explicit expression of the spectrum in the equation

$$E_{k_1} = \gamma E_{k_2}$$
$$2J \cos\left(\frac{k_1\pi}{N+1}\right) = 2J \cos\left(\frac{k_2\pi}{N+1}\right).$$

This equation can be simplified by dividing both sides by $2J$, and using Euler's complex exponential expression for the trigonometric functions:

$$\exp\left(i\,\frac{k_1\pi}{N+1}\right) = \gamma\exp\left(i\,\frac{k_2\pi}{N+1}\right).$$

We have to keep in mind though that we only demand the equality of the real parts. Since there is no such k value that $\cos\left(\frac{k}{N+1}\,\pi\right) = 0$, we may divide both sides of the equation above with the exponential on the right hand side:

$$\exp\left(i\,\frac{k_1-k_2}{N+1}\,\pi\right) = \gamma.$$

Raising both sides to the power of $(N+1)$ leads us to

$$e^{i(k_1-k_2)\pi} = \gamma^{N+1}. \tag{20}$$

Notice that $e^{i(k_1-k_2)\pi} = (e^{i\pi})^{(k_1-k_2)} = (-1)^{k_1-k_2}$. Since both k_1 and k_2 are integers their difference is also an integer number, thus the left hand side of equation (**??**) is ± 1 depending on the parity of (k_1-k_2). Meanwhile the right hand side of equation (**??**) is γ^{N+1}, where $|\gamma| > 1$, therefore $\left|\gamma^{N+1}\right| > 1$. Consequently this equation cannot have a solution triplet (k_1, k_2, γ), where k_1, k_2 are integers between 1 and N inclusively and γ is rational. ■

We have actually proven a much stronger statement than we needed. Here we showed that it is not possible to chose only two eigenvalues from E_k which are rational multiple of each other.

Hence, we have shown that all one-dimensional noninteracting systems with more than three lattice sites should not exhibit recurrence, which has implications for thermalisation in these systems. To the best of our knowledge, this is a novel result that has not previously been presented elsewhere.

9.5 Interacting one-dimensional systems

Adding multiple interacting particles introduces a number of interesting features in the thermalisation properties of our system. We have found that when weak interactions are present, thermalisation appears to occur in all one-dimensional systems, including those that exhibited clear and regular revival in the noninteracting case. We also note that with weak interactions the long-term average for the expectation value of the number operators all tend towards $\frac{P}{N}$, i.e., the particles become evenly distributed on the lattice. With stronger interactions, however, we observe localisation, which we will investigate in section **??**.

To see why the systems that exhibited revival in the noninteracting case thermalise once interactions are added, we consider the specific case of two bosons on a 3×1 lattice. In the absence of interactions, this is identical to a single boson on a 3×1 lattice, up to normalisation. We can see from figure 8that we have exact revival in this system. Once we have multiple particles with interactions in the system, we need a larger dimensional basis to represent all of the distinct number states, and thus we need a larger Hamiltonian. We need to pick a labelling convention for our number states in order to define the representation of the Hamiltonian matrix. In this project, we have chosen to label the states in such a way that the states with the lowest index have the

most particles on one particular site of the lattice. For example ion a 3×1 system with 2 particles the number of number states is

$$\mathcal{D}_{3\times 1} = \frac{(N+P-1)!}{P!(N-1)!} = \frac{(3+2-1)!}{2!(3-1)!} = \frac{4!}{2!2!} = 6$$

and the corresponding number states can be labelled as

$$|200\rangle = |1\rangle\,,\ |110\rangle = |2\rangle\,,\ |101\rangle = |3\rangle\,,\ |020\rangle = |4\rangle\,,\ |011\rangle = |5\rangle\,,\ |002\rangle = |6\rangle\,.$$

Using this basis, we can represent the Hamiltonian as

$$\hat{H}_{3\times 1}^{(P=2)} = \begin{pmatrix} U & -\sqrt{2}J & 0 & 0 & 0 & 0 \\ -\sqrt{2}J & 0 & -\sqrt{2}J & -J & 0 & 0 \\ 0 & -\sqrt{2}J & U & 0 & -\sqrt{2}J & 0 \\ 0 & -J & 0 & 0 & -J & 0 \\ 0 & 0 & -\sqrt{2}J & -J & 0 & -\sqrt{2}J \\ 0 & 0 & 0 & 0 & -\sqrt{2}J & U \end{pmatrix}. \tag{21}$$

The eigenvalues of this system are

$$\begin{aligned}
\lambda_1 &= U_0 \\
\lambda_2 &= \frac{1}{2}\left(U_0 - \sqrt{8J^2+U_0^2}\right) \\
\lambda_3 &= \frac{1}{2}(U_0 + \sqrt{8J^2+U_0^2}) \\
\lambda_4 &= \frac{U_0}{3} - \frac{-24J^2-U_0^2}{3\left(9J^2U_0+U_0^3+3\sqrt{3}\Lambda\right)^{\frac{1}{3}}} + \frac{1}{3}\left(9J^2U_0+U_0^3+3\sqrt{3}\Lambda\right)^{\frac{1}{3}} \\
\lambda_5 &= \frac{U_0}{3} + \frac{(1+i\sqrt{3})(-24J^2-U_0^2)}{6\left(9J^2U_0+U_0^3+3\sqrt{3}\Lambda\right)^{\frac{1}{3}}} - \frac{1}{6}(1-i\sqrt{3})\left(9J^2U_0+U_0^3+3\sqrt{3}\Lambda\right)^{\frac{1}{3}} \\
\lambda_6 &= \frac{U_0}{3} + \frac{(1-i\sqrt{3})(-24J^2-U_0^2)}{6\left(9J^2U_0+U_0^3+3\sqrt{3}\Lambda\right)^{\frac{1}{3}}} - \frac{1}{6}(1+i\sqrt{3})\left(9J^2U_0+U_0^3+3\sqrt{3}\Lambda\right)^{\frac{1}{3}}
\end{aligned}$$

where we introduced the temporary shorthand notation of

$$\Lambda = \sqrt{-512J^6 - 61J^4U_0^2 - 2J^2U_0^4}.$$

Whilst we have not proven that the above eigenvalues form a mutually irrational set, when we consider the number of square roots and third roots in the above set of eigenvalues, we see that it at least appears very unlikely that a particular combination of J and U_0 would result in a mutually rational set of eigenvalues.

When we run a simulation of this system, we find that the long term average for the particle to be on the same site that it started on approaches $\frac{P}{N} = \frac{2}{3}$, which is consistent with it thermalising.

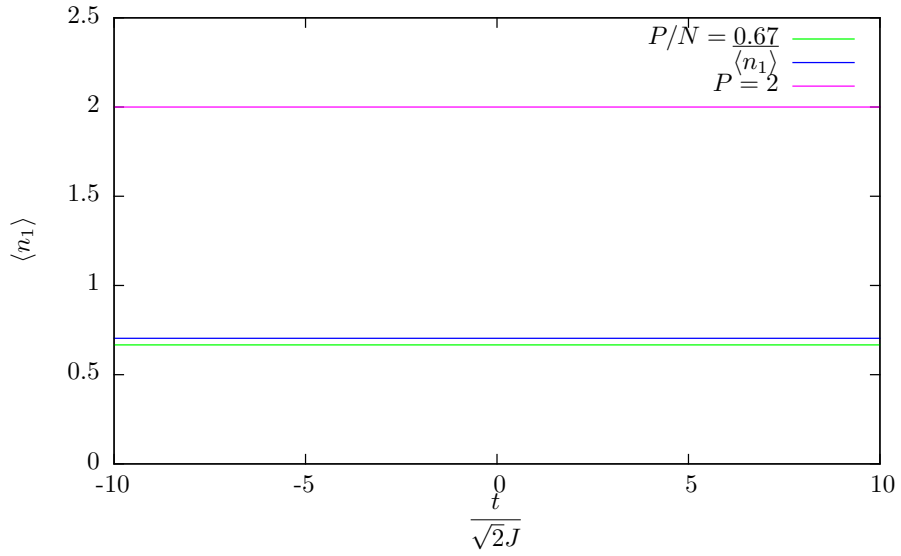

Figure 8: Thermalisation for a 3×1 lattice with two bosons and $U = 0.1$.

We observe something similar in the case of a 2×1 lattice with two bosons on it. Here we expect the long term average to be $\frac{P}{N} = \frac{2}{2} = 1$, which is consistent with what we see.

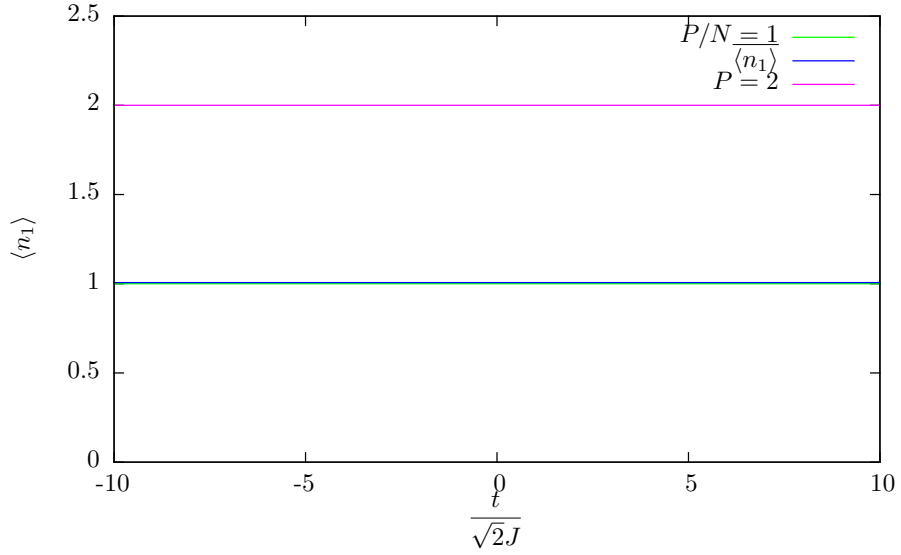

Figure 9: Thermalisation for a 2×1 lattice with two bosons and $U_0 = 0.1$.

We see a similar pattern with a 3×1 lattice with two particles, with the long-term average being $2/3$.

The agreement of the long-term average with a uniform spatial distribution is also clear for larger system sizes, such as a 10×1 lattice with two bosons, as demonstrated in figure **??**, where $\frac{P}{N} = 0.2$.

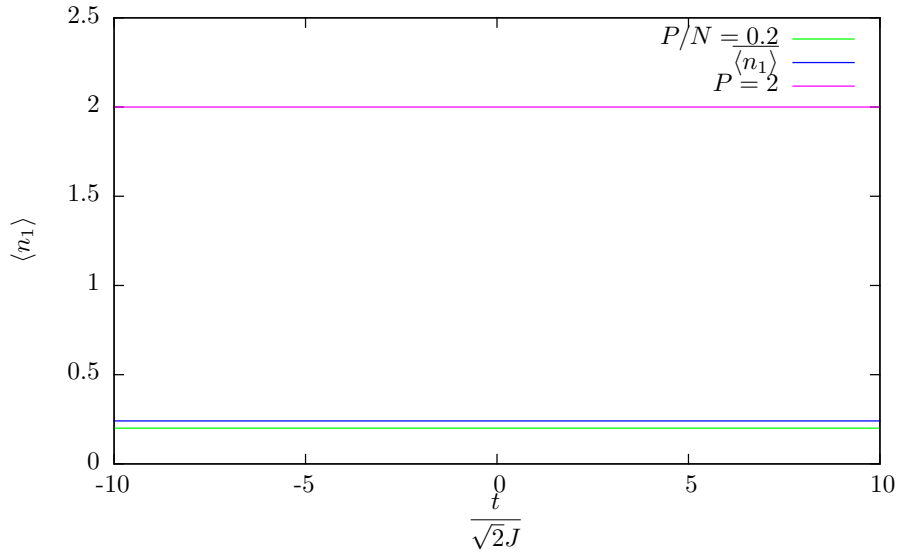

Figure 10: Thermalisation for a 10×1 lattice with two bosons and $U = 0.1$.

9.5.1 Effect of interaction strength

When the interaction strength is increased, we see that the long-term averages of the expectation values of the number operators are much greater for lattice sites that are closer to where to bosons are initially placed. This lack of independence of the long term states from the initial conditions suggests that having strong interparticle interactions can frustrate thermalisation, at least within the time scales that the simulations show. However, it is possible that these localised states are only metastable, in the sense that they would eventually thermalise if given an arbitrarily long time to do so. The following simulations are run for a 3×1 lattice with two bosons and $J = 1$.

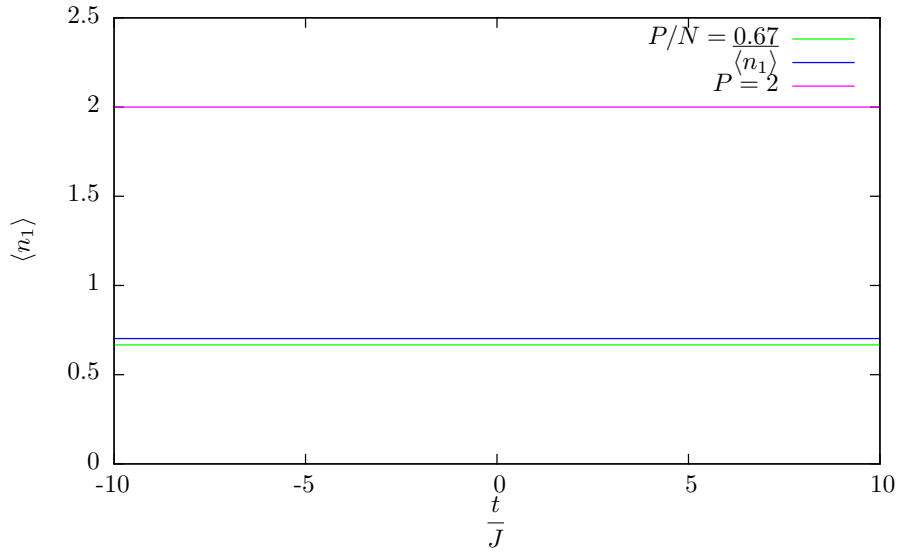

Figure 11: Frustrated thermalisation for a 3×1 lattice with two bosons and $U = 0.005$. The long time average of $\langle n_1 \rangle$ is $\overline{\langle n_1 \rangle} = 0.70245$.

The time average of the expectation value of the number operator for the first site, $\overline{\langle n_1 \rangle} = 0.70245$, is greater than $\frac{P}{N} = 0.67$. This may appear to be a result of the contributions to the time average of the early timesteps, as the bosons were on the first site at $t = 0$. However, running a simulation with the same parameters for 5 times as long gives an average that is nearly indistinguishable from this, suggesting that the early data is not skewing the result.

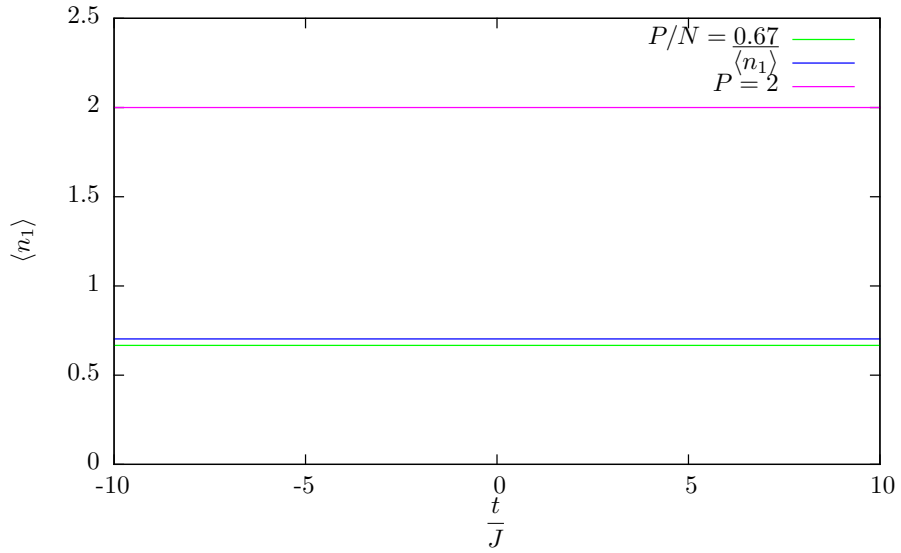

Figure 12: Thermalisation for a 3×1 lattice with two bosons and $U = 0.005$. The long time average of $\langle n_1 \rangle$ is $\overline{\langle n_1 \rangle} = 0.70280$.

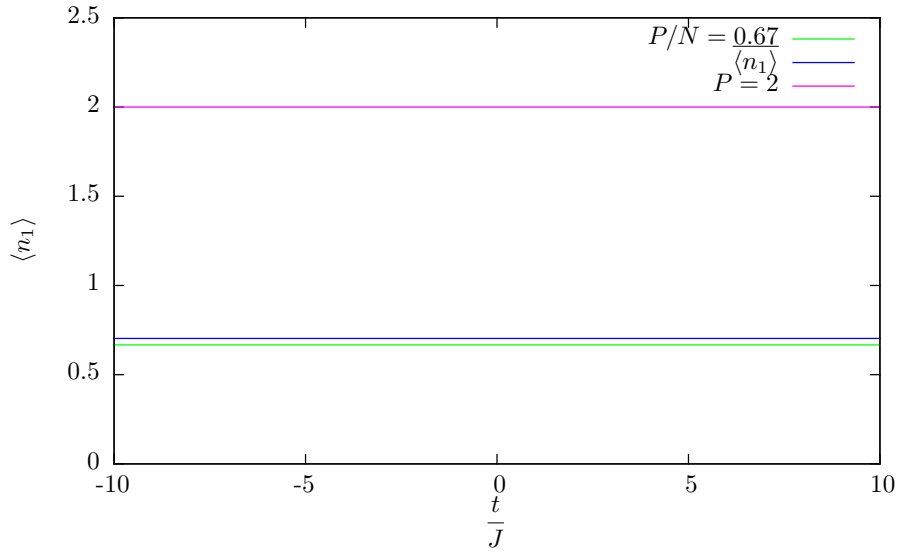

Figure 13: Thermalisation for a 3×1 lattice with two bosons and $U_0 = 0.01$. The long time average of $\langle n_1 \rangle$ is $\overline{\langle n_1 \rangle} = 0.70329$.

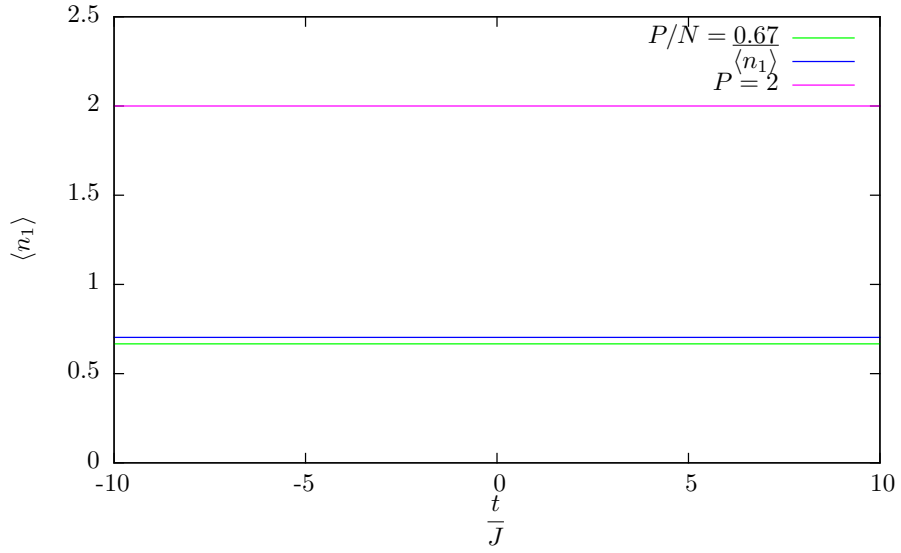

Figure 14: Thermalisation for a 3×1 lattice with two bosons and $U_0 = 0.01$. The long time average of $\langle n_1 \rangle$ is $\overline{\langle n_1 \rangle} = 0.70319$.

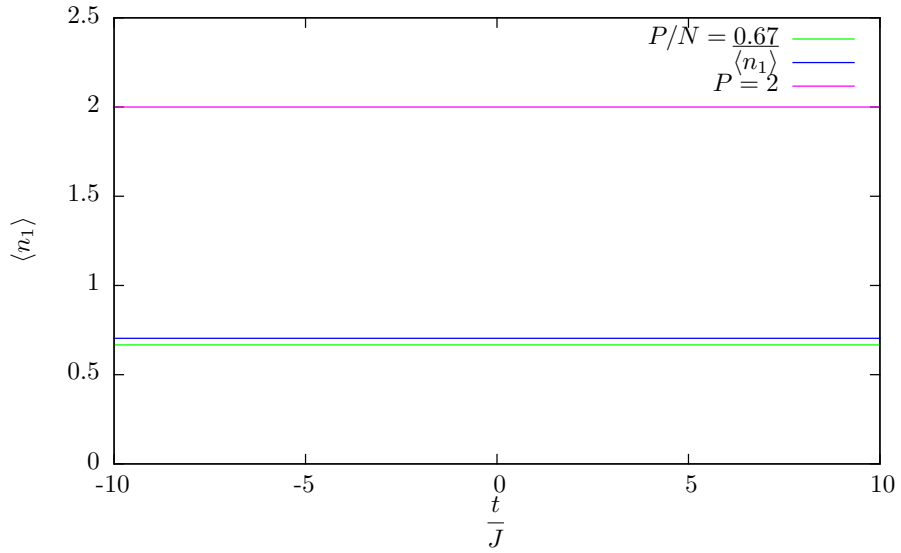

Figure 15: Thermalisation for a 3×1 lattice with two bosons and $U = 0.1$. The long time average of $\langle n_1 \rangle$ is $\overline{\langle n_1 \rangle} = 0.70390$.

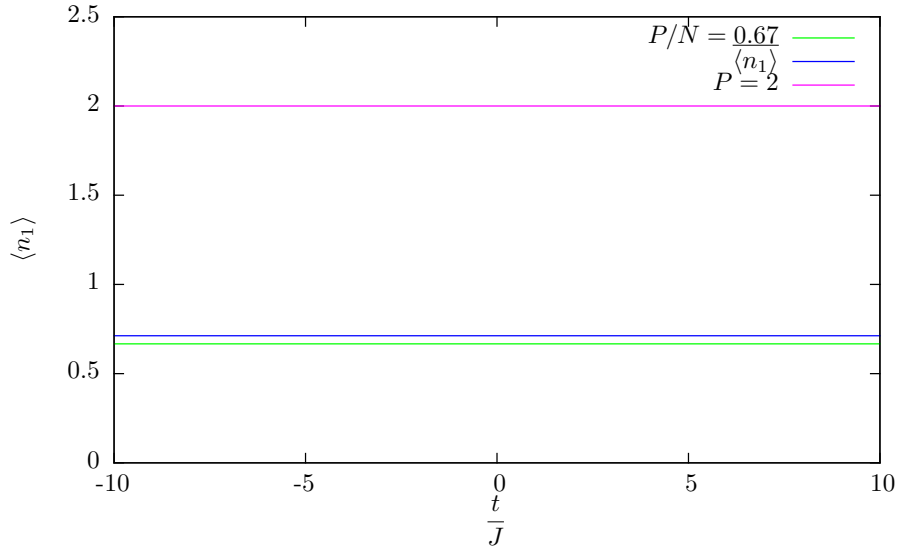

Figure 16: Thermalisation for a 3×1 lattice with two bosons and $U_0 = 0.5$. The long time average of $\langle n_1 \rangle$ is $\overline{\langle n_1 \rangle} = 0.71241$.

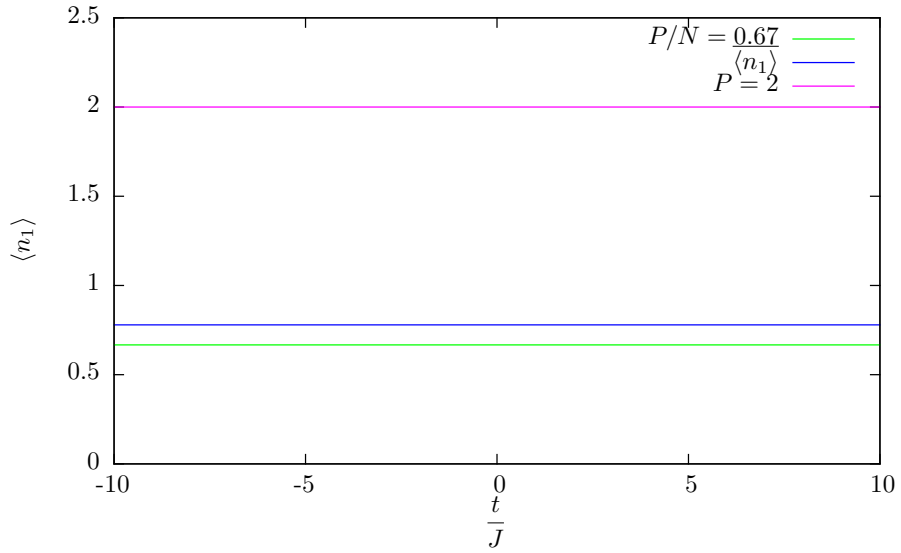

Figure 17: Thermalisation for a 3×1 lattice with two bosons and $U_0 = 2$. The long time average of $\langle n_1 \rangle$ is $\overline{\langle n_1 \rangle} = 0.77936$.

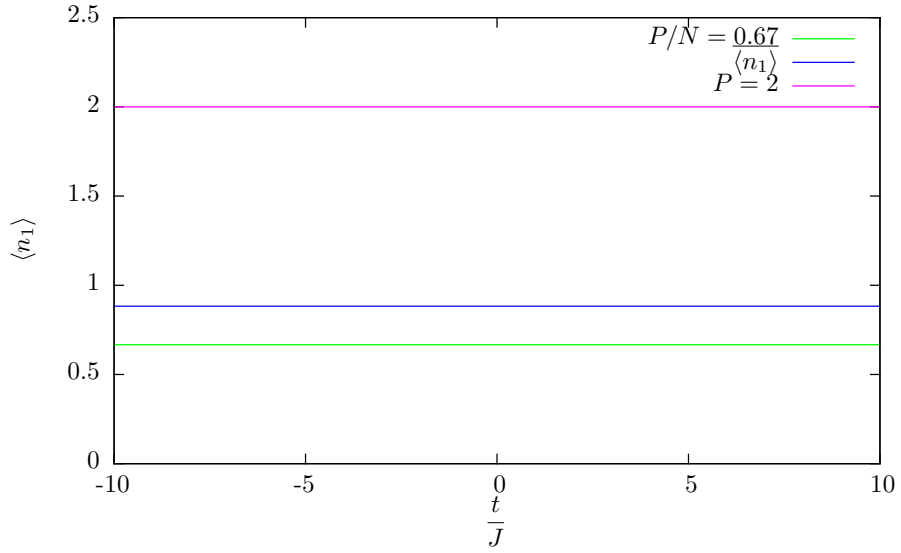

Figure 18: Thermalisation for a 3×1 lattice with two bosons and $U_0 = 5$. The long time average of $\langle n_1 \rangle$ is $\overline{\langle n_1 \rangle} = 0.88260$.

We can look at the long-term averages for the expectation value of the occupation of all of the lattice sites and not just the one that the boson started on. When we do this, a remarkable pattern emerges. If we start the boson on the first site, for low values of U_0 the average time spent on the second site is slightly lower than the outer lattice sites. We believe this to be due to the boundary conditions, as the effect becomes less pronounced when we look at systems with a greater number of lattice sites. However, once U_0 gets larger

(especially once it becomes greater than J), we find that the long-term average for the site furthest from the one that the boson begins on drops dramatically.

Figure 19: Long term averages for 3×1 systems with varying interparticle interaction strengths

We have run simulations for higher values of U_0 in which we see that $\overline{\langle n_1 \rangle}$ and $\overline{\langle n_2 \rangle}$ asymptotically approach unity, and $\overline{\langle n_3 \rangle}$ approaches zero.

One potential explanation for this behaviour is as follows. If the interparticle interactions are so powerful, beginning the system with both particles on the same site means that the system has very high energy. When one of the particles moves to the second lattice site, conservation of energy demands that the system still have high energy, but the interparticle interactions only apply to bosons on the same site. Hence, the boson must gain a large amount of kinetic energy. The kinetic energy is proportional to the curvature of the wavefunction ($\sim \nabla^2 \psi$), and hence the boson must be highly localised within the second lattice site. The stronger the interparticle interactions, the more kinetic energy this boson must have and thus the more localised it is. This "narrowness" of the boson's spatial wavefunction reduces its tendency to tunnel into the third lattice site, so $\overline{\langle n_3 \rangle}$ approaches zero. This behaviour suggests that the system undergoes a quantum phase transition from a superfluid (when U_0 is small) to a Mott insulator, when U_0 is large.

The suggestion that what we are observing is a quantum phase transition is inspired by work done by Greiner et al. [**?**], who state that for a system described by the Bose-Hubbard Hamiltonian

$$\hat{H} = J \sum_i (\hat{a}_i^\dagger \hat{a}_{i+1} + \text{h.c.}) + \frac{U_0}{2} \sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i,$$

in the limit where the tunnelling term dominates, the ground-state energy is minimised if each of the single-particle wavefunctions of P atoms are spread out over the entire lattice of N lattice sites. This is the superfluid phase, and is consistent with the values that we found for the long-term averages of number operator expectation values for $U_0 \ll J$, which were close to $\frac{P}{N}$.

They further note that if system is homogeneous (i.e., $\epsilon_i = \text{const}$), as our systems are, then the many-body ground state is given by

$$|\Psi_{\text{SF}}\rangle^{(U_0=0)} \propto \left(\sum_{i=1}^{N} \hat{a}_i^\dagger \right)^P |0\rangle \,. \tag{22}$$

This state is well described by a macroscopic wavefunction with long range phase coherence throughout the lattice.

On the other hand, if U_0 dominates the Hamiltonian, then the system acts as a Mott insulator. When in this phase, the ground state of the system is given by highly localised atomic wavefunctions with a *fixed number* of atoms per lattice site that minimise the interaction energy [**?**]. For a homogeneous lattice, this ground state is

$$|\Psi_{\text{MI}}\rangle^{(J=0)} \propto \prod_{i=1}^{N} \left(\hat{a}_i^\dagger \right)^{\frac{P}{N}} |0\rangle \,. \tag{23}$$

This state has very little phase coherence, but perfect correlations in particle number exist between lattice sites. The most important observation that we make about this Mott insulator state is that it cannot be described by a macroscopic wavefunction, and so when we later use the Gross-Pitaevskii equation we will not be able to legitimately consider systems with $U_0 \gg J$.

10 Two-dimensional systems

10.1 Single particle case

In the single particle case, which is identical to the many-particle non-interacting case up to normalisation, the Hamiltonian is given by

$$\hat{H}_{2D} = \left(J \sum_{i,j} \hat{a}^\dagger_{i,j} \hat{a}_{i,j+1} + J' \sum_{i,j} \hat{a}^\dagger_{i,j} \hat{a}_{i+1,j} \right) + \text{h.c.} \tag{24}$$

Similarly to the one-dimensional single-particle case, the Hamiltonian is an $N \times N$ square matrix. We see many similarities between these systems and one-dimensional single particle systems. We can attribute this to the fact that, in the absence of any interparticle interactions, the two-dimensional systems are separable. To demonstrate this, consider the Hamiltonian for a 3×3 lattice with a single boson on it, with hopping in the x-direction characterised by J and hopping in the y-direction characterised by J'

$$\hat{H}_{3\times 3} = \begin{pmatrix} 0 & -J & 0 & -J' & 0 & 0 & 0 & 0 & 0 \\ -J & 0 & -J & 0 & -J' & 0 & 0 & 0 & 0 \\ 0 & -J & 0 & 0 & 0 & -J' & 0 & 0 & 0 \\ -J' & 0 & 0 & 0 & -J & 0 & -J' & 0 & 0 \\ 0 & -J' & 0 & -J & 0 & -J & 0 & -J' & 0 \\ 0 & 0 & -J' & 0 & -J & 0 & 0 & 0 & -J' \\ 0 & 0 & 0 & -J' & 0 & 0 & 0 & -J & 0 \\ 0 & 0 & 0 & 0 & -J' & 0 & -J & 0 & -J \\ 0 & 0 & 0 & 0 & 0 & -J' & 0 & -J & 0 \end{pmatrix}. \tag{25}$$

We use this example rather than a 2×2 lattice because the 2×2 lattice is not strictly two-dimensional as it is equivalent to a 4×1 system with periodic boundary conditions. We note that this 3×3 system can be considered as a combination of two 3×1 systems, one with hopping J and the other with hopping J', i.e.,

$$\hat{H}_{3\times 3} = \hat{H}^{(J)}_{3\times 1} \otimes I_3 + I_3 \otimes H^{(J')}_{3\times 1}, \tag{26}$$

where

$$\hat{H}^{(J)}_{3\times 1} = \begin{pmatrix} 0 & -J & 0 \\ -J & 0 & -J \\ 0 & -J & 0 \end{pmatrix}, \quad H^{(J')}_{3\times 1} = \begin{pmatrix} 0 & -J' & 0 \\ -J' & 0 & -J' \\ 0 & -J' & 0 \end{pmatrix}, \tag{27}$$

and I_3 is the 3×3 identity matrix, while $\otimes$ is a Kronecker tensor product. Since the individual 3×1 systems exhibit revival, it is unsurprising that the two-dimensional one (almost always) does too. The revival time for the overall

system is simply the lowest common multiple of the revival times of the one-dimensional systems. Consequently, the case for which we do not see revival in a 3×3 noninteracting system is when J and J' are mutually irrational, as this renders their revival times mutually irrational.

The separability of these two-dimensional systems suggests that if either of the systems that it separates into have mutually irrational eigenvalues and thus do not exhibit revival, then the whole system will not revive either. In other words, if we have an $m \times n$ lattice, then we will see thermalisation if $\max\{m, n\} > 3$. We can now look at the simulation of several systems to demonstrate that the above condition for revival or thermalisation holds.

Consider first the time evolution, figure **??**, of a boson that starts in the top left corner ("first lattice site") of a 3×3 lattice with $J = J'$.

Figure 20: Revival for a 3×3 square lattice with a single boson and $J = J'$.

The eigenvalues for this system (with $J = J'$) are

$$\{0, \pm\sqrt{2}J, \pm 2\sqrt{2}J\} \quad \text{or after scaling} \quad \{0, \pm 1, \pm 2\}.$$

There are some eigenvalues in the above set with multiplicity greater than one, however, these energy eigenvalues are clearly mutually rational. We also note that we must have degeneracy in the eigenvalues now due to several symmetries of geometric origin (e.g., rotation by $\frac{\pi}{2}$), which was not possible in the one-dimensional case, as is clear from equation (**??**).

The presence of these symmetries has revealed what is almost certainly a bug in the many-body code that we developed to evolve these two-dimensional systems. When we run a simulation for a 3×3 lattice with a single boson and $J = J'$ and then calculate the long-term averages of the expectation values of the number operators, we find an asymmetry in these averages that we are unable to explain. This asymmetry can be seen from the averages displayed in table **??**, where we expect to have the average particle number on the lattice site $(1, 3)$ agree with that of the lattice site $(3, 1)$, yet they differ dramatically. The same is true of $(2, 1)$ and $(1, 2)$.

Lattice site positions			
Column number	Row 1	Row 2	Row 3
1	0.328	0.035	0.152
2	0.107	0.133	0.167
3	0.051	0.012	0.016

Table 1: Long term averages for a 3×3 noninteracting system

We suspect the error may lie in our map between the different orthogonal number states that our Hamiltonian is represented in and the number operator expectation values. Unfortunately, this asymmetry was discovered at a point sufficiently late that we have not been able to debug the code and run the simulations again.

However, the behaviour for the site on which the particle was started appears to have good agreement with what we predict from the separability argument, so it seems possible that whatever is going wrong with symmetry in our code has

not impacted the behaviour at this lattice site. If we consider a case identical to the previous one, except with $J = 1$ and $J' = \frac{3}{5}$ then we note that equation (**??**) predicts a revival time of $t^* = 10\pi$ here, which is consistent with the simulation.

Figure 21: Revival for a 3×3 square lattice with a single boson and $\{J, J'\}$ mutually rational.

If we now consider the case where J and J' are not mutually rational, then we see that we do not get full revival, see figure 24.

Figure 22: Absence of revival for a 3×3 lattice with a single boson and $\{J, J'\}$ mutually irrational: $J = 1$ and $J' = \frac{1}{\sqrt{2}}$

The principles discussed earlier lead us to expect revival to be absent from larger systems, such as the following 4×4 and 15×15 ones.

Figure 23: Absence of revival for a 4×4 lattice with a single boson and $J = J'$.

Figure 24: Absence of revival for a 15×15 lattice with a single boson and $J = J'$.

We finish this section by demonstrating that it is sufficient that either $m > 3$ or $n > 3$ for thermalisation to be frustrated in a $m \times n$ lattice. We do this by considering a 3×4 lattice with a single boson and $J = J'$.

Figure 25: Absence of revival for a 3×4 lattice with a single boson and $J = J'$.

It is not entirely clear from figure **??** that revival does not happen, but examination of the source data reveals that there are no times aside from the very beginning at which $\langle n_1 \rangle$ is greater than 0.985. Hence, in spite of unresolved issues with symmetry, we still observe much of the behaviour that we expect of these systems.

i don't see much value in including 2D interacting systems

11 Conclusions and further work

In this project, several distinct goals have been accomplished, while others remain as grounds for future investigation. A criterion for the exact revival of systems of noninteracting bosons in one dimension and two dimensions was deduced and proven analytically. This criterion relates to the mutual rationality or irrationality of the eigenvalues of the spectrum, and results from Ivan Niven's work on irrationality of trigonometric functions with rational arguments were supplemented by W. Yueh's results on the eigenvalues of tridiagonal matrices to prove that noninteracting $m \times n$ systems will only exhibit revival if $\max(\{m, n\}) \leq 3$. For systems with mutually rational eigenvalues, a formula for determining the exact time at which revival would occur was developed.

Our investigations into the thermalisation properties of interacting one-dimensional systems were suggestive of a quantum phase transition from a superfluid to a Mott insulator as the strength of the interactions increases relative to the hopping energy. This was argued on the basis of the long term averages of the expectation values of the number operators for each site.

The simulations that we ran to model the dynamics of two-dimensional systems with interactions have results from which it is much harder to draw confident conclusions. The code developed for many body analytic evolution agreed very well with the Gross-Pitaevskii approach in the noninteracting case. Both methods also appeared to demonstrate thermalisation for systems with larger lattices, though more efficient code needs to be developed to run simulations of these systems for longer before we can say anything with confidence here. The two methods did not agree well for smaller system sizes.

A possible direction for further work on these systems could involve attempting to predict the long term averages of observables for the noninteracting (integrable) systems that we studied using the generalised Gibbs ensemble. We could also attempt to prove whether or not any of the systems that we have studied satisfy Deutsch and Srednicki's Eigenstate Thermalisation Hypothesis, which provides a necessary and sufficient condition for thermalisation.