Thermalisation of Ultracold Bose Gases on Optical Lattices

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Abstract

Systems of ultra-cold gases in light-induced periodic potentials (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 BECs in an optical lattice and condensed matter systems, where electrons can be modelled as moving on a lattice generated by the periodic array of atom cores [1]. 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 main focus is on determining how the tunnelling energies and the strength of the interparticle interactions influence whether or not the system exhibits relaxation to a thermal state. For systems in which revival to the initial state occurs regularly (those which don't thermalise), a method for calculating the revival period is developed. For the systems which exhibit thermalisation, we attempt to characterise the long term states using [ETH, entropy of entanglement, whatever I actually end up doing].

rewrite this when rest done, David/-Danny ignore the abstract for now please

1 Introduction

[Want to include some of the stuff from section 7.3 at the start here] 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 is understood to emerge from the chaotic dynamics of sufficiently unconstrained systems. However, the time evolution of quantum systems is strictly linear, and 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 [2].

see square brackets

I'd rather not repeat "understood" twice in same sentence.

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. From

hence?

here, we look at some larger systems with a more approximate method that revolves around using an adaptive Runge-Kutta-Feldberg method to evolve the system wavefunction according to the Gross-Pitaevskii equation. We then look for similarities in the results of the simulations run according to each method to see what similarities in behaviour are retained as we move from small, exactly solved systems to large, numerically approximated systems.

2 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 [1]. 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 [1]. 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 [3], makes ultracold bosons on optical lattices an excellent arena in which to explore various model Hamiltonians for condensed matter systems and quantum optics. There are further advantages

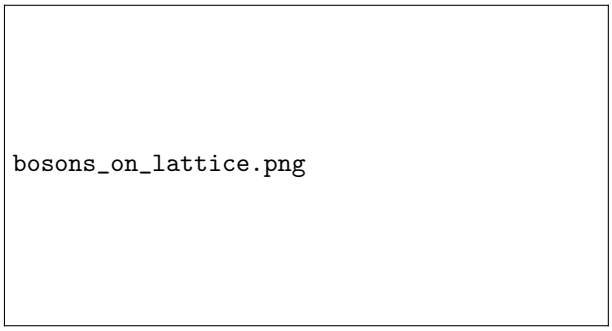

Figure 1: Bosons on a two-dimensional optical lattice. Figure is taken from `www.uibk.ac.at/th-physik/qo/research/opticallattices.html.en`

which can make conducting experiments with ultracold bosons on optical lattices more attractive than working with solids directly. One is that there are always impurities present in the solids we find in nature. These impurities can have significant impacts on the properties of the solid which cannot necessarily be accounted for by a perturbative approach which assumes these effects to be small. For large-enough detunings from an atomic transition frequency, optical lattices can be considered to be purely conservative and defect-free potentials [1], so when dealing with bosons on optical lattices this problem of impurities does not arise.

reference this at some point from the book I meant to get from David

Another benefit of working with bosons on optical lattices is that we can easily control the state of each of the particles on the lattice. Furthermore, the potential can be altered or switched off entirely during the experiment, which is a feature that is not available in any solid state experiment [4].

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

4 Effect of indistinguishability

The Hamiltonian in the previous section would act on a bosonic many-particle wave function. A single particle wave function $\psi(\mathbf{r})$ is defined within a Hilbert space $\mathcal{H}$, which is the space of complex, square integrable functions. It must satisfy $\int d^3\mathbf{r}|\psi(\mathbf{r})|^2 < \infty$. A wave function that represents the state of N

indistinguishable particles, $\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ is defined within $\mathcal{H}^N$, where $\mathcal{H}^N$ is constructed as the tensor product N single-particle Hilbert spaces:

$$\mathcal{H}^N = \mathcal{H} \otimes \mathcal{H} \otimes \cdots \otimes \mathcal{H}. \tag{3}$$

The wave functions in this space are also subject to normalisation constraints, i.e.,

$$\int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \ldots d^3\mathbf{r}_N |\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2 < \infty.$$

Whilst all functions satisfying the above constraints can be legitimately defined mathematically, only a small subset are found to occur in nature – those which are either entirely symmetric or anti-symmetric under particle exchange. The set of indistinguishable particles which are entirely symmetric under particle exchange are called bosons. This project will not investigate scenarios involving the particles that display exchange anti-symmetry (fermions), so we will be working within the space $S_N\mathcal{H}^N$. Here S_N projects onto the subspace of square-integrable functions that are unchanged by permuting the order of the variables. As an illuminating example one may construct the two-particle space, $S_2\mathcal{H}^2$ for bosons as

$$S_2\mathcal{H}^2 = \{\psi \mid \psi = \psi_1 \otimes \psi_2 + \psi_2 \otimes \psi_1, \quad \text{where } \psi_1, \psi_2 \in \mathcal{H}\}$$

It is apparent that $S_2\mathcal{H}^2 \neq \mathcal{H} \otimes \mathcal{H}$ since in this case we would be able to distinguish particles or states. We can formally extend this notion of exchange symmetry for larger systems and express the requirement of exchange symmetry for bosonic systems as [5]

$$\psi(\mathbf{r}_{\mathcal{P}_1}, \mathbf{r}_{\mathcal{P}_2}, \ldots, \mathbf{r}_{\mathcal{P}_N}) = \psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N),$$

where $\{\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_N\}$ represents any permutation, $\mathcal{P}$, of the set $\{1, 2, \ldots, N\}$.

Let us first consider the case of two indistinguishable bosons. We have not yet determined the energy eigenstates of our Hamiltonian, but if we suppose we have the set of normalised single-particle wave functions $\{|\lambda\rangle\}$, and we have one boson in state $|\lambda_1\rangle$ and another in state $|\lambda_2\rangle$, then we can write the two-particle wave function as

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}\big(\langle \mathbf{r}_1|\lambda_1\rangle \langle \mathbf{r}_2|\lambda_2\rangle + \langle \mathbf{r}_1|\lambda_2\rangle \langle \mathbf{r}_2|\lambda_1\rangle \big), \tag{4}$$

or in Dirac bra-ket notation, the two-body states would be represented as

$$|\lambda_1, \lambda_2\rangle = \frac{1}{\sqrt{2}}\big(|\lambda_1\rangle \otimes |\lambda_2\rangle + |\lambda_2\rangle \otimes |\lambda_1\rangle \big). \tag{5}$$

The number of permutations that one must account for grows extremely quickly as particle number increases. A properly symmetrised and normalised N-body state can be represented [6] as

$$|\lambda_1, \lambda_2, \ldots, \lambda_N\rangle = \frac{1}{\sqrt{N! \prod_{\lambda=0}^{\infty} n_\lambda}} \sum_{\mathcal{P}} |\lambda_{\mathcal{P}_1}\rangle \otimes |\lambda_{\mathcal{P}_2}\rangle \otimes \cdots \otimes |\lambda_{\mathcal{P}_N}\rangle, \tag{6}$$

where n_λ is the number of particles in state λ, and the summation runs over all $N!$ permutations $\mathcal{P}$ of the set of quantum numbers $\{\lambda_1, \ldots, \lambda_N\}$.

This formalism has a number of shortcomings. The most important of these for this project is that it is extremely cumbersome for practical computation because of the large number of entities that need to be represented. To avoid this, we shall adopt the second quantised formalism, which is much better suited to dealing concisely with large numbers of indistinguishable particles.

5 Second Quantisation

5.1 The Occupation Number Representation

The formalism that we have hitherto discussed explicitly represents a significant amount of redundant information, in the sense that it deals separately with the scenarios "particle 1 in state λ_1 and particle 2 in state λ_2" and "particle 2 in state λ_1 and particle 1 in state λ_2". Taking into account the indistinguishability of the particles, it is clear that these two scenarios are identical. A more efficient approach consists of describing the number of particles in a particular state λ_i, i.e., using the occupation number representation. When doing this, a general state can be written as a linear superposition

$$|\Psi\rangle = \sum_{n_1,n_2,\ldots} c_{n_1,n_2,\ldots} |n_1, n_2, \ldots\rangle. \tag{7}$$

In the scenario which this project will be working with, the occupation numbers refer to the number of bosons on a particular site of the lattice. Having established this, we can define creation and annihilation operators that create and annihilate particles from number eigenstates, that is

$$\hat{a}_j^\dagger |n_1, n_2, \ldots, n_j, \ldots\rangle = \sqrt{n_j + 1} |n_1, n_2, \ldots, n_j + 1, \ldots\rangle \tag{8}$$

and

$$\hat{a}_j |n_1, n_2, \ldots, n_j, \ldots\rangle = \sqrt{n_j} |n_1, n_2, \ldots, n_j - 1, \ldots\rangle . \tag{9}$$

These operators have very important commutation relations

$$[\hat{a}_j^\dagger, \hat{a}_k^\dagger] = 0, \quad [\hat{a}_j, \hat{a}_k] = 0, \quad [\hat{a}_j, \hat{a}_k^\dagger] = \delta_{jk}. \tag{10}$$

We can also define the number operator $hatn_j = \hat{a}_j^\dagger \hat{a}_j$ that has the property that

$$\hat{n}_j |n_1, n_2, \ldots, n_j, \ldots\rangle = n_j |n_1, n_2, \ldots, n_j, \ldots\rangle . \tag{11}$$

The occupation number eigenstates form the basis of the N-particle Hilbert space that we are working in (the Fock space $\mathcal{F}^N$), and it is useful to observe that any occupation number eigenstate can be created from the empty (or "vacuum") state $|0\rangle$ by repeated action of creation operators [6]

$$|n_1, n_2, \ldots\rangle = \prod_i \frac{1}{\sqrt{n_i!}} (\hat{a}_i^\dagger)^{n_i} |0\rangle . \tag{12}$$

It may seem that the state space $S_N \mathcal{H}^N$ that we have constructed is not robust enough to accommodate these operators. Indeed, the creation and annihilation operators take us from the N-particle Hilbert space to the $(N+1)$- and $(N-1)$-particle Hilbert spaces, respectively. In order to account for these differences in particle number, we must really be working within the symmetric Fock states $\mathcal{F}_S(\mathcal{H})$, defined by the direct sum [7]

$$\mathcal{F}_S(\mathcal{H}) = \oplus_{N=0}^{\infty} S_N \mathcal{H}^N. \tag{13}$$

However, we will be working in systems in which the particle number is conserved. Each combination of creation and annihilation operators that appears

in the Hamiltonian will create an equal number of particles to the number destroyed. So for practical purposes we are just working within $S_N \mathcal{H}^N$.

Having established the space and states that we are operating with, we now need to rewrite the Hamiltonian in number state representation, i.e., we need to "second quantise" it.

5.2 Second Quantisation of the Hamiltonian

We can second quantise the Hamiltonian initially used to describe our system through the boson field operators, $\hat{\psi}^\dagger(x)$ and $\hat{\psi}(x)$, which create and destroy particles at particular spatial locations (we will define these more explicitly later). The two terms in $\hat{h}_1$ are single-particle operators for the kinetic and potential energy contributions, and can be transformed to

$$\hat{H}_1 = \int \hat{\psi}^\dagger(x) \hat{h}_1 \hat{\psi}(x)\, dx. \tag{14}$$

The one-dimensional Bloch's theorem states [8, 9] that the eigenstates of a particle in a periodic potential have the form

$$\phi_q(x) = e^{iqx} u_q(x), \tag{15}$$

where q is the quasi-momentum and $u_q(x)$ is periodic with the same period as the lattice, d. We will be considering scenarios in which the strength of the lattice potential is such that the bosons are not completely localised, but such that the overlap between the wave functions of particles on particular lattice sites have effectively zero overlap with non-nearest neighbours. Under these conditions, the wave functions can be conveniently described by the localised Wannier functions

$$\psi(R; r) = \frac{1}{d} \int dq\, e^{iRq} \phi_q(x) \tag{16}$$

which are superposition of Bloch functions [9, 10]. This is a useful description because the Wannier functions are both orthonormal and, more importantly, complete. We can use this to rewrite the field operators as

$$\hat{\psi} = \sum_j \hat{a}_j \psi(R_j - x). \tag{17}$$

With this in mind, we can write

Time-dependence in a?

$$\int \sum_j \hat{a}_j^\dagger \psi^*(R_j - x) \hat{h}_1 \sum_l \hat{a}_l \psi(R_l - x)\, dx = \sum_{j,l} J_{j,l} \hat{a}_j^\dagger \hat{a}_l. \tag{18}$$

Here we have introduced a shorthand notation

$$J_{j,l} = \int \psi^*(R_j - x) \hat{h}_1 \psi(R_l - x)\, dx \tag{19}$$

for the numerical values of these integrals. Notice that the integration –at least numerically– can indeed be carried out and characterises the strength of the hopping between sites j and l. It is typically described as characterising the overlap of the single-particle spatial wave functions (see figure below). This is

need references!

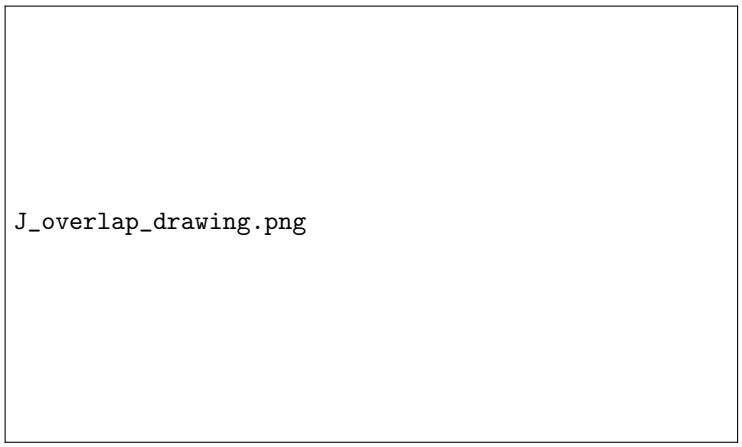

Figure 2: The strength of hopping J is considered as the overlap of localised Wannier functions centred at neighbouring lattice sites.

not entirely accurate, as the Wannier states are orthonormal and so the integral over their inner product is zero. More precisely, $J_{j,l}$ takes the inner product between a Wannier state $\psi(R_j - x)$ and the state produced by the action of $\hat{h}_1$ on the Wannier state $\psi(R_l - x)$, which does not have to be zero. However, the depiction in figure 2 can still be useful for developing an intuition for what J is, since J depends on the combination of the lattice depth (and width) and the kinetic energy and so would the overlap of the spatial wave functions if they were not orthonormal. It is also clear from the figure that computing overlap integrals using wave functions on non-neighbouring sites does not add much accuracy to our model, so we neglect these. For the hopping interactions that are permitted, we assume that each has identical strength. This assumption allows us to write

$$\hat{H}_1 = \int \hat{\psi}^\dagger(x)\left(\sum_i -\frac{\hbar^2}{2m}\partial_{x_i}^2 + \sum_j V_{\text{lattice}}(R_j)\right)\hat{\psi}(x)\,dx = J\sum_i (\hat{a}_i^\dagger \hat{a}_{i+1} + h.c.), \tag{20}$$

where $h.c.$ denotes the hermitian conjugate. We can go through a similar process for the contributions of the external potential and on-site interactions between bosons. The external potential gives an on-site energy that can vary at different locations in the lattice

$$\hat{H}_{\text{ext}} = \int \hat{\psi}^\dagger(x) V_{\text{ext}}(x)\hat{\psi}(x)\,dx = \sum_i \epsilon_i \hat{a}_i^\dagger \hat{a}_i. \tag{21}$$

The term for on-site interaction between bosons is a two-particle operator, thus second quantisation requires integration between two sets of boson field operators

$$\hat{H}_{\text{int}} = \int \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\frac{U_0}{2}\sum_{i,j}\delta(x_i - x_j)\hat{\psi}(x)\hat{\psi}(x)dx = \frac{U_0}{2}\sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i \tag{22}$$

Putting these terms together, we arrive at the Bose-Hubbard model described in the next section.

6 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 $\hat{H}_{\text{int}}$:

$$\hat{H}_{\text{1D}} = J\sum_i (\hat{a}_i^\dagger \hat{a}_{i+1} + h.c.) + \frac{U_0}{2}\sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i + \sum_i \epsilon_i \hat{a}_j^\dagger \hat{a}_j, \tag{23}$$

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

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

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

$$\hat{H}_{2D} = \left(J\sum_{i,j} \hat{a}_{i,j+1}^\dagger \hat{a}_{i,j} + J'\sum_{i,j} \hat{a}_{i,j}^\dagger \hat{a}_{i+1,j} \right) + \text{h.c.} + \frac{U_0}{2}\sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i, \tag{24}$$

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.

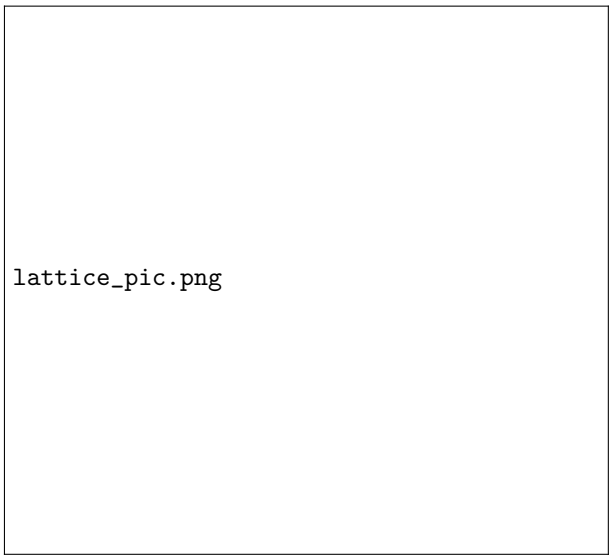

Figure 3: The blue circles here represent lattice sites and the crosses denote individual bosons. Hopping between any two neighbouring sites on the same chain is characterised by J, whereas hopping between chains is characterised by J'. A three by three lattice is shown here, but the system can be extended to arbitrary size.

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

7 Thermalisation

7.1 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 [2]. 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.

7.2 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. Classical systems exhibit chaotic dynamics, which are strongly non-linear and allow the system to quickly and essentially uniformly explore the constant-energy manifold irrespective of the initial conditions. This promotes ergodicity, which is implicit in the fundamental assumption of statistical mechanics - all accessible microstates are equiprobable. This is what leads us to expect our classical systems to thermalise.

get Kinoshita's definition of ergodicity

Do I need to elaborate on this further?

7.3 Draft: from Danny

It is our everyday experience that a hot tea or coffee cools and reaches the temperature of its surrounding, or in general when a system or its environment undergo a change, the system of interest usually respond but after a while it reaches a new state where no further macroscopic change takes place and an observer may conclude that the system reached its *thermodynamic equilibrium*. However, this phenomenon raises the question: how does the system approach its new equilibrium state?

Need to explicitly link ergodicity and thermalisation, otherwise this is just free-floating and its relevance is not obvious. What is this link?

While Ludwig Boltzmann developed the theory of entropy based on notions of statistics and probability theory [11, 12, 13]. During the derivation of the aesthetically pleasing relationship $S = k_B \ln(W)$ for an ideal gas consisting of N particles, Boltzmann a priori considered that each realisation of particles is equally probable. However, the evolution of the system would lead to a distribution of macroscopic quantities for which there are more possible microscopic realisations.

Although Boltzmann established the connection between the micro- and macroscopic world, even his contemporaries, e.g., Lord Kelvin [14, 15] and Johann Josef Loschmidt [13], raised two philosophically hard questions: reversibility and recurrence.

The former relies on the time-reversal symmetry of classical mechanics, thus one may expect processes with decreasing entropy occurring as often as ones which increase the entropy of a system. We note here that the same objection cannot be raised if one replaces classical mechanics as the description of the microscopic world with quantum mechanics. The basic equation of non-relativistic quantum mechanics is the Schödinger equation, which is *not* invariant under time-reveral symmetry.

The second objection was raised by Planck's student, Ernst Zermelo [16, 17]. His argument was based on Henri Poincare's fresh result [18, 19], namely that a mechanical system returns or almost returns to its initial state. Zermelo argued that if this is the case then entropy must decrease in some portion of the time evolution.

This second argument, however, is at the heart of this dissertation as well, since unitary time evolution forms the basis of quantum mechanics. The incongruence between the notions of thermalisation and unitary time evolution inspired a vibrant research field [20, 21, 22, 23]. One of the emerging ideas is the *eigenstate thermalisation hypothesis* (ETH) []. If the conditions of ETH are satisfied then it leads to thermalisation, as it has been proven [], i.e., ETH is sufficient for guaranteeing thermalisation. Recently G. de Palma et al. also argued [23] that ETH is also necessary for thermalisation.

7.4 Quantum systems

Quantum systems do not exhibit dynamic chaos [Rigol's line is "dynamical chaos itself cannot occur in an isolated quantum system, in which the time evolution is linear and the spectrum is discrete" How does that argument work?], so it is not obvious how one would justify applying the assumption of ergodicity in these systems. Because of this, 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.

usually?

see square brackets

8 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 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. 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 [22].

[Maybe fall back on "All 1D systems with conserved energy are integrable" for U!=0, referencing page 6 of the handout Danny gave me. I don't really know where to go for 2D at this point.]

half? according to handout this seems to be the case

reference handout Danny gave me, I can't see anywhere where its from

see square brackets

9 Experimental studies

9.1 A quantum Newton's cradle

Kinoshita et. al. investigated [24] 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

write more about red-detuned and blue-detuned lasers from what I learned talking to David.

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 diagram below)

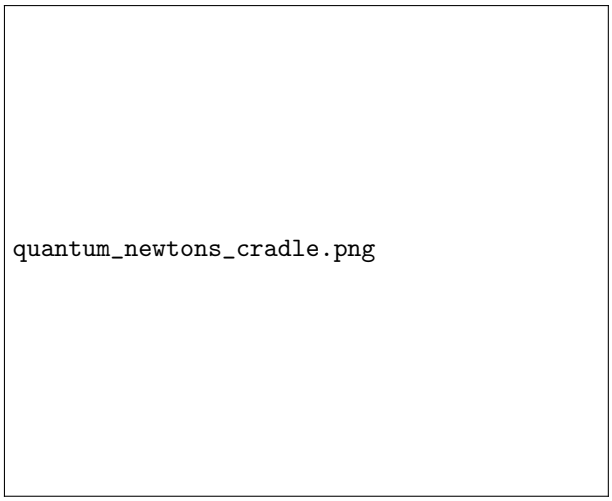

Figure 4: Sketches at various times of two out of equilibrium clouds of atoms in a one-dimensional anharmonic trap. At time $t = 0$ the atoms are put into a momentum superposition with $2\hbar k$ to the right and $2\hbar k$ to the left. The two parts of the wave function oscillate out of phase with each 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 [24].

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

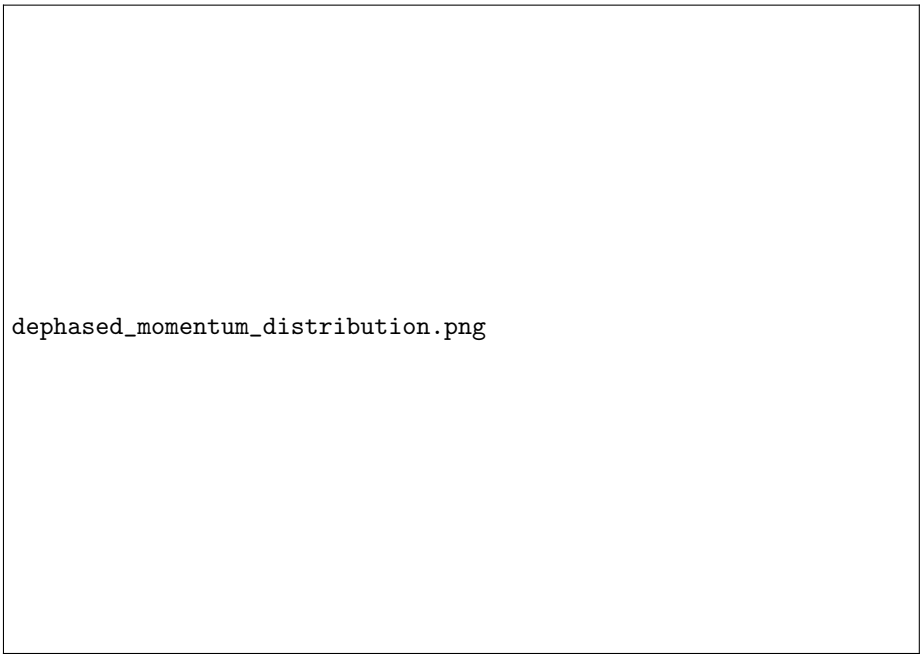

Figure 5: The blue and green curves in the above figure are projections from models that take into account loss and heating. The red line is the actual distribution observed. The dashed line is a Gaussian with the same number of atoms and r.m.s. width as the actual distribution.

To the extent that the actual distribution in figure 5 conforms to the projected distribution rather than to the Gaussian, the atoms have not thermalised.

These observations 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.

9.2 Relaxation in a Completely 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. In this experiment, hard-core bosons on a one-dimensional lattice were used. The authors, Rigol et. al [22], started with a one-dimensional bosonic Hamiltonian with no interactions and periodic boundary conditions for a lattice with L lattice sites.

$$\hat{H} = -J \sum_{i=1}^{L} (\hat{a}_i^\dagger \hat{a}_{i+1} + h.c.) \tag{25}$$

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

$$\hat{H} = -J \sum_{i=1}^{L} (\hat{c}_i^\dagger \hat{c}_{i+1} + \text{h.c.}) \tag{26}$$

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 properties of the state that the system relaxed to were not given by the grand-canonical ensemble, but rather by a generalised Gibbs ensemble, in which the partition function is extended to include all of the integrals of motion.

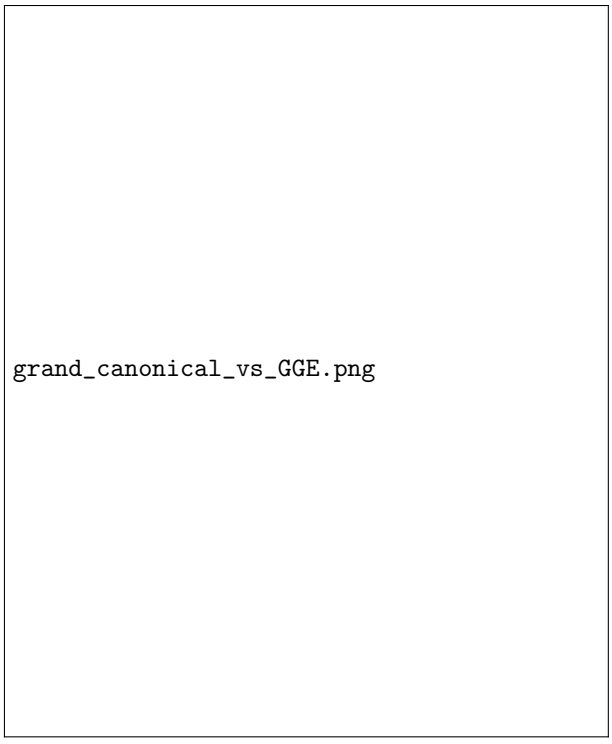

Figure 6: Equilibrium (quasi-)momentum distribution after relaxation in comparison with the predictions of the grand-canonical and of the fully constrained thermodynamic ensembles. The prediction of the fully constrained ensemble is virtually indistinct from the results of the dynamical simulation. Image taken from [22].

They further showed that their generalised equilibrium state carries more memory of the initial conditions than the usual thermodynamic one.

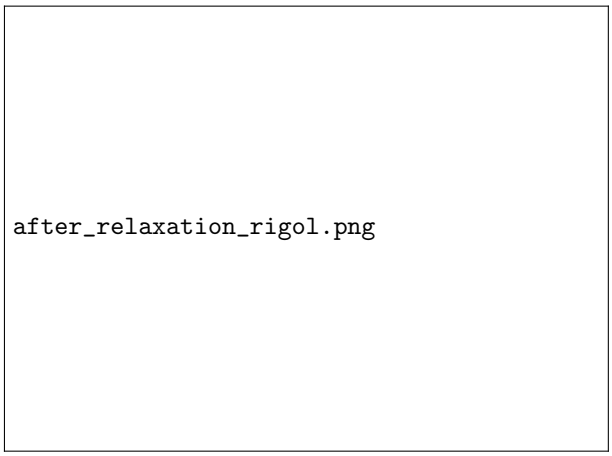

Figure 7: The actual quasi-momentum distribution after relaxation versus predictions of the generalised Gibbs ensemble and the grand canonical ensemble. Image taken from [22].

The momentum peaks remain clear and distinct during the whole duration of propagation; $t_{\text{fin}} = 3000\hbar/J$.

9.3 Measuring entanglement entropy in a quantum many-body system

- I still don't see how this is supposed to relate to what I'm doing. I can write down the definition of the nth order Rényi entropy, and describe what purity is. I imagine that I could construct a system that is a $2 \times N$ lattice and split it into two one-dimensional lattices of length N, then evaluate their purity (which must be zero for one of the chains and 1 for the other if I'm starting with all bosons on one site, right?), then do some second order Renyi entropy calculation based on that. Then I could evolve the system in time and note that this entropy changes. How does that relate to thermalisation? What can I find out from this approach that I don't already get from just looking at expectation values of number operators?

10 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 behaviour of the small systems is preserved in the larger ones.

10.1 Small 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 12 for details):

$$|\psi(t)\rangle = \sum_j e^{iE_j t} |E_j\rangle \langle E_j|\psi(0)\rangle. \tag{27}$$

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

$$\mathcal{D} = \frac{(N+P-1)!}{P!(N-1)!}, \tag{28}$$

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 is a $\mathcal{D}\times\mathcal{D}$ square matrix, and diagonalising it and then evolving the system according to equation (28) quickly becomes impractical for systems with large numbers of particles and lattice sites. We can use another familiar tool from elementary statistical mechanics –Stirling's approximation– to clarify the rate of growth of the dimensionality of the system. Stirling's approximation [25] is

$$N! \approx N^N e^{-N} \sqrt{2\pi N}. \tag{29}$$

All of the following assumptions (including Stirling's approximation) are valid only for large N.

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

Now applying Stirling's approximation to each factorial:

$$\mathcal{D} \approx \frac{(P+N)^{P+N} e^{-(P+N)} \sqrt{2\pi(P+N)}}{P^P e^{-P} N^N e^{-N} 2\pi\sqrt{PN}} = \frac{(P+N)^{P+N} \sqrt{2\pi(P+N)}}{P^P N^N 2\pi\sqrt{PN}}.$$

The exponentials are much more significant than the multiplicative factors, so we have

$$\mathcal{D} \approx \frac{(P+N)^{P+N}}{P^P N^N}.$$

In order to get a more concrete idea of how quickly the dimensionality of a typical system would grow, consider the case where we have roughly one boson per lattice site ($N \approx P$). In this case,

$$\mathcal{D} \approx \frac{(2P)^{2P}}{P^P P^P} = 2^{2P} = 4^P.$$

This means that when we increase the size of the system by one lattice site with one boson on it, the dimensionality roughly quadruples. In light of this exponential increase in dimensionality for large systems, a different approach to time evolution is required. We have chosen to use a Gross-Pitaevskii equation to reduce the dimensionality of the system. Doing this forces us to take an iterative approach to time evolution rather than an analytic one. A Runge-Kutta-Feldberg algorithm [26] was written for this purpose.

10.2 The Gross-Pitaevskii Equation

The Gross-Pitaevskii Equation (GPE) is a classical mean-field equation for describing Bose-Einstein condensates (BECs) in the zero-temperature limit. In the smaller systems that we consider with the analytic method, it is rare for us to have more than two particles on a lattice, and hence the concept of "macroscopic occupation of the ground state" that is integral to Bose-Einstein condensation has little importance here.

The validity of some of the assumptions that we make in this method will rely on there being a large number of particles. When second quantising our Hamiltonian earlier, in equation (17) we decomposed the field operators into linear combinations of single-particle Wannier position states. However, it is possible to decompose the field operators into any complete single-particle basis. If we chose the single particle energy basis $\{\phi_i\}$, then we get

$$\hat{\Psi}(\mathbf{r}) = \sum_{i=0}^{\infty} \hat{a}_i \phi_i(\mathbf{r}) = \hat{a}_0 \phi_0(\mathbf{r}) + \sum_{i=1}^{\infty} \hat{a}_i \phi_i(\mathbf{r}). \tag{30}$$

Since the GPE is a tool for investigating near-zero temperature BECs (very low energy systems), we now assume that the occupancy of energy modes other than the ground modes is negligible, i.e.,

$$\hat{\Psi}(\mathbf{r}) = \hat{a}_0 \phi_0(\mathbf{r}). \tag{31}$$

Next we note that when there are a large number of particles in the ground state $|N_0\rangle$ then the action of the creation and destruction operators on the ground state approximately commute:

$$\hat{a}_0 \hat{a}_0^\dagger |N_0\rangle = N_0 \sqrt{1 + \frac{1}{N_0}} |N_0\rangle \approx N_0 |N_0\rangle = \hat{a}_0^\dagger \hat{a}_0 |N_0\rangle \tag{32}$$

It is this property of commutation that leads us to replace the creation and annihilation operators by $\sqrt{N_0}$, which allows us to approximate the field operator $\hat{Psi}(\mathbf{r})$ with a wave function

$$\hat{\Psi}(\mathbf{r}) = \hat{a}_0 \phi_0(\mathbf{r}) \approx N_0 \phi_0(\mathbf{r}) = \psi_0(\mathbf{r}). \tag{33}$$

10.3 Runge-Kutta-Feldberg Method

The nonlinear term in the GPE prevents us from being able to represent the Hamiltonian in matrix form. Hence we cannot find the eigenvectors and eigenvalues of the system directly, which prevents us from using the 'analytic' approach to time evolution that we used for smaller system sizes. One method that we could use in its pace is to simply expand the time evolution operator $e^{-i\hat{H}t}$ in a Taylor series, truncated at an appropriate order, i.e.,

$$|\psi(t)\rangle = e^{-i\hat{H}t}\,|\psi(0)\rangle = \left(1 + (-i\hat{H}t) + \frac{1}{2}(-i\hat{H}t)^2 + \frac{1}{6}(-i\hat{H}t)^3 + \dots\right)|\psi(0)\rangle\,. \tag{34}$$

When we are working with systems in which $U_0 \neq 0$, the nonlinearity that is present quickly causes inaccuracies in any low-order (≤ 3) Taylor method. This can be observed by calculating the norm of $|\psi(t)\rangle$ at each timestep (it quickly grows significantly greater than 1). Using a higher-order Taylor method is slow, due to the computation time required to calculate the derivatives of $e^{-i\hat{H}t}$ at each timestep.

check this is exactly correct

A standard Runge-Kutta method speeds up the calculation by avoiding calculating these derivatives while retaining high-order truncation error. One of the most frequently used Runge-Kutta methods is a fourth order method, which has truncation error of $\mathcal{O}(h^4)$, where h is the size of the timestep.

For a given differential equation

$$y' = f(t, y) \tag{35}$$

with initial condition $y(t = 0) = \alpha$, we can approximate the value of y at N successive times (each separated by timestep h) by w, where

$$\begin{aligned}
w_0 &= \alpha \\
k_1 &= hf(t_i, w_i) \\
k_2 &= hf\left(t_i + \frac{h}{2}), w_i + \frac{1}{2}k_1\right) \\
k_3 &= hf\left(t_i + \frac{h}{2}), w_i + \frac{1}{2}k_2\right) \\
k_4 &= hf(t_{i+1}, w_{i+k_3}) \\
w_{i+1} &= w_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}$$

for each $i = 0, 1, \dots, N-1$. Setting $y = |\psi(t)\rangle$, $w_0 = \psi(t = 0)$ and $f(t, y) = i\hat{H}$.

blarg. need to work through this again to get it right

Even when using this method, we are concerned about the effect of the nonlinear term on our error. Hence we adopt a more sophisticated algorithm (the Runge-Kutta-Feldberg method). This method incorporates a estimate of the truncation error and adapts the step size as it goes to ensure that the error stays below a certain tolerance set by the user.

Specifically, it uses a Runge-Kutta method of order five to estimate the local error in a Runge-Kutta method of order four. If the estimated error is greater than the tolerance, then the timestep is shortened and the error is estimated again. The interested reader may refer to chapter 5 of *Numerical Analysis* by R. Burden and J. Faires [26] for the precise details of the algorithm used.

11 Results

12 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

$$|\psi(t)\rangle = e^{i\hat{H}t} |\psi(0)\rangle . \tag{36}$$

Now noting that we can use the completeness relation for the energy eigenstates to expand the initial state in the energy basis, and incorporating the $\hbar^{-1}$ into the time scale,

$$\begin{aligned} |\psi(t)\rangle &= e^{i\hat{H}t} \sum_j |E_j\rangle \langle E_j|\psi(0)\rangle \\ &= \sum_j e^{i\hat{H}t} |E_j\rangle \langle E_j|\psi(0)\rangle \\ &= \sum_j e^{iE_j t} |E_j\rangle \langle E_j|\psi(0)\rangle \\ &= \sum_j c_j e^{iE_j t} |E_j\rangle \end{aligned} \tag{37}$$

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_r 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.

12.1 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

$$t^* = \frac{2\pi Q_{\text{LCM}}}{P_{\text{HCF}}}, \tag{38}$$

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 13).

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

$$\hat{H}_{3\times 1} = \begin{pmatrix} 0 & -J & 0 \\ -J & 0 & -J \\ 0 & -J & 0 \end{pmatrix}. \tag{39}$$

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 8: 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 $\langle n_1 \rangle \sim \|\psi(t)\|^2$.

12.2 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

$$\hat{H}_{5\times 1} = \begin{pmatrix} 0 & -J & 0 & 0 & 0 \\ -J & 0 & -J & 0 & 0 \\ 0 & -J & 0 & -J & 0 \\ 0 & 0 & -J & 0 & -J \\ 0 & 0 & 0 & -J & 0 \end{pmatrix}. \tag{40}$$

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 [22]. Note that the eigenvalues of a system with 4 lattice sites are also mutually irrational (they are $\frac{J}{2}\{-1-\sqrt{5}, 1+\sqrt{5}, 1-\sqrt{5}, -1+\sqrt{5}\}$) 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 9: 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.

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.

12.3 The Poincaré Recurrence Theorem

In 1890, Henri Poincaré proved [18, 19] 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 [27], 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 $\alpha^2(t^*) = \| |\psi(t^*)\rangle - |\psi(t_0)\rangle \|^2$.

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

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 the case according to a standard result of the theory of the almost-periodic functions [28].

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

$$\sum_{n=1}^{\mathcal{D}} \left(1 - \cos\left(E_n\tau\right)\right) < \epsilon', \tag{41}$$

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^*. ■

12.4 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 result about the eigenvalues of tridiagonal matrices proven by W. Yueh [29]. A tridiagonal matrix has the form

$$A_{N\times N} = \begin{pmatrix} b & c & 0 & 0 & \dots & 0 \\ a & b & c & 0 & \dots & 0 \\ 0 & a & b & c & \dots & 0 \\ 0 & 0 & a & b & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & c \\ 0 & 0 & 0 & 0 & a & b \end{pmatrix}. \tag{42}$$

It was shown that the eigenvalues of a matrix of this form are given by

$$\lambda_k = -b + 2\sqrt{ac}\cos\left(\frac{k\pi}{N+1}\right) \tag{43}$$

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

$$\hat{H}_N = \begin{pmatrix} 0 & -J & 0 & 0 & \ldots & 0 \\ -J & 0 & -J & 0 & \ldots & 0 \\ 0 & -J & 0 & -J & \ldots & 0 \\ 0 & 0 & -J & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & -J \\ 0 & 0 & 0 & 0 & -J & 0 \end{pmatrix}, \tag{44}$$

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

$$E_k = 2J\cos\left(\frac{k\pi}{N+1}\right). \tag{45}$$

This result is particularly interesting when combined with Niven's theorem [30].

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:* $\sin\theta, \cos\theta = 0, \pm\frac{1}{2}, \pm 1; \sec\theta, \csc\theta = \pm 1, \pm 2;$
$\tan\theta, \cot\theta = 0, \pm 1.$

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 (45) becomes

$$E_k = 2J\cos\left(\frac{180k}{N+1}\right). \tag{46}$$

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 (45). 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

$$e^{i(k_1-k_2)\pi} = \gamma^{N+1}. \tag{47}$$

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 (47) is ± 1 depending on the parity of $(k_1 - k_2)$. Meanwhile the right hand side of (47) 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. ∎

Hence, we have shown that all one-dimensional noninteracting systems with more than three lattice sites should not exhibit recurrence, and are thus expected to thermalise.

12.5 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

Should I talk about dimensionality of Hamiltonian and/or having to choose a numbering convention for

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 12.5.1.

confirm this happens the same way for lots of different initial conditions.

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 12.1 that 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 an ordering convention for our number states in order to define the representation of the Hamiltonian matrix. In this project, we have chosen to order the states in such a way that the states with the lowest index have the most particles on one particular side of the lattice, i.e.,

$$|200\rangle = |1\rangle\,,\ |110\rangle = |2\rangle\,,\ |101\rangle = |3\rangle\,,\ |020\rangle = |4\rangle\,,\ \ldots,\ |002\rangle = |10\rangle\,.$$

Using this basis, we can represent the Hamiltonian as

$$\hat{H}^{(P=2)}_{3\times1} = \begin{pmatrix} U & -\sqrt{2}J & 0 & 0 & 0 & 0 \\ -\sqrt{2}J & 0 & -\sqrt{2}J & -J & 0 & 0 \\ 0 & -\sqrt{2}J & U & 0 & -\sqrt{2}J & 0 \\ 0 & -J & 0 & 0 & -J & 0 \\ 0 & 0 & -\sqrt{2}J & -J & 0 & -\sqrt{2}J \\ 0 & 0 & 0 & 0 & -\sqrt{2}J & U \end{pmatrix}. \tag{48}$$

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 10: 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.

on reflection, this looks a bit like revival. Look at data file to test.

Figure 11: 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 (12), where $\frac{P}{N} = 0.2$.

Figure 12: Thermalisation for a 10×1 lattice with two bosons and $U = 0.1$.

12.5.1 Effect of interaction strength

When the interaction strength is increased, we notice an increasing dependence of the long-term averages of the expectation values of the number operators. This suggests that having strong interparticle interactions can frustrate thermalisation. All of the following simulations are run for a 3×1 lattice with two bosons. U=0.005 (short term)

add more words here

Figure 13: Demonstrating 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 14: 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 15: 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 16: 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 17: 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 18: 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 19: 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 20: 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 (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 a result of the repulsive contact interactions. However, once U_0 gets larger (especially once it becomes greater than 1), we find that the long-term average for the site furthest from the one that the boson begins on drops dramatically.

Figure 21: 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 $\overline{\langle n_3 \rangle}$ goes to 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).

This suggestion that what we are observing is a quantum phase transition is inspired by work doneby Greiner et al. [31], who state that for a system described by the Bose-Hubbard Hamiltonian

this is in their introduction, not their experiment. So is "work done" the right terminology?

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

in the limit where the tunnelling term dominates the Hamiltonian, 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 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

$$|\Psi_{SF}\rangle^{(U_0=0)} \propto \left(\sum_{i=1}^{N} \hat{a}_i^\dagger\right)^P |0\rangle\,. \tag{49}$$

[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 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 [32]. For a homogeneous lattice, this ground state is

$$|\Psi_M I\rangle^{(J=0)} \propto \prod_{i=1}^{N} \left(\hat{a}_i^\dagger\right)^{\frac{P}{N}} |0\rangle\,. \tag{50}$$

This state has very little phase coherence, but perfect correlations in particle number exist between lattice sites. [does this mean that when P¡N each lattice site has either one particle on it or zero? If so, then point out that this is consistent with the data in figure 12.5.1]. 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 $U_0 > J$.

ask exactly what sentence in "[]" means, then reword

maybe I can talk about Tonks-Girardeau gas somewhere in here, see highlighted paper

see square brackets

13 Two-dimensional systems

13.1 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

$$\hat{H}_{2D} = \left(J\sum_{i,j} \hat{a}_{i,j+1}^\dagger \hat{a}_{i,j} + J'\sum_{i,j} \hat{a}_{i,j}^\dagger \hat{a}_{i+1,j}\right) + h.c. \tag{51}$$

Like in 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'

$$\hat{H}_{3\times 3} = \begin{pmatrix} 0 & -J & 0 & -J' & 0 & 0 & 0 & 0 & 0 \\ -J & 0 & -J & 0 & -J' & 0 & 0 & 0 & 0 \\ 0 & -J & 0 & 0 & 0 & -J' & 0 & 0 & 0 \\ -J' & 0 & 0 & 0 & -J & 0 & -J' & 0 & 0 \\ 0 & -J' & 0 & -J & 0 & -J & 0 & -J' & 0 \\ 0 & 0 & -J' & 0 & -J & 0 & 0 & 0 & -J' \\ 0 & 0 & 0 & -J' & 0 & 0 & 0 & -J & 0 \\ 0 & 0 & 0 & 0 & -J' & 0 & -J & 0 & -J \\ 0 & 0 & 0 & 0 & 0 & -J' & 0 & -J & 0 \end{pmatrix}. \tag{52}$$

We use this example rather than a 2×2 lattice because the 2×2 lattice is not strictly two-dimensional (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.

$$\hat{H}_{3\times 3} = \hat{H}^{(J)}_{3\times 1} \otimes I_3 + I_3 \otimes H^{(J')}_{3\times 1}, \tag{53}$$

where

$$\hat{H}^{(J)}_{3\times 1} = \begin{pmatrix} 0 & -J & 0 \\ -J & 0 & -J \\ 0 & -J & 0 \end{pmatrix}, \quad H^{(J')}_{3\times 1} = \begin{pmatrix} 0 & -J' & 0 \\ -J' & 0 & -J' \\ 0 & -J' & 0 \end{pmatrix}, \tag{54}$$

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 22, of a boson that starts in the top left corner ("first lattice site") of a 3×3 lattice with $J = J'$.

Need to finish this argument off here, am too tired to do it atm

quasi-two-dimensional

Figure 22: Revival for a 3×3 square lattice with a single boson and $J = J'$.

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

should I get rid of this text

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

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 (45).

Now consider a case identical to the previous one, except with $J = 1$ and $J' = \frac{3}{5}$. Note that equation (38) predicts a revival time of $t^* = 10\pi$ here, which is consistent with the simulation.

should t^* be over $\sqrt{2}$?

Figure 23: 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 13.1.

Figure 24: 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 4×4 systems, such as the following one with $J = J'$.

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

Is it worth putting in a larger system, like the following one? 15×15 with $J = J'$.

Figure 26: 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 27: Absence of revival for a 3×4 lattice with a single boson and $J = J'$.

It is not entirely clear from figure 27 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.

14 Two-dimensional interacting systems

We will now look at two-dimensional systems where the particles have repulsive interactions ($U_0 > 0$). Like in the one-dimensional case,

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