Honours Research Project progress report

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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[2]. 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 tunneling 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].

I think I should include some "flavour" here with vaguely interesting general statements about thermodynamics

1 Experimental advantages of working with bosons on optical lattices

Bosons on optical lattices are an excellent arena in which to explore various model Hamiltonians [for condensed matter systems, or is it broader than that? want something linking this to solids, or my later line about impurities lacks context], due to the fine degree of experimental control attainable in generating these systems. The shape, depth and spacing of the potential can be easily varied in optical lattices of BECs[5]. The strength of the interparticle interaction can also be easily varied. Moreover, there are always impurities present in the solids we find in nature, which 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. Optical lattices are highly uniform, so when dealing with BECs on optical lattices this problem of impurities does not arise.

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

2 First quantised representation

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 (we will assume this only occurs if they occupy the same lattice sites), and there may also be an external potential imposed that can vary in strength from site to site. From this reasoning, we can construct a first quantised Hamiltonian for a 1D system of interacting bosons on an optical lattice, in the presence of an external potential V_{ext}

$$\hat{H} = \sum_i -\frac{\hbar^2}{2m}\partial_{x_i}^2 + \sum_j V_{lattice}(R_j) + V_{ext}(x) + \frac{U}{2}\sum_{i,j}\delta(x_i - x_j). \qquad (1)$$

should mention the aspect of control compared to solids (can't put all electrons on a single atom)

Similar Hamiltonians are frequently used to describe systems of electrons on atomic lattices.

should I include this external potential, given that I won't use it? And is it still the Bose-Hubbard model if we have no external potential?

3 Many-particle wavefunctions and identical particles [6, 3, 1]

The Hamiltonian in the previous section would act on a bosonic many-particle wavefunction. A system of identical bosons must be symmetric under particle exchange, and this has implications for how we must write our many-particle wavefunctions. Let us first consider the case of two indistinguishable bosons. We have not yet determined the eigenstates of our Hamiltonian, but if we suppose we have the set of normalised single-particle wavefunctions $|\lambda\rangle$, and we have one boson in state $|\lambda_1\rangle$ and another in state $|\lambda_2\rangle$, then we can write the two-particle wavefunction as

Should spread these references throughout the following sections?

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}\big(\langle x_1|\lambda_1\rangle \langle x_2|\lambda_2\rangle + \langle x_1|\lambda_2\rangle \langle x_2|\lambda_1\rangle \big), \tag{2}$$

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

$$|\lambda_1, \lambda_2\rangle = \frac{1}{\sqrt{2}}\big(|\lambda_1\rangle \otimes |\lambda_2\rangle + |\lambda_2\rangle \otimes |\lambda_1\rangle \big) \tag{3}$$

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 as

$$|\lambda_1, \lambda_2, ..., \lambda_N\rangle = \frac{1}{\sqrt{N! \prod_{\lambda=0}^{\infty} n_\lambda}} \sum_{\mathcal{P}} \lambda_{\mathcal{P}1} \otimes \lambda_{\mathcal{P}2} \otimes ... \otimes \lambda_{\mathcal{P}N} \tag{4}$$

where n_λ is the number of particles in state λ, and the summation runs over all $N!$ permutations 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.

4 Second Quantisation

4.1 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

$$|\Psi\rangle = \sum_{n_1, n_2, \ldots} c_{n_1, n_2, \ldots} |n_1, n_2, ...\rangle \tag{5}$$

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

$$\hat{a}_j^\dagger |n_1, n_2, \ldots, n_j, \ldots\rangle = \sqrt{n_j + 1}\, |n_1, n_2, \ldots, n_j + 1, \ldots\rangle \tag{6}$$

and

$$\hat{a}_j |n_1, n_2, \ldots, n_j, \ldots\rangle = \sqrt{n_j}\, |n_1, n_2, \ldots, n_j - 1, \ldots\rangle \tag{7}$$

These operators have very important commutation relations

$$[\hat{a}_j^\dagger, \hat{a}_k^\dagger] = 0, \qquad [\hat{a}_j, \hat{a}_k] = 0, \qquad [\hat{a}_j, \hat{a}_k^\dagger] = \delta_{jk}. \tag{8}$$

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

$$\hat{n}_j \left|n_1, n_2, \ldots, n_j, \ldots\right\rangle = n_j \left|n_1, n_2, \ldots, n_j, \ldots\right\rangle \tag{9}$$

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

$$\left|n_1, n_2, \ldots\right\rangle = \prod_i \frac{1}{\sqrt{n_i!}} (\hat{a}_i^\dagger)^{n_i} \left|0\right\rangle \tag{10}$$

The N-particle Hilbert space is built up from N single-particle Hilbert spaces $\mathcal{H}$.

$$\mathcal{H}^N = \mathcal{H} \otimes \mathcal{H} \otimes \cdots \otimes \mathcal{H} \tag{11}$$

The Fock space $\mathcal{F}^N$ is a subspace of $\mathcal{H}^N$ subject to certain symmetry constraints.

Now that we have established the space and states that we are operating within, we now need to rewrite the Hamiltonian in such a form that it can operate on number eigenstates i.e. we "second quantise" it.

is this true? Needs to account for different values of N?

4.2 Second Quantisation of the Hamiltonian

We can second quantise the Hamiltonian initially used to describe our system through the use of 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 first two terms in (1),the kinetic and potential energy contributions, can be transformed to

$$\int \hat{\psi}^\dagger(x) \left(\sum_i -\frac{\hbar^2}{2m} \partial_{x_i}^2 + \sum_j V_{lattice}(R_j) \right) \hat{\psi}(x) dx \tag{12}$$

how to reference this equation in a way that will autoupdate?

In a weak lattice, Bloch's theorem (in 1D) tells us that the eigenstates of a particle in a periodic potential has the form

$$\phi_q(x) = e^{iqx} u_q(x) \tag{13}$$

is transformed the correct term?

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 wavefunctions of particles on particular lattice sites have effectively zero overlap with non-nearest neighbours. Under these conditions, the wavefunctions can be described by the localised Wannier functions

$$\psi(R; r) = \frac{1}{d} \int dq \, e^{iRq} \phi_q(x) \tag{14}$$

which are superpositions of Bloch functions. We can use this to rewrite the field operators as

$$\hat{\psi}(x) = \sum_j \hat{a}_j(t)\psi(R_j - x) \tag{15}$$

With this in mind, we can write

$$\int \sum_j \hat{a}_j^\dagger \psi^*(R_j - x)\Big(\sum_i -\frac{\hbar^2}{2m}\partial_{x_i}^2 + \sum_i V_{lattice}(R_i)\Big)\sum_l \hat{a}_l \psi(R_l - x)dx = \sum_{j,l} J_{j,l}\hat{a}_j^\dagger \hat{a}_l \tag{16}$$

Where

$$J_{j,l} = \int \psi^*(R_j - x)\Big(\sum_i -\frac{\hbar^2}{2m}\partial_{x_i}^2 + \sum_j V_{lattice}(R_j))\Big)\psi(R_l - x)dx \tag{17}$$

characterises the strength of the hopping between sites l and j, which (intuitively) depends on the combination of the lattice depth and the kinetic energy. We take this this hopping strength to be negligible for sites which are not nearest-neighbours. Of the permitted hopping interactions, we assume that each has identical strength. This allows us to write

$$\int \hat{\psi}^\dagger(x)\Big(\sum_i -\frac{\hbar^2}{2m}\partial_{x_i}^2 + \sum_j V_{lattice}(R_j)\Big)\hat{\psi}(x)dx = J\sum_i(\hat{a}_i^\dagger \hat{a}_{i+1} + c.c.). \tag{18}$$

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

$$\int \hat{\psi}^\dagger(x)V_{ext}(x)\hat{\psi}(x)dx = \sum_i \epsilon_i \hat{a}_i^\dagger \hat{a}_i. \tag{19}$$

Second quantising the term for on-site interaction between bosons (which is a two-particle operator) requires integration between two sets of boson field operators

$$\int \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\frac{U}{2}\sum_{i,j}\delta(x_i - x_j)\hat{\psi}(x)\hat{\psi}(x)dx = \frac{U}{2}\sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i \tag{20}$$

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

5 The Bose-Hubbard model

The Hamiltonian for a weakly interacting BEC in an 1-dimensional optical lattice and subject to harmonic trapping potential is given by

$$\hat{H} = J\sum_i(\hat{a}_i^\dagger\hat{a}_{i+1} + c.c.) + \frac{U}{2}\sum_i \hat{a}_i^\dagger\hat{a}_i^\dagger\hat{a}_i\hat{a}_i + \sum_i \epsilon_i\hat{a}_j^\dagger\hat{a}_j, \tag{21}$$

The ϵ_i's refer to on-site energies at each lattice site (influenced by the harmonic trap), and the middle term gives an interaction energy when there is more than one particle on a particular site.

Should I have a diagram here or elsewhere where I actually draw in the laser beam and the wavefunction overlap?

This project will look at scenarios where there is no external harmonic potential which produces different on-site energies for different sites. Under these conditions, the Hamiltonian in one dimension reduces to

$$\hat{H} = J\sum_i(\hat{a}_i^\dagger\hat{a}_{i+1} + c.c.\ ) + \frac{U}{2}\sum_i \hat{a}_i^\dagger\hat{a}_i^\dagger\hat{a}_i\hat{a}_i. \tag{22}$$

The atoms in the lattice are still subject to the lattice potential. We can see this from the definition of J as the "hopping integral" in terms of the Hamiltonian of the system in the wavefunction representation.

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

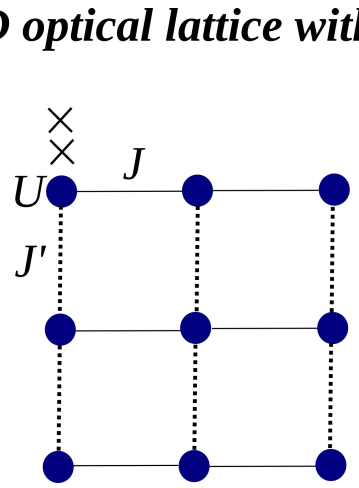
$$\hat{H} = (J\sum_{i,j}\hat{a}_{i,j+1}^\dagger\hat{a}_{i,j} + J'\hat{a}_{i,j}^\dagger\hat{a}_{i+1,j}) + c.c. + \frac{U}{2}\sum_i \hat{a}_i^\dagger\hat{a}_i^\dagger\hat{a}_i\hat{a}_i, \tag{23}$$

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; it characterises the overlap between adjacent Wannier states on different chains.

factcheck: should this be Bloch states? or neither?

get the captioning sorted out

Figure 2: *



The blue circles here represent lattice sites and the crosses individual bosons. Hopping between any two 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 any arbitrary size.

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

6 Thermalisation

6.1 Overview

To say that a system thermalises means that it relaxes 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, are there are strong theoretical reasons for anticipating thermalisation here. 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 Integrable systems

[Flesh this section out quite a bit, start with some generic stuff for classical systems, then should I try to do the Jordan-Wigner mapping from Rigol+Olshanii 2007 to prove my 1D U=0 system is integrable? Maybe fall back on "All 1D systems with conserved energy are integrable" for U!=0, referencing the handout Danny gave me. I don't really know where to go for 2D at this point.] An integrable system is one for which the number of independent constraints is equal to the number of degrees of freedom. Since the system we are dealing with is closed, it is subject to the constraints of constant energy and particle number. For a single atom in 1 dimension, its degrees of freedom are its 1D position and

see square brackets

I don't think I can use particle number

momentum. So we expect this system to be completely integrable. Once more particles are added, or the system is extended to two dimensions, then if we do not introduce a commensurate number of new constraints, integrability will be broken.

8 Experimental studies

8.1 A Quantum Newton's Cradle[4]

This study investigated the thermalisation of an out-of-equilibrium 1D Bose gases, which are nearly-integrable systems. The authors prepared of out-of-equilibrium arrays of trapped one-dimensional (1D) Bose gases, each containing from 40 to 250 ^{87}Rb atoms, and found them to not noticeably equilibrate, even after thousands of collisions.

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.

8.2 Relaxation in a Completely Integrable Many-Body Quantum System [7]

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 (which cannot occupy the same state and so behave like fermions, but without exchange antisymmetry) on a 1D lattice were used. The authors found that the system can 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. They further showed that their generalized equilibrium state carries more memory of the initial conditions than the usual thermodynamic one.

9 Results

10 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. The dividing line between systems for which we see revival and those in which we don't is whether the eigenvalues of the system are mutually rational. To demonstrate this, consider the initial state of the system $|\psi(0)\rangle$, which evolves in time according to

$$|\psi(t)\rangle = e^{i\hat{H}t}\,|\psi(0)\rangle\,, \tag{24}$$

noting that we can use the completeness relation for the energy eigenstates to

should expand what I currently have have, Kinoshita and Rigol2007 could definitely be a couple of paragraphs each. Possibly include diagrams.

should the citation of Kinoshita be in the main body of the paragraph instead of the title? If so, where?

section on ETH seems advisable

need to introduce Greiner's entanglement entropy stuff somewhere, probably around here

should this section come within results or background?

Is this a

expand the initial state in the energy basis,

$$|\psi(t)\rangle = e^{i\hat{H}t} \sum_j |E_j\rangle \langle E_j|\psi(0)\rangle \tag{25}$$

$$= \sum_j e^{i\hat{H}t} |E_j\rangle \langle E_j|\psi(0)\rangle \tag{26}$$

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

$$\tag{28}$$

From here it can be seen that the only time dependence is in the complex exponential, and that if we can find some time t_r such that $E_j t_r = 2\pi k_j$, where $k_j \in \mathbf{Z}$ for all j, we will recover the initial state i.e. $|\psi(t_r)\rangle = |\psi(0)\rangle$.

10.1 Exact and regular 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. 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 $E_j = \frac{p_j}{q_j}, p_j, q_j \in \mathbf{Z}$. The revival time is then given by $t_r = 2\pi Q_{LCM}$, where Q_{LCM} is the lowest common multiple of q_j.

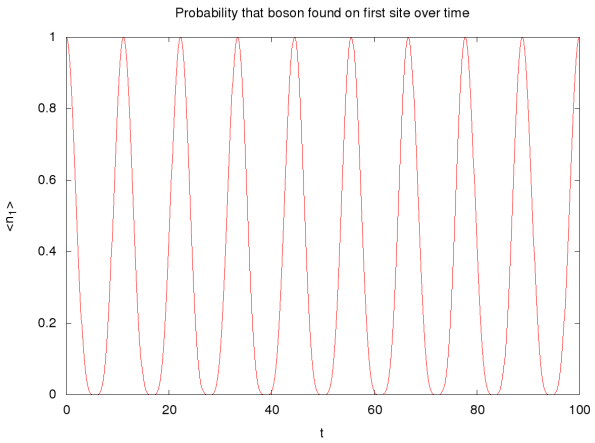
We are yet to find any systems with nonzero interparticle interaction that have mutually rational eigenvalues. In one dimension, the only systems that we have found that meet the criterion of mutually irrational eigenvalues are those with fewer than 4 lattice sites. In two dimensions, .

do a comprehensive batch of simulations to determine what is and isn't ok in 2D

To see this exact revival, consider the following system: A one dimensional lattice with three sites, a single boson and a hopping constant of $J = 0.4$. So the Hamiltonian is

$$\hat{H} = \begin{bmatrix} 0 & -0.4 & 0 \\ -0.4 & 0 & -0.4 \\ 0 & -0.4 & 0 \end{bmatrix}$$

. Diagonalising this matrix yields the eigenvalues $\{-\frac{2\sqrt{2}}{5}, 0, \frac{2\sqrt{2}}{5}\}$. These are mutually rational (If we divide them all by $\sqrt{2}$ they are all rational). Ignoring the $\sqrt{2}$ factor for a moment, our formula for the revival time gives $t_r = 10\pi$, or taking into account the square root of two factor $t_r = 10\sqrt{2}\pi \approx 44.43$. We can see from the graph of the simulation below that this matches up with a return to the initial state.



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 $< n_1 >= 1$, whereas the revival time that is calculated in our method corresponds to exact revival of the initial wavefunction.

10.2 Mutually irrational eigenvalues

The range of systems for which the spectrum is 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 spectrum will be irrational. We can demonstrate this by considering a single chain of five sites, with one boson and $J = -1$. The Hamiltonian for this system is

$$\hat{H} = \begin{bmatrix} 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 \end{bmatrix}$$

.

is it inaccurate to describle the spectrum (as opposed to the eigenvalues) as mutually irrational?

do I need to include this?

need mathematica for the rest of this section?

do I need to prove this?

11 The Poincaré Recurrence Theorem

12 Arbitrarily close but arbitrarily long

References

[1] A. Altland and B.D. Simons. *Condensed Matter Field Theory*. Cambridge books online. Cambridge University Press, 2010.

[2] Immanuel Bloch, Jean Dalibard, and Sylvain Nascimbène. Quantum simulations with ultracold quantum gases. *Nature Physics*, 8(4):267–276, Apr 2012.

[3] J.C. Inkson. *Many-body theory of solids: an introduction*. Plenum Press, 1984.

[4] Toshiya Kinoshita, Trevor Wenger, and David S. Weiss. A quantum Newton's cradle. *Nature*, 440(7086):900–903, Apr 2006.

[5] Oliver Morsch and Markus Oberthaler. Dynamics of Bose-Einstein condensates in optical lattices. *Reviews of Modern Physics*, 78(1):179–215, Feb 2006.

[6] J.W. Negele and H. Orland. *Quantum many-particle systems*. Frontiers in physics. Addison-Wesley Pub. Co., 1988.

[7] Marcos Rigol, Vanja Dunjko, Vladimir Yurovsky, and Maxim Olshanii. Relaxation in a completely integrable many-body quantum system: Anab initiostudy of the dynamics of the highly excited states of 1D lattice hard-core bosons. *Physical Review Letters*, 98(5), Feb 2007.