Simulating experimental error with the Bose–Hubbard model

Dmitri Iouchtchenko

21 October 2016

Contents

1 Background

In principle, everything should be done in three spatial dimensions, but for the sake of simplicity, we work in one dimension.

1.1 Wannier functions

For a potential $V(x)$ which is periodic with lattice spacing a_0 (*i.e.* $V(x + ja_0) = V(x)$ for $j \in \mathbb{Z}$), the Bloch theorem guarantees that the one-body Hamiltonian

$$\hat{h} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{1.1}$$

has eigenfunctions of the form

$$\psi_{nk}(x) = e^{ikx} u_{nk}(x), \tag{1.2}$$

where the $u_{nk}(x)$ have the same periodicity as $V(x)$. Here k is a pseudomomentum that may take on values in the first Brillouin zone ($-\pi/a_0 < k \leq \pi/a_0$). The corresponding eigenvalues are ε_{nk}.

An equivalent way to model such a system is with a collection of Hamiltonians

$$\hat{h}_k = \frac{(\hat{p} + \hbar k)^2}{2m} + V(\hat{x}), \tag{1.3}$$

indexed by the pseudomomentum. This makes it clear that for each k there is a ladder of eigenvalues indexed by n. Since the eigenvalues vary continuously with k, this leads to "band structure", with a band of energies for each n.

If we only have L periods in our lattice, we only get L evenly-spaced values of k in the first Brillouin zone: $k_\alpha = 2\pi\alpha/La_0$ for $\alpha \in \mathbb{Z}$ and $-L/2 < \alpha \leq L/2$. For each band, we may take the eigenfunctions $\psi_{nk}(x)$ and construct the Wannier functions

$$w_j^{(n)}(x) = w^{(n)}(x - X_j) = \frac{1}{\sqrt{L}} \sum_\alpha e^{ik_\alpha(x - X_j)} u_{nk_\alpha}(x) = \frac{1}{\sqrt{L}} \sum_\alpha e^{2\pi i\alpha(x - X_j)/La_0} u_{n\alpha}(x), \tag{1.4}$$

where each X_j lies at the same position in each lattice site. That is, $X_j = ja_0 + b$, where $0 \leq b < a_0$. The Wannier functions are orthonormal within a band (forming a basis) and each is localized fairly well inside its site.

1.2 Second-quantized operators

Starting with a one-body basis of wavefunctions $\varphi_k(x)$, also known as "orbitals", we may define the operators $a_k^\dagger$ and a_k (we omit the hats from some operators) which create particles in and annihilate particles from orbital k. These operators in operating in succession give rise to the number operator

$$n_k = a_k^\dagger a_k, \tag{1.5}$$

which counts the number of particles in orbital k. Summing over the orbitals, we may construct the field operators

$$\hat{\psi}^\dagger(x) = \sum_k \varphi_k^*(x) a_k^\dagger \tag{1.6a}$$

and

$$\hat{\psi}(x) = \sum_k \varphi_k(x) a_k, \tag{1.6b}$$

which allow us to create and annihilate a particle at some location x.

The second-quantized form of a one-body operator

$$\hat{O} = \sum_{i=1}^N \hat{o}_i \tag{1.7}$$

is

$$\hat{O} = \sum_{k,\ell} \langle k|\hat{o}|\ell\rangle \, a_k^\dagger a_\ell, \tag{1.8a}$$

which may also be written as

$$\hat{O} = \int \mathrm{d}x \int \mathrm{d}x' \, \hat{\psi}^\dagger(x) \left\langle x\middle|\hat{o}\middle|x'\right\rangle \hat{\psi}(x'). \tag{1.8b}$$

Of particular interest are operators diagonal in position, such as

$$\hat{V} = \int \mathrm{d}x \, \hat{\psi}^\dagger(x) V(x) \hat{\psi}(x) \tag{1.9}$$

and the kinetic energy operator

$$\hat{K} = \int \mathrm{d}x\, \hat{\psi}^\dagger(x) \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \hat{\psi}(x). \tag{1.10}$$

The second-quantized form of a two-body operator

$$\hat{O} = \sum_{i=1}^{N} \sum_{i=j+1}^{N} \hat{o}_{ij} \tag{1.11}$$

is

$$\hat{O} = \frac{1}{2} \sum_{i,j,k,\ell} \langle i\, j | \hat{o} | k\, \ell \rangle\, a_i^\dagger a_j^\dagger a_\ell a_k, \tag{1.12a}$$

which may also be written as

$$\hat{O} = \frac{1}{2} \int \mathrm{d}x \int \mathrm{d}x' \int \mathrm{d}x'' \int \mathrm{d}x'''\, \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') \left\langle x\, x' \middle| \hat{o} \middle| x''\, x''' \right\rangle \hat{\psi}(x''') \hat{\psi}(x''). \tag{1.12b}$$

For operators diagonal in position, this is simply

$$\hat{V} = \frac{1}{2} \int \mathrm{d}x \int \mathrm{d}x'\, \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') V(x, x') \hat{\psi}(x') \hat{\psi}(x), \tag{1.13}$$

while for a contact interaction $V(x - x') = g\delta(x - x')$, it is the even simpler

$$\hat{V} = \frac{g}{2} \int \mathrm{d}x\, \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x) \hat{\psi}(x) \hat{\psi}(x). \tag{1.14}$$

1.3 Bosonic occupation basis

Consider a system of L orbitals and N bosons which may occupy these orbitals without restriction. Because the particles are indistinguishable, we can't use a simple product basis that describes the state of each particle. Instead, such a system may be described using the bosonic occupation basis $\mathcal{B}(L, N)$, which has all possible states of the form

$$|\mathbf{n}\rangle \equiv |n_1\, n_2\, \cdots\, n_L\rangle \tag{1.15}$$

subject to

$$\sum \mathbf{n} \equiv \sum_{\ell=1}^{L} n_\ell = N. \tag{1.16}$$

For example, when $L = 3$ and $N = 2$, the necessary basis $\mathcal{B}(3, 2)$ is

$$\left\{ |2\,0\,0\rangle, |0\,2\,0\rangle, |0\,0\,2\rangle, |1\,1\,0\rangle, |1\,0\,1\rangle, |0\,1\,1\rangle \right\}. \tag{1.17}$$

In general, the number of required states is

$$\left| \mathcal{B}(L, N) \right| = \binom{N + L - 1}{L - 1} = \binom{N + L - 1}{N}. \tag{1.18}$$

This does not scale very well! At unit filling (one particle per orbital, $L = N$), we get

$$\left|\mathcal{B}(1,1)\right| = 1 \tag{1.19a}$$
$$\left|\mathcal{B}(2,2)\right| = 3 \tag{1.19b}$$
$$\left|\mathcal{B}(4,4)\right| = 35 \tag{1.19c}$$
$$\left|\mathcal{B}(8,8)\right| = 6435 \tag{1.19d}$$
$$\left|\mathcal{B}(16,16)\right| = 300\,540\,195 \tag{1.19e}$$
$$\left|\mathcal{B}(32,32)\right| = 916\,312\,070\,471\,295\,267 \tag{1.19f}$$
$$\left|\mathcal{B}(64,64)\right| = 11\,975\,573\,020\,964\,041\,433\,067\,793\,888\,190\,275\,875, \tag{1.19g}$$

where the last values have 18 and 38 digits, respectively. Doubling the number of particles and orbitals approximately doubles the number of digits, which suggests exponential scaling. This is still better than the distinguishable case, where the number of states is given by L^N and has 116 digits for $L = N = 64$.

1.4 Bose–Hubbard model

We start with a familiar first-quantized one-dimensional Hamiltonian for N particles (each of mass m) in a lattice potential $\hat{V}_i$ and with pair-wise interactions $\hat{V}_{ij}$:

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \sum_{i=1}^{N} \hat{V}_i + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \hat{V}_{ij}. \tag{1.20}$$

We assume that the particles are sufficiently trapped in the other spatial dimensions that we may disregard those motions. The lattice potential has spacing a_0 and contains L sites, for a total length La_0. Such a lattice has the recoil energy

$$E_{\mathrm{R}} = \frac{\hbar^2}{2m} k_{\max}^2 = \frac{\pi^2 \hbar^2}{2m a_0^2}; \tag{1.21}$$

this is the top of the first band for a free particle.

Rewriting the above Hamiltonian in bosonic second-quantized notation (now without a fixed number of particles), we find

$$\hat{H} = \int_0^{La_0} \mathrm{d}x\, \hat{\psi}^\dagger(x) \hat{h} \hat{\psi}(x) + \frac{1}{2} \int_0^{La_0} \mathrm{d}x \int_0^{La_0} \mathrm{d}x'\, \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') V(x,x') \hat{\psi}(x') \hat{\psi}(x), \tag{1.22}$$

where

$$\hat{h} = -\frac{\hbar^2}{2m} \nabla^2 + V(x). \tag{1.23}$$

For an optical lattice of ultracold atoms, it is typical to choose

$$V(x) = V_0 \cos^2\left(\frac{\pi x}{a_0}\right) \tag{1.24a}$$

and

$$V(x,x') = g\delta(x - x'), \tag{1.24b}$$

where V_0 is the depth of the lattice and g is the integrated strength of the interaction potential. This choice of interaction potential is easily justified by considering that the lattice spacing a_0 is typically on the order

of 100 nm, while the interactions are relevant on scales of the order of 1 Å = 0.1 nm. The Hamiltonian is then just

$$\hat{H} = \int_0^{La_0} \mathrm{d}x\, \hat{\psi}^\dagger(x)\hat{h}\hat{\psi}(x) + \frac{g}{2}\int_0^{La_0} \mathrm{d}x\, \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x). \tag{1.25}$$

We may expand the field operators in an arbitrary basis of one-body orbitals to find

$$\hat{H} = \sum_{k,\ell}\left[\int_0^{La_0} \mathrm{d}x\, \varphi_k^*(x)\hat{h}\varphi_\ell(x)\right] a_k^\dagger a_\ell + \frac{1}{2}\sum_{i,j,k,\ell}\left[g\int_0^{La_0} \mathrm{d}x\, \varphi_i^*(x)\varphi_j^*(x)\varphi_k(x)\varphi_\ell(x)\right] a_i^\dagger a_j^\dagger a_k a_\ell, \tag{1.26}$$

which we write as

$$\hat{H} = -\sum_{k,\ell} J_{k\ell} a_k^\dagger a_\ell + \frac{1}{2}\sum_{i,j,k,\ell} U_{ijk\ell} a_i^\dagger a_j^\dagger a_k a_\ell, \tag{1.27}$$

where

$$J_{k\ell} = -\langle k|\hat{h}|\ell\rangle \tag{1.28a}$$

$$= -\int_0^{La_0} \mathrm{d}x\, \varphi_k^*(x)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0\cos^2\left(\frac{\pi x}{a_0}\right)\right)\varphi_\ell(x) \tag{1.28b}$$

and

$$U_{ijk\ell} = g\,\langle i\, j|\delta(x-x')|k\,\ell\rangle \tag{1.29a}$$

$$= g\int_0^{La_0} \mathrm{d}x\, \varphi_i^*(x)\varphi_j^*(x)\varphi_k(x)\varphi_\ell(x). \tag{1.29b}$$

For a sufficiently cold lattice, only the first band will be occupied, so we may choose the Wannier functions from the first band as the basis of orbitals in which we expand the field operators, yielding

$$J_{k\ell} = -\int_0^{La_0} \mathrm{d}x\, w_k^*(x)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0\cos^2\left(\frac{\pi x}{a_0}\right)\right) w_\ell(x) \tag{1.30a}$$

and

$$U_{ijk\ell} = g\int_0^{La_0} \mathrm{d}x\, w_i^*(x)w_j^*(x)w_k(x)w_\ell(x). \tag{1.30b}$$

In a deep lattice, tunnelling across more than one barrier and overlap between different sites are strongly suppressed, so only terms with $J_{k(k\pm1)}$ and U_{kkkk} contribute appreciably to the Hamiltonian. Since all Wannier functions are identical up to translation, these coefficients are independent of k, and we define

$$J = -\int_0^{La_0} \mathrm{d}x\, w_1^*(x)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0\cos^2\left(\frac{\pi x}{a_0}\right)\right) w_2(x) \tag{1.31a}$$

and

$$U = g\int_0^{La_0} \mathrm{d}x\, w_1^*(x)w_1^*(x)w_1(x)w_1(x), \tag{1.31b}$$

which we use in the Bose–Hubbard Hamiltonian

$$\hat{H} = -J\sum_{\langle k,\ell\rangle} a_k^\dagger a_\ell + \frac{U}{2}\sum_k n_k(n_k-1). \tag{1.32}$$

Because the orbitals we have chosen are well localized on the sites of the optical lattice, we may identify each orbital with a single physical site, so terms of the form $a_k^\dagger a_\ell$ correspond to a particle hopping between sites. The notation $\sum_{\langle k,\ell\rangle}$ means summation over all pairs of neighbouring sites k and ℓ. This Hamiltonian therefore covers both periodic and open boundary conditions, depending on whether sites 1 and L are considered to be neighbouring.

We may make this model even more abstract by considering that the energy scale doesn't affect the shape of the wavefunctions. After dividing by J, we get the dimensionless Hamiltonian

$$\hat{H}/J = -\sum_{\langle k,\ell\rangle} a_k^\dagger a_\ell + \frac{U}{2J}\sum_k n_k(n_k-1) \tag{1.33}$$

that only depends on a single parameter U/J which dictates how important the interactions are relative to the tunnelling. In an experiment, the interaction strength U is often determined by the choice of atoms and the J parameter may be varied by changing the depth of the lattice.

We may consider the Hamiltonian matrix in an explicit bosonic occupation basis for some system sizes. In the simplest non-trivial case, $L = 2$ and $N = 1$, so the Hamiltonian matrix is

$$\underline{\mathbf{H}}/J = \begin{pmatrix} & -1 \\ -1 & \end{pmatrix} \tag{1.34}$$

in the basis $\{|1\,0\rangle, |0\,1\rangle\}$. There is clearly no possibility for interactions, and tunnelling is possible back and forth. With one more particle ($L = N = 2$), the basis is $\{|2\,0\rangle, |1\,1\rangle, |0\,2\rangle\}$ and the Hamiltonian matrix is

$$\underline{\mathbf{H}}/J = \begin{pmatrix} U/J & -\sqrt{2} & \\ -\sqrt{2} & & -\sqrt{2} \\ & -\sqrt{2} & U/J \end{pmatrix}. \tag{1.35}$$

1.5 Hong–Ou–Mandel effect

A 50:50 beam splitter with two input modes and two output modes (described by the operators $a^\dagger$ and $\tilde{a}^\dagger$) acting on photons may be modelled by the mapping

$$a^\dagger \to \frac{1}{\sqrt{2}}(a^\dagger + i\tilde{a}^\dagger) \qquad\qquad \tilde{a}^\dagger \to \frac{1}{\sqrt{2}}(ia^\dagger + \tilde{a}^\dagger). \tag{1.36}$$

This means that if we start with the state

$$a^\dagger |\mathrm{vac}\rangle = |1\,0\rangle, \tag{1.37}$$

application of the beam splitter results in the superposition

$$\frac{1}{\sqrt{2}}(a^\dagger + i\tilde{a}^\dagger)|\mathrm{vac}\rangle = \frac{|1\,0\rangle + i\,|0\,1\rangle}{\sqrt{2}}, \tag{1.38}$$

as we might expect.

If we start with a photon in each of the input modes ($a^\dagger\tilde{a}^\dagger$), the beam splitter gives us

$$\frac{1}{2}(a^\dagger + i\tilde{a}^\dagger)(ia^\dagger + \tilde{a}^\dagger) = \frac{i}{2}\left((a^\dagger)^2 + (\tilde{a}^\dagger)^2\right), \tag{1.39}$$

which is a superposition of states with both photons on the same side. This may be more clear in the following form:

$$a^\dagger\tilde{a}^\dagger|\mathrm{vac}\rangle = |1\,1\rangle \tag{1.40a}$$

$$\frac{i}{2}\left((a^\dagger)^2 + (\tilde{a}^\dagger)^2\right)|\mathrm{vac}\rangle = \frac{i}{2}(a^\dagger)^2|\mathrm{vac}\rangle + \frac{i}{2}(\tilde{a}^\dagger)^2|\mathrm{vac}\rangle = \frac{i}{\sqrt{2}}(|2\,0\rangle + |0\,2\rangle). \tag{1.40b}$$

The lack of any contribution from $|1\,1\rangle$ in the output state due to interference is known as the Hong–Ou–Mandel effect.

This effect may be observed in a double well, which may be modelled as a simple Bose–Hubbard system with hopping terms and no interaction terms. If two particles start on opposite sides of the well ($|1\,1\rangle$) and are allowed to tunnel back and forth, after doing so for the appropriate amount of time, they will be found in an even superposition of $|2\,0\rangle$ and $|0\,2\rangle$, with no amplitude for $|1\,1\rangle$. A parity measurement would deterministically find an even number of particles in each well. This is referred to as an "atomic beam splitter".

1.6 Spatial entanglement entropy

For a bipartite system ϱ_{AB}, we may find the reduced density operator

$$\varrho_A = \operatorname{Tr}_B \varrho_{AB}. \tag{1.41}$$

The second Rényi entropy is then given by

$$S_2(\varrho_A) = -\log\Big(\operatorname{Tr} \varrho_A^2\Big) \tag{1.42}$$

and provides a measure of entanglement between subsystems A and B. The degrees of freedom contained in A and B are arbitrary and may be, for example, particle labels or spatial regions.

For a system composed of discrete sites, we may choose to put some of them in A and the rest in B. It then makes sense to call the collection of sites found in A "region A" and likewise for B. Because these are spatial degrees of freedom, this results in a spatial entanglement entropy.

Clearly, if $\varrho = \tilde{\varrho}$, we may think of the trace $\operatorname{Tr} \varrho_A^2$ as the overlap between two copies of the same state: $\operatorname{Tr} \varrho_A \tilde{\varrho}_A$. If we define the permutation operator $\hat{\Pi}_A$ which swaps the particles in region A between the two copies, we find that

$$\begin{aligned}
\operatorname{Tr} \varrho_A \tilde{\varrho}_A &= \sum_{\mathbf{n}_A} \sum_{\tilde{\mathbf{n}}_A} \langle \mathbf{n}_A | \varrho_A | \tilde{\mathbf{n}}_A \rangle \, \langle \tilde{\mathbf{n}}_A | \tilde{\varrho}_A | \mathbf{n}_A \rangle && \text{(1.43a)} \\
&= \sum_{\mathbf{n}_A} \sum_{\mathbf{n}_B} \sum_{\tilde{\mathbf{n}}_A} \sum_{\tilde{\mathbf{n}}_B} \langle \mathbf{n}_A \, \mathbf{n}_B | \varrho | \tilde{\mathbf{n}}_A \, \mathbf{n}_B \rangle \, \langle \tilde{\mathbf{n}}_A \, \tilde{\mathbf{n}}_B | \tilde{\varrho} | \mathbf{n}_A \, \tilde{\mathbf{n}}_B \rangle && \text{(1.43b)} \\
&= \sum_{\mathbf{n}_A} \sum_{\mathbf{n}_B} \sum_{\tilde{\mathbf{n}}_A} \sum_{\tilde{\mathbf{n}}_B} \langle \mathbf{n}_A \, \mathbf{n}_B \, \tilde{\mathbf{n}}_A \, \tilde{\mathbf{n}}_B | \varrho \otimes \tilde{\varrho} | \tilde{\mathbf{n}}_A \, \mathbf{n}_B \, \mathbf{n}_A \, \tilde{\mathbf{n}}_B \rangle && \text{(1.43c)} \\
&= \sum_{\mathbf{n}_A} \sum_{\mathbf{n}_B} \sum_{\tilde{\mathbf{n}}_A} \sum_{\tilde{\mathbf{n}}_B} \langle \mathbf{n}_A \, \mathbf{n}_B \, \tilde{\mathbf{n}}_A \, \tilde{\mathbf{n}}_B | (\varrho \otimes \tilde{\varrho}) \hat{\Pi}_A | \mathbf{n}_A \, \mathbf{n}_B \, \tilde{\mathbf{n}}_A \, \tilde{\mathbf{n}}_B \rangle && \text{(1.43d)} \\
&= \operatorname{Tr}\Big[(\varrho \otimes \tilde{\varrho}) \hat{\Pi}_A \Big]. && \text{(1.43e)}
\end{aligned}$$

Thus, to find the trace for the entropy, it is sufficient to find the expectation value of the permutation operator in a replicated system.

2 Entanglement experiment

In [Nature 528, 77 (2015)][‡], Islam *et al.* experimentally measure the entanglement entropy of a lattice of ultracold ^{87}Rb atoms using two copies (also: replicas, twins) of the system. Their protocol is roughly as follows:

1. Create a 2×4 plaquette of atoms (2 copies in the y direction of a 4-atom system in the x direction) at unit density in a very deep lattice ($\approx 50\, E_\mathrm{R}$).

[‡] doi:10.1038/nature15750

2. Adiabatically lower the lattice in x to the desired depth to set U/J ($26\,E_\mathrm{R}$ to $3\,E_\mathrm{R}$, which is $U/J \approx 100$ to $U/J \approx 1$).
3. Raise the lattice in x to prevent tunnelling, freezing the system ($45\,E_\mathrm{R}$).
4. Lower the lattice in y ($2\,E_\mathrm{R}$).
5. Wait for the beam splitter operation to take place.
6. Raise the lattice in y to prevent tunnelling, freezing the system ($45\,E_\mathrm{R}$).
7. Use fluorescence imaging to get the parity of the occupation at each site.

The preparation steps result in two non-interacting copies of the same system, whose density operators we will call ϱ and $\tilde{\varrho}$. These may be considered together as $\varrho \otimes \tilde{\varrho}$. The subsequent beam splitter operation $\hat{U}^\mathrm{BS}$ results in the state $\hat{U}^\mathrm{BS}(\varrho \otimes \tilde{\varrho})(\hat{U}^\mathrm{BS})^\dagger$. The averaged parity measurement on site k then amounts to the expectation value of $\hat{P}_k = (-1)^{n_k}$:

$$\langle \hat{P}_k \rangle = \mathrm{Tr}\Big[\hat{U}^\mathrm{BS}(\varrho \otimes \tilde{\varrho})(\hat{U}^\mathrm{BS})^\dagger \hat{P}_k\Big], \tag{2.1}$$

which results in -1 for an odd number of particles and 1 for an even number of particles (but may be an altogether different value if the parity at the site is not definite). In general, it is possible to perform measurements of the form

$$\langle \hat{f} \rangle = \mathrm{Tr}\Big[\hat{U}^\mathrm{BS}(\varrho \otimes \tilde{\varrho})(\hat{U}^\mathrm{BS})^\dagger f(\hat{P}_1, \ldots, \hat{P}_L, \hat{P}_{\tilde{1}}, \ldots, \hat{P}_{\tilde{L}})\Big] \tag{2.2}$$

for an arbitrary function f. For example,

$$\langle \hat{P}_1 \hat{P}_{\tilde{2}} \rangle = \mathrm{Tr}\Big[\hat{U}^\mathrm{BS}(\varrho \otimes \tilde{\varrho})(\hat{U}^\mathrm{BS})^\dagger \hat{P}_1 \hat{P}_{\tilde{2}}\Big] \tag{2.3}$$

2.1 Expectation of permutation operator

The site-local permutation operator $\hat{\Pi}$ swaps the particles in the two replicas at a site pair:

$$\hat{\Pi}\,|n\,\tilde{n}\rangle = |\tilde{n}\,n\rangle\,. \tag{2.4}$$

Another way to write this is as

$$a^\dagger \to \tilde{a}^\dagger \qquad\qquad \tilde{a}^\dagger \to a^\dagger. \tag{2.5}$$

Consider the operator $\hat{U}^\mathrm{FT}$ (FT stands for Fourier transform) acting on a single pair of sites which maps

$$a^\dagger \to \frac{a^\dagger + \tilde{a}^\dagger}{\sqrt{2}} \qquad\qquad \tilde{a}^\dagger \to \frac{a^\dagger - \tilde{a}^\dagger}{\sqrt{2}}. \tag{2.6}$$

This operator is its own inverse. Note that the beam splitter operation is related to this by

$$\hat{U}^\mathrm{BS} = \hat{\Theta}\hat{U}^\mathrm{FT}\hat{\Theta}, \tag{2.7}$$

where $\hat{\Theta}$ applies a relative phase shift of $\pi/2$:

$$a^\dagger \to a^\dagger \qquad\qquad \tilde{a}^\dagger \to e^{i\pi/2}\tilde{a}^\dagger. \tag{2.8}$$

Obviously,

$$\hat{U}^\mathrm{FT}(\hat{U}^\mathrm{FT})^\dagger = \hat{\mathbb{1}}. \tag{2.9}$$

Less obviously,

$$\hat{U}^{\mathrm{FT}}\hat{\Pi}(\hat{U}^{\mathrm{FT}})^\dagger = (-1)^{\tilde{n}}. \tag{2.10}$$

This is easy to show. Starting from the above definition for $\hat{U}^{\mathrm{FT}}$, we see that $\hat{\Pi}(\hat{U}^{\mathrm{FT}})^\dagger$ maps

$$a^\dagger \to \frac{a^\dagger + \tilde{a}^\dagger}{\sqrt{2}} \qquad\qquad \tilde{a}^\dagger \to -\frac{a^\dagger - \tilde{a}^\dagger}{\sqrt{2}} \tag{2.11}$$

and $\hat{U}^{\mathrm{FT}}\hat{\Pi}(\hat{U}^{\mathrm{FT}})^\dagger$ maps

$$a^\dagger \to a^\dagger \qquad\qquad \tilde{a}^\dagger \to -\tilde{a}^\dagger, \tag{2.12}$$

which is the same as the action of $(-1)^{\tilde{n}}$:

$$\hat{U}^{\mathrm{FT}}\hat{\Pi}(\hat{U}^{\mathrm{FT}})^\dagger \left|n\,\tilde{n}\right\rangle = \hat{U}^{\mathrm{FT}}\hat{\Pi}(\hat{U}^{\mathrm{FT}})^\dagger \frac{(a^\dagger)^n(\tilde{a}^\dagger)^{\tilde{n}}}{\sqrt{n!\tilde{n}!}}\left|\mathrm{vac}\right\rangle \tag{2.13a}$$

$$= \frac{(a^\dagger)^n(-\tilde{a}^\dagger)^{\tilde{n}}}{\sqrt{n!\tilde{n}!}}\left|\mathrm{vac}\right\rangle \tag{2.13b}$$

$$= (-1)^{\tilde{n}}\frac{(a^\dagger)^n(\tilde{a}^\dagger)^{\tilde{n}}}{\sqrt{n!\tilde{n}!}}\left|\mathrm{vac}\right\rangle \tag{2.13c}$$

$$= (-1)^{\tilde{n}}\left|n\,\tilde{n}\right\rangle. \tag{2.13d}$$

The operator

$$\hat{P}_{\tilde{A}} = \prod_{k\in A}\hat{P}_{\tilde{k}} = \prod_{k\in A}(-1)^{\tilde{n}_k} \tag{2.14}$$

gives the total parity of particle number in region $\tilde{A}$. Because all the full system operators are tensor products of one-site operators, above argument is trivially extended to all sites, and we find that

$$\hat{U}^{\mathrm{FT}}\hat{\Pi}_A(\hat{U}^{\mathrm{FT}})^\dagger = \hat{P}_{\tilde{A}} \tag{2.15a}$$

or

$$(\hat{U}^{\mathrm{FT}})^\dagger\hat{P}_{\tilde{A}}\hat{U}^{\mathrm{FT}} = \hat{\Pi}_A. \tag{2.15b}$$

Thus, measuring the average parity in region $\tilde{A}$ is equivalent to finding

$$\langle\hat{P}_{\tilde{A}}\rangle = \mathrm{Tr}\Big[\hat{U}^{\mathrm{BS}}(\varrho\otimes\tilde{\varrho})(\hat{U}^{\mathrm{BS}})^\dagger\hat{P}_{\tilde{A}}\Big] \tag{2.16a}$$

$$= \mathrm{Tr}\Big[\hat{\Theta}\hat{U}^{\mathrm{FT}}\hat{\Theta}(\varrho\otimes\tilde{\varrho})\hat{\Theta}^\dagger(\hat{U}^{\mathrm{FT}})^\dagger\hat{\Theta}^\dagger\hat{P}_{\tilde{A}}\Big] \tag{2.16b}$$

$$= \mathrm{Tr}\Big[\hat{\Theta}(\varrho\otimes\tilde{\varrho})\hat{\Theta}^\dagger(\hat{U}^{\mathrm{FT}})^\dagger\hat{\Theta}^\dagger\hat{P}_{\tilde{A}}\hat{\Theta}\hat{U}^{\mathrm{FT}}\Big]. \tag{2.16c}$$

The parity measurement is insensitive to relative phases and the two copies of the system have no definite phase relation, so we are left with just

$$\langle\hat{P}_{\tilde{A}}\rangle = \mathrm{Tr}\Big[(\varrho\otimes\tilde{\varrho})(\hat{U}^{\mathrm{FT}})^\dagger\hat{P}_{\tilde{A}}\hat{U}^{\mathrm{FT}}\Big] \tag{2.17a}$$

$$= \mathrm{Tr}\Big[(\varrho\otimes\tilde{\varrho})\hat{\Pi}_A\Big]. \tag{2.17b}$$

Since the two copies are identical, it does not matter which one we use for the parity measurement, and we find that

$$\langle\hat{P}_A\rangle = \mathrm{Tr}\,\varrho_A^2, \tag{2.18}$$

meaning that parity measurements are sufficient to find the entanglement entropy.

3 Simulating experimental error

We may make an attempt at modelling the results of the paper using a simple Bose–Hubbard Hamiltonian, whose ground state we find using an exact diagonalization approach. This ground state may then be manipulated arbitrarily, including finding its entanglement entropy. However, this turns out to be insufficient.

The paper provides a discussion on experimental sources of error. In particular, they provide data for loading error (where the wrong number of particles is loaded into the initial plaquette) and for contrast reduction in the beam splitter.

3.1 Loading error

3.1.1 Fitting

In the preparation step, the lattice is sufficiently deep that double occupation of sites is extremely unlikely. Thus, the authors claim that all sites with even parity immediately after preparation should be empty. They provide the following statistics:

n atoms	loading probability $P(n)$
8	0.66(1)
7	0.27(1)
6	0.052(4)

If we expect a total of N particles, but assume that the probability of a hole at any particular site is p, we may use the binomial distribution to model the total number of particles present:

$$P(n) = \binom{N}{n}(1-p)^n p^{N-n}. \tag{3.1}$$

For the data presented in the paper, we may perform a least-squares analysis with a simple cost function of the form

$$J(p) = \frac{1}{2}\sum_{n=6}^{8}(P(n) - y_n)^2, \tag{3.2}$$

which has an extremum around $p = 0.0497219$. We interpret this as a probability of approximately 5 % for a hole at any site.

These holes will result in finding the incorrect ground states in addition to the correct one. We will label these $|\Psi_0\rangle$, $|\Psi_1\rangle$, …, $|\Psi_N\rangle$ and combine them with the appropriate statistical weights into the effective mixed state generated in the experiment:

$$\varrho = \sum_{n=0}^{N}\binom{N}{n}(1-p)^n p^{N-n}\,|\Psi_n\rangle\langle\Psi_n|\,. \tag{3.3}$$

Computationally, we must be careful to express these wavefunctions in their respective bases: $\mathcal{B}(L,0)$, $\mathcal{B}(L,1)$, …, $\mathcal{B}(L,N)$. We will refer to the union of all these bases as

$$\overline{\mathcal{B}}(L,N) = \bigcup_{n=0}^{N}\mathcal{B}(L,n), \tag{3.4}$$

with

$$\left|\overline{\mathcal{B}}(L,N)\right| = \sum_{n=0}^{N} \binom{n+L-1}{L-1} = \binom{N+L}{L}. \tag{3.5}$$

Conveniently, ϱ is block diagonal, since each ground state wavefunction lives in its own subspace. Since the partial trace operation must remove the same number of particles on either side, ϱ_A also can't couple states with different particle number and must be block diagonal.

3.2 Beam splitter contrast reduction

3.2.1 Derivation

It is claimed in the paper that the amplitude of the Rabi oscillations of a single particle in the beam splitter double well are reduced by about 5 %. Based on the given plot, it appears that the time evolution due to the beam splitter is unitary, at least for short times, which means that there is a Hamiltonian which generates the dynamics. In order to model the Rabi oscillations, we only need a two-level system, so we can do everything analytically.

A two-level system with the simple Hamiltonian

$$\underline{\mathbf{H}} = J \begin{pmatrix} & -1 \\ -1 & \end{pmatrix}, \tag{3.6}$$

which only has tunnelling between the levels, exhibits Rabi oscillations of the form

$$\left| \langle 1|\hat{U}(t)|0\rangle \right|^2 = \sin^2\!\left(\frac{Jt}{\hbar}\right), \tag{3.7}$$

where $\hat{U}(t) = e^{-\frac{i\hat{H}t}{\hbar}}$ is the time propagator. What sort of Hamiltonian gives us Rabi oscillations of the form

$$\left| \langle 1|\hat{U}(t)|0\rangle \right|^2 = (1-\delta)^2 \sin^2\!\left(\frac{Jt}{\hbar}\right), \tag{3.8}$$

with reduced amplitude?

In a two-dimensional Hilbert space, given a general normalized state

$$|A\rangle = \alpha\,|0\rangle + e^{i\theta}\sqrt{1-\alpha^2}\,|1\rangle \tag{3.9}$$

(with $\theta \in [0, 2\pi)$ and $\alpha \in [0, 1]$), there is a unique (up to global phase) state

$$|B\rangle = \sqrt{1-\alpha^2}\,|0\rangle - e^{i\theta}\alpha\,|1\rangle\,. \tag{3.10}$$

that is orthogonal to $|A\rangle$. In the most general case, we have a Hamiltonian with real (and possibly equal) eigenvalues A and B, and which is diagonal in the orthonormal basis $\{|A\rangle, |B\rangle\}$. Since

$$|0\rangle = \alpha\,|A\rangle + \sqrt{1-\alpha^2}\,|B\rangle \tag{3.11a}$$

$$|1\rangle = e^{-i\theta}\sqrt{1-\alpha^2}\,|A\rangle - e^{-i\theta}\alpha\,|B\rangle\,, \tag{3.11b}$$

we have

$$\hat{U}(t)\,|0\rangle = \left(e^{-\frac{iAt}{\hbar}}\alpha^2 + e^{-\frac{iBt}{\hbar}}(1-\alpha^2)\right)|0\rangle + e^{i\theta}\alpha\sqrt{1-\alpha^2}\left(e^{-\frac{iAt}{\hbar}} - e^{-\frac{iBt}{\hbar}}\right)|1\rangle\,. \tag{3.12}$$

It is convenient to introduce $E = (B+A)/2$ and $\Delta E = (B-A)/2$ (so that $A = E - \Delta E$ and $B = E + \Delta E$), using which we get

$$\left| \langle 1|\hat{U}(t)|0\rangle \right|^2 = 4\alpha^2(1-\alpha^2)\sin^2\left(\frac{\Delta E t}{\hbar}\right). \tag{3.13}$$

Without loss of generality, we require $A \leq B$, so $0 \leq \Delta E$. To get the desired oscillation frequency, we must maintain an energy splitting of $2J$. The phase θ doesn't matter, but to reduce the amplitude to $(1-\delta)^2$, we must have

$$(1-\delta)^2 = 4\alpha^2(1-\alpha^2), \tag{3.14}$$

so

$$\alpha = \sqrt{\frac{1 \pm \sqrt{\delta(2-\delta)}}{2}}. \tag{3.15}$$

After some tedious manipulations, we find that the necessary Hamiltonian is

$$\underline{\mathbf{H}} = \begin{pmatrix} E \mp \sqrt{\delta(2-\delta)}\Delta E & -e^{-i\theta}(1-\delta)\Delta E \\ -e^{i\theta}(1-\delta)\Delta E & E \pm \sqrt{\delta(2-\delta)}\Delta E \end{pmatrix}. \tag{3.16}$$

That has too many moving pieces for our needs, so we simplify it to just

$$\underline{\mathbf{H}} = J \begin{pmatrix} -\sqrt{\delta(2-\delta)} & -(1-\delta) \\ -(1-\delta) & \sqrt{\delta(2-\delta)} \end{pmatrix}. \tag{3.17}$$

This may be written in second-quantized form as

$$\hat{H}/J = -(1-\delta)(a^\dagger \tilde{a} + \tilde{a}^\dagger a) - \sqrt{\delta(2-\delta)}(n - \tilde{n}). \tag{3.18}$$

Of course, if there are multiple particles, they will interact, so we must also include the interaction terms:

$$\hat{H}/J = -(1-\delta)(a^\dagger \tilde{a} + \tilde{a}^\dagger a) + \frac{U}{2J}\left(n(n-1) + \tilde{n}(\tilde{n}-1)\right) - \sqrt{\delta(2-\delta)}(n - \tilde{n}). \tag{3.19}$$

We call this the reduced contrast beam splitter Hamiltonian.

3.2.2 Implementation

To implement the beam splitter operation and parity measurement, we have to work in an enlarged basis. Each replica exists in $\overline{\mathcal{B}}(L, N)$, but both replicas together have twice as many sites and up to twice as many particles, so the relevant basis is $\overline{\mathcal{B}}(2L, 2N)$. We will refer to states in this basis as $|\mathbf{N}\rangle$.

Our goal is to find

$$\langle \hat{P}_A \rangle = \mathrm{Tr}\Big[\hat{U}^{\mathrm{BS}}(\varrho \otimes \tilde{\varrho})(\hat{U}^{\mathrm{BS}})^\dagger \hat{P}_A\Big], \tag{3.20}$$

which we may do explicitly in the replicated basis:

$$\langle \hat{P}_A \rangle = \sum_{\mathbf{M},\mathbf{N}} \langle \mathbf{M}|\hat{U}^{\mathrm{BS}}(\varrho \otimes \tilde{\varrho})(\hat{U}^{\mathrm{BS}})^\dagger|\mathbf{N}\rangle \ \langle \mathbf{N}|\hat{P}_A|\mathbf{M}\rangle \tag{3.21a}$$

$$= \sum_{\mathbf{N}} (-1)^{\sum \mathbf{n}_A} \langle \mathbf{N}|\hat{U}^{\mathrm{BS}}(\varrho \otimes \tilde{\varrho})(\hat{U}^{\mathrm{BS}})^\dagger|\mathbf{N}\rangle\,. \tag{3.21b}$$

Since

$$\mathrm{Tr}\Big[\hat{U}^{\mathrm{BS}}(\varrho\otimes\tilde{\varrho})(\hat{U}^{\mathrm{BS}})^\dagger\Big]=\sum_{\mathbf{N}}\langle\mathbf{N}|\hat{U}^{\mathrm{BS}}(\varrho\otimes\tilde{\varrho})(\hat{U}^{\mathrm{BS}})^\dagger|\mathbf{N}\rangle=1, \tag{3.22}$$

we find that

$$\langle\hat{P}_A\rangle=1-2\sum_{\substack{\mathbf{N}\\ \text{odd number of particles in }\mathbf{n}_A}}\langle\mathbf{N}|\hat{U}^{\mathrm{BS}}(\varrho\otimes\tilde{\varrho})(\hat{U}^{\mathrm{BS}})^\dagger|\mathbf{N}\rangle\,. \tag{3.23}$$

This is extremely convenient, since we would like to avoid constructing matrices in this basis explicitly if we can avoid it. Even for a small system with $L=N=4$, the basis has 12 870 states, which leads to complex-valued matrices that are about 2.5 GB. That's not unreasonable, but it is quite wasteful and scales very poorly.

Recall that the mixed states ϱ are block diagonal, so we have

$$\langle\mathbf{m}|\varrho|\mathbf{n}\rangle=\binom{N}{\sum\mathbf{n}}(1-p)^{\sum\mathbf{n}}p^{N-\sum\mathbf{n}}\left\langle\mathbf{m}\middle|\Psi_{\sum\mathbf{n}}\right\rangle\left\langle\Psi_{\sum\mathbf{n}}\middle|\mathbf{n}\right\rangle\delta_{\sum\mathbf{m},\sum\mathbf{n}}. \tag{3.24}$$

Since $\varrho\otimes\tilde{\varrho}$ acts on a subspace of the total space spanned by the replicated basis, we also have

$$\langle\mathbf{M}|\varrho\otimes\tilde{\varrho}|\mathbf{N}\rangle=\begin{cases}\langle\mathbf{m}\,\tilde{\mathbf{m}}|\varrho\otimes\tilde{\varrho}|\mathbf{n}\,\tilde{\mathbf{n}}\rangle & \text{if } \sum\mathbf{n},\sum\tilde{\mathbf{n}}\le N\\ 0 & \text{otherwise}\end{cases}. \tag{3.25}$$

For the beam splitter, we need to find the matrix elements

$$\langle\mathbf{M}|\hat{U}(t)|\mathbf{N}\rangle=\prod_{k=1}^{L}\langle m_k\,\tilde{m}_k|e^{-\frac{i\hat{H}_k t}{\hbar}}|n_k\,\tilde{n}_k\rangle\,, \tag{3.26}$$

where $\hat{H}_k$ is the reduced contrast beam splitter Hamiltonian acting on site k. This simple structure is possible because the operator acts independently on each site:

$$\hat{U}(t)=\bigotimes_{k=1}^{L}\hat{U}_k(t)=\bigotimes_{k=1}^{L}e^{-\frac{i\hat{H}_k t}{\hbar}}. \tag{3.27}$$

Since the Hamiltonian is the same for all sites, we only need to construct the $(2N+1)^2\times(2N+1)^2$ matrix once in the simple product basis $\{|n\,\tilde{n}\rangle\}_{n=0,\tilde{n}=0}^{2N,2N}$ and diagonalize it.

Putting everything together and rearranging, we find

$$\langle\mathbf{N}|\hat{U}^{\mathrm{BS}}(\varrho\otimes\tilde{\varrho})(\hat{U}^{\mathrm{BS}})^\dagger|\mathbf{N}\rangle=\sum_{n'=0}^{N}\sum_{\tilde{n}'=0}^{N}C_{pn'}C_{p\tilde{n}'}\left|\sum_{\mathbf{n}'}\sum_{\tilde{\mathbf{n}}'}\left\langle\mathbf{n}\,\tilde{\mathbf{n}}\middle|\hat{U}^{\mathrm{BS}}\middle|\mathbf{n}'\,\tilde{\mathbf{n}}'\right\rangle\left\langle\mathbf{n}'\middle|\Psi_{n'}\right\rangle\left\langle\tilde{\mathbf{n}}'\middle|\Psi_{\tilde{n}'}\right\rangle\right|^2, \tag{3.28}$$

where

$$C_{pn}=\binom{N}{n}(1-p)^n p^{N-n}. \tag{3.29}$$

3.3 Example code

The following is a Julia implementation of the entropy calculation using the error models outlined above. It is not a complete program, but it captures the relevant aspects.

```
# Construct the one-site beam splitter.
A = 0.5*Ut_bs
B = sqrt(delta*(2-delta))
C = (1-delta)
bs_H = zeros((2N+1)^2, (2N+1)^2)
# For this, we work in the product basis {0, ..., 2N} x {0, ..., 2N}.
for m=0:2N
    for mp=0:2N
        i = 1+m*(2N+1)+mp
        for n=0:2N
            for np=0:2N
                j = 1+n*(2N+1)+np
                if m == n && mp == np
                    bs_H[i, j] += A*(n*(n-1)+np*(np-1))
                    bs_H[i, j] -= B*(n-np)
                elseif m == n+1 && mp == np-1
                    bs_H[i, j] -= C*sqrt((n+1)*np)
                elseif m == n-1 && mp == np+1
                    bs_H[i, j] -= C*sqrt(n*(np+1))
                end
            end
        end
    end
end
bs_op = expm(-im * bs_H * time)

bases = [Szbasis(M, n) for n in 0:N]
big_bases = [Szbasis(2M, n) for n in 0:2N]

# Calculate the overlap.
overlap = 1.
for big_basis in big_bases
    for v in big_basis
        # First replica.
        v1 = v[1:2:end]
        sum(v1[1:Asize]) % 2 != 0 || continue
        # Second replica.
        v2 = v[2:2:end]

        for n1 in 0:N
            C1 = binomial(N, n1) * (1-p)^n1 * p^(N-n1)
            for n2 in 0:N
                C2 = binomial(N, n2) * (1-p)^n2 * p^(N-n2)

                coef = 0.
                for (i, w1) in enumerate(bases[n1+1])
                    for (j, w2) in enumerate(bases[n2+1])
                        k = 1.
                        for site=1:M
                            x = 1+v1[site]*(2N+1)+v2[site]
                            y = 1+w1[site]*(2N+1)+w2[site]
                            k *= bs_op[x, y]
                        end
                        coef += k*wfs[n1+1][i]*wfs[n2+1][j]
                    end
                end

                overlap -= 2*C1*C2*abs2(coef)
            end
        end
    end
end

s2_spatial = -log(overlap)
```