

The Role of Mutually Attractive Interaction Between Neutral Atoms: A Split-Operator Method Analysis

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1 Abstract

An optical lattice is a crystal of light formed from counter-propagating laser beams in which one can hold and control a nearly perfect array of atoms floating in a vacuum chamber. By changing the shape of the optical lattice, it is possible to split the wavefunctions of individual atoms so that they are put into a quantum superposition of two different locations within the optical lattice at the same time. When there are two atoms at the same location in the optical lattice, their mutual interaction will influence the wave function splitting process. This physics has been studied for pairs of repelling atoms, but I have shown it is possible to create new types of quantum states of matter from atoms that attract each other, a possibility not previously explored. I have designed a computer simulation based on the split-operator method to model the splitting of such pairs of atoms and have demonstrated that this interaction can result in two atom NOON-state superpositions.

2 Background Information

An optical lattice system is an experimental setup used to study the fundamental quantum properties of atoms and multi-atom systems. Such a setup consists of an evacuated ultra-cold region (on the order of microkelvins above absolute zero) intersected by standing waves of laser light. Lasers are orthogonally directed and reflected back and forth through the field creating three dimensional potential wells that act to hold neutral atoms in a regularly spaced grid that is easy to profile mathematically. Typical grid spacings are about 400 nm, half a wavelength of the light typically emitted by the laser. Because these atoms have little thermal energy, one can assume each is in a ground state energy configuration, and thus exists in the ground state wavefunction consistent with the profile of the potential well.

By manipulating the wavelength of the lasers forming the lattice, an experimenter can change the size and shape of the potential wells. Wells may be split from a single trap per site to a double well with two traps per site. [1] Done slowly, this process is adiabatic. Further these splittings and merging are reversible and may be used to incite interactions between atoms in adjacent wells, so one may probe the results of such interaction between atoms. It has been previously shown that when double well splitting in one dimension is performed while an atom is trapped in the well, the atom's wavefunction is split into a superposition – the particle is localized in the left sub-well, $-x_0$ and in the right sub-well x_0 . Henceforth, I will denote this state by $|1, 0\rangle + |0, 1\rangle$ where the general state $|a, b\rangle$ represents a atoms in the left sub-well and b atoms in right sub-well. Given the minimum of the original well is centered around the origin and a symmetrical splitting, such a state would display $\langle x \rangle = 0$ upon measurement, with $x = -x_0$ with probability $P = 0.50$ and $x = x_0$ with probability $P = 0.50$. Here, x_0 depends on the laser's wavelength, and the axis of the splitting is x .

3 Research Thrust

A NOON state is a superposition of an arbitrary number of atoms, $|N, 0\rangle + |0, N\rangle$. Such a state may represent a macroscopic superposition, the implications of which are often discussed and debated. The goal of this research is to create a two atom NOON state, i.e. $|2, 0\rangle + |0, 2\rangle$. The theory about how to do this not yet developed, but it is understood that the inter-atomic interaction must play a role. Suppose one simultaneously loads two atoms into the original symmetrically splitting potential well site. Throughout this splitting, the two atoms have a chance to interact. We hypothesize that if the atoms feel an attractive force, the wavefunctions

of the atoms will not split independently into $|1, 0\rangle + |0, 1\rangle \otimes |1, 0\rangle + |0, 1\rangle$; rather the result may be instead $|2, 0\rangle + |0, 2\rangle$. The creation of such a state would be the first step toward the creation of a $|N, 0\rangle + |0, N\rangle$ state.

4 Simulation

I used a computer simulation to construct a model of the time-evolution of two atoms in a splitting potential well. Solving for the evolution of a wavefunction in a time dependent potential requires a different approach than is sufficient for solving the case of a static potential. Iteratively calculating the Hamiltonian at each time step and solving the Schrödinger equation is computationally intensive and proves prohibitive. Instead, another general method called the split-operator method, allows for more efficient time evolution.[2] This technique involves first solving for the initial state of the system by solving the time independent Schrödinger equation at $t = 0$ and $V(\vec{r}, 0)$. To do this, one must first construct the two particle Hamiltonian operator and solve the resulting differential equation for the eigenfunctions of $\hat{\mathcal{H}}$. The conventional Hamiltonian operator is then transformed mathematically such that time evolution becomes unitary rotation of the state within the Hilbert space by kinetic and potential energy evolution operators.[3]

4.1 Construct the Two-Particle Hamiltonian

The Hamiltonian Operator is defined like the classical Hamiltonian, $\mathcal{H} = K + V$, but with canonical substitutions made for the elements of K and V , such that $\hat{\mathcal{H}} = \hat{K} + \hat{V}$.

4.1.1 The Kinetic Energy Operators

Each atom has a kinetic energy operator defined by $\frac{\hat{p}_i^2}{2m_i}$ where $\hat{p}_i \rightarrow \frac{\hbar}{i} \frac{\partial}{\partial x_i}$ and m_i is the mass of atom i . This makes the kinetic energy operator for two atoms

$$\hat{K} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2}. \quad (1)$$

4.1.2 The Potential Energy Operator

Any potential with a minimum at the origin, expanded around the origin, may be approximated by a harmonic oscillator. First expand the 1D potential in a Taylor polynomial series

$$V(x, t) = V(0, t) + \frac{V'(x, t)}{1!}x + \frac{V''(x, t)}{2!}x^2 + \frac{V^{(3)}(x, t)}{3!}x^3 \dots \quad (2)$$

The linear term, $(V'(x, t)x)/1!$ disappears because $V'(x, t) = 0$ at any minimum. The constant level of potential energy is arbitrary, so we may also discard $V(0, t)$. This leaves

$$V(x, t) = \frac{V''(x, t)}{2!}x^2 + \frac{V^{(3)}(x, t)}{3!}x^3 \dots \quad (3)$$

with the behavior of the well dominated by the first term. The approximation then involves ignoring these higher order terms so that

$$V(x, t) = \frac{V''(x, t)}{2!}x^2 = \frac{1}{2}kx_i^2 \quad (4)$$

is the potential of the well and is of the form of the classical 1D harmonic oscillator with uniform restoring force. In the absence of interpartical interaction, this would make the potential energy operator for both atoms

$$\hat{V}(x, t) = \frac{1}{2}kx_1^2 + \frac{1}{2}kx_2^2 \quad (5)$$

I will return to add interaction potential to potential energy operator after explaining the Split Operator Algorithm.

4.1.3 Hamiltonian Operator

Adding these pieces together, we arrive at the Hamiltonian Operator for the two atoms,

$$\hat{\mathcal{H}} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + \frac{1}{2}kx_1^2 + \frac{1}{2}kx_2^2 \quad (6)$$

Pausing for a moment, we notice this operator is identical in form to the Hamiltonian Operator for one atom in a 2D harmonic oscillator; subscripts 1 and 2 would represent two arbitrary cartesian coordinates instead of delineating separate atoms.

4.2 Solve the Schrödinger Equation

Solving the time independent Schrödinger equation consistent with the above Hamiltonian operator amounts to solving the following equation:

$$\left(\frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + \frac{1}{2}kx_1^2 + \frac{1}{2}kx_2^2 \right) \psi_n = E_n \psi_n \quad (7)$$

where E_n is the energy eigenvalue of the n^{th} stationary state. This is a separable partial differential equation with a completely understood set of eigenfunctions and eigenvalues. The joint wavefunction solution to the system of two identical 1D particles in a harmonic oscillator is identical in form to the solution to one particle in a two-dimensional well, namely

$$\psi_n(x_1, x_2) = \sqrt{\frac{1}{2\pi}} e^{-\left(\frac{x_1^2}{2} + \frac{x_2^2}{2}\right)} \quad (8)$$

with canonical natural unit substitution $\hbar = m_i = k = 1$. One may derive these solutions by either series recursion or by the raising and lowering operator method of Dirac. This is the only time during the implementation of the algorithm when the Schrödinger equation must be solved. Henceforth, all time evolution is performed by multiplication of the state by unitary evolution operators.

4.3 Create the Unitary Evolution Operators

We derive the Unitary Evolution Operators through the following argumentation. Given a one dimensional state of a single particle, $\Psi(x, t)$, the wavefunction at a later time, $t + dt$, is given by

$$\Psi(x, t + dt) = \Psi(x, t) + d\Psi(x, t) \quad (9)$$

where $d\Psi(x, t) = f(x, t)dt$. This is correct in the limit that $dt \rightarrow 0$; otherwise, errors compound by $O(dt)$ per timestep.

Rewriting the Time Dependent Schrödinger Equation in terms of these differentials gives

$$i\hbar \left[\frac{\Psi(x, t + dt) - \Psi(x, t)}{dt} \right] = \hat{\mathcal{H}}\Psi(x, t). \quad (10)$$

Rearranging this equation gives

$$\Psi(x, t + dt) = \Psi(x, t) + \frac{-i\hat{\mathcal{H}}}{\hbar}\Psi(x, t)dt = \Psi(x, t) + d\Psi. \quad (11)$$

Then,

$$d\Psi = \left[\frac{-i\hat{\mathcal{H}}}{\hbar}dt \right] \Psi(x, t) \quad (12)$$

or

$$\frac{d\Psi}{\Psi} = \frac{-i\hat{\mathcal{H}}}{\hbar}dt. \quad (13)$$

Solving this differential equation by integrating back via

$$\int_{\Psi_i}^{\Psi_f} \frac{d\Psi}{\Psi} = \int_{t_i}^{t_f} \frac{-i\hat{\mathcal{H}}}{\hbar}dt \quad (14)$$

gives

$$\frac{\Psi_i}{\Psi_f} = e^{\frac{-i\hat{\mathcal{H}}}{\hbar}(t_f - t_i)} \quad (15)$$

Noting that

$$\Psi_f = e^{\frac{-i\hat{\mathcal{H}}}{\hbar}(t_f - t_i)}\Psi_i \quad (16)$$

we see that the exponential acts to evolve the state through time, taking $\Psi_i \rightarrow \Psi_f$. If timesteps are small but not infinitesimal, we can take $t_f - t_i = \Delta t$ and the Unitary Time Evolution Operator becomes

$$\hat{U} = e^{\frac{-i\hat{\mathcal{H}}}{\hbar}\Delta t} \quad (17)$$

4.4 Applying the Evolution Operators

Generally, the state of a quantum system, $|\Psi\rangle$ can be represented by an N -dimensional vector in Hilbert space, the infinite dimensional vector space of square integrable functions, \mathbb{L}^2 . Time evolution of this state can be thought of as a rotation of this vector within the space. Applying the previously derived operator accomplishes this rotation.

This operator may be applied to an arbitrary function f by substituting $-i\hat{\mathcal{H}}\Delta t/\hbar$ for x in the Taylor expansion of e^x around $x = 0$, yielding

$$e^{\frac{-i\hat{\mathcal{H}}}{\hbar}\Delta t} = 1 - \frac{-i\hat{\mathcal{H}}}{\hbar}\Delta t + \frac{(\frac{-i\hat{\mathcal{H}}\Delta t}{\hbar})^2}{2!} + \frac{(\frac{-i\hat{\mathcal{H}}\Delta t}{\hbar})^3}{3!} \dots \quad (18)$$

It is also easy to generalize the evolution to an arbitray number of timesteps N by

$$\Psi(x, t + n\Delta t) = e^{\frac{-i\hat{\mathcal{H}}_n}{\hbar}\Delta t} \dots e^{\frac{-i\hat{\mathcal{H}}_1}{\hbar}\Delta t}\Psi(x, t). \quad (19)$$

4.4.1 Splitting the Operator

In the previous section, it was shown that the Unitary Evolution Operator, $\hat{U} = \exp[\frac{-i\hat{H}}{\hbar}\Delta t]$, evolves an arbitrary quantum state through time. Using the properties of exponentials, we can separate the kinetic and potential energy operator components of the hamiltonian by

$$\hat{U} = e^{\frac{-i}{\hbar}(\frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m})\Delta t} e^{\frac{-i}{\hbar}\hat{V}(x,t)\Delta t} + O(dt^2) \quad (20)$$

where $O(dt^2)$ errors arise because \hat{p} and \hat{x} do not commute. It has been shown that splitting the operator one step further, to

$$\hat{U} = e^{\frac{-i}{\hbar}(\frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m})\frac{\Delta t}{2}} e^{\frac{-i}{\hbar}\hat{V}(x,t)\Delta t} e^{\frac{-i}{\hbar}(\frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m})\frac{\Delta t}{2}} + O(dt^3) \quad (21)$$

is effective in reducing compounded error per time-step from $O(dt^2) \rightarrow O(dt^3)$. This reduction makes the time evolution accurate enough for reliable numerical computation.

4.4.2 Transforming Bases

Applying each exponential component of the Unitary Operator is most easily achieved by changing the basis in which the state $|\Psi\rangle$ is represented. Given gridded - thus discretized - momentum and configuration spaces, applying each component of the operator amounts to matrix-vector multiplication of the operator evaluated at each grid point (in momentum space for the kinetic energy operator exponentials, configuration space for the potential energy operator exponentials) with the state to undergo evolution. This requires re-expression of the state in the relevant basis for each multiplication. Fortunately, the Fast-Fourier Transform, FFT , and the Inverse Fast Fourier Transform, FFT^{-1} , provide numerically optimized methods to perform these tasks.

These transforms are usually included in and optimized for computational software packages, so even with these extra transform steps included the split-operator method is much more efficient than calculating the Hamiltonian, eigenfunctions, and eigenenergies at every time-step. After adding these additional steps, the complete time evolution expression is

$$\Psi(x, t + \Delta t) = FFT^{-1} e^{\frac{-i}{\hbar}(\frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m})\frac{\Delta t}{2}} FFT e^{\frac{-i}{\hbar}\hat{V}(x,t)\Delta t} FFT^{-1} e^{\frac{-i}{\hbar}(\frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m})\frac{\Delta t}{2}} FFT[\Psi(x, t)] \quad (22)$$

4.5 Modeling the Physical System

4.5.1 Visualization

The single-atom NOON state system is created when a particle is held within a splitting single potential well. When the single well becomes a full double well, the particle's state evolves by $|1\rangle \rightarrow |1, 0\rangle + |0, 1\rangle$. Mathematically, in configuration space, we want to establish a single well potential grid akin to the harmonic oscillator potential (for ease of ground state wavefunction determination) and represent the ground state wavefunction on that grid. Splitting this well in time amounts to evaluating the changing potential function at each point on the grid. These evolved points are used in the Unitary Operator.

The research hypothesis is that by adding attractive interaction between two one dimensional particles in a splitting single well, one can create a two atom NOON state, $|1, 0\rangle + |0, 1\rangle$. An operational issue then becomes the establishment and modeling of the second particle's configuration and momentum space grids. We may accomplish this by modeling the joint two particle wavefunction, $\Psi(x_1, x_2)$, as a two dimensional space with the position of x_1 on the conventional

“x-axis” and the position of x_2 on the conventional “y axis.” (In actuality, each is an x-axis, plotting the x positions of x_1 and x_2 .) In this way, one can use the third graphical dimension’s amplitude as the value of the joint probability density of finding particle one at x_1 and finding particle two at x_2

This idea is illustrated in Figure 1. In the figure shown, both particles have position to the right of $x = 0$. This type of visualization also makes the interpretation of particle superpositions easier. Depicted in Figure 2, is a state in which both particle one and particle two are in a superposition of both sides of the double well. Quadrant one represents the state with both particles to the right, i.e. $|0, 1\rangle \otimes |0, 1\rangle$. Quadrant three represents the state of both particles left, i.e. $|1, 0\rangle \otimes |1, 0\rangle$. Quadrants two and four represents states in which the particles are antigruped, i.e. $|1, 0\rangle \otimes |0, 1\rangle$ and $|0, 1\rangle \otimes |1, 0\rangle$, respectively.

4.5.2 Interaction

Adding an attractive interaction is most easily achieved by modifying the Hamiltonian, $\hat{\mathcal{H}}$, to include an extra term, a deep potential well when the position of atom one is that of atom two. A delta function potential accomplishes this,

$$V_{total}(x_1, x_2, t) = V_{well}(x_1, x_2, t) - \alpha\delta(x_1 - x_2), \quad (23)$$

where α is the depth of the well. This establishes a tendency for the particles to stay and move together, graphically along the line where $x_1 = x_2$. When plotted on the potential grid, this additional interaction appears as a trench in the potential along this line. See Figure 3.

4.6 Results

When the time evolution simulation is performed in the absence of inter-particle interaction, predictably each particle splits into an equal superposition given by $|1, 0\rangle + |0, 1\rangle \otimes |1, 0\rangle + |0, 1\rangle$. This result is depicted in Figure 6.

When weak interactions between particles are included, the splitting is not entirely independent. The particles are more likely to be split into a state where both inhabit the same subwell of the split well, i.e.

$$|\Psi\rangle = \alpha[|1, 0\rangle + |0, 1\rangle \otimes |1, 0\rangle + |0, 1\rangle] + \beta[|2, 0\rangle + |0, 2\rangle] \quad (24)$$

where $\alpha + \beta = 1$ and $\beta > \alpha$. The superposition is biased toward the state in which the particles split into the same well.

For strong interactions, (Figure 7) we note that the superposition has become entirely one for which the particles split together, namely

$$|\Psi\rangle = |2, 0\rangle + |0, 2\rangle. \quad (25)$$

This is the realization of the two atom NOON state, and we have found the initial hypothesis to be true. It is, in fact, possible to create such a state using attractive inter-particle interactions.

5 Future Research

While we have succeeded in creating the two-particle NOON state, more work can and should be done to investigate this system. Of interest is the correlation of interaction strength to

the entanglement of the particles. We know that a sufficiently strong interaction causes the two-particle NOON state, but it would be of interest to know exactly where that threshold occurs and whether such an interaction is experimentally realizable. Similarly, analyzing the model with scale parameters might prove illustrious.

Generalizing the result to higher dimensions and a greater number of particles is also a natural extension, but for this case, significantly more computing power would be required.

References

- [1] M. Anderlini, J. Sebby-Strabley, J. Kruse, J.V. Porto, and W.D. Phillips. Controlled atom dynamics in a double-well optical lattice. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 39:S199, 2006.
- [2] K. Kormann, S. Holmgren, and H.O. Karlsson. Accurate time propagation for the Schrödinger equation with an explicitly time-dependent Hamiltonian. *The Journal of chemical physics*, 128:184101, 2008.
- [3] R. Kosloff. Propagation methods for quantum molecular dynamics. *Annual Review of Physical Chemistry*, 45(1):145–178, 1994.

6 Appendix: Figures

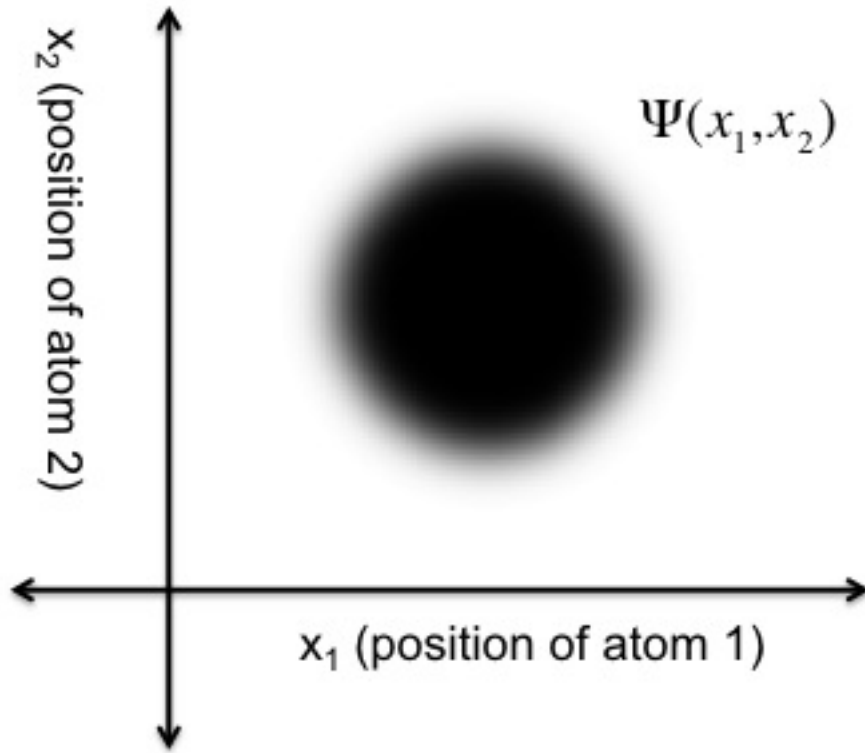


Figure 1: A Gaussian joint wavefunction with both particles to the right of the origin.

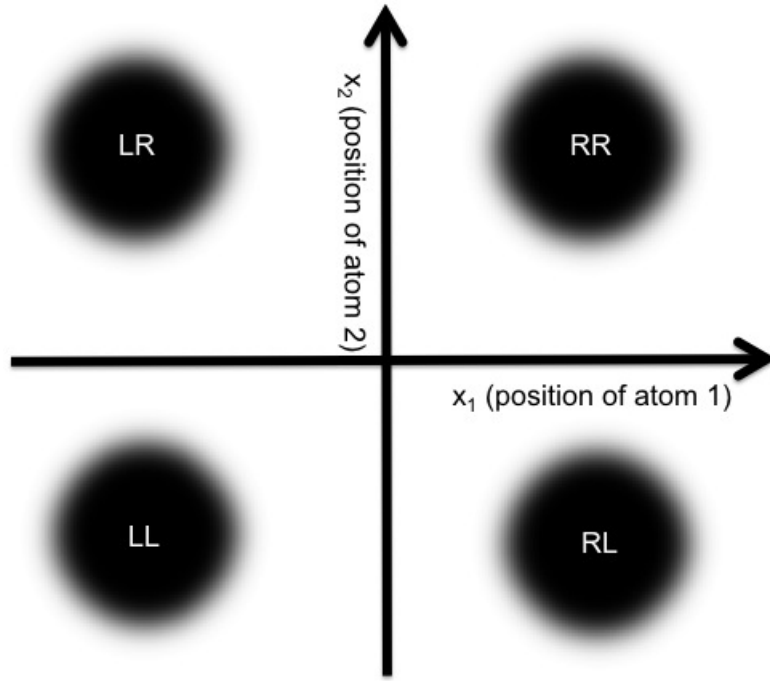


Figure 2: A joint wavefunction depicting a $|1, 0\rangle + |0, 1\rangle \otimes |1, 0\rangle + |0, 1\rangle$ state.

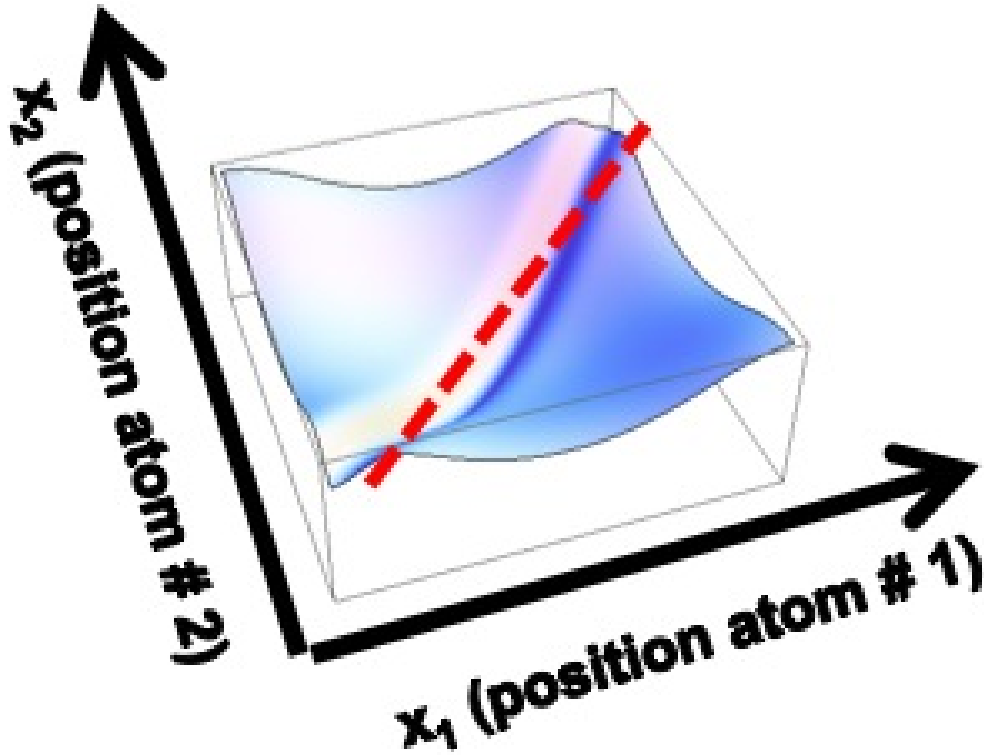


Figure 3: The full potential of the pre-split single well with inter-particle interaction.

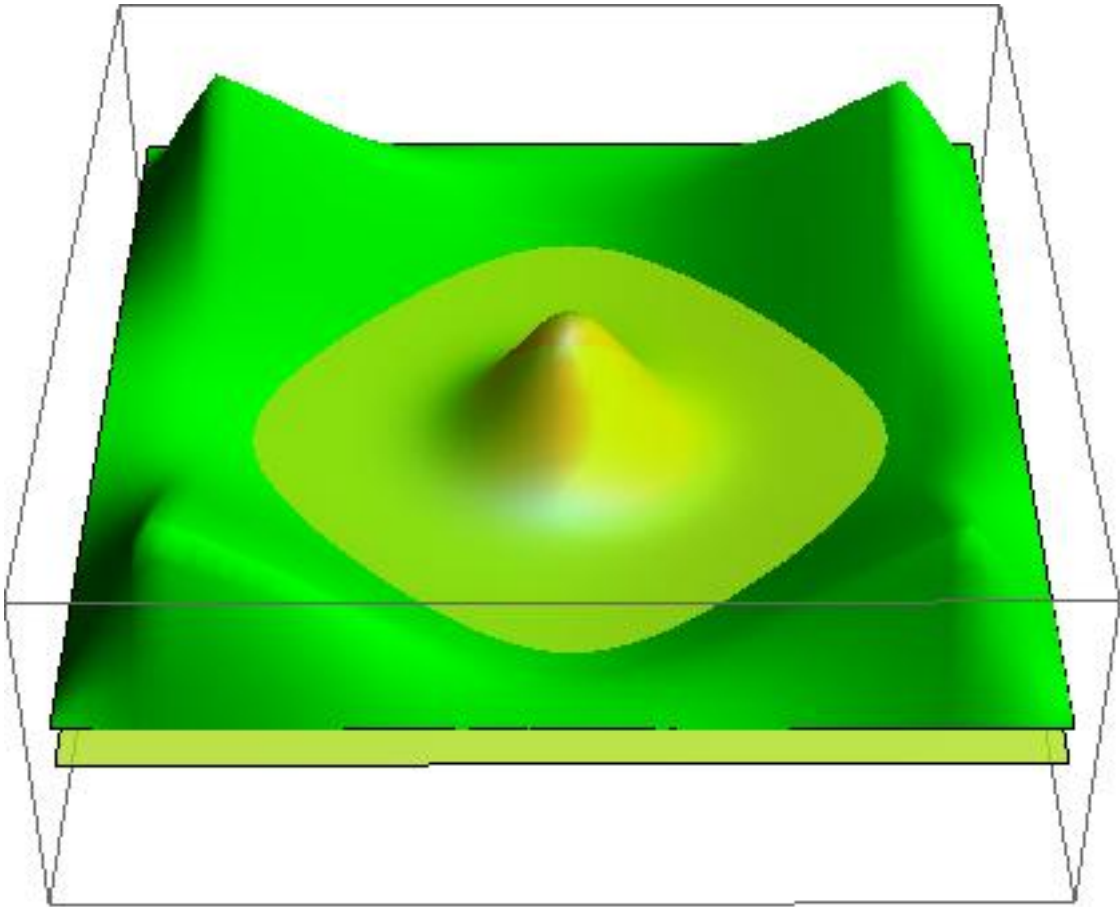


Figure 4: Each particle's wavefunction starts centered around $x = 0$ in the single well.

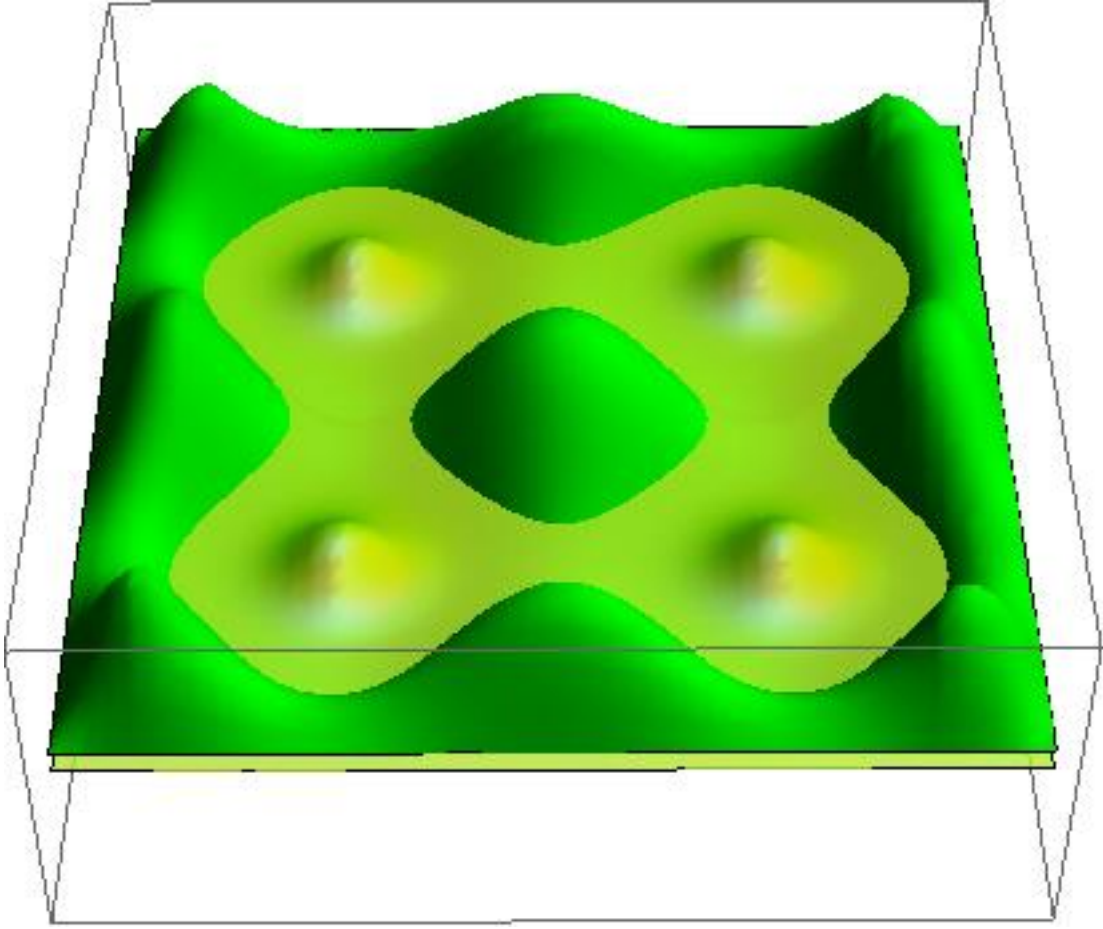


Figure 5: Here, each particle's wavefunction has split into a superposition of $|1, 0\rangle + |0, 1\rangle \otimes |1, 0\rangle + |0, 1\rangle$. There was no inter-particle interaction during this evolution.

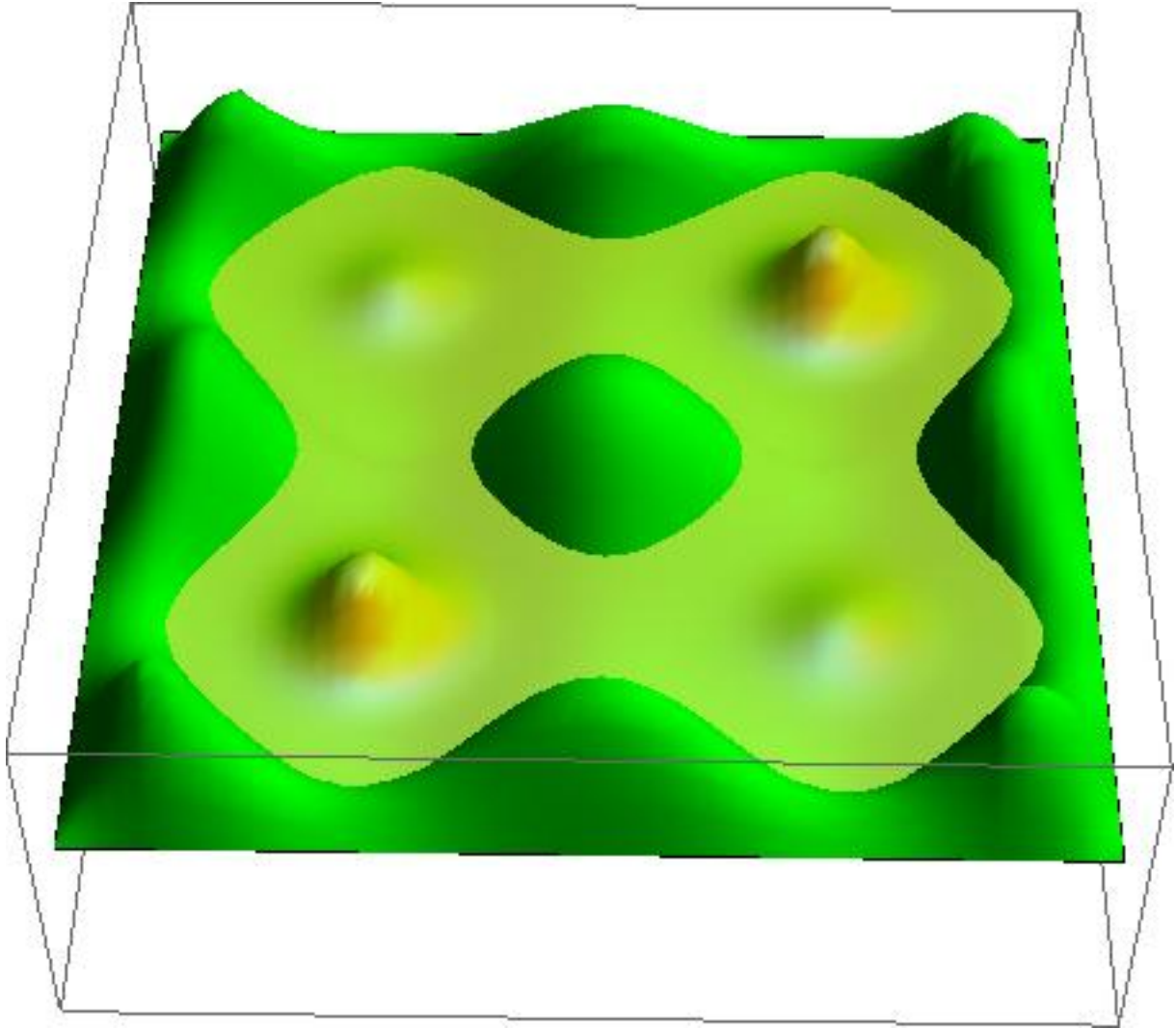


Figure 6: With weak inter-particle interaction, the superposition is more complicated.

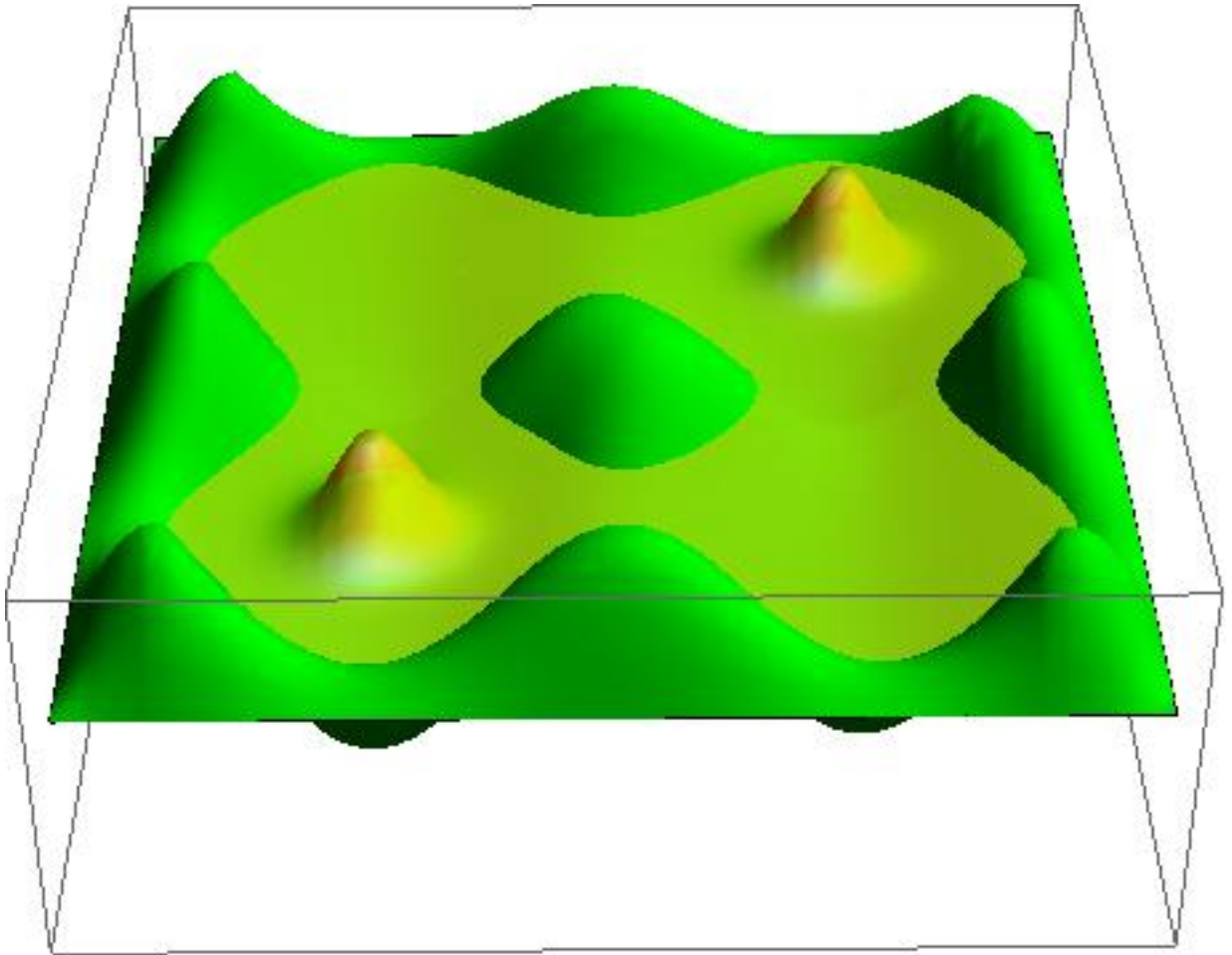


Figure 7: With strong inter-particle interaction, we observe a two-atom NOON state.