Double well potentials and quantum gates

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Abstract:

The quantum system of particles in a double well potential is a widely studied and extremely useful example for understanding quantum mechanics. This simple system has recently been used in theoretical proposals and related experiments as a way to make quantum logic gates for ultra-cold atoms confined in optical lattices (periodic potentials arising from the interaction of atoms with standing waves of laser light). Such quantum gates are the fundamental building blocks for quantum information processing; in this context the regular array of cold atoms in the optical lattice serves as the quantum register. The purpose of this paper is to explain how this current research can be understood in terms of well-known principles for systems of identical particles, and hence furnish an up-to-date example for the teaching of quantum mechanics.

I. INTRODUCTION

A system with two particles in a double well potential has been studied in recent experiments with ultra-cold atoms. The atoms were confined in optical lattice potentials; these are periodic potentials created by standing waves of laser light. These experiments were remarkable as they were able to simultaneously prepare a large number of copies of the double well system, each with a well defined and almost identical quantum state; this quantum state could then be manipulated. Furthermore, there has recently been a related theoretical proposal to make a quantum logic gate with neutral atoms held in double well potentials, for the purposes of quantum information processing.

In this paper we explain the basic principles underlying this current research using simple quantum mechanics, in order to furnish an up-to-date example for the teaching of quantum theory. We shall write out the states of the system explicitly in terms of multi-particle wave functions, rather than using the more compact formulation of creation and annihilation operations (second quantized notation) as in most of the research papers. In order to establish the notation and background, we first consider the system of two particles in a single well—the reader who is familiar with this background material could skip to section IV.
II. TWO PARTICLES IN A POTENTIAL WELL

The well-known example of two particles in the same potential well illustrates the important pedagogical point that the energy levels of quantum systems do not depend on whether or not the particles are identical. The occupation of those energy levels, however, is influenced by quantum statistics if, and only if, the particles are identical.

The Schrödinger equation for a system of two particles of mass $m$ moving in one dimension is

$$\left\{-\frac{\hbar^2}{2m} \frac{d^2}{dx_1^2} + V(x_1) - \frac{\hbar^2}{2m} \frac{d^2}{dx_2^2} + V(x_2)\right\} \Psi(x_1, x_2) = E \Psi(x_1, x_2)$$ (1)

where we take the potential $V(x)$ to be the same for both particles. For this case where the particles do not interact, $\Psi$ can be written as the product of the wave functions for the individual particles

$$\Psi(x_1, x_2) = \psi(x_1)\psi(x_2).$$ (2)

To provide a simple example we shall consider an infinite square well, i.e. $V(x) = 0$ for $0 < x \leq L$ and $V(x) = \infty$ elsewhere. Note, however, that the form of the potential makes no difference to our subsequent arguments. The single-particle wave functions for an infinite square well are

$$\psi(x_1) = \alpha_n \sin\left(\frac{n\pi x_1}{L}\right),$$ (3)

for $n$ integer, where $\alpha_n$ is a normalisation constant; and similarly for $\psi(x_2)$. It is convenient to express the eigenenergies as $E_n = n^2 E_g$ where the ground state energy is given by

$$E_g = \frac{\hbar^2 \pi^2}{2mL^2}.$$ (4)

The lowest configuration of the two-particle system has energy $E_a = 2E_g$, and wave function

$$\Psi_{g,g} = \alpha_g^2 \sin\left(\frac{\pi x_1}{L}\right) \sin\left(\frac{\pi x_2}{L}\right) = \psi_g(x_1)\psi_g(x_2).$$ (5)

Here $\psi_g(x_i)$ is the wave function the $i$th particle in the ground state. Particles in the first excited state have the wave function $\psi_e(x_i)$ with energy eigenvalue $E_e$ (where $E_e = 4E_g$ for a square well). The first excited level of the two-particle system has energy $E_{g,e} = E_g + E_e$, and the two possible wave functions are

$$\psi_g(x_1)\psi_e(x_2) \quad \text{or} \quad \psi_e(x_1)\psi_g(x_2).$$ (6)

The degeneracy of the first excited state (and higher lying ones) arises from the symmetry of the system under the exchange of particle labels, i.e. the energy of two particles of the same mass in the same potential does not depend on which particle is in the excited state. To determine the effect of an interaction we therefore need to use degenerate perturbation theory.
A. The effect of an interaction between the particles

We now consider the effect of an interaction between the particles so that the Hamiltonian becomes

\[ \hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x_2) + V(x_1) + V'(x_1 - x_2). \]  

(7)

The potential \( V'(x_1 - x_2) \) represents the interaction between the two particles, which we shall consider as a perturbation. We only consider potentials that are a function of the distance between the two particles \( |x_1 - x_2| \), e.g. the Coulomb potential between charged particles.

At this stage those who have encountered similar situations before, e.g. in solving the helium atom, are inclined to anticipate the result and exploit the freedom arising from the degeneracy to rewrite the two-particle wave functions as linear combinations the original wave functions which are symmetric or antisymmetric under exchange of particle labels. This may be prompted by the knowledge that both spatial and spin wavefunctions will be either symmetric or antisymmetric for systems of identical particles. However, for now we keep the discussion to distinguishable particles, to see the natural emergence of symmetric and antisymmetric states, without explicitly invoking the exchange symmetry operator.

The effect of \( V'(x_1 - x_2) \) on the non-degenerate ground state is given straightforwardly by the first-order perturbation:

\[ \Delta E_{g,g} = \int dx_1 \int dx_2 |\psi_g(x_1)|^2 |\psi_g(x_2)|^2 V'(x_1 - x_2). \]  

(8)

To evaluate the effect of the perturbation on the degenerate states (of eqn 6) we write a general wave function in the basis of the two states as

\[ \Psi(x_1, x_2) \approx a\psi_g(x_1)\psi_e(x_2) + b\psi_e(x_1)\psi_g(x_2). \]  

(9)

This projection of the wave function onto two states is a good approximation when the perturbation is sufficiently small that is does not mix in significant amplitudes of other states. It is convenient to represent these two degenerate basis states as vectors:

\[ \psi_g(x_1)\psi_e(x_2) \mapsto \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \psi_e(x_1)\psi_g(x_2) \mapsto \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \]  

(10)

In this truncated basis the Schrödinger equation \( \hat{H}\Psi = E\Psi \) reduces to a matrix equation (with eigenvalue \( E \)):

\[ \begin{pmatrix} E_{g,e} + J & K \\ K & E_{g,e} + J \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = E \begin{pmatrix} a \\ b \end{pmatrix}. \]  

(11)
The eigenvalues are determined by the roots of the equation

\[(E_{g,e} + J - E)^2 - K^2 = 0.\]  \hspace{1cm} (12)

as

\[E = E_{g,e} + J \pm K.\]  \hspace{1cm} (13)

Here \(J\) is the direct integral given by

\[J = \int dx_1 \int dx_2 |\psi_g(x_1)|^2 |\psi_e(x_2)|^2 V'(x_1 - x_2),\]  \hspace{1cm} (14)

and \(K\) is the exchange integral (it may appear strange to call this the exchange integral when the particles are distinguishable, but it has exactly the same form for identical particles). This is given by

\[K = \int dx_1 \int dx_2 \psi_g(x_1)\psi_e^*(x_1)\psi_g^*(x_2)\psi_e(x_2)V'(x_1 - x_2).\]  \hspace{1cm} (15)

This is real (the symmetry of the integral for interchange of variables \(x_1 \leftrightarrow x_2\) implies that \(K^* = K\)). Unlike the direct integral, the exchange integral \(K\) cannot be interpreted in terms of a simple classical picture; attempts to explain it classically lead to nonsensical concepts, e.g. ‘exchange forces’, which are contrived and completely fictional. (For example, the gross structure of the helium atom is determined by electrostatic interactions and nothing else.)

The two eigenvectors and corresponding spatial wave functions are:

\[
\begin{pmatrix}
  a \\
  b
\end{pmatrix}
= \begin{pmatrix}
  1/\sqrt{2} \\
  -1/\sqrt{2}
\end{pmatrix} \mapsto \frac{1}{\sqrt{2}} \left\{ \psi_g(x_1)\psi_e(x_2) - \psi_e(x_1)\psi_g(x_2) \right\} \text{ for } E_{g,e} + J - K,  
\]

\[
\begin{pmatrix}
  1/\sqrt{2} \\
  1/\sqrt{2}
\end{pmatrix} \mapsto \frac{1}{\sqrt{2}} \left\{ \psi_g(x_1)\psi_e(x_2) + \psi_e(x_1)\psi_g(x_2) \right\} \text{ for } E_{g,e} + J + K.
\]  \hspace{1cm} (16)

The eigenstates of the Hamiltonian with an interaction between the distinguishable particles are antisymmetric and symmetric combinations of the original wave functions, as in the case of indistinguishable particles. To reinforce this point one can consider the case where the two particles differ slightly in their mass (or other property affecting their energies), and show that this tends to the above result as the masses become equal.

### B. A delta-function interaction

The interaction between two ultracold neutral atoms can be represented, a good approximation, by a delta-function potential

\[V'(x_1 - x_2) = a \delta(x_2 - x_1)\]  \hspace{1cm} (18)
where $a$ is a constant, and $a > 0$ for a repulsive interaction. For this so-called contact interaction, the direct and exchange integrals are the same:

$$J = K = \int dx \left| \psi_g(x) \right|^2 \left| \psi_e(x) \right|^2 a$$  \hspace{1cm} (19)

Since $J - K = 0$ the interaction does not change the energy of the antisymmetric wave function in eqn [16] which is an obvious consequence of the function being equal to zero when $x_1 = x_2$. By a similar argument the triplet terms of the helium atom have lower energy than the singlets, because the expectation value of the electrostatic repulsion between the two electrons is lower for the spatial wave function in which the two parts have opposite sign.

**III. IDENTICAL PARTICLES AND SPIN STATISTICS**

When the two particles are identical their spin has an influence on the occupancy of the energy levels. In particular the requirements of overall exchange antisymmetry for fermions, and symmetry for bosons, introduces a connection between the spin and spatial wave functions. Consequently states with different spin have different energies, e.g. the singlet and triplet terms in helium; it is tempting to think that the energies themselves depend on spin, although they do not. The wave functions for two fermions have the form

$$\Psi_{\text{fermions}} = \Psi_{\text{space}}^{(S)} \Psi_{\text{spin}}^{(A)} \text{ or } \Psi_{\text{space}}^{(A)} \Psi_{\text{spin}}^{(S)}$$ \hspace{1cm} (20)

where $(A)$ denotes antisymmetric with respect to exchange of the particle labels 1 $\leftrightarrow$ 2, and $(S)$ denotes symmetric. This subset of all the possible two-particle wave functions has overall antisymmetry with respect to exchange of particle labels as required for identical fermions. The spin wave functions are written out in Table II (right-hand column); there is a singlet for $\Psi_{\text{spin}}^{(A)}$ and a triplet for $\Psi_{\text{spin}}^{(S)}$ making a total of 4 functions. A well-known example of this physics is the helium atom: for the ground configuration (1s$^2$) there is only a symmetric spatial wave function $\Psi_{\text{space}}^{(S)} = \psi_{1s}^2$ associated with a spin singlet; the first excited configuration (1s2s) is split into two terms: a singlet ($^1S$) and a triplet ($^3S$) whose energy separation is twice the exchange integral given by

$$K = \frac{e^2}{4\pi\epsilon_0} \int dr_1^2 \int dr_2^3 \psi_{1s}^*(r_1)\psi_{2s}^*(r_2) \frac{1}{|r_2 - r_1|} \psi_{2s}(r_1)\psi_{1s}(r_2)$$ \hspace{1cm} (21)

where $e^2/4\pi\epsilon_0|r_2 - r_1|$ is the Coulomb repulsion between the electron at $r_1$ and the electron at $r_2$; see Footnote for further details. For two bosons the wave function is symmetric with respect to exchange of the particle labels:

$$\Psi_{\text{bosons}} = \Psi_{\text{space}}^{(S)} \Psi_{\text{spin}}^{(S)} \text{ or } \Psi_{\text{space}}^{(A)} \Psi_{\text{spin}}^{(A)}$$ \hspace{1cm} (22)
FIG. 1: The wave functions of a single particle in a double well potential are illustrated using a square well with a high barrier for simplicity. a) The wave function \( \phi(x) \) of lowest energy has even parity. b) The lowest wave function with odd parity \( \tilde{\phi}(x) \) lies slightly higher in energy than \( \phi \), and the energy difference between them increases as the tunneling rate increases. c) and d) show the combinations of \( \phi \) and \( \tilde{\phi} \) given in eqns 23 and 24 which represent the particle localized in the left and right well respectively.

This brief review of the physics of two particles in a single well serves as an introduction for the treatment of a double system in the following sections.

IV. DOUBLE WELL POTENTIAL

A. A single particle in a double well

We consider double wells that have symmetry with respect to inversion \( (x \rightarrow -x) \), so that the eigenfunctions of particles in this potential have definite parity (the Hamiltonian of the system commutes with the parity operator \( \hat{P} \), i.e. \( [\hat{H}, \hat{P}] = 0 \), so these operators have simultaneous eigenfunctions). The even and odd parity wave functions for a single particle in a double square well potential with a thin barrier are illustrated in Fig. 1.

The state whose wave function \( \phi \) has even parity lies lower in energy than the wave function with odd parity \( \tilde{\phi} \)—the barrier has less effect on the odd wave function since \( \tilde{\phi} \) has a node at
\( x = 0 \) no matter what the height of the barrier, whereas the energy of the even parity wave function decreases as the barrier height decreases. For the simple case of square well potentials, when the barrier is reduced from \( \infty \) to zero, so that the well becomes twice its original length, the ground state energy reduces to \( 1/4 \) of its original value (see eqn 4). A qualitatively similar argument holds for any double well (with reflection symmetry); the solution of the Schrödinger equation with no nodes has the lowest eigenenergy.

We can form linear superpositions of the energy eigenstates

\[
\langle x|L \rangle = \frac{1}{\sqrt{2}} \left\{ \phi(x) + \tilde{\phi}(x) \right\}
\]

\[ (23) \]

\[
\langle x|R \rangle = \frac{1}{\sqrt{2}} \left\{ \phi(x) - \tilde{\phi}(x) \right\}
\]

which correspond to wave functions in which the particle is located predominantly in the left, or right, well respectively, as illustrated in Fig. 1. These are not eigenstates of the system, so the wave function of a particle initially prepared in the left well (at \( t = 0 \)) evolves according to

\[
\psi(x, t) = \frac{1}{\sqrt{2}} \left\{ \phi(x)e^{-iE_t/\hbar} + \tilde{\phi}(x)e^{-i\tilde{E}_t/\hbar} \right\}
\]

\[ (25) \]

where \( \Omega = (\tilde{E} - E)/\hbar \) is the tunneling rate between the wells. When \( \Omega t = 2\pi n \), for \( n \) integer, the wave function is proportional to \( \langle x|L \rangle \), and when \( \Omega t = (2n-1)\pi \) the wave function is proportional to \( \langle x|R \rangle \) corresponding to the particle having tunneled across into the other well. For negligible tunneling between the wells (very high barrier) it is possible to describe the particle as being either in the left or right well—this is obviously true when the wells are very far apart so that the particle is localised in one of the wells. This is the situation at the start of the experiments we shall describe.

### B. Two interacting particles in a double well

The previous sections have prepared all the mathematical tools we need to understand the behavior of two particles in a double well. We choose a potential with a high barrier so that initially the system is close to the limit of two separate wells. There is an antisymmetric spatial wave function \( \Psi_{\text{space}}^{(A)} \) which can be expressed in terms of the Left/Right wave functions of the individual particles as:

\[
\Psi_{\text{space}}^{(-)}(x_1, x_2) = \frac{1}{\sqrt{2}} \left\{ \langle x_1|L \rangle \langle x_2|R \rangle - \langle x_1|R \rangle \langle x_2|L \rangle \right\}.
\]

\[ (26) \]
This can be rewritten using the ket notation to represent \( \Psi_{\text{space}}^{(-)} \):

\[
\Psi_{\text{space}}^{(-)} = \frac{1}{\sqrt{2}} \{ |LR\rangle - |RL\rangle \}.
\] (27)

Similarly, the three possible symmetric wave functions (\( \Psi_{\text{space}}^{(S)} \)) are

\[
|LL\rangle, \quad |RR\rangle, \quad \text{and} \quad \Psi_{\text{space}}^{(+)} = \frac{1}{\sqrt{2}} \{ |LR\rangle + |RL\rangle \}.
\] (28)

Writing the 4 spatial wave functions in this way highlights their similarity with the form of the 4 spin wave functions for two spin-1/2 particles; both have one \( \Psi^{(A)} \) and three \( \Psi^{(S)} \). Combining space and spin functions with the restriction of overall antisymmetry, as in eqn (20), we find by inspection of Table III that there are 6 two-particle wave functions for identical spin-1/2 particles.

Now consider the effect of a repulsive contact interaction between the particles. Clearly this has very little effect on the energy when the two particles are localized in different wells (with small overlap of their wave functions), i.e. for \( \Psi_{\text{space}}^{(-)} \) and \( \Psi_{\text{space}}^{(+)} \); however, for the wave functions containing \( \psi_R(x_1)\psi_R(x_2) \) (i.e. \( |RR\rangle \)) and \( \psi_L(x_1)\psi_L(x_2) \) (i.e. \( |LL\rangle \)), the interaction raises the energy by a positive quantity which we denote as \( U \). The integral for \( U \) resembles eqn (19):

\[
U = \int dx \ |\psi_R(x)|^4 a
\] (29)

and analogously for \( \psi_L(x) \). Figure 2 and Table III shows the eigenenergies and associated fermionic eigenstates for a double well with a repulsive interaction.

In the following we shall mainly consider the sub-set of states with the particles in different wells. These are separated by the energy gap \( U \) from the higher lying states \( |LL\rangle\chi^{(-)} \) and \( |RR\rangle\chi^{(-)} \).

C. Quantum gate for two fermions

In quantum computing notation the state in which both particles are spin-up \( |\uparrow\uparrow\rangle \) can be written as \( |00\rangle \) and conversely \( |\downarrow\downarrow\rangle \equiv |11\rangle \). The state of the system is encoded in terms of the four basis states as:

\[
\Psi = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle
\]

where \( a, b, c \) and \( d \) are complex coefficients. The state \( |00\rangle \) corresponds to a spin-up particle in each well for which the antisymmetrised wave function (unnormalised) is

\[
|00\rangle \propto \langle x_1 |L\rangle |\uparrow_1\rangle \langle x_2 |L\rangle |\uparrow_2\rangle - \langle x_1 |R\rangle |\uparrow_1\rangle \langle x_2 |L\rangle |\uparrow_2\rangle
\]
TABLE I: The spatial and spin wave functions for two particles can be those which are antisymmetric (A) with respect to exchange of the particle labels 1 ↔ 2, and others are symmetric (S). For a pair of fermions these can be combined to give 6 two-particle wave functions of the form \(\Psi_{\text{space}}^{(A)} \Psi_{\text{spin}}^{(S)}\) or \(\Psi_{\text{space}}^{(S)} \Psi_{\text{spin}}^{(A)}\), i.e. each of the 6 symmetric functions in the bottom row is associated with one of the functions in the top row. This subset (of the 16 possible product states) has overall antisymmetry with respect to exchange of particle labels as required for identical fermions.

| \(\Psi_{\text{space}}^{(A)}\) | \(\Psi_{\text{spin}}^{(A)}\) | \(\Psi_{\text{space}}^{(S)}\) | \(\Psi_{\text{spin}}^{(S)}\) |
|-----------------|-----------------|-----------------|-----------------|
| \(\frac{1}{\sqrt{2}} \{ |LR\rangle - |RL\rangle \}\) | \(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\rangle\) | \(|LL\rangle\) | \(|\uparrow\uparrow\rangle\) |
| \(\frac{1}{\sqrt{2}} \{ |LR\rangle + |RL\rangle \}\) | \(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\rangle\) | \(|\uparrow\downarrow\rangle\) | \(|\downarrow\downarrow\rangle\) |

This can be expressed in terms of the energy eigenstates found above as

\[
|00\rangle \propto ( |LR\rangle - |RL\rangle ) |\uparrow\uparrow\rangle, \nonumber
\]
\[
\propto \Psi_{\text{space}}^{(-)} |\uparrow\uparrow\rangle. \quad (30)
\]

The state \(|01\rangle\) corresponds to spin-up in the left well and spin-down on the right for which the antisymmetrised wave function (unnormalised) is

\[
|01\rangle \propto \langle x_1|L| \uparrow_1 \rangle \langle x_2|R| \downarrow_2 \rangle - \langle x_1|R| \downarrow_1 \rangle \langle x_2|L| \uparrow_2 \rangle. \quad (31)
\]

This can be expressed in terms of the energy eigenstates found above as

\[
|01\rangle \propto \langle LR| |\uparrow\downarrow\rangle - \langle RL| |\uparrow\downarrow\rangle, \nonumber
\]
\[
\propto \left( \Psi_{\text{space}}^{(-)} + \Psi_{\text{space}}^{(+)\text{space}} \right) |\uparrow\downarrow\rangle + \left( \Psi_{\text{space}}^{(-)} - \Psi_{\text{spin}}^{(+)\text{spin}} \right) |\downarrow\uparrow\rangle, \nonumber
\]
\[
\propto \Psi_{\text{space}}^{(-)} ( |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle ) + \Psi_{\text{spin}}^{(+)\text{spin}} ( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle ). \quad (32)
\]
and similarly for $|10\rangle$ and $|11\rangle$. Thus we write the quantum computational basis states in terms of the 4 eigenstates of two spin-1/2 particles (which are degenerate for zero tunnelling) as:

$$
|00\rangle = \Psi_{\text{space}}^{(-)}|\uparrow\uparrow\rangle \\
|01\rangle = \left\{ \Psi_{\text{space}}^{(-)}|\uparrow\downarrow\rangle + \Psi_{\text{space}}^{(+)}|\downarrow\uparrow\rangle \right\} / \sqrt{2} \\
|10\rangle = \left\{ \Psi_{\text{space}}^{(-)}|\downarrow\uparrow\rangle - \Psi_{\text{space}}^{(+)}|\uparrow\downarrow\rangle \right\} / \sqrt{2} \\
|11\rangle = \Psi_{\text{space}}^{(-)}|\downarrow\downarrow\rangle. 
$$

When the barrier is lowered slowly, $\Psi_{\text{space}}^{(-)}$ and $\Psi_{\text{space}}^{(+)}$ adiabatically evolve into $\Psi_a$ and $\Psi_b$ respectively, which are no longer degenerate. Further details are given in Hayes et al\(^2\) (see also Table II), but to understand the operation of the gate all we need to know that a phase difference accumulates between these states as they have different eigenenergies during the gate operation. Thus if the barrier is lowered for a certain period and then raised again (to switch off the tunneling), the wave function that starts as $|01\rangle$ becomes

$$
\Psi(t) = e^{-i\varphi} \left\{ \Psi_{\text{space}}^{(-)}|\uparrow\downarrow\rangle + e^{i\Delta\varphi} \Psi_{\text{space}}^{(+)}|\downarrow\uparrow\rangle \right\} / \sqrt{2}. 
$$

Controlling the process so that the accrued phase shift $\Delta\varphi = \pi$ causes this state to evolve into

$$
\Psi(t_\pi) = e^{-i\varphi} \left\{ \Psi_{\text{space}}^{(-)}|\uparrow\downarrow\rangle + e^{i\pi\Delta\varphi} \Psi_{\text{space}}^{(+)}|\downarrow\uparrow\rangle \right\} / \sqrt{2} \\
= e^{-i\varphi} \left\{ \Psi_{\text{space}}^{(-)}|\uparrow\downarrow\rangle - \Psi_{\text{space}}^{(+)}|\downarrow\uparrow\rangle \right\} / \sqrt{2} \\
= e^{-i\varphi} |10\rangle. 
$$

The global phase factor $e^{-i\varphi}$ is not important; all other combinations pick up this phase too, therefore it does not affect the relative phase. It can be seen that a system initialised in $|01\rangle$ evolves into $|10\rangle$ and vice versa which implements the SWAP operation $|01\rangle \leftrightarrow |10\rangle$. When $\Delta\varphi = 2\pi$ the system cycles back to its initial state. More generally, the states $|01\rangle$ and $|10\rangle$ evolve into a coherent superposition, while the $|00\rangle$ and $|11\rangle$ states remain unaffected. The SWAP operation can be written as the $4 \times 4$ matrix:

$$
U_{\text{SWAP}} = 
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
\end{pmatrix}
$$

for the basis states in eqn [33].

It is the so-called square-root-of-SWAP gate that performs a useful entangling operation in quantum computation; this operation is represented by the matrix such that

$$
U_{\sqrt{\text{SWAP}}}U_{\sqrt{\text{SWAP}}} = U_{\text{SWAP}}.
$$
Hence we find that

\[ U_{\sqrt{\text{SWAP}}} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{2}(1 + i) & \frac{1}{2}(1 - i) & 0 \\
0 & \frac{1}{2}(1 - i) & \frac{1}{2}(1 + i) & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}. \]

Clearly to implement \( \sqrt{\text{SWAP}} \) the system undergoes 1/2 of the phase evolution for SWAP. The entangled state obtained by operating on \(|01\rangle\) with \( \sqrt{\text{SWAP}} \) is

\[ U_{\sqrt{\text{SWAP}}} |01\rangle = \frac{1}{2} (|01\rangle + |10\rangle) + \frac{i}{2} (|01\rangle - |10\rangle). \]

The square-root-of-SWAP gate cannot be broken down into a combination of single qubit gates, i.e. gates operating on one qubit at a time (whereas \( U_{\text{SWAP}} \) can). Single qubit gates would be implemented in this system by the rotation of the atomic spin orientation in of one of the wells; this may be accomplished relatively simply by optical (Raman) or microwave pulses. The square-root-of-SWAP gate, used alongside single-qubit operations, is sufficient to provide a universal set of gates for quantum computation\(^5\). The implementation of these powerful ideas with fermionic atoms in optical lattices is described by Hayes et al\(^3\). Similar principles can also be applied to a system of two bosons (selecting just two out of the possible spin states to form a suitable basis). More details of a gate for bosons are given in the theoretical paper of Vaucher et al\(^6\) and the experimental papers\(^1,2\).

V. CONCLUSION

This paper shows how recent experimental and theoretical research on ultracold atoms in double well potentials can be understood in terms of simple quantum mechanics. The experiments have been carried out with bosonic atoms (the isotope Rb-87) for technical reasons but for simplicity the fermionic case has been used to expound the principles. This system described by Hayes et al\(^3\) is particularly intriguing for the way in which influence of the nuclear spin on the spatial wave functions is exploited.

For a more general solution, second quantized notation tends to be used, as in most of the papers we cite; this notation becomes more efficient in keeping track of exchange symmetry as the number of particles in the system increases.

There is great current interest in using cold atoms in optical lattices for quantum information processing, including the direct quantum simulation of strongly correlated many particle systems (such as those in Condensed Matter Physics). The simple approach outlined in this
paper gives an intuitive way of understanding aspects of these systems.

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**TABLE II**: The four lowest energy eigenstates of the two-atom double well system, as shown in Fig.2. Only states a and b are used in the quantum logic gate; these are degenerate in the limit of an infinite barrier. (In this limit states c and d are also degenerate, both having energy $U$ greater than a and b.) As the barrier height is decreased a and b evolve into states with an energy splitting between them and a phase difference accumulates which is an essential part of the operation gate described in the text. The localized eigenstates $\langle x|L \rangle$ and $\langle x|R \rangle$ are not appropriate for a low barrier (high tunneling rate between wells), and one should use products of the even and odd parity wave functions $\phi$ and $\tilde{\phi}$ (see eqns. 23 and 24)—these states are included for completeness in the right column.

| State | Spin | Exchange | Parity | Eigenfunctions for a high barrier | Eigenfunctions for a low barrier |
|-------|------|----------|--------|-----------------------------------|----------------------------------|
| a     | singlet | +       | +      | $\frac{1}{\sqrt{2}} \left\{ |LR\rangle + |RL\rangle \right\} \equiv \Psi^{(+)}_{\text{space}}$ | $|\phi\phi\rangle$ |
| b     | triplet | −       | −      | $\frac{1}{\sqrt{2}} \left\{ |LR\rangle - |RL\rangle \right\} \equiv \Psi^{(-)}_{\text{space}}$ | $\frac{1}{\sqrt{2}} \left\{ |\phi\tilde{\phi}\rangle - |\tilde{\phi}\phi\rangle \right\}$ |
| c     | singlet | +       | +      | $\frac{1}{\sqrt{2}} \left\{ |LL\rangle + |RR\rangle \right\}$ | $|\tilde{\phi}\tilde{\phi}\rangle$ |
| d     | singlet | +       | −      | $\frac{1}{\sqrt{2}} \left\{ |LL\rangle - |RR\rangle \right\}$ | $\frac{1}{\sqrt{2}} \left\{ |\phi\tilde{\phi}\rangle + |\tilde{\phi}\phi\rangle \right\}$ |
FIG. 2: A schematic diagram of the operation of a quantum gate for two atoms in a double well potential. The energies of the four lowest states (see Table II) of the 2-atom double well system are shown as a function of time as the height of the barrier is lowered and then raised. For the initial and final conditions (marked A and C) tunneling is negligible, whereas during operation (e.g. at B) the barrier is much lower—indeed the barrier can be reduced to zero so that both atoms are in a single well for a certain time before the barrier is raised. The phase $\Delta \varphi$ of the gate is the integral of the shaded region between paths a and b (divided by $\hbar$). The barrier is altered slowly and smoothly to ensure the adiabatic evolution of the states along the given paths (otherwise states a and c mix). The condition for adiabatic evolution dictates that the gate must take place over a time significantly longer than $\hbar/U$. The states have been labeled to be consistent with Hayes et al.3

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