Analysing a SWAP gate for atoms in a double well potential

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This question uses simple quantum mechanics (wave functions rather than creation operators) to look at the physics of a so-called SWAP gate. Such an entangling gate in combination with single-qubit operations can be used to create a system suitable for measurement-based quantum computation with atoms in optical lattices. This question examines the gate for fermions proposed by Hayes *et al* (2007) PRL **98**, 070501, which is readily understandable because of its similarities with the physics of the helium atom (antisymmetrised wave functions for two identical particles etc), and this paper may help with part (c). Similar principles are used in gates for bosons, e.g. Rb-87 (Vaucher, Nunnenkamp and Jaksch (2008) New J. Phys. **10**, 023005 and experiments at NIST, Gaithersburg reported in Anderlini *et al.* (2007) Nature **448**, 452, which are recommended for further reading).

We build up to the full system in the following steps: (a) two particles in a potential well, (b) one particle in a double well, (c) two spin-1/2 particles in a double well.

Parts (a) and (b) are 'revision' of elementary quantum mechanics as a preliminary to part (c). The physical principles do not depend on the shape of the potential so it is simplest to consider simple square wells. Familiarity with the wave functions for a particle of mass m in an infinite square well of length L (sine waves) is assumed.

(a) Two particles in a potential well.

- **(i)** Write down the wave functions for the ground and first excited energy levels of a system of two non-interacting particles in the same well.
- **(ii)** What is the effect of a contact interaction $a\,\delta(x_2 - x_1)$ which acts as a perturbation on these eigenstates ($a > 0$)? (You do not need to evaluate any integrals but only to establish whether the integrals are zero, or not. Take account the degeneracy of the first excited eneryg level arising from exchange symmetry.)
- **(iii)** Consider the two particles to be identical fermions with spin-1/2. What are the possible spin states associated with the each of the energy levels of the perturbed system in part ii). Make a comparison with the singlet and triplet terms of the helium atom arising from the configurations 1s^2 and 1s2s.
- **(iv)** (optional) If the two particles are not identical (but almost exactly the same mass) what difference, if any, does it make to the energy levels.

(b) One particle in a double well.

For definiteness consider two square wells with $V(x) = 0$ for $-L - \frac{w}{2} < x < -\frac{w}{2}$ and $\frac{w}{2} < x < L + \frac{w}{2}$; a constant potential $V(x) = V$ for $-\frac{w}{2} < x < \frac{w}{2}$, and $V(x) = \infty$ elsewhere. (Assume that the barrier is thin $w \ll L$). The particle has energy E.

- **(i)** Sketch the single-particle wave functions for the ground and first excited states for the case of a high barrier $V \gg E$, i.e. almost separate wells. Describe the behaviour of the system in a linear superposition of these two wave functions with equal amplitudes.
- **(ii)** For the extreme case where for the tunnelling goes to zero (infinite barrier) the two states found previously are degenerate, so that we can combine them together and still have an energy eigenfunction. Sketch the wave functions corresponding to the particle being in the left well ψ_L, or the right well ψ_R respectively.

(c) Two spin-1/2 particles in a double well.

(i) Spatial wave functions for two particles in a double well are of the form

$$\psi_L(x_1)\psi_R(x_2),\ \psi_R(x_1)\psi_R(x_2), \ldots$$

Write down the 6 two-particle wave functions which have the form $\Psi^{(\mathrm{S})}_{\mathrm{space}}\Psi^{(\mathrm{A})}_{\mathrm{spin}}$ or $\Psi^{(\mathrm{A})}_{\mathrm{space}}\Psi^{(\mathrm{S})}_{\mathrm{spin}}$, where (A) denotes antisymmetric with respect to exchange of the particle labels $1 \leftrightarrow 2$, and (S) denotes symmetric. This subset has overall antisymmetry w.r.t. exchange of particle labels as required for identical fermions. The following spatial part of the wave functions of the helium atom are a useful guide:

$$u_{1\mathrm{s}}(r_1)u_{1\mathrm{s}}(r_2),\ \frac{1}{\sqrt{2}}\{u_{1\mathrm{s}}(r_1)u_{2\mathrm{s}}(r_2) \pm u_{2\mathrm{s}}(r_1)u_{1\mathrm{s}}(r_2)\}.$$

(ii) Interaction between the particles causes the two wave functions containing $\psi_R(1)\psi_R(2) \equiv |RR\rangle$, and $|LL\rangle$ to have an energy U greater than the wave functions corresponding to particles in separate wells. What is the effect of a lowering the barrier to allow tunnelling at a rate $J \ll U$ on the four states of lowest energy?

(iii) The system is intialised in a state with spin-up in the left well and spin-down on the right, which corresponds the antisymmetrised wavefunction (unnormalised)

$$\psi_L(x_1)|\uparrow\rangle_1\psi_R(x_2)|\downarrow\rangle_2 - \psi_R(x_1)|\downarrow\rangle_1\psi_L(x_2)|\uparrow\rangle_2$$

Express this as superposition of energy eigenstates found in ii).

(v) In quantum computing notation the state with spin-up in the left well and spin-down on the right is written as $|01\rangle$. When $J \neq 0$ a system initialised in state $|01\rangle$ evolves into $|10\rangle$ and then cycles back to the initial state. Explain why. [This is the method which Hayes *et al* use to implement the SWAP operation $|01\rangle \leftrightarrow |10\rangle$.]

(iv) In quantum computing notation the state in which both particles are spin-up is written as $|00\rangle$ and conversely both spin-down is $|11\rangle$. A general wave function can be expressed in terms of the four basis states:

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

In this basis the SWAP operation is the 4×4 matrix:

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

Find the matrix representing the so-called $\sqrt{\mathrm{SWAP}}$ gate, such that

$$U_{\sqrt{\mathrm{SWAP}}}U_{\sqrt{\mathrm{SWAP}}} = U_{\mathrm{SWAP}}$$

Clearly to implement $\sqrt{\mathrm{SWAP}}$ the system undergoes $\frac{1}{2}$ of the phase evolution for SWAP.

(v) Show that the entangled state obtained by operating on $|01\rangle$ with $\sqrt{\mathrm{SWAP}}$ is

$$U_{\sqrt{\mathrm{SWAP}}}|01\rangle = \frac{1}{2}\,(\,|01\rangle + |10\rangle\,) + \frac{\mathrm{i}}{2}\,(\,|01\rangle - |10\rangle\,)\,.$$

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