4. *Quantum Mechanics* (Spring 2003)

Consider two electrons which are constrained to live on two sites. There is an interaction energy U when both electrons are on the same site. When they are on different sites, there is no interaction energy. There is an amplitude t for an electron to hop from one site to the other. In other words, the Hamiltonian is of the form:

$$H = -t(|1\uparrow,1\downarrow\rangle\langle 1\uparrow,2\downarrow| + \text{h.c.} + |2\uparrow,2\downarrow\rangle\langle 1\uparrow,2\downarrow| + \text{h.c.}) + U(|1\uparrow,1\downarrow\rangle\langle 1\uparrow,1\downarrow| + |2\uparrow,2\downarrow\rangle\langle 2\uparrow,2\downarrow|)$$

where $|1\sigma, 2\sigma'\rangle$ is the state with an electron of spin $\sigma = \uparrow,\downarrow$ at site 1 and an electron of spin $\sigma' = \uparrow,\downarrow$ at site 2 while $|1\sigma, 1\ -\sigma\rangle$ is the state with two electrons (of spins σ and $-\sigma$) at site 1. What are the energies and degeneracies of the ground and first excited states of the system to lowest order in t for $t \ll U$?

Note that there can't be two of the same spin in one site by the Pauli exclusion principle, and there is nothing to cause the spins to flip, so we assume that one electron is always spin up and the other is always spin down. Thus there are 4 distinct states $|1\uparrow,1\downarrow\rangle, |1\uparrow,2\downarrow\rangle, |1\downarrow,2\uparrow\rangle, |2\uparrow,2\downarrow\rangle$, so $|\Psi\rangle = \begin{pmatrix}\langle 1\uparrow,1\downarrow|\Psi\rangle\\ \langle 1\uparrow,2\downarrow|\Psi\rangle\\ \langle 1\downarrow,2\uparrow|\Psi\rangle\\ \langle 2\downarrow,2\downarrow|\Psi\rangle\end{pmatrix}$

The Hamiltonian above seems to be missing transitions to and from the $|1\downarrow,2\uparrow\rangle$ state. We will assume this is an error. In the basis described above, H is

$$H \doteq -t\begin{pmatrix}0&1&1&0\\1&0&0&1\\1&0&0&1\\0&1&1&0\end{pmatrix} + U\begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&1\end{pmatrix} = \begin{pmatrix}U&-t&-t&0\\-t&0&0&-t\\-t&0&0&-t\\0&-t&-t&U\end{pmatrix}$$

We find the energy eigenvalues by solving $\det(H-\lambda I)=0$

$$0 = \det(H-\lambda I) = \begin{vmatrix}U-\lambda&-t&-t&0\\-t&-\lambda&0&-t\\-t&0&-\lambda&-t\\0&-t&-t&U-\lambda\end{vmatrix} = \begin{vmatrix}U-\lambda&-t&-t&0\\-t&-\lambda&0&-t\\0&\lambda&-\lambda&0\\0&-t&-t&U-\lambda\end{vmatrix}$$

$$= (U-\lambda)\begin{vmatrix}-\lambda&0&-t\\\lambda&-\lambda&0\\-t&-t&U-\lambda\end{vmatrix} + t\begin{vmatrix}-t&-t&0\\\lambda&-\lambda&0\\-t&-t&U-\lambda\end{vmatrix}$$

$$= (U-\lambda)\left[-\lambda\left(-\lambda(U-\lambda)\right) - t\left(-\lambda t - \lambda t\right)\right] + t(U-\lambda)(\lambda t + \lambda t)$$

$$= (U-\lambda)\left[\lambda^2(U-\lambda) + 4\lambda t^2\right]$$

$$\Rightarrow \lambda = U \text{ or } \lambda = 0 \text{ or } \lambda(U-\lambda) + 4t^2 = 0$$

$$\lambda^2 - \lambda U - 4t^2 = 0 \Rightarrow \lambda = \frac{1}{2}\left[+U \pm \sqrt{U^2+16t^2}\right] = \frac{U}{2} \pm \frac{U}{2}\sqrt{1+\frac{16t^2}{U^2}}$$

$$\text{or } \lambda \cong \frac{U}{2} \pm \frac{U}{2}\left(1 - \frac{8t^2}{U^2}\right) = \frac{U}{2} \pm \frac{U}{2} \pm \frac{4t^2}{U}$$

The ground state energy is the lowest of $\left\{U, 0, U+\frac{4t^2}{U}, -\frac{4t^2}{U}\right\}$ which is $E_0 = -\frac{4t^2}{U}$ and the first excited state is $E_1 = 0$.
Both have degeneracy 1 because there are 4 states and 4 energies.