# 1 Quantum

## 1.1 Problem 3

**(a)** The hamiltonian can be written in matrix form by writing out the matrix elements in the suggested basis. Then Schrödinger's equation generates a characteristic equation:

$$|\boldsymbol{h} - \mu \boldsymbol{I}| = 0$$

where $\mu$ are the energy eigenvalues, $\boldsymbol{h}$ is the hamiltonian matrix, and $\boldsymbol{I}$ is the identity matrix in 3 dimensions. The equation turns out to be:

$$(\epsilon_0 - \mu)[(\epsilon_0 - \mu)^2 - t^2] + t[-t(\epsilon_0 - \mu) - \lambda t^2] - \lambda t[t^2 + \lambda t(\epsilon_0 - \mu)] = 0$$
$$(\epsilon_0 - \mu)^3 - (2 + \lambda^2)t^2(\epsilon_0 - \mu) - 2\lambda t^3 = 0$$

The first eigenvalue can be seen from inspection:

$$\mu_1 = \epsilon_0 + \lambda t$$

We can then divide the equation by $(\epsilon_0 - \mu + \lambda t)$, using, for example, Ruffini's rule (Wiki: Ruffini's rule), to obtain:

$$(\epsilon_0 - \mu)^2 - \lambda t(\epsilon_0 - \mu) - 2t^2 = 0$$

Using the quadratic equation, we can get:

$$\mu_{2,3} = \epsilon_0 - \frac{\lambda t \pm t\sqrt{\lambda^2 + 8}}{2}$$

With these you can find the eigenstates. From the first eigenvalue:

$$\psi_1 = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \tag{1}$$

This eigenvalue is antisymmetric upon interchange of $|1>$ and $|3>$, and $|2>$ is not involved at all, because it has a special spatial configuration. The other two eigenvalues are obtained in a similar way as we obtained the first one, i.e., by requiring that:

$$(\boldsymbol{h} - \mu_{2,3}\boldsymbol{I})\psi_{2,3} = 0$$

The answers are:

$$\psi_{2,3} = \begin{bmatrix} \frac{\lambda^2 \pm \lambda\sqrt{\lambda^2+8}+2}{3\lambda \pm \sqrt{\lambda^2+8}} \\ 1 \\ \frac{\lambda^2 \pm \lambda\sqrt{\lambda^2+8}+2}{3\lambda \pm \sqrt{\lambda^2+8}} \end{bmatrix} \tag{2}$$

or, equivalently:

$$\psi_{2,3} = \begin{bmatrix} 1 \\ \frac{-\lambda \pm \sqrt{\lambda^2+8}}{2} \\ 1 \end{bmatrix} \tag{3}$$

These states are symmetric with respect to interchange of states 1 and 3, and this time 2 plays a role in the eigenfunction, but it's still distinguished from the other two states. We are asked to make a sketch of the energies as a function $\lambda$. I cannot make a graph here, but basically $\mu_1$ climbs up linearly from $\epsilon_0$ to $\infty$, $\mu_2$ goes down with some mild curvature from $\epsilon_0 - 2t$ to $-\infty$, and $\mu_3$ goes down from $\epsilon_0 + \sqrt{2}t$, asymptotically approaching $\epsilon_0$. The ground state should be even, and the energy should be minimized, so only $\psi_2$ will be the only one occupied. Finally, in the special case $\lambda = 1$, there are only two eigenvalues: $\epsilon_0 - 2t$ (with degeneracy 1), and $\epsilon_0 + t$ (with degeneracy 2). The singly degenerate state is:

$$\psi_{\epsilon_0 - 2t} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \tag{4}$$

By the requirement that the other two states be orthogonal to this one and to each other, we can find two eigenstates with the other energy value. Any states will do, actually, for instance:

$$\psi_{(\epsilon_0+t),1} = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \tag{5}$$

$$\psi_{(\epsilon_0+t),2} = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} \tag{6}$$

**(b)** This problem is solved by waving your hands really hard. Look first at the A configuration. It has three eigenvalues: $\epsilon_0$, $\epsilon_0 - t$ and $\epsilon_0 + t$. The adiabatic approximation says that as the configuration changes from A to B and then to C, the state with the lowest eigenvalue will remain in the lowest, the intermediate will remain in the intermediate, and similarly for the highest. For simplicity we'll study the intermediate eigenvalue, which in configuration A corresponds to the eigenstate:

$$\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

The intermediate state will also have an intermediate eigenvalue $\epsilon_0$, and its corresponding eigenvector will be, up to a negative sign:

$$\begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

Then in the B configuration, there will also be a similar eigenvalue, with eigenvector:

$$\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

Now, our assumption will be that in order to go from 1 to 0, the state should not go through -1. Then the intermediate state will actually be the negative of what we obtained, and the final B state will also be the negative of what we obtained. Continuing this procedure we get back to A, but with a relative minus sign.