HAMILTONIAN AND OBSERVABLES IN THREE-STATE SYSTEM

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 3.38.

Suppose we have a three-state hamiltonian whose matrix elements, relative to a certain basis, are

$$\mathsf{H}=\hbar\omega\left[\begin{array}{ccc}1 & 0 & 0\\0 & 2 & 0\\0 & 0 & 2\end{array}\right] \tag{1}$$

We also have two other observables A and B, represented by the matrices

$$\mathsf{A}=\lambda\left[\begin{array}{ccc}0 & 1 & 0\\1 & 0 & 0\\0 & 0 & 2\end{array}\right] \tag{2}$$

$$\mathsf{B}=\mu\left[\begin{array}{ccc}2 & 0 & 0\\0 & 0 & 1\\0 & 1 & 0\end{array}\right] \tag{3}$$

Here, ω, λ and μ are positive real numbers.

The hamiltonian is already diagonal, so we can read its eigenvalues from the matrix. We find for H:

$$E = \hbar\omega,2\hbar\omega \tag{4}$$

where the $2\hbar\omega$ eigenvalue is degenerate (occurs twice). The eigenvector is $[1,0,0]$ for $E=\hbar\omega$. For $E=2\hbar\omega$, the eigenvectors span a two-dimensional space, so we can choose any two linearly independent vectors in that space. The simplest choice is $[0,1,0]$ and $[0,0,1]$.

The eigenvalues and eigenvectors of A and B are found in the usual way by calculating determinants and solving the resulting polynomial equation.

For A, the eigenvalues are $a=2\lambda$ and $a=\pm\lambda$. The eigenvectors are $[0,0,1]$ for $a=2\lambda$, $[1,1,0]/\sqrt{2}$ for $a=\lambda$ and $[1,-1,0]/\sqrt{2}$ for $a=-\lambda$.

For B, the eigenvalues are $b=2\mu$ and $b=\pm\mu$. The eigenvectors are $[1,0,0]$ for $b=2\mu$, $[0,1,1]/\sqrt{2}$ for $b=\mu$ and $[0,1,-1]/\sqrt{2}$ for $b=-\mu$.

Now suppose that the system starts in the state

$$|\mathscr{S}(0)\rangle=\left[\begin{array}{c}c_1\\c_2\\c_3\end{array}\right] \tag{5}$$

where the state is assumed to be normalized so that $|c_1|^2+|c_2|^2+|c_3|^2=1$.

We can find the expectation values of the three observables at this time most easily if we can express $|\mathscr{S}(0)\rangle$ as a linear combination of the eigenvectors for each operator. In the case of H, this is easy, and we get

$$|\mathscr{S}(0)\rangle=c_1H_1+c_2H_2+c_3H_3 \tag{6}$$

where we have labelled each of the eigenvectors of H as H_1, etc in the order in which they were calculated above. The expectation value of H is then

$$\begin{aligned}
\langle H\rangle &= \langle\mathscr{S}(0)|\mathsf{H}|\mathscr{S}(0)\rangle && (7)\\
&= |c_1|^2\hbar\omega+2\hbar\omega\left(|c_2|^2+|c_3|^2\right) && (8)\\
&= \hbar\omega\left(2-|c_1|^2\right) && (9)
\end{aligned}$$

For A, we have

$$|\mathscr{S}(0)\rangle=\frac{c_1}{\sqrt{2}}(A_2+A_3)+\frac{c_2}{\sqrt{2}}(A_2-A_3)+c_3A_1 \tag{10}$$

The expectation value is therefore

$$\begin{aligned}
\langle A\rangle &= \langle\mathscr{S}(0)|\mathsf{A}|\mathscr{S}(0)\rangle && (11)\\
&= 2\lambda|c_3|^2+\lambda\left(c_1^*c_2+c_2^*c_1\right) && (12)\\
&= 2\lambda\left(|c_3|^2+\Re(c_1^*c_2)\right) && (13)
\end{aligned}$$

For B, we have

$$|\mathscr{S}(0)\rangle=\frac{c_2}{\sqrt{2}}(B_2+B_3)+\frac{c_3}{\sqrt{2}}(B_2-B_3)+c_1B_1 \tag{14}$$

Note that this is a cyclic permutation of the c_i coefficients from 10, so since the B_i are orthonormal, we can read the value for $\langle B\rangle$ from that for $\langle A\rangle$ by cyclically permuting the indices:

$$\langle B\rangle = 2\mu\left(|c_1|^2 + \Re(c_2^* c_3)\right) \tag{15}$$

From 6 we can get the time dependent form:

$$|\mathscr{S}(t)\rangle = c_1 e^{-i\omega t} H_1 + e^{-2i\omega t}(c_2 H_2 + c_3 H_3) \tag{16}$$

so a measurement of energy will give $\hbar\omega$ with probability $|c_1|^2$ and $2\hbar\omega$ with probability $|c_2|^2 + |c_3|^2$.

To work out possible values of the other two observables, we note that

$$H_1 = \frac{1}{\sqrt{2}}(A_2 + A_3) \tag{17}$$

$$H_2 = \frac{1}{\sqrt{2}}(A_2 - A_3) \tag{18}$$

$$H_3 = A_1 \tag{19}$$

so from 10, we can write

$$|\mathscr{S}(t)\rangle = \frac{c_1}{\sqrt{2}} e^{-i\omega t}(A_2 + A_3) + \frac{c_2}{\sqrt{2}} e^{-2i\omega t}(A_2 - A_3) + c_3 e^{-2i\omega t} A_1 \tag{20}$$

$$= c_3 e^{-2i\omega t} A_1 + \frac{1}{\sqrt{2}}(c_1 e^{-i\omega t} + c_2 e^{-2i\omega t}) A_2 + \frac{1}{\sqrt{2}}(c_1 e^{-i\omega t} - c_2 e^{-2i\omega t}) A_3 \tag{21}$$

A measurement of A will give 2λ with probability $|c_3|^2$. The second eigenvalue of $+\lambda$ will be obtained with probability

$$p_\lambda = \frac{1}{\sqrt{2}}(c_1^* e^{i\omega t} + c_2^* e^{2i\omega t}) \frac{1}{\sqrt{2}}(c_1 e^{-i\omega t} + c_2 e^{-2i\omega t}) \tag{22}$$

$$= \frac{1}{2}\left(|c_1|^2 + |c_2|^2 + 2\Re(c_1^* c_2 e^{-i\omega t})\right) \tag{23}$$

and the probability of the third eigenvalue $-\lambda$ is

$$p_{-\lambda} = \frac{1}{\sqrt{2}}(c_1^* e^{i\omega t} - c_2^* e^{2i\omega t}) \frac{1}{\sqrt{2}}(c_1 e^{-i\omega t} - c_2 e^{-2i\omega t}) \tag{24}$$

$$= \frac{1}{2}(|c_1|^2 + |c_2|^2 - 2\Re(c_1^* c_2 e^{-i\omega t})) \tag{25}$$

Note that the sum of all three probabilities is $|c_1|^2 + |c_2|^2 + |c_3|^2 = 1$.

For B, we can reason the same way

$$H_1 = B_1 \tag{26}$$

$$H_2 = \frac{1}{\sqrt{2}}(B_2 + B_3) \tag{27}$$

$$H_3 = \frac{1}{\sqrt{2}}(B_2 - B_3) \tag{28}$$

so

$$|\mathscr{S}(t)\rangle = c_1 e^{-i\omega t} B_1 + \frac{c_2}{\sqrt{2}} e^{-2i\omega t}(B_2 + B_3) + \frac{c_3}{\sqrt{2}} e^{-2i\omega t}(B_2 - B_3) \tag{29}$$

$$= c_1 e^{-i\omega t} B_1 + \frac{1}{\sqrt{2}} e^{-2i\omega t}(c_2 + c_3) B_2 + \frac{1}{\sqrt{2}} e^{-2i\omega t}(c_2 - c_3) B_3 \tag{30}$$

The probability of a measurement of B giving the first eigenvalue of 2μ is therefore $|c_1|^2$. For the second eigenvalue of $+\mu$ the probability is $\frac{1}{2}|c_2 + c_3|^2$ and for the third eigenvalue of $-\mu$ the probability is $\frac{1}{2}|c_2 - c_3|^2$.

Note that $|c_2 + c_3|^2 = |c_2|^2 + |c_3|^2 + 2\Re(c_2^* c_3)$ and $|c_2 - c_3|^2 = |c_2|^2 + |c_3|^2 - 2\Re(c_2^* c_3)$ so again the sum of the three probabilities is $|c_1|^2 + |c_2|^2 + |c_3|^2 = 1$. Note also that only the measurements of A are time dependent.