Energy Level Crossing and Entanglement

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We consider a Hamilton operator in a finite dimensional Hilbert space with energy level crossing. We discuss the question how energy level crossing and entanglement of states in this Hilbert space are intertwined. Since energy level crossing is related to symmetries of the Hamilton operator we also derive these symmetries and give the reduction to the invariant Hilbert subspaces.

Key words: Energy Level Crossing; Symmetries; Group Theory; Entanglement.

1. Introduction

A basic problem in quantum mechanics is the calculation of the energy spectrum of a given (hermitian) Hamilton operator $\hat{H}$. It is assumed that the hermitian Hamilton operator acts in a Hilbert space $\mathcal{H}$. Here we assume we have a finite dimensional Hilbert space. Thus the spectrum is discrete. In many cases the Hamilton operator depends on a real parameter. The question whether or not energy levels can cross by changing the parameter was first discussed by Hund [1]. He studied examples only and conjectured that, in general no crossing of energy levels can occur. In 1929 von Neumann and Wigner [2] investigated this question more rigorously and found the following theorem: Real symmetric matrices (respectively the hermitian matrices) with a multiple eigenvalue form a real algebraic variety of codimension 2 (respectively 3) in the space of all real symmetric matrices (respectively all hermitian matrices). This implies the famous "non-crossing rule" which asserts that a "generic" one parameter family of real symmetric matrices (or two-parameter family of hermitian matrices) contains no matrix with multiple eigenvalue. "Generic" means that if the Hamilton operator $\hat{H}$ admits symmetries the underlying Hilbert space has to be decomposed into invariant Hilbert subspaces using group theory [3]. Meanwhile a large number of researcher have studied energy level crossing (see [4] and references therein).

Entanglement of states in finite-dimensional Hilbert spaces $(\dim \mathcal{H} \geq 4)$ has been investigated by many authors (see [5], [6] and references therein). The measure of entanglement for bipartite states are the von Neumann entropy, concurrence and the 2-tangle.

2. Theory

We consider the Hilbert space $\mathbb{C}^4$ and the Hamilton operator

$$\hat{H} = \hbar\omega(\sigma_z \otimes \sigma_z) + \Delta(\sigma_x \otimes \sigma_x),$$

where $\omega > 0$ and $\Delta > 0$. The Hamilton operator shows energy level crossing and the unitary operator $U(t) = \exp(-\mathrm{i}\hat{H}t/\hbar)$ can generate entangled states from unentangled states.

The eigenvalues of $\hat{H}$ are given by

$$E_1 = \hbar\omega + \Delta, \quad E_2 = -(\hbar\omega + \Delta),$$
$$E_3 = -\hbar\omega + \Delta, \quad E_4 = \hbar\omega - \Delta$$

with the corresponding normalized eigenvectors

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}, \quad |\Psi^-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix},$$

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix}, \quad |\Phi^-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix}.$$

Note that the states do not depend on the parameters ω and Δ. These states are the Bell states [4]. The Bell states are fully entangled. As a measure of entanglement we can apply the tangle which is the squared concurrence. The concurrence $\mathcal{C}$ for a pure state $|\psi\rangle$ in $\mathcal{H} = \mathbb{C}^4$ is given by

$$\mathcal{C} = 2\left|\det\begin{pmatrix} c_{00} & c_{01} \\ c_{10} & c_{11} \end{pmatrix}\right|$$

with the state $|\psi\rangle$ written in the form

$$|\psi\rangle = \sum_{j,k=0}^{1} c_{jk}|j\rangle \otimes |k\rangle,$$

and $|j\rangle$ $(j = 0,1)$ denotes the standard basis in $\mathbb{C}^2$.

Energy level crossing occurs if $\Delta = \hbar\omega$. Then we have the eigenvalues $E_1 = 2\hbar\omega$, $E_3 = 0$, $E_4 = 0$, $E_2 = -2\hbar\omega$. For the degenerate eigenvalue 0 we have the eigenvectors

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \quad |\Phi^-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}.$$

Since we have energy level crossing the Hamilton operator $\hat{H}$ admits a symmetry. We have

$$[\sigma_x \otimes \sigma_x, \sigma_z \otimes \sigma_z] = 0.$$

Thus

$$[\hat{H}, \sigma_x \otimes \sigma_x] = 0, \quad [\hat{H}, \sigma_z \otimes \sigma_z] = 0.$$

Now both $\{I_2 \otimes I_2, \sigma_x \otimes \sigma_x\}$ and $\{I_2 \otimes I_2, \sigma_z \otimes \sigma_z\}$ form a group under matrix multiplication, where I_2 is the 2×2 identity matrix. Both can be used to find the reduction to Hilbert subspaces. Consider first the group $\{I_2 \otimes I_2, \sigma_x \otimes \sigma_x\}$. The character table provides the projection operators

$$\Pi_1 = \frac{1}{2}(I_2 \otimes I_2 + \sigma_x \otimes \sigma_x),$$
$$\Pi_2 = \frac{1}{2}(I_2 \otimes I_2 - \sigma_x \otimes \sigma_x).$$

The projection operator Π_1 projects into a two-dimensional Hilbert space spanned by the Bell states

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$

with the corresponding matrix for the Hamilton operator

$$\begin{pmatrix} \hbar\omega - \Delta & 0 \\ 0 & -\hbar\omega - \Delta \end{pmatrix}.$$

The projection operator Π_2 projects into a two-dimensional Hilbert space spannded by the Bell states

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$$

with the corresponding matrix for the Hamilton operator

$$\begin{pmatrix} \hbar\omega + \Delta & 0 \\ 0 & -\hbar\omega + \Delta \end{pmatrix}.$$

Consider now the group $\{I_2 \otimes I_2, \sigma_z \otimes \sigma_z\}$. The character table provides the projection operators

$$\Pi_1 = \frac{1}{2}(I_2 \otimes I_2 + \sigma_z \otimes \sigma_z),$$
$$\Pi_2 = \frac{1}{2}(I_2 \otimes I_2 - \sigma_z \otimes \sigma_z).$$

The projection operator Π_1 projects into a two-dimensional Hilbert space spanned by elements of the standard basis

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

with the corresponding matrix for the Hamilton operator

$$\begin{pmatrix} \hbar\omega & \Delta \\ \Delta & \hbar\omega \end{pmatrix}.$$

The projection operator Π_2 projects into a two-dimensional Hilbert space spanned by the elements of the standard basis

$$\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

with the corresponding matrix for the Hamilton operator

$$\begin{pmatrix} -\hbar\omega & \Delta \\ \Delta & -\hbar\omega \end{pmatrix}.$$

Note that the elements of these two groups are elements of the Pauli group $\mathcal{P}_2$ which is defined by

$$\mathcal{P}_n := \{I_2, \sigma_x, \sigma_y, \sigma_z\}^{\otimes n} \otimes \{\pm 1, \pm i\}$$

where I_2 is the 2×2 identity matrix.

Next we look at the time evolution $U(t) = \exp(-\mathrm{i}\hat{H}t/\hbar)$. We obtain

$$\exp(-\mathrm{i}\hat{H}t/\hbar) = \mathrm{e}^{-\mathrm{i}\omega t(\sigma_z\otimes\sigma_z)}\mathrm{e}^{-\mathrm{i}t\Delta(\sigma_x\otimes\sigma_x)/\hbar}.$$

Since

$$\mathrm{e}^{-\mathrm{i}\omega t(\sigma_z\otimes\sigma_z)} = I_4\cos(\omega t) + \mathrm{i}(\sigma_z\otimes\sigma_z)\sin(\omega t)$$

and

$$\mathrm{e}^{-\mathrm{i}\Delta t(\sigma_x\otimes\sigma_x)/\hbar)} = I_4\cos(t\Delta/\hbar) + \mathrm{i}(\sigma_x\otimes\sigma_x)\sin(t\Delta/\hbar)$$

we obtain

$$\begin{aligned}\mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar} = {} & I_4\cos(\omega t)\cos(t\Delta/\hbar) \\ & + \mathrm{i}(\sigma_z\otimes\sigma_z)\sin(\omega t)\cos(t\Delta/\hbar) \\ & + \mathrm{i}(\sigma_x\otimes\sigma_x)\cos(\omega t)\sin(t\Delta/\hbar) \\ & - (\sigma_z\sigma_x)\otimes(\sigma_z\sigma_x)\sin(\omega t)\sin(t\Delta/\hbar).\end{aligned}$$

Applying $U(t)$ to the unentangled state $(1\,0\,0\,0)^T$ yields

$$U(t)\begin{pmatrix}1\\0\\0\\0\end{pmatrix} = \begin{pmatrix}\cos(\omega t)\cos(t\Delta/\hbar) + \mathrm{i}\sin(\omega t)\cos(t\Delta/\hbar) \\ 0 \\ 0 \\ -\sin(\omega t)\sin(\Delta t/\hbar) + \mathrm{i}\cos(\omega t)\sin(t\Delta/\hbar)\end{pmatrix}.$$

Depending on t, ω and Δ we can obtain entangled states using the concurrence as measure. For the case $\hbar\omega = \Delta$ (level crossing) the state reduces to

$$\begin{pmatrix}\cos^2(\omega t) + \mathrm{i}\sin(\omega t)\cos(\omega t) \\ 0 \\ 0 \\ -\sin^2(\omega t) + \mathrm{i}\cos(\omega t)\sin(\omega t)\end{pmatrix}.$$

The results given above can be extend to the Hamilton operator

$$\hat{H} = \hbar\omega(\overbrace{\sigma_z\otimes\sigma_z\otimes\cdots\otimes\sigma_z}^{N\text{-factors}}) + \Delta(\overbrace{\sigma_x\otimes\sigma_x\otimes\cdots\otimes\sigma_x}^{N\text{-factors}})$$

with $N > 2$ and N even. For this case we also have

$$[\sigma_x\otimes\sigma_x\otimes\cdots\otimes\sigma_x, \sigma_z\otimes\sigma_z\otimes\cdots\otimes\sigma_z] = 0.$$

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