

# Spin Hamilton Operators, Symmetry Breaking, Energy Level Crossing and Entanglement

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**Abstract** We study finite-dimensional product Hilbert spaces, coupled spin systems, entanglement and energy level crossing. The Hamilton operators are based on the Pauli group. We show that swapping the interacting term can lead from unentangled eigenstates to entangled eigenstates and from an energy spectrum with energy level crossing to avoided energy level crossing.

## 1 Introduction

Let  $\mathcal{H}_1, \mathcal{H}_2$  be Hilbert spaces and  $\mathcal{H}_1 \otimes \mathcal{H}_2$  be the tensor product Hilbert space [1,2]. Quite often a self-adjoint Hamilton operator acting on the the tensor product Hilbert space  $\mathcal{H}_1 \otimes \mathcal{H}_2$  can be written as

$$\hat{H} = \hat{H}_1 \otimes I_2 + I_1 \otimes \hat{H}_2 + \epsilon \hat{V} \quad (1)$$

where the self-adjoint Hamilton operator  $\hat{H}_1$  acts in the Hilbert space  $\mathcal{H}_1$ , the self-adjoint Hamilton operator  $\hat{H}_2$  acts in the Hilbert space  $\mathcal{H}_2$ ,  $I_1$  is the identity operator acting in the Hilbert space  $\mathcal{H}_1$  and  $I_2$  is the identity operator acting in the Hilbert space  $\mathcal{H}_2$ . The self-adjoint operator  $\hat{V}$  acts in the product Hilbert space and  $\epsilon$  is a real parameter. The main task would be to find the spectrum of  $\hat{H}$ .

In the following we consider the finite-dimensional Hilbert space  $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^n$  and then  $\otimes$  denotes the Kronecker product [3,4,5,6]. Let  $I_n$  be the  $n \times n$  identity matrix. We consider the two hermitian Hamilton operators

$$\hat{H} = \alpha A \otimes I_n + I_n \otimes \beta B + \epsilon(A \otimes B) \quad (2)$$

$$\hat{K} = \alpha A \otimes I_n + I_n \otimes \beta B + \epsilon(B \otimes A) \quad (3)$$

where  $A, B$  are nonzero  $n \times n$  hermitian matrices and  $\alpha, \beta, \epsilon$  are real parameters with  $\epsilon \geq 0$ . We assume that  $[A, B] \neq 0$ . The vector space of the  $n \times n$  matrices over  $\mathbb{C}$  form a Hilbert space with the scalar product  $\langle X, Y \rangle := \text{tr}(XY^*)$ . We also assume that  $\langle A, B \rangle = 0$ , i.e. the nonzero  $n \times n$  hermitian matrices  $A$  and  $B$  are orthogonal to each other. Of particular interest would be the case where  $A$  and  $B$  are elements of a semi-simple Lie algebra. We discuss the eigenvalue problem for the two Hamilton operators and its connection with entanglement and energy level crossings for specific choices of  $A$  and  $B$ . In the following the matrices  $A$  and  $B$  are realized by Pauli spin matrices. The Hamilton operator will be a linear combination of elements of the Pauli group  $\mathcal{P}_n$ . The Pauli group [7] is defined by

$$\mathcal{P}_n := \{ I_2, \sigma_x, \sigma_y, \sigma_z \}^{\otimes n} \otimes \{ \pm 1, \pm i \}. \quad (4)$$

Such two-level and higher level quantum systems and their physical realization have been studied by many authors (see [8] and references therein). The thermodynamic behaviour is determined by the partition functions

$$Z_{\hat{H}}(\beta) = \text{tr}(\exp(-\beta\hat{H})), \quad Z_{\hat{K}}(\beta) = \text{tr}(\exp(-\beta\hat{K})).$$

Since

$$\text{tr}(\hat{H}) = \text{tr}(\hat{K}) = \alpha n \text{tr}(A) + \beta n \text{tr}(B) + \epsilon (\text{tr}(A))(\text{tr}(B))$$

the sum of the eigenvalues of the operators  $\hat{H}$  and  $\hat{K}$  are the same. However, in general, the partition functions will be different.

## 2 Commutators, Eigenvalues and Eigenvectors

Let us first summarize the equations we utilize in the following. Let  $A, B$  be  $n \times n$  matrices over  $\mathbb{C}$ . First note that we have the following commutators

$$[A \otimes I_n, I_n \otimes B] = 0, \quad [A \otimes I_n, A \otimes B] = 0, \quad [I_n \otimes B, A \otimes B] = 0$$

and

$$[A \otimes I_n, B \otimes A] = ([A, B]) \otimes A, \quad [I_n \otimes B, B \otimes A] = B \otimes ([B, A]).$$

The last two commutators would be 0 if  $[A, B] = 0$ . There is an  $n^2 \times n^2$  permutation matrix  $P$  (swap gate) such that

$$P(A \otimes B)P^{-1} = B \otimes A.$$

This implies that  $P(A \otimes I_n)P^{-1} = I_n \otimes A$  and  $P(I_n \otimes B)P^{-1} = B \otimes I_n$ .

Now let  $A$  and  $B$  be  $n \times n$  hermitian matrices. If the eigenvalues and normalized eigenvectors of  $A$  and  $B$  are  $\lambda_j, \mathbf{u}_j, \mu_j, \mathbf{v}_j, (j = 1, 2, \dots, n)$ , respectively, then the eigenvalues and normalized eigenvectors of the Hamilton operator (2) are given by [3, 4, 5, 6]

$$\alpha\lambda_j + \beta\mu_k + \epsilon\lambda_j\mu_k, \quad \mathbf{u}_j \otimes \mathbf{v}_k \quad j, k = 1, 2, \dots, n.$$

Thus the eigenvectors are not entangled since they can be written as product states. These results can be extended to the Hamilton operator

$$\hat{H} = \alpha(A \otimes I_n \otimes I_n) + \beta(I_n \otimes B \otimes I_n) + \gamma(I_n \otimes I_n \otimes C) + \epsilon(A \otimes B \otimes C)$$

and higher dimensions.

### 3 Pauli Spin Matrices and Entanglement

Since we realize the linear operators  $A$  and  $B$  by Pauli spin matrices we summarize some results for the Pauli spin matrices and their Kronecker products. Consider the Pauli spin matrices  $\sigma_z, \sigma_x, \sigma_y$ . The eigenvalues are given by  $+1$  and  $-1$  with the corresponding normalized eigenvectors

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

for  $\sigma_z, \sigma_x$  and  $\sigma_y$ , respectively. Consider now the three hermitian and unitary  $4 \times 4$  matrices  $\sigma_x \otimes \sigma_x, \sigma_y \otimes \sigma_y, \sigma_z \otimes \sigma_z$ . These matrices appear in Mermin's magic square [9] for the proof of the Bell-Kochen-Specker theorem. Since the eigenvalues of the Pauli matrices are given by  $+1$  and  $-1$ , the eigenvalues of the  $4 \times 4$  matrices  $\sigma_x \otimes \sigma_x, \sigma_y \otimes \sigma_y, \sigma_z \otimes \sigma_z$  are  $+1$  (twice) and  $-1$  (twice). The eigenvectors can be given as product states (unentangled states), but also as entangled states (i.e. they cannot be written as product states). Obviously

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

are four normalized product eigenstates of  $\sigma_z \otimes \sigma_z$ . The normalized product eigenstates of  $\sigma_x \otimes \sigma_x$  are

$$\frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad \frac{1}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \frac{1}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

The normalized product eigenstates of  $\sigma_y \otimes \sigma_y$  are

$$\frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix} \otimes \begin{pmatrix} i \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix} \otimes \begin{pmatrix} -i \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \end{pmatrix} \otimes \begin{pmatrix} i \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \end{pmatrix} \otimes \begin{pmatrix} -i \\ 1 \end{pmatrix}.$$

All three  $4 \times 4$  matrices also admit the Bell basis

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

as normalized eigenvectors which are maximally entangled. As measure for entanglement the tangle [5, 7, 10, 11] will be utilized.

Consider now the hermitian and unitary  $4 \times 4$  matrices  $\sigma_x \otimes \sigma_z$ ,  $\sigma_z \otimes \sigma_x$ . Since the eigenvalues of the Pauli matrices are given by  $+1$  and  $-1$ , the eigenvalues of the  $4 \times 4$  matrices  $\sigma_x \otimes \sigma_z$  and  $\sigma_z \otimes \sigma_x$ , are  $+1$  (twice) and  $-1$  (twice). The eigenvectors can be given as product states (unentangled states), but also as entangled states (i.e. they cannot be written as product states). The normalized product eigenstates of  $\sigma_x \otimes \sigma_z$  are

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

The normalized product eigenstates of  $\sigma_z \otimes \sigma_x$  are

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

The two  $4 \times 4$  matrices also admit

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

as normalized eigenvectors which are maximally entangled. Note that  $\sigma_y \otimes \sigma_y$  also admits these maximally entangled eigenvectors besides the Bell basis as eigenvectors and the product eigenvectors.

For the triple spin interaction term  $\sigma_x \otimes \sigma_y \otimes \sigma_z$  we obtain the eigenvalues  $+1$  (fourfold) and  $-1$  (fourfold) and all the eight product states as eigenstates given

by the eigenstates of  $\sigma_x, \sigma_y, \sigma_z$ . Owing to the degeneracies of the eigenvalues we also find fully entangled states such as

$$\frac{1}{2} (1 \ 1 \ 0 \ 0 \ 0 \ 0 \ i \ -i)^T$$

with the three-tangle as measure [11].

## 4 Examples

Consider now a specific example for  $\alpha A$  and  $\beta B$  with  $n = 2$  and  $\epsilon > 0$ . Utilizing the Pauli spin matrices

$$\alpha A = \hbar\omega_1\sigma_z, \quad \beta B = \hbar\omega_2\sigma_x$$

where  $\alpha = \hbar\omega_1$ ,  $\beta = \hbar\omega_2$  and  $\omega_1, \omega_2$  are the frequencies. Note that  $[\sigma_z, \sigma_x] = 2i\sigma_y$  and  $\text{tr}(\hat{H}) = 0$ ,  $\text{tr}(\hat{K}) = 0$ . The elements of the set

$$\{ I_2 \otimes I_2, \sigma_z \otimes I_2, I_2 \otimes \sigma_x, \sigma_z \otimes \sigma_x \}$$

form a commutative subgroup of the Pauli group  $\mathcal{P}_2$ . The elements  $\sigma_z \otimes I_2, I_2 \otimes \sigma_x, \sigma_x \otimes \sigma_z$  are generators of the Pauli group  $\mathcal{P}_2$ . Now the eigenvalues and eigenvectors of  $\alpha A$  are given by

$$\lambda_1 = \hbar\omega_1, \quad \mathbf{u}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \lambda_2 = -\hbar\omega_1, \quad \mathbf{u}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and the eigenvalues and eigenvectors of  $\beta B$  are given by

$$\mu_1 = \hbar\omega_2, \quad \mathbf{u}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \mu_2 = -\hbar\omega_2, \quad \mathbf{u}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

The Hamilton operator  $\hat{H}$  is given by the  $4 \times 4$  matrix which can be written as direct sum of two  $2 \times 2$  matrices

$$\tilde{H} = \begin{pmatrix} \hbar\omega_1 & \hbar\omega_2 + \epsilon & 0 & 0 \\ \hbar\omega_2 + \epsilon & \hbar\omega_1 & 0 & 0 \\ 0 & 0 & -\hbar\omega_1 & \hbar\omega_2 - \epsilon \\ 0 & 0 & \hbar\omega_2 - \epsilon & -\hbar\omega_1 \end{pmatrix}.$$

The eigenvalues of  $\tilde{H}$  are

$$\begin{aligned} E_1(\omega_1, \omega_2, \epsilon) &= \hbar\omega_1 + \hbar\omega_2 + \epsilon, & E_2(\omega_1, \omega_2, \epsilon) &= \hbar\omega_1 - \hbar\omega_2 - \epsilon \\ E_3(\omega_1, \omega_2, \epsilon) &= -\hbar\omega_1 + \hbar\omega_2 - \epsilon, & E_4(\omega_1, \omega_2, \epsilon) &= -\hbar\omega_1 - \hbar\omega_2 + \epsilon \end{aligned}$$

with the corresponding eigenvectors (which can be written as product states)

$$\begin{aligned} & \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \\ & \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \end{aligned}$$

The Hamilton operator  $\hat{K}$  is given by the  $4 \times 4$  matrix

$$\tilde{K} = \begin{pmatrix} \hbar\omega_1 & \hbar\omega_2 & \epsilon & 0 \\ \hbar\omega_2 & \hbar\omega_1 & 0 & -\epsilon \\ \epsilon & 0 & -\hbar\omega_1 & \hbar\omega_2 \\ 0 & -\epsilon & \hbar\omega_2 & -\hbar\omega_1 \end{pmatrix}$$

with the four eigenvalues

$$\begin{aligned} k_1(\omega_1, \omega_2, \epsilon) &= -\sqrt{\hbar^2(\omega_1 + \omega_2)^2 + \epsilon^2}, \\ k_2(\omega_1, \omega_2, \epsilon) &= \sqrt{\hbar^2(\omega_1 + \omega_2)^2 + \epsilon^2}, \\ k_3(\omega_1, \omega_2, \epsilon) &= -\sqrt{\hbar^2(\omega_1 - \omega_2)^2 + \epsilon^2}, \\ k_4(\omega_1, \omega_2, \epsilon) &= \sqrt{\hbar^2(\omega_1 - \omega_2)^2 + \epsilon^2} \end{aligned}$$

and the corresponding unnormalized eigenvectors

$$\begin{aligned} & \begin{pmatrix} \epsilon \\ \epsilon \\ k_1 - \hbar(\omega_1 + \omega_2) \\ k_2 + \hbar(\omega_1 + \omega_2) \end{pmatrix}, \quad \begin{pmatrix} \epsilon \\ \epsilon \\ k_2 - \hbar(\omega_1 + \omega_2) \\ k_1 + \hbar(\omega_1 + \omega_2) \end{pmatrix}, \\ & \begin{pmatrix} \epsilon \\ -\epsilon \\ k_3 - \hbar(\omega_1 - \omega_2) \\ k_4 - \hbar(\omega_1 - \omega_2) \end{pmatrix}, \quad \begin{pmatrix} \epsilon \\ -\epsilon \\ k_4 - \hbar(\omega_1 - \omega_2) \\ k_3 + \hbar(\omega_1 - \omega_2) \end{pmatrix}. \end{aligned}$$

Thus for the Hamilton operator  $\hat{H}$  we have energy level crossing [10,12] which is due to the discrete symmetry of the Hamilton operator  $\hat{H}$ . For the Hamilton operator  $\hat{K}$  we have no energy level crossing for  $\epsilon > 0$ . The symmetry is broken. For  $\epsilon \rightarrow \infty$  and fixed frequencies the eigenvalues for the two Hamilton operators approach  $\epsilon$  (twice) and  $-\epsilon$  (twice). The four eigenvectors are entangled for  $\epsilon > 0$ .

Extensions to higher order spin systems are straightforward. An extension is to study the Hamilton operators with triple spin interactions

$$\begin{aligned}\hat{H} = & \hbar\omega_1(\sigma_x \otimes I_2 \otimes I_2) + \hbar\omega_2(I_2 \otimes \sigma_y \otimes I_2) + \hbar\omega_3(I_2 \otimes I_2 \otimes \sigma_z) \\ & + \gamma_{12}(\sigma_x \otimes \sigma_y \otimes I_2) + \gamma_{13}(\sigma_x \otimes I_2 \otimes \sigma_z) + \gamma_{23}(I_2 \otimes \sigma_y \otimes \sigma_z) \\ & + \epsilon(\sigma_x \otimes \sigma_y \otimes \sigma_z)\end{aligned}$$

and

$$\begin{aligned}\hat{K} = & \hbar\omega_1(\sigma_x \otimes I_2 \otimes I_2) + \hbar\omega_2(I_2 \otimes \sigma_y \otimes I_2) + \hbar\omega_3(I_2 \otimes I_2 \otimes \sigma_z) \\ & + \gamma_{12}(\sigma_x \otimes \sigma_y \otimes I_2) + \gamma_{13}(\sigma_x \otimes I_2 \otimes \sigma_z) + \gamma_{23}(I_2 \otimes \sigma_y \otimes \sigma_z) \\ & + \epsilon(\sigma_z \otimes \sigma_y \otimes \sigma_x).\end{aligned}$$

Triple spin interacting systems have been studied by several authors [13,14,15]. For  $\hat{H}$  we find the eight product states given by the eigenstates of  $\sigma_x, \sigma_y, \sigma_z$ . We also have energy level crossing owing to the symmetry of the Hamilton operator  $\hat{H}$ . For the Hamilton operator  $\hat{K}$  the symmetry is broken and no level crossing occurs. We also find entangled states for this Hamilton operator. As an entanglement measure the three-tangle can be used [11]. Also the permutations  $\sigma_z \otimes \sigma_x \otimes \sigma_y, \sigma_y \otimes \sigma_z \otimes \sigma_x$  of the interacting term could be investigated.

The question discussed in the introduction could also be studied for Bose systems with a Hamilton operator such as

$$\hat{H} = \alpha(b^\dagger b \otimes I) + \beta(I \otimes (b^\dagger + b)) + \gamma(b^\dagger b \otimes (b^\dagger + b))$$

where  $I$  is the identity operator and  $\otimes$  denotes the tensor product.

In conclusion we have shown that swapping the terms in the interacting part of Hamilton operators acting in a product Hilbert space breaks the symmetry and thus the behaviour about entanglement and energy level crossing will change.

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