Application of the Kronecker product to simple spin systems

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Abstract

We show that the well known Kronecker product is a suitable tool for the construction of matrix representations of widely used spin Hamiltonians. In this way we avoid the explicit use of basis sets for the construction of the matrix elements. As illustrative examples we discuss two isotropic models and an anisotropic one.

1 Introduction

In a recent paper we discussed two different operator products in quantum mechanics [1]. We showed that one of them, the Kronecker or direct product, is particularly useful for treating the coupling of spin systems and for the study of the structure of NMR lines. In this paper we are interested in the application of this product to another spin model of practical utility.

The Breit-Rabi Hamiltonian provides a reasonable description of the behaviour of a one-electron atom in a magnetic field. Earlier pedagogical articles focused on the crossings and avoided crossings between pairs of energy levels predicted by this model [2][3]. The purpose of this paper is to illustrate the util-

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ity of the Kronecker product in the construction of the matrix representation of the Breit-Rabi Hamiltonian as well as of other spin models.

In section 2 we outline the necessary equations based on the Kronecker product. In sections 3 and 4 we apply the technique to two isotropic models with nuclear spin 1/2 and 3/2, respectively. In section 5 we briefly consider an anisotropic model and in section 6 we summarize the main results and draw conclusions.

2 The Kronecker product

Here we just summarize that part of the direct product that is relevant for present purposes. For further details the reader is referred to our earlier paper [1]. The Kronecker product $A \otimes B$ of an $N \times N$ matrix $A$ and an $M \times M$ matrix $B$ is an $NM \times NM$ matrix with elements $A_{ni}B_{mj}$, $n, i = 1, 2, \ldots N$, $m, j = 1, 2, \ldots , M$. In order to construct the Kronecker product $A \otimes B$ we just follow a simple and straightforward rule: substitute $A_{ij}B$ for every element $A_{ij}$ of $A$; for example:

$$
\begin{pmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{pmatrix}
\otimes
\begin{pmatrix}
B_{11} & B_{12} \\
B_{21} & B_{22}
\end{pmatrix} =
\begin{pmatrix}
A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12} \\
A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{12}B_{22} \\
A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12} \\
A_{21}B_{21} & A_{21}B_{22} & A_{22}B_{21} & A_{22}B_{22}
\end{pmatrix}.
$$

(1)

3 First isotropic model

The Breit-Rabi formula [4] for the interaction between an electron and a nucleus in a magnetic field is commonly derived from the Hamiltonian

$$
H_{BR} = AI \cdot S + B (aS_z + bI_z),
$$

(2)

where $I$ and $S$ are the nuclear and electronic spins, respectively, the magnetic field of intensity $B$ is supposed to be along the $z$ axis, $A$ is a measure of the cou-
pling between the nuclear and electronic magnetic moments and the constants \(a\) and \(b\) are related to the electronic and nuclear gyromagnetic ratios and the Bohr magneton \([2, 3]\).

In order to obtain a suitable matrix representation of the Hamiltonian \([2]\) most authors resort to a basis set given by the direct product of nuclear and electronic spin eigenvectors \([3, 5, 6]\)

\[
|m_s, m_I\rangle = |S, m_S\rangle \otimes |I, m_I\rangle, \quad m_S = -S, -S+1, \ldots, S; \quad m_I = -I, -I+1, \ldots, I.
\]

In this expression \(|S, m_S\rangle\) is an eigenvector of \(S^2\) and \(S_z\) and \(|I, m_I\rangle\) an eigenvector of \(I^2\) and \(I_z\). In order to calculate the matrix elements \(\langle m_s, m_I | I \cdot S | m'_s, m'_I \rangle\) one can, for example, express the operators \(I_x, I_y, S_x\) and \(S_y\) in terms of ladder operators. However, the straightforward application of the Kronecker product appears to be simpler as shown in what follows.

The matrix representation of the operator \(H_{BR}\) is straightforwardly given by

\[
H_{BR} = A (I_x \otimes S_x + I_y \otimes S_y + I_z \otimes S_z) + B [a I_d (2I + 1) \otimes S_z + b I_z \otimes I_d (2)],
\]

where \(I_d (n)\) is the identity matrix of dimension \(n\) and \(I_u\) and \(S_u\) are the well known nuclear and electronic spin matrices. Obviously, for the electron we have the Pauli matrices

\[
S_x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
\]

in units of \(\hbar\). In what follows we consider two cases with different nuclear spin.

In the simplest case \(I = 1/2\) the nuclear spin matrices are identical to \([5]\)

\[
I_x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad I_y = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad I_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
\]
and the straightforward application of the Kronecker formula (4) leads to

\[ H_{BR} = \frac{1}{4} \begin{pmatrix} A + 2B(a + b) & 0 & 0 & 0 \\ 0 & 2B(b - a) - A & 2A & 0 \\ 0 & 2A & 2B(a - b) - A & 0 \\ 0 & 0 & 0 & A - 2B(a + b) \end{pmatrix}. \]  

(7)

This matrix does not agree with those shown by Bhattacharya [3] and Oh et al [6] which also differ from each other. The three matrices are, however, equivalent; for example

\[ U_1 H_{BR} U_1^T = H_{BR}^B, \]

where \( H_{BR}^B \) is Bhattacharya’s matrix and \( U_1 \) is the orthogonal one

\[ U_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} = U_1^T = U_1^{-1}, \]  

(8)

where \( T \) stands for transpose. Analogously, the relation with the matrix of Oh et al is

\[ U_2 H_{BR} U_2^T = H_{BR}^{OHKP}, \]

where

\[ U_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = U_2^T = U_2^{-1}. \]  

(9)

Clearly, \( H_{BR}, H_{BR}^B \) and \( H_{BR}^{OHKP} \) are isospectral and, consequently, equivalent representations of the same Hamiltonian \( H_{BR} \). Note that the straightforward application of the Kronecker product is equivalent to choosing a particular order in the basis set [3] which does not agree with the order chosen by those other authors. The unitary transformations given by the matrices (8) and (9) are just two particular permutations of the basis functions.

The matrix (7) is the direct sum of two \( 1 \times 1 \) and one \( 2 \times 2 \) matrices. A matrix with this property is commonly called block-diagonal and it is well known that its determinant is the product of the determinants of each block. Therefore, the
characteristic polynomial \( P(E) = \det (H_{BR} - E I_d(4)) \) has a particularly simple form:

\[
P(E) = \frac{1}{256} [4E - A - 2B (a + b)] [4E - A + 2B (a + b)] \times \\
[16E^2 + 8AE - 3A^2 - 4B^2 (a - b)^2]
\]

(10)

We realize that the problem of obtaining the four eigenvalues of \( H_{BR} \) reduces to solving a quadratic equation because two eigenvalues are already known. The eigenvalues of this matrix were discussed in detail in earlier papers [3][4]; here we are mainly interested in a simpler construction of the matrix representation of the Hamiltonian operator.

4 Second isotropic model

The next example is the case of a nucleus with spin \( I = 3/2 \). The spin matrices are given by

\[
I_x = \frac{1}{2} \begin{pmatrix}
0 & \sqrt{3} & 0 & 0 \\
\sqrt{3} & 0 & 2 & 0 \\
0 & 2 & 0 & \sqrt{3} \\
0 & 0 & \sqrt{3} & 0
\end{pmatrix},
\]

\[
I_y = \frac{1}{2i} \begin{pmatrix}
0 & \sqrt{3} & 0 & 0 \\
-\sqrt{3} & 0 & 2 & 0 \\
0 & -2 & 0 & \sqrt{3} \\
0 & 0 & -\sqrt{3} & 0
\end{pmatrix},
\]

\[
I_z = \frac{1}{2} \begin{pmatrix}
3 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -3
\end{pmatrix}.
\]

(11)

Straightforward application of the Kronecker formula (4) yields
\[ H_{BB} = \frac{1}{4} \begin{pmatrix}
3A + 2B(a + 3b) & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2B(b - a) - 3A & 2\sqrt{3}A & 0 & 0 & 0 & 0 \\
0 & 2\sqrt{3}A & A + 2B(a + b) & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 3B(b - a) - A & 4A & 0 & 0 \\
0 & 0 & 0 & 4A & 2B(a - b) - A & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & A - 2B(a + b) & 2\sqrt{3}A \\
0 & 0 & 0 & 0 & 0 & 2\sqrt{3}A & 2B(a - 3b) - 3A \\
0 & 0 & 0 & 0 & 0 & 0 & 3A - 2B(a + 3b)
\end{pmatrix} \]
This matrix differs from the one shown by Bhattacharya and Raman \[5\] in the order of some matrix elements. Both matrices are, however, equivalent since they are related by the orthogonal matrix

$$ U = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}. $$ \(13\)

The matrix \(12\) is the direct sum of two \(1 \times 1\) and three \(2 \times 2\) matrices and, consequently, its characteristic polynomial can be written as the product of polynomials of smaller degree:

$$ P(E) = \frac{1}{65536} [4E - 3A - 2B (a + 3b)] [4e - 3A + 2B (a + 3b)] \times [16E^2 + 8AE - 15A^2 - 4B^2 (a - b)^2] \times [16E^2 + 8E (A + 4Bb) - 15A^2 + 4B (2Aa + B (a + b) (3b - a))] \times \left[16E^2 + 8E (A - 4Bb) - 15A^2 - 4B (2Aa + B (a + b) (a - 3b))\right]. $$ \(14\)

Once again, the calculation of the eigenvalues of the matrix representation \(H_{BR}\) reduces to the calculation of the roots of quadratic equations.

### 5 Anisotropic model

In the examples above we have just considered isotropic cases, but the application of the Kronecker-product approach to anisotropic models is straightforward. For example, suppose that

$$ H = \beta_1 S^T \cdot g \cdot B + S^T \cdot A \cdot I - \beta_n I^T \cdot g_n \cdot B, $$ \(15\)
where $S$ and $I$ are column matrices with components $S_x$, $S_y$, $S_z$ and $I_x$, $I_y$ and $I_z$, respectively, and $g$, $A$, and $g_n$ are $3 \times 3$ matrices \([2]\). In order to apply the Kronecker product we rewrite it as
\[
H = a_1 I_x + a_2 I_y + a_3 I_z + b_1 S_x + b_2 S_y + b_3 S_z + c_{11} I_x S_x + c_{12} I_x S_y + c_{13} I_x S_z + c_{23} I_y S_z,
\]
where we have omitted the identity operators in the linear terms; for example $I_u \otimes \hat{1}_S$ or $\hat{1}_I \otimes S_u$ (see our earlier paper for more details \([1]\)).

The matrix representation of the Hamiltonian can then be easily obtained from
\[
H_A = \frac{1}{4} \begin{pmatrix}
2 (a_3 + b_3) & 2b_1 - 2ib_2 & 2a_1 + c_{13} - i(2a_2 + c_{23}) & c_{11} - ic_{12} \\
2b_1 + 2ib_2 & 2(a_3 - b_3) & c_{11} + ic_{12} & 2a_1 - c_{13} + i(c_{23} - 2a_2) \\
2a_1 + c_{13} + i(2a_2 + c_{23}) & c_{11} - ic_{12} & 2(b_3 - a_3) & 2b_1 + 2ib_2 \\
c_{11} + ic_{12} & 2a_1 - c_{13} + i(c_{23} - 2a_2) & 2(b_3 - a_3) & -2(a_3 + b_3)
\end{pmatrix}
\]
that contains the matrix (7) as a particular case. In this case the matrix $H_A - EI_d(4)$ is not block-diagonal and the characteristic polynomial will not exhibit a simple form; consequently, we will have to solve the characteristic polynomial of fourth order. However, the point is that the construction of the matrix representation of the Hamiltonian (16) is greatly facilitated by the straightforward application of the Kronecker product.

6 Conclusions

The aim of this sequel of our earlier paper \([1]\) is to show that one can easily obtain the matrix representation of a wide variety of spin Hamiltonians without resorting to a basis set and ladder operators for the calculation of the matrix elements. The straightforward application of the Kronecker product yields the desired result. To this end it is only necessary to have the matrix
representations of the spin matrices of all the particles in the Hamiltonian operator. This approach is particularly appealing if one has a suitable program for the calculation of the Kronecker product within a computer algebra system. In the present case we resorted to the computer algebra system Derive (https://education.ti.com/en/us/home) and one of the Kronecker-product programs contributed to the Derive User Group (http://www.austromath.at/dug/).

The examples discussed in the preceding sections clearly illustrate the remarkable simplicity of the Kronecker-product method. Note that we used basically the same formula for the isotropic cases with $I = 1/2$ and $I = 3/2$ and we easily adapted it to the anisotropic case with $I = 1/2$.

The spin matrices necessary for the application of the Kronecker product are easily obtained by means of the commutation properties of the spin operators. The analytic expressions for the matrix elements are well known and therefore available from several sources (see, for example, [http://easyspin.org/documentation/spinoperators.html](http://easyspin.org/documentation/spinoperators.html)).

**References**

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