SYMmetric Kronecker Products and Semiclassical wave packets

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abstract. we investigate the iterated kronecker product of a square matrix with itself and prove an invariance property for symmetric subspaces. This motivates the definition of an iterated symmetric kronecker product as a restriction of the iterated product on a symmetric subspace and the derivation of an explicit formula for its action on vectors. we apply our result for describing a linear change in the matrix parametrization of semiclassical wave packets.

1. introduction

the kronecker product of matrices is known to be ubiquitous \[vl00\], and our aim here is to investigate the \(n\)-fold kronecker product of a complex square matrix \(M \in \mathbb{C}^{d \times d}\) with itself,

\[
M^n \otimes = M \otimes \cdots \otimes M \tag{1}
\]

\(n \times \) times \(n \in \mathbb{N}\),

and to apply our findings to the parametrization of semiclassical wave packets.

1.1. the motivation. we encountered a variant of the \(n\)-fold kronecker product when studying linear changes in the parametrization of semiclassical wave packets. semiclassical wave packets have first been proposed in \[hag85\] as a multivariate non-isotropic generalization of the hermite functions. see also \[hag98\]. a family of semiclassical wave packets

\[
\{ \varphi_k[A, B; a, \eta] : k \in \mathbb{N}^d \}
\]

is parametrized by two invertible complex matrices \(A, B \in \text{GL}(d, \mathbb{C})\) and two real vectors \(a, \eta \in \mathbb{R}^d\). it forms an orthonormal basis of the hilbert space of square integrable functions. here, we focus on the more delicate dependence on the parametrizing matrices \(A\) and \(B\). we therefore take \(a = \eta = 0\) and simply write \(\varphi_k[A, B]\) for the corresponding wave packet. a wave packet with \(|k| = n\) is the product of a multivariate polynomial of order \(n\) times a complex-valued gaussian.

if the parameter matrix \(A\) has real entries only, then the polynomial can be factorized into univariate hermite polynomials. a linear change of the parametrization,

\[
A' = AM, \quad B' = BM
\]

for some \(M \in \text{GL}(d, \mathbb{C})\),

results in a formula for the wave packet \(\varphi_k[A', B']\) involving wave packets in the old parametrization weighted by coefficients stemming from the \(n\)-fold kronecker product \(M^n \otimes\). the following analysis will reveal the relevant symmetric subspaces.

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and corresponding orthogonal projections such that the resulting \( n \)-fold symmetric Kronecker product explicitly describes the wanted change of the parametrization.

1.2. Two-fold symmetric Kronecker products. In semidefinite programming (See for example [AHO98] or [Kle02, Appendix E]), the two-fold Kronecker product has notably occurred in combination with subspaces of a particular symmetry property. One considers the space

\[
X_2 = \{ x \in \mathbb{C}^{d^2} : x = \text{vec}(X), X = X^t \in \mathbb{C}^{d \times d} \},
\]

that contains those vectors that can be obtained by the row-wise vectorization of a complex symmetric \( d \times d \) matrix, that is, a complex matrix coinciding with its transpose matrix. The dimension of the space \( X_2 \) is

\[
L_2 = \frac{1}{2} d (d + 1).
\]

One can prove that this space is invariant under Kronecker products, in the sense that for all matrices \( M \in \mathbb{C}^{d \times d} \), one has

\[
(M \otimes M) x \in X_2, \quad \text{whenever} \quad x \in X_2.
\]

Now one uses the standard basis of \( \mathbb{C}^{d^2} \) for constructing an orthonormal basis of the subspace \( X_2 \) and defines a corresponding sparse \( L_2 \times d^2 \) matrix \( P_2 \) that has the basis vectors as its rows. The symmetric Kronecker product of \( M \) with itself is then the \( L_2 \times L_2 \) matrix

\[
S_2(M) = P_2 (M \otimes M) P_2^*.
\]

1.3. \( n \)-fold symmetric Kronecker products. How does one extend this construction to symmetrizing \( n \)-fold Kronecker products? It is instructive to revisit the second order space in two dimensions and to write a vector \( x \in X_2 \) as

\[
x = (x_{(2,0)}, x_{(1,1)}, x_{(1,1)}, x_{(0,2)})^t.
\]

This labelling uses the multi-indices \( k = (k_1, k_2) \in \mathbb{N}^2 \) with \( k_1 + k_2 = 2 \) in the redundant enumeration

\[
\nu_2 = ((2, 0), (1, 1), (1, 1), (0, 2)).
\]

This description allows for a straightforward extension to higher order \( n \) and dimension \( d \). One works with a redundant enumeration of the multi-indices \( k = (k_1, \ldots, k_d) \in \mathbb{N}^d \) with \( k_1 + \cdots + k_d = n \), collects them in a row vector \( \nu_n \), and defines

\[
X_n = \{ x \in \mathbb{C}^{d^n} : \text{For all } j, j' \in \{1, \ldots, d^n\}, x_j = x_{j'} \text{ if } \nu_n(j) = \nu_n(j') \}.
\]

The dimension of \( X_n \) equals the number of multi-indices in \( \mathbb{N}^d \) of order \( n \), that is the binomial coefficient

\[
L_n = \binom{n + d - 1}{n}.
\]

And again, we can prove invariance in the sense that for all \( M \in \mathbb{C}^{d \times d} \)

\[
M^\otimes n \otimes x \in X_n, \quad \text{whenever} \quad x \in X_n.
\]

See Proposition[2]. Then, we use the standard basis of \( \mathbb{C}^{d^n} \) to build an orthonormal basis of \( X_n \) and assemble the corresponding sparse \( L_n \times d^n \) matrix \( P_n \). All this motivates the definition of the \( n \)-fold symmetric Kronecker product as

\[
S_n(M) = P_n M^\otimes n P_n^*.
\]
The matrix $S_n(M)$ is of size $L_n \times L_n$ and inherits structural properties as invertibility or unitarity from the matrix $M$. See Lemma 5.

Our main result Theorem 1 provides an explicit formula for the action of the matrix $S_n(M)$ in terms of multinomial coefficients and powers of the entries of the original matrix $M$. Labelling the components of a vector $y \in \mathbb{C}^{L_n}$ by multi-indices of order $n$, we obtain for all $k \in \mathbb{N}^d$ with $|k| = n$ that

$$(S_n(M)y)_k = \frac{1}{\sqrt{k!}} \sum_{|\alpha_1| = k_1} \cdots \sum_{|\alpha_d| = k_d} \binom{k_1}{\alpha_1} \cdots \binom{k_d}{\alpha_d} m_1^{\alpha_1} \cdots m_d^{\alpha_d} \times \sqrt{(\alpha_1 + \cdots + \alpha_d)!} \ y_{\alpha_1 + \cdots + \alpha_d},$$

where $m_1, \ldots, m_d \in \mathbb{C}^d$ denote the row vectors of $M$. The summations range over multi-indices $\alpha_1, \ldots, \alpha_d \in \mathbb{N}^d$ with $|\alpha_1| = k_1, \ldots, |\alpha_d| = k_d$. They are weighted with multinomial coefficients stemming from the $n$-fold Kronecker product $M^n \otimes$, whereas the square roots of the factorials originate in the orthonormalization of the row vectors of the matrix $P_n$.

1.4. Application to semiclassical wave packets. We consider semiclassical wave packets $\varphi_k[A, B]$, $k \in \mathbb{N}^d$, parametrized by two matrices $A, B \in \text{GL}(d, \mathbb{C})$. The $k$th wave packet is the product of a multivariate polynomial $p_k[A]$ and the complex-valued Gaussian function

$$\varphi_0[A, B](x) = (\pi \hbar)^{-d/4} \ det(A)^{-1/2} \exp \left( -\frac{\langle x, BA^{-1}x \rangle}{2 \hbar} \right), \quad x \in \mathbb{R}^d,$$

where $\hbar > 0$ is the semiclassical parameter used for the overall scaling. See Definition 2. The polynomial family

$$\{p_k[A] : k \in \mathbb{N}^d\}$$

obeys a three-term recurrence relation and a Rodrigues type representation. See [LT14] Proposition 4 and [Hag15] Theorem 4.1. It is orthogonal with respect to the Gaussian weight function $|\varphi_0[A, B](x)|^2$, but differs from the standard Hermite polynomials on $\mathbb{R}^d$ that are biorthogonal and not orthogonal. See for example [IZ17] §6. If the matrix $A$ is real, then the polynomials $p_k[A]$ are real and factorize into univariate scaled Hermite polynomials. In the complex case, we encounter a more intricate structure that we wish to explore both for theoretical and numerical reasons.

We consider a change of parametrization

$$A' = AM, \quad B' = BM$$

induced by a suitably chosen invertible matrix $M \in \text{GL}(d, \mathbb{C})$. Collecting all wave packets $\varphi_k[A, B]$ of order $|k| = n$ as the components of a formal vector of wave functions $\varphi_n[A, B]$, the formula of Theorem 1 allows us to identify the change of parametrization explicitly as

$$\varphi_n[A', B'] = \det(M)^{-1/2} S_n(M) \varphi_n[A, B],$$

see Corollary 1 in Section 5.3. That is, the $n$-fold symmetric Kronecker product explicitly transforms one parametrization into another one.
Recently, E. Faou, V. Gradinaru, and C. Lubich \([\text{FGL09, Lub08}]\) have used semiclassical wave packets for the numerical discretization of semiclassical quantum dynamics. See also \([\text{GH14}]\). The computationally demanding step of this method is the assembly of the Galerkin matrix for the potential function \(V : \mathbb{R}^d \rightarrow \mathbb{R}\) according to

\[
\langle \varphi_{\mathbf{k}}[A, B], V \varphi_{\mathbf{l}}[A, B] \rangle = \int_{\mathbb{R}^d} \varphi_{\mathbf{k}}[A, B](x) V(x) \varphi_{\mathbf{l}}[A, B](x) \, dx,
\]

where the multi-indices \(\mathbf{k}, \mathbf{l} \in \mathbb{N}^d\) are bounded in modulus by some truncation value \(N \in \mathbb{N}\), that determines the dimension of the Galerkin space. If the wave packets are parametrized by a matrix \(A\) that has only real entries, then they factorize into univariate Hermite functions, and the multi-dimensional integral becomes the product of one-dimensional ones. \([\text{B17, Chapter 5.9}]\) presents a two-dimensional numerical test case, transforming a linear combination of semiclassical wave packets of order \(n = 4\) from one parametrization to another one using a tree-based implementation of the \(n\)-fold symmetric Kronecker product. The transformation error is in the order of machine precision. This experiment suggests a new numerical method for semiclassical quantum dynamics using the change of parametrization via \(n\)-fold symmetric Kronecker products. Such a method assembles the Galerkin matrix in terms of univariate Hermite functions. Then, the known large order asymptotics of the Hermite functions should allow one to stabilize the numerical evaluation of the integrands \([\text{TTO16}]\), such that larger values of the truncation value \(N\) become feasible.

1.5. **Organization of the paper.** In the next Section, we start with some combinatorics for explicitly relating the lexicographic enumeration of multi-indices of order \(n\) with the redundant enumeration \(\mathbf{\nu}_n\). Then we introduce the symmetric subspaces \(X_n\) in Section 3 and construct an orthonormal basis together with the corresponding matrix \(P_n\). There we also discuss symmetric subspaces and our basis construction in tensor terminology. In Section 4 we define the \(n\)-fold symmetric Kronecker product and prove our main results Proposition 2 and Theorem 1. An introduction to semiclassical wave packets and the description of linear changes in their parametrization by symmetric Kronecker products is given in Section 5.

1.6. **Notation.** Vectors and multi-indices are bold. On some occasions we shall use the binomial coefficient

\[
\binom{n}{j} = \frac{n!}{(n-j)!j!}, \quad \text{for non-negative integers } n \geq j.
\]

We write a multi-index \(\mathbf{k} \in \mathbb{N}^d\) as a row vector \(\mathbf{k} = (k_1, \ldots, k_d)\). We use the modulus \(|\mathbf{k}| = k_1 + \cdots + k_d\), and the multinomial coefficient

\[
\binom{|\mathbf{k}|}{\mathbf{k}} = \frac{|\mathbf{k}|!}{k_1! \cdots k_d!}, \quad \text{for } \mathbf{k} \in \mathbb{N}^d.
\]

We adopt the convention that any multinomial coefficient with any negative argument is defined to be 0. We also use the \(k^{\text{th}}\) power of a vector,

\[
\mathbf{x}^k = x_1^{k_1} \cdots x_d^{k_d}, \quad \mathbf{x} \in \mathbb{C}^d.
\]
2. Combinatorics

2.1. Reverse Lexicographic ordering. First we enumerate the set multi-indices of order \( n \) in \( d \) dimensions,

\[
\{ \mathbf{k} \in \mathbb{N}^d : |\mathbf{k}| = n \}, \quad n \in \mathbb{N},
\]

in reverse lexicographic ordering and collect them as components of a formal row vector denoted by \( \ell_n \). The length of the vector \( \ell_n \) is the binomial coefficient

\[
L_n = \binom{n + d - 1}{n}
\]

One can think of this in the following way [JHT]: The multi-indices \( \mathbf{k} \) of order \( n \) in \( d \) dimensions are in a one-to-one correspondence with the sequence \( s \) of \( n \) identical balls and \( d - 1 \) identical sticks. The sticks partition the line into \( d \) bins into which one can insert the \( n \) balls. (The first bin is to the left of all the sticks, and contains \( k_1 \) balls; the last bin is to the right of all the sticks, and contains \( k_d \) balls; for \( 2 \leq j \leq d - 1 \), the \( j \)th bin is between sticks \( j - 1 \) and \( j \), and it contains \( k_j \) balls.) E.g., the multi-index \((3, 2, 0, 1)\) in four dimensions corresponds to

\[
\bullet \bullet \bullet | \bullet \bullet | \bullet | \bullet
\]

If all these objects were distinguishable, there would be \((n + d - 1)!\) permutations, but since the balls are all identical, one must divide by \( n! \), and since the sticks are all identical, one must divide by \((d - 1)!\).

2.2. A redundant enumeration. Next we redundantly enumerate and collect multi-indices of modulus \( n \) in a vector \( \nu_n \) of length \( d^n \). Each entry of the vector \( \nu_n \) is a multi-index of modulus \( n \). Some of these entries occur repeatedly, since our enumeration is redundant. We proceed recursively and set

\[
\nu_0 = ((0, \ldots, 0)), \quad \nu_1 = (e_1^t, \ldots, e_d^t),
\]

and

\[
\nu_{n+1} = \text{vec}\left( \begin{array}{c}
\nu_n(1) + e_1^t & \cdots & \nu_n(d^n) + e_1^t \\
\vdots & \ddots & \vdots \\
\nu_n(1) + e_d^t & \cdots & \nu_n(d^n) + e_d^t
\end{array} \right), \quad n \geq 0,
\]

where \( e_1, \ldots, e_d \in \mathbb{C}^d \) are the standard basis vectors of \( \mathbb{C}^d \), and vec denotes the row-wise vectorization of a matrix into a row vector.

For example, for \( d = 2 \), we have

\[
\ell_1 = ((1, 0), (0, 1)), \\
\nu_1 = ((1, 0), (0, 1)), \\
\ell_2 = ((2, 0), (1, 1), (0, 2)), \\
\nu_2 = ((2, 0), (1, 1), (1, 1), (0, 2)), \\
\ell_3 = ((3, 0), (2, 1), (1, 2), (0, 3)), \\
\nu_3 = ((3, 0), (2, 1), (2, 1), (1, 2), (2, 1), (1, 2), (1, 2), (0, 3)).
\]

We observe that the multi-index \((1, 1)\) appears twice in \( \nu_2 \), since

\[
(1, 1) = \nu_1(1) + e_2^t = \nu_1(2) + e_1^t.
\]
The modulus three multi-index \((2, 1)\) can be generated as
\[
(2, 1) = \nu_2(1) + e_2^t = \nu_2(2) + e_1^t = \nu_2(3) + e_1^t,
\]
and therefore appears three times in \(\nu_3\).

2.3. A partition. For relating the lexicographic and the redundant enumeration, we define the mapping
\[
\sigma_n : \{1, \ldots, L_n\} \to \mathcal{P}(\{1, \ldots, d^n\})
\]
so that for all \(i \in \{1, \ldots, L_n\}\) and \(j \in \{1, \ldots, d^n\}\) the following holds:
\[
j \in \sigma_n(i) \iff \nu_n(j) = \ell_n(i).
\]

For example, for \(d = 2\), we have
\[
\sigma_2(1) = \{1\}, \quad \sigma_2(2) = \{2, 3\}, \quad \sigma_2(3) = \{4\}
\]
and
\[
\sigma_3(1) = \{1\}, \quad \sigma_3(2) = \{2, 3, 5\}, \quad \sigma_3(3) = \{4, 6, 7\}, \quad \sigma_3(4) = \{8\}.
\]

We observe the following partition property.

**Lemma 1.** We have
\[
\#\sigma_n(i) = \binom{n}{\ell_n(i)}, \quad i = 1, \ldots, L_n,
\]
and
\[
\bigcup_{i=1,\ldots,L_n} \sigma_n(i) = \{1, \ldots d^n\}, \text{ where the union is pairwise disjoint.}
\]

**Proof.** We first prove that we have a partition property. For any \(j \in \{1, \ldots, d^n\}\) there exists \(i \in \{1, \ldots, L_n\}\) so that \(\nu_n(j) = \ell_n(i)\). So, we clearly have
\[
\bigcup_{i=1,\ldots,L_n} \sigma_n(i) = \{1, \ldots, d^n\}.
\]
Moreover, since \(j \in \sigma_n(i) \cap \sigma_n(i')\) is equivalent to \(\ell_n(i) = \ell_n(i')\), that is, \(i = i'\), the union is disjoint.

For proving the claimed cardinality, we argue by induction. For \(n = 0\), we have
\[
\ell_0 = ((0, \ldots, 0)) = \nu_0, \quad \sigma_0(1) = \{1^0\}, \quad \#\sigma_0(1) = 1.
\]

For the inductive step, we observe that in the redundant enumeration \(\nu_n\), the multi-index \(k = (k_1, \ldots, k_d)\) can be generated from \(d\) possible entries in \(\nu_{n-1}\),
\[
(k_1 - 1, k_2, \ldots, k_d), \ldots, (k_1, \ldots, k_{d-1}, k_d - 1)
\]
by adding \(e_1^t, \ldots, e_d^t\), respectively. Of course, such an entry only belongs to \(\nu_{n-1}\) if all its components are non-negative. For each of these indices with all entries non-negative, there is a unique number \(j \in \{1, 2, \ldots, L_{n-1}\}\), such that \(\ell_{n-1}(j)\) is the given index. If one of these indices has a negative entry, we define \(j = -1\) and \(\sigma_{n-1}(-1)\) to be the empty set, \(i.e.,\)
\[
\sigma_{n-1}(-1) = \{\}, \quad \text{whose cardinality is 0.}
\]
We list the \(d\) numbers defined this way as \(i_1, \ldots, i_d\), and note that all the positive values in this list must be distinct. Then,

\[
\#\sigma_n(i) = \sum_{m=1}^{d} \#\sigma_{n-1}(i_m)
\]

\[
= \sum_{m=1}^{d} \binom{n-1}{k_1, \ldots, k_m-1, \ldots, k_d}
\]

\[
= \sum_{m=1}^{d} \left\{ \frac{(n-1)!}{k_1! \cdots (k_m-1)! \cdots k_d!} : k_m > 0 \right\}
\]

\[
= \frac{(n-1)! (k_1 + \cdots + k_d)}{k_1! \cdots k_d!}
\]

\[
= \binom{n}{k}.
\]

Remark 1. Consider \(i \in \{1, \ldots, L_n\}\). A number \(j \in \{1, \ldots, d^n\}\) is contained in the set \(\sigma_n(i)\), if the multi-index \(\nu_n(j)\) coincides with the multi-index \(\ell_n(i)\). The previous Lemma 1 verifies that the cardinality \#\(\sigma_n(i)\) is the number of unique permutations of the multi-index \(\ell_n(i)\).

3. Symmetric subspaces

We next analyze the symmetric spaces

\[X_n = \{ x \in \mathbb{C}^{d^n} : \text{For all } j, j' \in \{1, \ldots, d^n\}, \ x_j = x_{j'} \ \text{if } \nu_n(j) = \nu_n(j') \}\]

for \(n \in \mathbb{N}\). We have \(X_0 = \mathbb{C}\) and \(X_1 = \mathbb{C}^d\), whereas \(X_n\) is a proper subset of \(\mathbb{C}^{d^n}\) for \(n \geq 2\).

For example, for \(d = 2\),

\[X_2 = \{ x \in \mathbb{C}^4 : x_2 = x_3 \}, \]

\[X_3 = \{ x \in \mathbb{C}^8 : x_2 = x_3 = x_5, \ x_4 = x_6 = x_7 \}.\]

Any vector \(x \in X_n\) has \(d^n\) components, but the components that correspond to the same multi-index in the redundant enumeration \(\nu_n(1), \ldots, \nu_n(d^n)\) have the same value. Hence, at most \(L_n\) components of \(x \in X_n\) are different. They may be labelled by the multi-indices \(\ell_n(1), \ldots, \ell_n(L_n)\), and we often refer to them by \(x_{\ell_n(i)}, \ i = 1, \ldots, L_n\).

The symmetric subspaces \(X_n, n \in \mathbb{N}\), can also be obtained as the vectorization of symmetric tensor spaces, and we next relate this alternative point of view to ours.
3.1. The symmetric spaces in tensor terminology. The second order subspace

\[ X_2 = \left\{ x \in \mathbb{C}^{d^2} : x_j = x_{j'} \text{ if } \nu_2(j) = \nu_2(j') \right\} \]

can also be described in terms of matrices. Since

\[ \nu_2 = \text{vec} \begin{pmatrix} e_1^t + e_1^t & \cdots & e_d^t + e_1^t \\
\vdots & & \vdots \\
e_1^t + e_d^t & \cdots & e_d^t + e_d^t \end{pmatrix}, \]

we may write

\[ X_2 = \left\{ x \in \mathbb{C}^{d^2} : x = \text{vec}(X), \ X = X^t \in \mathbb{C}^{d \times d} \right\}. \]

Alternatively, as in [VLV15 §2.3], one may permute the standard basis vectors \( e_1, \ldots, e_d \in \mathbb{C}^d \) according to the \( d^2 \times d^2 \) permutation matrix

\[ \Pi_{dd} = (e_1 + 0 \cdot d, e_1 + 1 \cdot d, \ldots, e_1 + (d - 1) \cdot d, \ldots, e_d + 0 \cdot d, e_d + 1 \cdot d, \ldots, e_d) \]

and characterize the symmetric subspace as

\[ X_2 = \left\{ x \in \mathbb{C}^{d^2} : \Pi_{dd} x = x \right\}. \]

More generally, the higher order symmetric spaces \( X_n \) can also be described in terms of higher order tensors. A tensor \( X \in \mathbb{C}^{d_1 \times \cdots \times d_\alpha} \) of order \( n \) is called symmetric, if

\[ X_{i_1, \ldots, i_n} = X_{\sigma(i_1), \ldots, \sigma(i_n)}, \quad \text{for any permutation } \sigma \in S_d, \]

see for example [KB09 Section 2.2] or [Hack12 Chapter 3.5], and an inductive argument with respect to \( n \) shows that

\[ X_n = \left\{ x \in \mathbb{C}^{d^n} : x = \text{vec}(X), \ X \in \mathbb{C}^{d \times \cdots \times d} \text{ symmetric} \right\}. \]

3.2. Relation between the subspaces. Due to the recursive definition of the redundant multi-index enumeration, the symmetric subspaces of neighboring order can be easily related to each other as follows.

**Lemma 2.** The symmetric subspace \( X_{n+1} \) is contained in the \( d \)-ary Cartesian product of the symmetric subspace \( X_n \),

\[ X_{n+1} \subseteq X_n \times \cdots \times X_n, \quad n \in \mathbb{N}. \]

**Proof.** We decompose a vector

\[ x = (x^{(1)}, \ldots, x^{(d)})^t \in X_{n+1} \]

into \( d \) subvectors with \( d^n \) components each. The \( d^{n+1} \) components of \( x \) can be labelled by the multi-indices

\[ \nu_n(1) + e_1^t, \ldots, \nu_n(d^n) + e_1^t, \nu_n(1) + e_d^t, \ldots, \nu_n(d^n) + e_d^t, \]

so that the components of the subvector \( x^{(m)} \), \( m = 1, \ldots, d \), can be labelled by

\[ \nu_n(1) + e_m^t, \ldots, \nu_n(d^n) + e_m^t. \]

Hence,

\[ x^{(m)}_j = x^{(m)}_{j'} \quad \text{if} \quad \nu_n(j) = \nu_n(j'), \]

and \( x^{(m)} \in X_n \) for all \( m = 1, \ldots, d \). \( \square \)
The two-dimensional examples

\[ X_1 = \mathbb{C}^2 \quad \text{and} \quad X_2 = \{ x \in \mathbb{C}^4 : x_2 = x_3 \} \]

show that the inclusion of Lemma 2 is in general not an equality.

3.3. An orthonormal basis. We now use the standard basis of \( \mathbb{C}^{d^n} \) to construct an orthonormal basis of the symmetric subspace \( X_n \).

**Lemma 3.** Let \( e_1, \ldots, e_{d^n} \) be the standard basis vectors of \( \mathbb{C}^{d^n} \), and define the vectors

\[
 p_i = \frac{1}{\sqrt{\#\sigma_n(i)}} \sum_{j \in \sigma_n(i)} e_j, \quad i = 1, \ldots, L_n.
\]

Then, \( \{ p_1, \ldots, p_{L_n} \} \) forms an orthonormal basis of the space \( X_n \).

**Proof.** For all \( i = 0, \ldots, L_n \) and \( j, j' = 1, \ldots, d^n \), we have

\[
 (p_i)_j = \begin{cases} 
 (\#\sigma_n(i))^{-1/2}, & \text{if } j \in \sigma_n(i), \\
 0, & \text{otherwise}.
\end{cases}
\]

Since \( j \in \sigma_n(i) \) if and only if \( \nu_n(j) = \ell_n(i) \), we have

\[
 (p_i)_j = (p_i)_{j'} \quad \text{if} \quad \nu_n(j) = \nu_n(j'),
\]

and thus \( p_i \in X_n \). We also observe, that for all \( i, i' = 1, \ldots, L_n \),

\[
 \langle p_i, p_{i'} \rangle = \frac{1}{\sqrt{\#\sigma_n(i) \cdot \#\sigma_n(i')}} \sum_{j \in \sigma_n(i)} \sum_{j' \in \sigma_n(i')} \langle e_j, e_{j'} \rangle = \delta_{i,i'}.
\]

Hence, the vectors \( p_1, \ldots, p_{L_n} \) are orthonormal. Moreover, for all \( x \in X_n \), we have

\[
 \langle p_i, x \rangle = \frac{1}{\sqrt{\#\sigma_n(i)}} \sum_{j \in \sigma_n(i)} \langle e_j, x \rangle = \sqrt{\#\sigma_n(i)} x_{\ell_n(i)},
\]

and therefore

\[
 x = \sum_{j=1}^{d^n} \langle e_j, x \rangle e_j = \sum_{i=1}^{L_n} \sum_{j \in \sigma_n(i)} \langle e_j, x \rangle e_j = \sum_{i=1}^{L_n} x_{\ell_n(i)} \sqrt{\#\sigma_n(i)} p_i = \sum_{i=1}^{L_n} \langle p_i, x \rangle p_i.
\]

The orthonormal basis \( \{ p_1, \ldots, p_{L_n} \} \) of the symmetric subspace \( X_n \) may be viewed as a normalized version of an orthogonal basis

\[ \{ X^{(1)}, \ldots, X^{(L_n)} \} \]

of the space of \( d \)-dimensional symmetric tensors of order \( n \) constructed as follows: For each \( i = 1, \ldots, L_n \) the multi-index \( \ell_n(i) = (k_1, \ldots, k_d) \) defines the non-zero elements of the corresponding basis tensor \( X^{(i)} \in \mathbb{C}^{d \times \cdots \times d} \) according to

\[
 X^{(i)}_{j_1, \ldots, j_d} \neq 0 \quad \text{if} \quad (j_1, \ldots, j_d) \text{ comprises } k_1 \text{ times } 1, \ldots, k_d \text{ times } d.
\]
Moreover, by symmetry, all non-vanishing entries of the tensor $X^{(i)}$ have to be the same. The following Table 1 illustrates this alternative line of thought for the third order symmetric subspace in dimension $d = 2$.

| $i$ | $\ell_3(i)$ | $p_i$ | non-zero elements of $X^{(i)}$ | $\#\sigma_3(i)$ |
|-----|-------------|-------|-------------------------------|-----------------|
| 1   | (3, 0)      | $e_1$ | (1, 1, 1)                     | 1               |
| 2   | (2, 1)      | $\frac{1}{\sqrt{3}}(e_2 + e_3 + e_5)$ | (2, 1, 1), (1, 2, 1), (1, 1, 2) | 3               |
| 3   | (1, 2)      | $\frac{1}{\sqrt{3}}(e_4 + e_6 + e_7)$ | (2, 2, 1), (2, 1, 2), (1, 2, 2) | 3               |
| 4   | (0, 3)      | $e_8$  | (2, 2, 2)                     | 1               |

**Table 1.** The table lists the orthonormal basis $\{p_1, \ldots, p_4\}$ of the third symmetric subspace $X_3$ for dimension $d = 2$. It also specifies the non-vanishing entries of a corresponding basis $\{X_1^{(1)}, \ldots, X_4^{(4)}\}$ of the space of symmetric tensors of size $2 \times 2 \times 2$.

### 3.4. An orthonormal matrix.

The orthonormal basis vectors $p_1, \ldots, p_{L_n} \in X_n$ allow us to define the sparse rectangular $L_n \times d^n$ matrix

$$P_n = \begin{pmatrix} p_1^t \\ \vdots \\ p_{L_n}^t \end{pmatrix}$$

that has the $L_n$ basis vectors as its rows. For example, for $d = 2$, we have

$$P_2 = \begin{pmatrix} e_1^t \\ \frac{1}{\sqrt{2}}(e_2^t + e_3^t) \\ e_4^t \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$P_3 = \begin{pmatrix} e_1^t \\ \frac{1}{\sqrt{3}}(e_2^t + e_3^t + e_5^t) \\ \frac{1}{\sqrt{3}}(e_4^t + e_6^t + e_7^t) \\ e_8^t \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

We summarize some properties of the matrix $P_n$ and of its adjoint $P_n^*$ and calculate explicit formulas for their actions on vectors.

**Proposition 1.** The $L_n \times d^n$ matrix $P_n$ and its adjoint $P_n^*$ satisfy

$$P_n P_n^* = \text{Id}_{L_n \times L_n}, \quad \text{range}(P_n^*) = X_n.$$

Moreover, for all $x \in X_n$,

$$(P_n x)_i = \sqrt{\#\sigma_n(i)} \ x_{\ell_n(i)}, \quad i = 1, \ldots, L_n,$$
and for all \( y \in \mathbb{C}^{L_n} \),
\[
(P_n^* y)_{\ell_n(i)} = \frac{1}{\sqrt{\# \sigma_n(i)}} y_i, \quad i = 1, \ldots, L_n.
\]
In particular,
\[
P_n^* P_n x = x, \quad \text{whenever } x \in X_n.
\]

Proof. The two properties \( P_n P_n^* = \text{Id}_{L_n \times L_n} \) and \( \text{range}(P_n^*) = X_n \) equivalently say, that the row vectors of \( P_n \) build an orthonormal basis of \( X_n \).

For any \( y \in \mathbb{C}^{L_n} \), the vector \( P_n^* y \) is a linear combination of the column vectors \( p_1, \ldots, p_{L_n} \) and therefore in \( X_n \). Labelling its components by \( \ell_n(1), \ldots, \ell_n(L_n) \), we obtain
\[
(P_n^* y)_{\ell_n(i)} = \frac{1}{\sqrt{\# \sigma_n(i)}} y_i, \quad i = 1, \ldots, L_n.
\]

For \( x \in X_n \) and \( i = 1, \ldots, L_n \), we obtain
\[
(P_n x)_i = \frac{1}{\# \sigma_n(i)} \sum_{j=1}^{L_n} (p_i)_{\ell_n(j)} x_{\ell_n(j)} = \sqrt{\# \sigma_n(i)} x_{\ell_n(i)},
\]
since \( \# \sigma_n(i) \) components of \( p_i \) do not vanish. In particular,
\[
(P_n^* P_n x)_{\ell_n(i)} = \frac{1}{\sqrt{\# \sigma_n(i)}} (P_n x)_i = x_{\ell_n(i)}.
\]

4. Symmetric Kronecker products

4.1. Iterated Kronecker products. We next investigate the action of an \( n \)-fold Kronecker product on the symmetric subspace \( X_n \), \( n \in \mathbb{N} \). First, we prove the invariance of the symmetric spaces under multiplication with iterated Kronecker products.

Lemma 4. For all \( M \in \mathbb{C}^{d \times d} \) we have \( M^n \otimes x \in X_n \) whenever \( x \in X_n \).

Proof. Applying \( M^n \otimes \) to a tensor \( X \in \mathbb{C}^{d \times \ldots \times d} \) of order \( n \), we obtain the tensor
\[
(M^n \otimes X)_{i_1, \ldots, i_n} = \sum_{j_1=1}^{d} \cdots \sum_{j_n=1}^{d} M_{i_1, j_1} \cdots M_{i_n, j_n} X_{j_1, \ldots, j_n}.
\]

For a symmetric tensor \( X \), we then have
\[
(M^n \otimes X)_{\sigma(i_1), \ldots, \sigma(i_n)} = \sum_{j_1=1}^{d} \cdots \sum_{j_n=1}^{d} M_{\sigma(i_1), j_1} \cdots M_{\sigma(i_n), j_n} X_{j_1, \ldots, j_n}
\]
\[
= \sum_{k_1=1}^{d} \cdots \sum_{k_n=1}^{d} M_{i_1, k_1} \cdots M_{i_n, k_n} X_{k_1, \ldots, k_n}
\]
\[
= (M^n \otimes X)_{i_1, \ldots, i_n}.
\]
That is, $M^{n \otimes} X$ is a symmetric tensor, too. By vectorisation we then obtain that $M^{n \otimes} \mathbf{x} \in X_n$ whenever $\mathbf{x} \in X_n$.

We now derive an explicit formula for the components of a vector $M^{n \otimes} \mathbf{x}$ in terms of the row vectors of the matrix $M$.

**Proposition 2.** Let $M \in \mathbb{C}^{d \times d}$, and denote by $\mathbf{m}_1, \ldots, \mathbf{m}_d \in \mathbb{C}^d$ the row vectors of the matrix $M$. Then, for all $\mathbf{x} \in X_n$, the components of the vector $M^{n \otimes} \mathbf{x} \in X_n$ can be labelled by multi-indices $k \in \mathbb{N}^d$ with $|k| = n$ and satisfy

\[
(M^{n \otimes} \mathbf{x})_k = \sum_{|\alpha_1| = k_1} \cdots \sum_{|\alpha_d| = k_d} \binom{k_1}{\alpha_1} \cdots \binom{k_d}{\alpha_d} \mathbf{m}_1^{\alpha_1} \cdots \mathbf{m}_d^{\alpha_d} \mathbf{x}_{\alpha_1 + \cdots + \alpha_d},
\]

where the summation ranges over $\alpha_1, \ldots, \alpha_d \in \mathbb{N}^d$ with $|\alpha_1| = k_1, \ldots, |\alpha_d| = k_d$.

**Proof.** For $n = 1$, we have $M^{n \otimes} = M$ and $X_n = \mathbb{C}^d$, and our formula reduces to usual matrix-vector multiplication written as

\[
(M \mathbf{x})_{ek} = \sum_{j=1}^d m_{ej} \mathbf{x}_j, \quad k = 1, \ldots, d.
\]

For the inductive step, we consider $\mathbf{x} = (\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(d)}) \in X_{n+1}$ decomposed as in Lemma 2 with $\mathbf{x}^{(j)} \in X_n$. We compute

\[
M^{(n+1) \otimes} \mathbf{x} = \left( \begin{array}{ccc}
M^{n \otimes} & \cdots & M^{n \otimes} \\
\vdots & \ddots & \vdots \\
\vdots & \vdots & \ddots \\
M^{n \otimes} & \cdots & M^{n \otimes}
\end{array} \right)
\left( \begin{array}{c}
\mathbf{x}^{(1)} \\
\vdots \\
\vdots \\
\mathbf{x}^{(d)}
\end{array} \right)
= \left( \begin{array}{c}
M^{n \otimes} \mathbf{x}^{(1)} + \cdots + m_{1d} M^{n \otimes} \mathbf{x}^{(d)} \\
\vdots \\
M^{n \otimes} \mathbf{x}^{(1)} + \cdots + m_{dd} M^{n \otimes} \mathbf{x}^{(d)}
\end{array} \right).
\]

By Lemma 2, we have for all $j = 1, \ldots, d$, that

\[
m_{j1} M^{n \otimes} \mathbf{x}^{(1)} + \cdots + m_{jd} M^{n \otimes} \mathbf{x}^{(d)} \in X_n.
\]

The components of these vectors can be labelled by $k \in \mathbb{N}^d$ with $|k| = n$, and we have

\[
\left( m_{j1} M^{n \otimes} \mathbf{x}^{(1)} + \cdots + m_{jd} M^{n \otimes} \mathbf{x}^{(d)} \right)_k
= \sum_{|\alpha_1| = k_1} \cdots \sum_{|\alpha_d| = k_d} \binom{k_1}{\alpha_1} \cdots \binom{k_d}{\alpha_d} \left( m_{j1} \mathbf{m}_1^{\alpha_1} \cdots \mathbf{m}_d^{\alpha_d} \mathbf{x}_{\alpha_1 + \cdots + \alpha_d} + \cdots + m_{jd} \mathbf{m}_1^{\alpha_1} \cdots \mathbf{m}_d^{\alpha_d} \mathbf{x}_{\alpha_1 + \cdots + \alpha_d} \right).
\]

□
The \( j \)th of these sums can be rewritten as
\[
\sum_{|\alpha_j| = k_j} \binom{k_j}{\alpha_j} \left( m_j^{\alpha_j+\epsilon_1} x_{\alpha_1+\cdots+\alpha_d}^{(1)} + \cdots + m_j^{\alpha_j+\epsilon_d} x_{\alpha_1+\cdots+\alpha_d}^{(d)} \right)
\]
\[
= \sum_{|\beta_j-\epsilon_1| = k_j} \binom{k_j}{\beta_j-\epsilon_1} m_j^{\beta_j} x_{\alpha_1+\cdots+\beta_j+\cdots+\alpha_d}^{(1)} + \cdots + \sum_{|\beta_j-\epsilon_d| = k_j} \binom{k_j}{\beta_j-\epsilon_d} m_j^{\beta_j} x_{\alpha_1+\cdots+\beta_j+\cdots+\alpha_d}^{(d)}.
\]
Now we observe that for all \( r = 1, \ldots, d \),
\[
x_{\alpha_1+\cdots+(\beta_j-\epsilon_r)+\cdots+\alpha_d}^{(r)} = x_{\alpha_1+\cdots+\beta_j+\cdots+\alpha_d},
\]
so that
\[
\sum_{|\alpha_j| = k_j} \binom{k_j}{\alpha_j} \left( m_j^{\alpha_j+\epsilon_1} x_{\alpha_1+\cdots+\alpha_d}^{(1)} + \cdots + m_j^{\alpha_j+\epsilon_d} x_{\alpha_1+\cdots+\alpha_d}^{(d)} \right)
\]
\[
= \sum_{|\beta_j-\epsilon_1| = k_j} \binom{k_j}{\beta_j-\epsilon_1} m_j^{\beta_j} x_{\alpha_1+\cdots+\beta_j+\cdots+\alpha_d}^{(1)} + \cdots + \sum_{|\beta_j-\epsilon_d| = k_j} \binom{k_j}{\beta_j-\epsilon_d} m_j^{\beta_j} x_{\alpha_1+\cdots+\beta_j+\cdots+\alpha_d}^{(d)}.
\]
Since all multi-indices \( \beta_j \in \mathbb{N}^d \) with \( |\beta_j| = k_j + 1 \) satisfy
\[
\binom{k_j + 1}{\beta_j} = \binom{k_j}{\beta_j-\epsilon_1} + \cdots + \binom{k_j}{\beta_j-\epsilon_d},
\]
we can write
\[
\sum_{|\alpha_j| = k_j} \binom{k_j}{\alpha_j} \left( m_j^{\alpha_j+\epsilon_1} x_{\alpha_1+\cdots+\alpha_d}^{(1)} + \cdots + m_j^{\alpha_j+\epsilon_d} x_{\alpha_1+\cdots+\alpha_d}^{(d)} \right)
\]
\[
= \sum_{|\beta_j| = k_j + 1} \binom{k_j + 1}{\beta_j} m_j^{\beta_j} x_{\alpha_1+\cdots+\beta_j+\cdots+\alpha_d}
\]
and obtain
\[
\left( m_{j_1} M^{\epsilon_1 \otimes x^{(1)}} + \cdots + m_{j_d} M^{\epsilon_d \otimes x^{(d)}} \right) = \sum_{|\alpha_1| = k_1} \cdots \sum_{|\alpha_j| = k_j + 1} \cdots \sum_{|\alpha_d| = k_d} \binom{k_1}{\alpha_1} \cdots \binom{k_j + 1}{\alpha_j} \cdots \binom{k_d}{\alpha_d} m_{1}^{\alpha_1} \cdots m_{d}^{\alpha_d} x_{\alpha_1+\cdots+\alpha_d}.
\]
Hence, \( M^{(n+1) \otimes x} \) has at most \( L_{n+1} \) distinct components that can be labelled by \( k \in \mathbb{N}^d \) with \( |k| = n + 1 \). They satisfy
\[
\left( M^{(n+1) \otimes x} \right) = \sum_{|\alpha_1| = k_1} \cdots \sum_{|\alpha_d| = k_d} \binom{k_1}{\alpha_1} \cdots \binom{k_d}{\alpha_d} m_{1}^{\alpha_1} \cdots m_{d}^{\alpha_d} x_{\alpha_1+\cdots+\alpha_d}.
\]
Remark 2. The invariance property of Lemma 4 can also be proved alongside the inductive argument given in the proof of Proposition 2 without using tensor terminology.

4.2. Symmetric Kronecker products. Having proven that n-fold Kronecker products leave the nth symmetric subspace invariant, we define the n-fold symmetric Kronecker product as follows:

**Definition 1.** For \( M \in \mathbb{C}^{d \times d} \) and \( n \in \mathbb{N} \), we define the \( L_n \times L_n \) matrix

\[
S_n(M) = P_n^* M^{n\otimes} P_n
\]

and call it the n-fold symmetric Kronecker product of the matrix \( M \).

The n-fold symmetric Kronecker product has useful structural properties.

**Lemma 5.** The n-fold symmetric Kronecker product \( S_n(M) \) of a matrix \( M \in \mathbb{C}^{d \times d} \) satisfies \( S_n(M)^* = S_n(M^*) \). If \( M \in \text{GL}(d, \mathbb{C}) \), then

\[
S_n(M) \in \text{GL}(L_n, \mathbb{C}) \quad \text{with} \quad S_n(M)^{-1} = S_n(M^{-1}).
\]

In particular, if \( M \in U(d) \), then \( S_n(M) \in U(L_d) \).

**Proof.** Since \((M \otimes M)^* = M^* \otimes M^* \) and \((M^{n\otimes})^* = (M^*)^{n\otimes}\), we have

\[
S_n(M^*) = P_n^* (M^{n\otimes})^* P_n^*
= S_n(M^*).
\]

If \( M \) is invertible, then \( M \otimes M \) is invertible with \((M \otimes M)^{-1} = M^{-1} \otimes M^{-1}\). By Proposition 2,

\[
(M^{n\otimes})^{-1} p_j \in X_n, \quad j = 1, \ldots, L_n.
\]

Proposition 1 yields \( P_n^* P_n x = x \) for all \( x \in X_n \) and

\[
P_n p_j = e_j, \quad j = 1, \ldots, L_n,
\]

where \( e_1, \ldots, e_{L_n} \in \mathbb{C}^{L_n} \) are the standard basis vectors. Therefore,

\[
S_n(M) S_n(M^{-1}) e_j = P_n^* M^{n\otimes} P_n^* P_n (M^{n\otimes})^{-1} p_j
= P_n p_j
= e_j,
\]

that is,

\[
S_n(M) S_n(M^{-1}) = \text{Id}_{L_n \times L_n}.
\]

4.3. The main result. The explicit formula of Proposition 2 for the n-fold Kronecker product also allows a detailed description of the n-fold symmetric Kronecker product.

**Theorem 1.** Let \( M \in \mathbb{C}^{d \times d} \) and denote by \( m_1, \ldots, m_d \in \mathbb{C}^d \) the row vectors of the matrix \( M \). Then, the n-fold symmetric Kronecker product satisfies for all \( y \in \mathbb{C}^{L_n} \) and \( k \in \mathbb{N}^d \) with \(|k| = n\),

\[
(S_n(M) y)_k = \frac{1}{\sqrt{k!}} \sum_{|\alpha_1| = k_1} \cdots \sum_{|\alpha_d| = k_d} \binom{k_1}{\alpha_1} \cdots \binom{k_d}{\alpha_d} m_1^{\alpha_1} \cdots m_d^{\alpha_d} \times \sqrt{(\alpha_1 + \cdots + \alpha_d)!} y_{\alpha_1 + \cdots + \alpha_d},
\]
where the summations range over \( \alpha_1, \ldots, \alpha_d \in \mathbb{N}^d \) with \( |\alpha_1| = k_1, \ldots, |\alpha_d| = k_d \), and the components of \( y \in \mathbb{C}^{L_n} \) are denoted by multi-indices of order \( n \).

Proof. By Lemma 1 we have
\[
\# \sigma_n(i) = \binom{n}{\ell_n(i)}, \quad \text{for } i = 1, \ldots, L_n.
\]

By Proposition 1 we have \( P_n^* y \in X_n \) and
\[
(P_n^* y)_{\ell_n(i)} = \frac{1}{\sqrt{\binom{n}{\ell_n(i)}}} y_i, \quad \text{for } i = 1, \ldots, L_n.
\]

This can be reformulated as
\[
(P_n^* y)_\alpha = \sqrt{\frac{\alpha!}{n!}} y_\alpha, \quad \text{for } \alpha \in \mathbb{N}^d \text{ with } |\alpha| = n.
\]

By Lemma 3 the \( n \)-fold Kronecker product leaves \( X_n \) invariant, and by Proposition 2 we have for all \( k \in \mathbb{N}^d \) with \( |k| = n \),
\[
(M_n^\otimes P_n^* y)_k
= \sum_{|\alpha_1|=k_1} \cdots \sum_{|\alpha_d|=k_d} \binom{k_1}{\alpha_1} \cdots \binom{k_d}{\alpha_d} m_1^{\alpha_1} \cdots m_d^{\alpha_d} (P_n^* y)_{\alpha_1+\cdots+\alpha_d}
= \sum_{|\alpha_1|=k_1} \cdots \sum_{|\alpha_d|=k_d} \binom{k_1}{\alpha_1} \cdots \binom{k_d}{\alpha_d} m_1^{\alpha_1} \cdots m_d^{\alpha_d}
\times \sqrt{\frac{(\alpha_1+\cdots+\alpha_d)!}{n!}} y_{\alpha_1+\cdots+\alpha_d}.
\]

By Proposition 4 we have for all \( x \in X_n \)
\[
(P_n x)_i = \sqrt{\binom{n}{\ell_n(i)}} x_{\ell_n(i)}, \quad \text{for } i = 1, \ldots, L_n,
\]
so that
\[
(P_n M_n^\otimes P_n^* y)_k
= \sqrt{\frac{n!}{k!}} \sum_{|\alpha_1|=k_1} \cdots \sum_{|\alpha_d|=k_d} \binom{k_1}{\alpha_1} \cdots \binom{k_d}{\alpha_d} m_1^{\alpha_1} \cdots m_d^{\alpha_d}
\times \sqrt{\frac{(\alpha_1+\cdots+\alpha_d)!}{n!}} y_{\alpha_1+\cdots+\alpha_d}
= \frac{1}{\sqrt{k!}} \sum_{|\alpha_1|=k_1} \cdots \sum_{|\alpha_d|=k_d} \binom{k_1}{\alpha_1} \cdots \binom{k_d}{\alpha_d} m_1^{\alpha_1} \cdots m_d^{\alpha_d}
\times \sqrt{(\alpha_1+\cdots+\alpha_d)!} y_{\alpha_1+\cdots+\alpha_d}.
\]

\(\square\)
5. Application to semiclassical wavepackets

5.1. Parametrizing Gaussians. We consider two complex invertible matrices \(A, B \in \text{GL}(d, \mathbb{C})\) that satisfy the conditions

\[
\begin{align*}
A^t B - B^t A &= 0, \\
A^* B + B^* A &= 2 \text{Id}_{d \times d}.
\end{align*}
\]

These two conditions imply that \(B A^{-1}\) is a complex symmetric matrix such that its real part

\[
\text{Re}(B A^{-1}) = (A A^*)^{-1}
\]

is a Hermitian and positive definite matrix, see [Hag80]. Let \(\hbar > 0\) and define the multivariate complex-valued Gaussian function

\[
\varphi_0[A, B](x) = (\pi \hbar)^{-d/4} \det(A)^{-1/2} \exp\left(-\frac{\langle x, B A^{-1} x \rangle}{2 \hbar}\right).
\]

Then, \(\varphi_0[A, B]\) is a square-integrable function, and the constant factor \(\det(A)^{-1/2}\) ensures normalization according to

\[
\int_{\mathbb{R}^d} |\varphi_0[A, B](x)|^2 \, dx = 1.
\]

Changing the parametrization by a unitary matrix changes the Gaussian function only by constant multiplicative factor of modulus one:

**Lemma 6.** Let \(A, B \in \text{GL}(d, \mathbb{C})\) satisfy the conditions \(1\&2\). Then, for all unitary matrices \(U \in U(d)\), the matrices \(A' = AU\) and \(B' = BU\) also satisfy the conditions \(1\&2\). Moreover,

\[
\varphi_0[A', B'] = \det(U)^{-1/2} \varphi_0[A, B].
\]

**Proof.** We observe that

\[
\begin{align*}
(A')^t B' - (B')^t A' &= U^t (A^t B - BA) U = 0, \\
(A')^* B' + (B')^* A' &= U^* (A^* B + BA) U = 2 \text{Id}_{d \times d}.
\end{align*}
\]

and \(B' (A')^{-1} = BU U^* A^{-1} = BA^{-1}\). Therefore,

\[
\varphi_0[A', B'] = (\pi \hbar)^{-d/4} \det(A U)^{-1/2} \exp\left(-\frac{\langle x, B A^{-1} x \rangle}{2 \hbar}\right)
= \det(U)^{-1/2} \varphi_0[A, B].
\]

\[\square\]

5.2. Semiclassical wave packets. Following the construction of [Hag98], we consider \(A, B \in \text{GL}(d, \mathbb{C})\) satisfying the conditions \(1\&2\) and introduce the vector of raising operators

\[
\mathcal{R}[A, B] = \frac{1}{\sqrt{2\hbar}} \left( B^* x - iA^*(-i\hbar \nabla_x) \right)
\]

that consists of \(d\) components,

\[
\mathcal{R}[A, B] = \begin{pmatrix} \mathcal{R}_1[A, B] \\ \vdots \\ \mathcal{R}_d[A, B] \end{pmatrix}.
\]
The raising operator acts on Schwartz functions \( \psi : \mathbb{R}^d \to \mathbb{C} \) as
\[
(\mathcal{R}[A, B] \psi)(x) = \frac{1}{\sqrt{2\hbar}} (B^* x \psi(x) - iA^* (-i\hbar \nabla_x \psi)(x)), \quad x \in \mathbb{R}^d.
\]

Powers of the raising operator now generate the semiclassical wave packets.

**Definition 2** (Semiclassical wave packet). Let \( A, B \in \text{GL}(d, \mathbb{C}) \) satisfy the conditions (1–2) and \( \varphi_0[A, B] \) denote the Gaussian function of \( \mathbb{R}^d \). Then, the \( k \)-th semiclassical wave packet is defined by
\[
\varphi_k[A, B] = \frac{1}{\sqrt{k!}} \mathcal{R}[A, B]^k \varphi_0[A, B], \quad k \in \mathbb{N}^d.
\]

We note that the \( k \)-th power of the raising operator
\[
\mathcal{R}[A, B]^k = \mathcal{R}_1[A, B]^{k_1} \cdots \mathcal{R}_d[A, B]^{k_d}
\]
does not depend on the ordering, since the components commute with one another due to the compatibility conditions (1–2). The set
\[
\{ \varphi_k[A, B] : k \in \mathbb{N}^d \}
\]
forms an orthonormal basis of the space of square-integrable functions \( L^2(\mathbb{R}^d, \mathbb{C}) \).

5.3. **Hermite polynomials.** By its construction, the \( k \)-th semiclassical wave packet is a multivariate polynomial of degree \(|k|\) in \( x \) times the complex-valued Gaussian function \( \varphi_0[A, B] \), that is,
\[
\varphi_k[A, B](x) = \frac{1}{\sqrt{2^{|k|} k!}} p_k[A](x) \varphi_0[A, B](x), \quad x \in \mathbb{R}^d,
\]
The polynomials \( p_k[A] \) are determined by the matrix \( A \in \text{GL}(d, \mathbb{C}) \), see [Hag15], and satisfy the three-term recurrence relation
\[
(p_{k+e_j}[A])^d_{j=1} = \frac{2}{\sqrt{\hbar}} A^{-1} x p_k[A] - 2 A^{-1} A (k_j p_{k-e_j}[A])^d_{j=1},
\]
see [Lub08] Chapter V.2. Whenever the parameter matrix \( A \) has all entries real, \( A \in \text{GL}(d, \mathbb{R}) \), then the polynomials factorize according to
\[
p_k[A](x) = \prod_{j=1}^d H_n\left(\frac{1}{\sqrt{\hbar}} (A^{-1} x)_j\right), \quad x \in \mathbb{R}^d,
\]
where \( H_n \) is the \( n \)-th Hermite polynomial, \( n \in \mathbb{N} \), defined by the univariate three-term recurrence relation
\[
H_{n+1}(y) = 2y H_n(y) - 2n H_{n-1}(y), \quad y \in \mathbb{R}.
\]
The real parameter case, however, is rather exceptional when using semiclassical wave packets for their key application in molecular quantum dynamics. There, the parameter matrices \( A(t) \) and \( B(t) \), \( t \in \mathbb{R} \), are time-dependent and determined by a system of ordinary differential equations. For the particularly simple, but instructive example of harmonic oscillator motion, one can even write the solution explicitly as
\[
A(t) = \cos(t) A(0) + i \sin(t) B(0),
\]
\[
B(t) = i \sin(t) A(0) + \cos(t) B(0).
\]
Hence, the matrix $A(t)$ cannot be expected to have only real entries, and the crucial matrix factor $A(t)^{-1}A(t)$ in the three term recurrence relation generates multivariate polynomials beyond a tensor product representation.

5.4. Changing the parametrization. If $A, B \in \text{GL}(d, \mathbb{C})$ satisfy the compatibility conditions (1–2), then $|A| = \sqrt{AA^*}$ is a real symmetric, positive definite matrix, and the singular value decomposition of $A$,

$$A = V \Sigma W^* \quad \text{with} \quad \Sigma = \text{diag}(\sigma_1, \ldots, \sigma_d) \quad \text{positive definite},$$

is given by an orthogonal matrix $V \in O(d)$ and a unitary matrix $W \in U(d)$. This provides two natural ways for transforming $A' = AU$ with $A' \in \text{GL}(d, \mathbb{R})$ and $U \in U(d)$. One may work with the polar decomposition of $A$,

$$A' = |A| = V \Sigma \quad \text{and} \quad U = WV^*,$$

or alternatively with

$$A' = V \Sigma \quad \text{and} \quad U = W.$$

Both choices provide a unitary transformation to the real case, and we ask how to relate different families of wave packets that correspond to unitarily linked parametrizations. For an explicit description, we collect the semiclassical wave packets of order $n$ in one formal vector

$$\varphi_n[A, B] = \begin{pmatrix} \varphi_{\ell_n(1)}[A, B] \\ \vdots \\ \varphi_{\ell_n(L_n)}[A, B] \end{pmatrix},$$

whose components are labelled by the multi-indices $\ell_n(1), \ldots, \ell_n(L_n)$. Then, we use the $n$-fold symmetric Kronecker product in the following way:

**Corollary 1.** Let $A, B \in \text{GL}(d, \mathbb{C})$ satisfy the conditions (1–2), and consider the matrices $A' = AU$, $B' = BU$ with $U \in U(d)$. Then,

$$\varphi_n[A', B'] = \det(U)^{-1/2} S_n(U) \varphi_n[A, B], \quad n \in \mathbb{N}.$$

**Proof.** We observe that the raising operators transform according to

$$\mathcal{R}[A', B'] = \mathcal{R}[AU, BU] = U^* \mathcal{R}[A, B],$$

which means for the components that

$$\mathcal{R}_j[A', B'] = \sum_{m=1}^d u_{mj} \mathcal{R}_m[A, B], \quad j = 1, \ldots, d.$$ 

Since all components of the raising operators commute which each other, we can use the multinomial theorem and obtain for all $n \in \mathbb{N}$ that

$$\mathcal{R}_j[A', B']^n = \sum_{|\alpha| = n} \binom{n}{\alpha} \overline{u_j^\alpha} \mathcal{R}[A, B]^\alpha,$$

where $u_1, \ldots, u_d \in \mathbb{C}^d$ denote the column vectors of the matrix $U$. This implies for any $k \in \mathbb{N}^d$ with $|k| = n$,

$$\mathcal{R}[A', B']^k = \sum_{|\alpha_1| = k_1} \cdots \sum_{|\alpha_d| = k_d} \binom{k_1}{\alpha_1} \cdots \binom{k_d}{\alpha_d} \overline{u_1^{\alpha_1}} \cdots \overline{u_d^{\alpha_d}} \mathcal{R}[A, B]^\alpha_1 + \cdots + \alpha_d,$$
where the $d$ summations run over $\alpha_1, \ldots, \alpha_d \in \mathbb{N}^d$. Together with Lemma 6, we therefore obtain
\[
\varphi_k[A', B'] = 1 \sqrt{k!} \mathcal{R}[A', B']^k \varphi_0[A', B']
\]
\[
= 1 \sqrt{\det(U)} k! \sum_{|\alpha_1| = k_1} \cdots \sum_{|\alpha_d| = k_d} \left( \frac{k_1}{\alpha_1} \right) \cdots \left( \frac{k_d}{\alpha_d} \right) \frac{u_{\alpha_1}}{\alpha_1} \cdots \frac{u_{\alpha_d}}{\alpha_d} \times \mathcal{R}[A, B]^{\alpha_1 + \cdots + \alpha_d} \varphi_0[A, B].
\]
By Theorem 1, we then obtain
\[
\varphi_n[A', B'] = \det(U)^{-1/2} S_n(U) \varphi_n[A, B].
\]

6. Conclusion

We have derived an explicit formula for the action of $n$-fold Kronecker products on symmetric subspaces. See Theorem 1. Our findings generalize results on two-fold symmetric Kronecker products discussed in the literature on semidefinite programming [AHO98], [Kle02, Appendix E]. The new formula allows one to write a linear change of the parametrization of semiclassical wave packets in terms of a $n$-fold symmetric Kronecker product. Semiclassical wave packets have an associated family of multivariate orthogonal polynomials. Our result provides an explicit transformation of these polynomials to a tensor products of scaled univariate Hermite polynomials. Moreover, semiclassical wave packets have been used in [FGL09], [Lub08, Chapter 5] and [GH14] for a Galerkin discretization of multi-dimensional molecular quantum dynamics. The explicit formula for the effect of a change of parametrization will allow to convert the multi-dimensional Galerkin integrals of the method to a product of one-dimensional integrals, resulting in a more accurate and stable numerical method, see [B17, Chapter 5] for numerical experiments in this direction.

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