Catalan numbers, Dyck language, and second quantization: An algorithm-oriented representation of second quantization chains

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Second quantization is a fundamental formalism in quantum chemistry and condensed matter physics for describing systems of bosonic and fermionic particles. For electrons, this formalism enables the systematic manipulation of Slater determinants and operators representing observables, based on the anti-commutation and hermiticity rules of creation and annihilation operators. Second quantization operators are used in methods to describe many-body systems, such as coupled-cluster theory or configuration interaction.

Evaluating the expectation value of a chain of second quantization operators is a central challenge. Wick's theorem makes it possible to simplify the evaluation of an expectation value of a chain, relative to a vacuum, by expressing it as the normal order of the chain plus a sum of all contractions of the chain taken in normal order. That expectation value, with respect to the physical or Fermi vacuum, is given by the sum of the expectation values of the fully contracted terms. In fact, the expectation value of any non-fully contracted term is zero. The main advantage of this formulation is that it reduces the problem to finding all fully contracted terms. These terms can be expressed in terms of products of Kronecker deltas. In other words, finding the expectation value becomes a problem of finding viable pairings of second quantization operators. If this procedure is well defined, the number of terms generated by the contractions grows rapidly, making the computations costly in terms of time and memory. In addition, a significant number of the fully contracted terms will be zero, so it seems necessary to find criteria to limit the calculations to the non-zero terms as much as possible.

In this talk we propose a translation of chains of second quantization operators into a Dyck language. A word in a Dyck language can be seen as a string of left and right parenthesis (and/or brackets). If a word corresponds to a balanced string, it is called a Dyck word. In a chain of second quantization operators, each operator is translated into left or right parenthesis. If the resulting string is a Dyck word, the expectation value of the chain is non-zero.

The enumeration of chains of operators with a non-zero expectation value then joins the large family of problems for which Catalan numbers are the solution. This family includes Dyck language, triangulation of polygons, or some graph problems. This analogy makes it possible to formulate non-nullity rules for the expectation value of chains of operators. At the same time, tools used to describe Dyck words, can be used to predict the number of non-zero terms in the sum after applying Wick's theorem. This relationship can be made from the vacuum state or a single determinant State.

The graphical representation of admissible chains has enabled us to develop an algorithm for symbolically evaluating the expectation value of a 1-body operator between two Slater determinants. The strength of this algorithm is to reduce as much as possible the number of second quantization operator pairings to be taken into account to obtain the result, thus reducing the complexity of the algorithm.

References

[1] T. Etienne, *arxiv repository*, 1811.08849v15, sec. 5.2 (2018).