



## SNEG – Mathematica package for symbolic calculations with second-quantization-operator expressions <sup>☆</sup>

Rok Žitko

*J. Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia*

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### ABSTRACT

In many-particle problems involving interacting fermions or bosons, the most natural language for expressing the Hamiltonian, the observables, and the basis states is the language of the second-quantization operators. It thus appears advantageous to write numerical computer codes which allow the user to define the problem and the quantities of interest directly in terms of operator strings, rather than in some low-level programming language. Here I describe a Mathematica package which provides a flexible framework for performing the required translations between several different representations of operator expressions: condensed notation using pure ASCII character strings, traditional notation (“pretty printing”), internal Mathematica representation using nested lists (used for automatic symbolic manipulations), and various higher-level (“macro”) expressions. The package consists of a collection of transformation rules that define the algebra of operators and a comprehensive library of utility functions. While the emphasis is given on the problems from solid-state and atomic physics, the package can be easily adapted to any given problem involving non-commuting operators. It can be used for educational and demonstration purposes, but also for direct calculations of problems of moderate size.

### Program summary

*Program title:* SNEG  
*Catalogue identifier:* AEJL\_v1\_0  
*Program summary URL:* [http://cpc.cs.qub.ac.uk/summaries/AEJL\\_v1\\_0.html](http://cpc.cs.qub.ac.uk/summaries/AEJL_v1_0.html)  
*Program obtainable from:* CPC Program Library, Queen's University, Belfast, N. Ireland  
*Licensing provisions:* GNU General Public License  
*No. of lines in distributed program, including test data, etc.:* 319808  
*No. of bytes in distributed program, including test data, etc.:* 1081247  
*Distribution format:* tar.gz  
*Programming language:* Mathematica  
*Computer:* Any computer which runs Mathematica  
*Operating system:* Any OS which runs Mathematica  
*RAM:* Problem dependent  
*Classification:* 2.9, 5, 6.2  
*Nature of problem:* Manipulation of expressions involving second-quantization operators and other non-commuting objects. Calculation of commutators, anticommutators, expectation values. Generation of matrix representations of the Hamiltonians expressed in the second-quantization language.  
*Solution method:* Automatic reordering of operator strings in some well specified canonical order; (anti)commutation rules are used where needed. States may be represented in occupation-number representation. Dirac bra–ket notation may be intermixed with non-commuting operator expressions.  
*Restrictions:* For very long operator strings, the brute-force automatic reordering becomes slow, but it can be turned off. In such cases, the expectation values may still be evaluated using Wick's theorem.

<sup>☆</sup> This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (<http://www.sciencedirect.com/science/journal/00104655>).

E-mail address: rok.zitko@ijs.si.

*Unusual features:* SNEG provides the natural notation of second-quantization operators (dagger for creation operators, etc.) when used interactively using the Mathematica notebook interface.

*Running time:* Problem dependent

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## 1. Introduction

Computational science has emerged as the third paradigm of science, complementing experiments and theory. Computers are now used to realistically simulate physical systems which are not accessible to experiments or would be simply too expensive to study directly. They also allow numerical treatment of theoretical models which cannot be solved by analytical means or by simple approximations. In this field, it is still common practice to quickly write ad-hoc computer codes for performing calculations for specific problems. In these rapidly developed computer programs the problem definition and the quantities of interest are typically hard-coded using the same low-level programming language which is also used to implement the method of solution. In more technical terms, the problem-domain and the solution-domain languages tend to coincide. As the scientific interests change with time, such codes often undergo successive modifications and adaptations, often leading to maintainability issues or even bugs. In software engineering, the proposed solution to such difficulties is to use a domain-specific language (DSL), i.e., a specification language adapted to a particular problem domain. Using a DSL, the problem can be expressed significantly more clearly than allowed by low-level languages. In the field of many-particle physics, such a language already exists: the language of strings of second-quantization operators (particle creation and annihilation operators) in terms of which it is possible to express the problem (the Hamiltonian), the quantities of interest (the observables), and the domain of definition (the basis states defined by the creation operators applied to some vacuum state). Using an appropriate notation is equally important: the operators are usually expressed as single-character symbols, possibly with further indexes, and a dagger is used to distinguish creation from annihilation operators. The computer algebra system Mathematica makes it possible to both easily define the DSLs and to establish a suitable notation for these DSLs. In this article I describe package SNEG, which implements a DSL for second-quantization expressions and provides the corresponding natural notation for its output and several syntactically different but semantically equivalent ways for entering the input expressions. In addition to facilitating the representation of the input to numerical codes, the package is powerful enough to perform some calculations directly (e.g., evaluation of the expectation values using Wick's theorem, calculation and simplification of operator commutators, etc.).

This paper is structured as follows. Section 2 is devoted to the specification of basic elements (operators), their concatenation (non-commutative multiplication) and their automatic reordering (according to the canonical commutation/anticommutation rules or some other specification); it also introduces the Dirac bra-ket notation which can be mixed with the second-quantization operator expressions, and the occupation-number-representation vectors. Section 3 presents some examples of higher-level routines for generating second-quantization expression (particle number and spin operators, etc.) and their manipulation (commutators and anticommutators, etc.). Section 4 details the utility routines for generating basis states which satisfy chosen symmetries (particle number conservation, rotational invariance in the spin space) as well as the routines for generating the matrix representations of operator expressions in given basis space; these routines are crucial for the applications of SNEG as an input preprocessor for lower-level numerical computer codes. The focus of Section 5 are symbolic sums

with dummy indexes and their automated simplification using pattern matching. Finally, Section 6 describes the successful use of SNEG in the numerical renormalization group package “NRG Ljubljana”.

The package SNEG comes with detailed documentation which integrates in the Mathematica interactive help system. Each SNEG function is carefully documented and examples are provided. For this reason, the function calls are not described in this article; instead, the focus here is on the basic concepts, design choices, conventions followed, and some applications.

SNEG is released under the GNU Public License (GPL) and the most recently updated version is available from <http://nrg.ljubljana.ijs.si/sneg>. The package comes with a standard battery of test cases which may be used as a regression test, but also to verify that the possible user's custom extensions do not interfere with the expected behavior of the library.

While there are other packages for symbolic calculations with non-commuting objects for Mathematica and for other computer algebra systems (supercalc [1], ccr\_car\_algebra [2], NCAAlgebra [3], NCComAlgebra [4], grassmann.m [5], grassmannOps.m [6]), none appears to have the scope of SNEG. Furthermore, the goal of SNEG is different from more specialized symbolic manipulation packages such as TCE [7,8] for performing many-body perturbation theory in quantum chemistry or FormCalc [9] for calculations in theoretical high-energy physics. Instead, SNEG is principally intended to provide a general framework in which more sophisticated solutions can be implemented or as a tool that provides a more natural interface to the user.

## 2. Foundations

The cornerstone of SNEG is a definition of non-commutative multiplication with automatic reordering of operators in some standard form (usually the conventional normal ordering with creation operators preceding the annihilation operators) which takes into account selected (anti)commutation rules. Use of the standard form reordering allows automatic simplifications of expressions.

### 2.1. Operator objects and numeric objects

In SNEG, operators are internally represented as Mathematica expressions (lists) with a chosen head (typically a single-letter symbol) and containing the necessary indexes as list elements, for example

$$a[], c[k, \text{sigma}]. \quad (1)$$

The symbols need to be explicitly declared before they are used. The declaration routines define the default (anti)commutation properties of the objects. They also establish the natural on-screen notation (“pretty printing”) when the package is used interactively with the Mathematica notebook interface. Both the (anti)commutation properties and the pretty printing can be modified according to user's requirements. For operators declared to be bosons or fermions, the first element of the list (i.e., the first “index”) has a special role: it distinguishes creation operators ( $CR = 0$ ) and annihilation operators ( $AN = 1$ ):

$$c[CR, k] \rightarrow c_k^\dagger, \quad c[AN, k] \rightarrow c_k. \quad (2)$$

In addition, for fermions, by default SNEG follows the convention that the last index is interpreted as the particle spin ( $DO = \downarrow = 0$

and  $UP = \uparrow = 1$ ); this convention is used when generating operator expressions using higher-level functions (see below) and when pretty printing the expressions on computer display:

$$c[CR, k, UP] \rightarrow c_{k\uparrow}^\dagger, \quad c[CR, k, DO] \rightarrow c_{k\downarrow}^\dagger. \quad (3)$$

In addition to the internal Mathematica representation and the pretty printing, SNEG supports a third way of expressing operators using a condensed notation in pure ASCII strings. Such strings start with the operator symbol, followed by a + sign in case of creation operators, then the arguments follow in the parenthesis. For example, the three following expressions are equivalent:

$$c + (k) \leftrightarrow c[CR, k] \leftrightarrow c_k^\dagger. \quad (4)$$

The translations between ASCII strings and Mathematica expressions need to be performed explicitly using suitable functions, while pretty printing is (by default) performed automatically to render an expression in internal representation using the conventional notation. In principle, it would be possible to use the conventional pretty-printed notation for input, but entering such expressions by hand or with the assistance of Mathematica palettes turns out to be cumbersome.

Fermionic operators with different symbols are assumed to anticommute, bosonic operators with different symbols are assumed to commute, and bosonic and fermionic are assumed to commute. If necessary, this default behavior can be overridden.

SNEG allows to explicitly declare certain symbols to be numeric quantities of specific kinds (integers, real, complex, or Grassmann numbers); this information is used to correctly factor out numeric objects from the operator strings. Grassmann variables are correctly anticommuted and  $z^2 = 0$ .

## 2.2. Non-commutative multiplication

In SNEG, the non-commutative multiplication is internally denoted by `nc`. In interactive sessions `nc` multiplications are pretty printed with centered dots between the terms, for example:

$$nc[c[CR, k, UP], c[N, k, UP]] \rightarrow c_{k\uparrow}^\dagger \cdot c_{k\uparrow}. \quad (5)$$

The dot is displayed in order to permit easy detection of possible errors arising from an inadvertent replacement of non-commutative with the usual commutative multiplication. Function `nc` is linear in all its arguments and associative. Furthermore, `nc[] = 1` and `nc[c] = c`; these two rules mimic the behavior of the standard Mathematica product function `Times` and imply the property of idempotency of multiplication. Function `nc`, unlike `Times`, does not have the pattern-matching attributes `Flat` and `OneIdentity`. Instead, the associativity property is explicitly implemented. This design choice was motivated by reasons of efficiency in pattern matching, and benchmarking has shown that the explicit rules perform better than the version using `Flat` and `OneIdentity` by up to 50%.

It is possible to convert Mathematica representation of operator expressions to (and from) ASCII strings. In ASCII strings, the non-commutative multiplication is implied. For example, `a + (k)a(1)` is converted to `nc[a[CR, k], a[AN, 1]]`.

## 2.3. Expression reordering

Computer algebra systems simplify expressions by ordering them in some canonical manner; in this way, the equivalent parts can be combined (or canceled out, if the prefactors sum to zero). This is how some simplifications are automatically effected in Mathematica. For this reason, SNEG also attempts to reorder multiplicands in the `nc` operator strings according to some canonical

order, using the associated canonical anticommutation and commutation rules for the operators.

By default, fermionic operators are sorted canonically (in the sense that creation operators are permuted to the left and annihilation operators to the right) and then by the remaining indexes, including spin as the last index. It has to be remarked, however, that the canonical order depends on the definition of the vacuum state. SNEG supports either an “empty band” vacuum with no particles present, or a “Fermi sea” vacuum with levels filled up to the Fermi level. In the default “empty band” ordering the value of the first index (`CR` or `AN`) fully determines whether an operator is a creation or an annihilation operator. In the case of “Fermi sea” ordering, the second index of the operator is tested by default. This index is assumed to be a “momentum” or “energy” index, with the Fermi level fixed at zero. If necessary, it is also possible to turn off the automatic reordering for a fermionic operator. This is useful for very long expressions which can be simplified more efficiently by explicitly using Wick’s theorem rather than by automatic operator reordering.

Internally, the operator ordering is tested with `sneqOrderedQ`, while the necessary transformations on the operator strings (when out-of-order parts are detected) are implemented as transformation rules for the function `nc`.

When operators of different types appear in the same product, they are disentangled. For example, bosonic operators are by default always commuted to the left of fermionic operators, Majorana fermionic operators are anticommuted to the left of the Dirac fermionic operators, etc.

SNEG will attempt to simplify expressions involving exponential functions of operators using the Baker–Hausdorff relations and the Mendaš–Milutinović relations [10].

## 2.4. Occupation-number representation

For fermionic operators, SNEG allows working with the occupation-number representation (ONR) of the states in a given Fock space. Second-quantized expressions can be applied to these states, one can compute the matrix elements of operators between pairs of states, etc. The states in the ONR are expressed in the form of Mathematica lists (“vectors”) with head `vc`, which contain the occupancies of all orbitals represented by zeros and ones. In interactive Mathematica notebooks, the ONR vectors are shown in the Dirac-ket-like format with boxes which are either empty or filled, according to the occupancy of various orbitals:

$$vc[0, 1, 0, 1] \rightarrow |\square \blacksquare \square \blacksquare\rangle. \quad (6)$$

If a vector is conjugated using `conj`, it behaves as the corresponding bra. If a bra and a ket are multiplied by `nc`, the corresponding scalar product is computed.

It is possible to convert an ONR vector to the string of creation operators which, applied to the vacuum state, would give back the same vector.

## 2.5. Dirac’s bra–ket notation

SNEG provides support for calculations with the Dirac bra–ket notation, which can be intermixed with the second-quantization expressions. This is convenient, for example, for mixed electron–phonon systems, where the fermions can be described using the second-quantization language, but the oscillator using some other convenient representation, such as coherent states. In mixed expressions, the bras and kets are by default always commuted to the right of the fermionic operators. In interactive Mathematica sessions, the bras and kets are displayed enclosed by appropriate angled brackets and bars.

A ket can be expressed using function `ket`, which can take one or several arguments (quantum numbers):

$$\text{ket}[m, n] \rightarrow |m, n\rangle. \quad (7)$$

Quantum numbers may also remain unspecified; this is signaled by the value `Null`; in interactive sessions it is displayed as a small centered circle:

$$\text{ket}[m, \text{Null}, n] \rightarrow |m, \circ, n\rangle. \quad (8)$$

This functionality can be used to multiply kets from orthogonal Hilbert spaces. All the preceding rules also apply to bras, defined using `bra`. With the Hermitian conjugation function `conj`, a bra can be transformed into ket and vice versa.

When a bra and a ket are multiplied by `nc`, a scalar product is computed by comparing the quantum numbers in equivalent positions using the Kronecker delta:

$$\text{nc}[\text{bra}[m, n], \text{ket}[i, j]] \rightarrow \delta_{m,i} \delta_{n,j}. \quad (9)$$

It is possible to mix occupation-number-representation vectors and Dirac bra–ket vectors. The two subspaces are assumed to be unrelated (i.e., tensor product space).

### 3. Generation of expressions and operations on expressions

SNEG includes higher-level functions for generating various physically relevant operators which can be expressed in terms of the second-quantization operators and for performing various operations upon the expressions. In many of the applications of SNEG, the package can be used at this higher level and the user does not need to be concerned with the inner working of the library.

- The number (occupancy) operator  $n = c^\dagger c$  can be generated with the function `number` which comes in different flavors depending on the function argument(s). It can automatically handle particles with spin and it is possible to generate the number operator for more complex objects such as linear combinations of orbitals.
- The inter-site hopping operator may be generated using `hop`, for example for a particle with spin:

$$\text{hop}[c[1], c[2]] \rightarrow \sum_{\sigma} c_{1,\sigma}^\dagger c_{2,\sigma} + c_{2,\sigma}^\dagger c_{1,\sigma}. \quad (10)$$

- The electron–electron repulsion operator  $n_{\downarrow} n_{\uparrow}$  may be generated using the SNEG function `hubbard`:

$$\text{hubbard}[c] \rightarrow -c_{\downarrow}^\dagger c_{\uparrow}^\dagger c_{\downarrow} c_{\uparrow}. \quad (11)$$

- Spin operator for orbitals described by fermionic operators can be generated by SNEG functions `snegx`, `snegy`, and `snegz`, which are defined for all values of particle spin (parameter `spinof`). For example,

$$\text{spinx}[c] \rightarrow \frac{1}{2}(c_{\downarrow}^\dagger c_{\uparrow} + c_{\uparrow}^\dagger c_{\downarrow}) \quad (12)$$

for a spin-1/2 operators. The exchange coupling (i.e., the scalar product of two spin operators,  $\mathbf{S}_1 \cdot \mathbf{S}_2$ ) can be generated using `spinspin`.

- An important application area of SNEG is the computation of the vacuum expectation values (VEV) of second-quantization-operator strings using `vev`. To speed up the evaluations, a number of simplification rules are defined in SNEG. Expressions can be “normal ordered” by subtracting their vacuum expectation values.

- Hermitian conjugates of operator strings can be computed using the function `conj`. The numerical constants and parameters are handled correctly depending on their nature (real or complex commuting numbers, or Grassmann anticommuting numbers). For complex fermionic and bosonic operator objects, the first index is modified (creation to annihilation, and vice versa), while real fermionic operator objects are left unchanged.
- Commutators and anticommutators can be computed trivially by forming the sums or differences of the products, or with the help of the provided auxiliary functions `commutator` and `anticommutator`.
- Projection operators can be generated, for example `projector0[c] → (1 - n↑)(1 - n↓)`.

This list is not exhaustive and further functionality is described in the bundled SNEG documentation.

Often it is necessary to proceed in the opposite direction: given a long complex operator-string expression, one has to rewrite it in terms of higher-level functions, such as number, hopping, repulsion, or spin operators. This might be used, for example, after performing a change-of-basis transformation on the creation and annihilation operators, if one requires a physical interpretation of the resulting long expression. There is, clearly, no unique mapping from an expression to the corresponding generation functions. Therefore, there are several specialized SNEG routines which apply heuristic rules in an attempt to rewrite the expression. The whole set of the rules can also be applied by `SnegSimplify` and `SnegFullSimplify`, although experience shows that such brute-force approach is not very efficient and that a guided consecutive application of suitably chosen specialized routines gives better results.

### 4. Generation of sets of basis states

One of the principal application areas of SNEG is the transformation of the operators expressed in the second-quantized notation into the corresponding matrix representation in a given Hilbert space. To simplify numerics, it is often important to take into account various symmetries of the problem, i.e., to determine the Hamiltonian matrices in the different invariant Hilbert subspaces. SNEG provides a number of functions for generating the basis-state sets with chosen well-defined quantum numbers (total charge, total spin, etc.).

The states can be represented in SNEG either as strings of second-quantization operators (implicitly applied to a vacuum state in which no particles are present) or as occupation-number-representation vectors.

The basis-state set that spans the full Fock space is represented as a list of pairs – the first member of each pair is a list of quantum numbers which fully characterizes the invariant subspace, while the second member of the pair is a list of all the basis states in the given subspace. Once the desired basis sets have been generated, the operators in the second-quantization language can be transformed into the corresponding matrix representations. An example of such a calculation for the two-site Hubbard model is shown in Fig. 1 in the form of an interactive Mathematica session. One can see how easy it is to extend such a model definition to larger cluster sizes, to add various interaction terms to the Hamiltonian, or to define basis sets which satisfy different symmetries. For example, in the presence of the magnetic field (added using the macro function `spinz`), one should replace the full spin quantum number  $S$  by a component of spin along the  $z$ -axis,  $S_z$ ; such a change is effectuated by replacing the call to `qsbasis` by a call to `qszbasis`, no other changes are required. This example makes

```

In[5]:= H = ε (number[c[1]] + number[c[2]]) +
          U (hubbard[c[1]] + hubbard[c[2]]) + t hop[c[1], c[2]]

Out[5]:= t (c1†↓ · c2↓ + c1†↑ · c2↑ + c2†↓ · c1↓ + c2†↑ · c1↑) +
          ε (c1†↓ · c1↓ + c1†↑ · c1↑ + c2†↓ · c2↓ + c2†↑ · c2↑) +
          U (-(c1†↓ · c1†↑ · c1↓ · c1↑) - c2†↓ · c2†↑ · c2↓ · c2↑)

In[6]:= MatrixForm[b = qsbasis[{c[1], c[2]}]]

Out[6]/MatrixForm=
(
  {-2, 0}      {1}
  {-1, 1/2}    {c2†↑, c1†↑}
  {0, 0}       {c2†↓ · c2†↑, (c1†↓ · c2†↑ - c1†↑ · c2†↓) / √2, c1†↓ · c1†↑}
  {0, 1}       {-(c1†↑ · c2†↑)}
  {1, 1/2}     {c1†↑ · c2†↓ · c2†↑, c1†↓ · c1†↑ · c2†↑}
  {2, 0}       {c1†↓ · c1†↑ · c2†↓ · c2†↑}
)

In[7]:= m = makematricesbzop[H, b];
          MatrixForm@Map[{First[#], MatrixForm[Last[#]]} &, m]

Out[8]/MatrixForm=
(
  {-2, 0}      (0)
  {-1, 1/2}    (ε t)
               (t ε)
  {0, 0}       (U + 2 ε  √2 t  0)
               (√2 t  2 ε  √2 t)
               (0  √2 t  U + 2 ε)
  {0, 1}       (2 ε)
  {1, 1/2}     (U + 3 ε  -t)
               (-t  U + 3 ε)
  {2, 0}       (2 (U + 2 ε))
)

```

**Fig. 1.** A screen-shot from an interactive SNEG session using the Mathematica notebook interface: definition of the Hamiltonian  $H$  for a two-site Hubbard model, generation of a basis with well-defined total occupancy (relative to the half-filling) and total spin, and conversion of the Hamiltonian to its matrix representations in each invariant subspace of the total Fock space. The index pairs in the first column of the table are the quantum numbers, for example  $\{1, 1/2\}$  corresponds to  $Q = 1$  (one particle above half-filling) and  $S = 1/2$  (i.e. a spin-doublet state).

it clear how easy it is to add various perturbation terms to the Hamiltonian; very often no programming is required.

### 5. Symbolic sums

SNEG allows calculations with symbolic sums over dummy indexes, which remain in their unevaluated forms. They are defined using the function `sum` taking two arguments: the first one is the expression that is being summed over, while the second one is the list of all summation indexes. The list of indexes is automatically sorted; this allows some automatic simplifications. Numeric quantities which do not depend on any of the summation indexes are factored out. Products of sums can be calculated using `nc`. SNEG automatically handles summation index collisions and renames the duplicated indexes. It is thus perfectly safe to use the same dummy index in different expressions. When commutators of sums are computed, the name replacement is always performed on the same sum in order to maximize the opportunities for automatic cancellation of equal terms.

Expressions with symbolic sums can be automatically simplified using `sumSimplify` which uses Mathematica function `Simplify` with additional transformation functions for expanding, simplifying, and collecting the terms.

### 6. Applications

SNEG has found many applications in the field of theoretical condensed-matter physics. It has been applied to perform exact diagonalizations on Hubbard clusters, small Heisenberg chains, and similar lattice models, calculations of commutators of complex operator expressions (to establish the presence of various symmetries, in the equation of motion method, etc.), and perturbation theory to higher orders. It is best suited for problems where the complexity is too high for paper-and-pencil calculations, yet still sufficiently low for a brute-force computer algebra approach (which SNEG essentially is). The package makes otherwise tedious calculations a routine operation. Most importantly, it prevents inauspicious sign errors which commonly arise when fermionic operators are (anti)commuted. For this reason, the package is also suitable for educational purposes, i.e., as a way of verifying the correctness of elementary calculations with operator quantities.

It should be remarked that the automatic-reordering approach does not scale well to very long strings of operators, since the computation time for automatic simplifications increases as a power law of the string length. This is due to the fact that SNEG internally makes use of Mathematica as a pattern matching and replacement engine. The pattern application time increases with the string length, but also the application of (anti)commutation rules

leads to the rapid growth of the total number of terms in the intermediate expressions before the terms can be eventually canceled out. For such problems, the automatic reordering can be turned off; the expression can still be reordered explicitly using a suitable direct calculation. For very long operator strings, it would be more appropriate to perform the expression reordering and simplification using a direct algorithm coded, perhaps, in some lower-level programming language.

The main major application of SNEG in its role of an “interface” between the user and the low-level numerical codes is the package “NRG Ljubljana” for performing the numerical renormalization group (NRG) calculations for quantum impurity models [11–13]. Using SNEG as the underlying library, both the model (Hamiltonian) and the observables (operators) may be defined in terms of high-level expressions. This enables a clear separation between the problem domain (coded in Mathematica and SNEG) and the solution domain (coded in C++). This is advantageous not only for reasons of performance, but especially for maintainability of the code. During the lifetime of the project, no major rewrites or design changes were necessary in either part of the code and the development could proceed incrementally without breaking the existing features. Furthermore, adapting the package to different problems and symmetries, or to calculate new quantities, is rather trivial.

## 7. Conclusion

The natural language of many-particle physics is the quantum field theory, more particularly the formalism of the second quantization. I have argued that the computational many-body physics should strive towards creating computer codes which allow defining problems – whenever possible – in their natural problem-

domain language. It is hoped that the approach (and the specific implementation, SNEG) will improve the productivity of users and the quality of scientific software, in particular reliability, reusability, maintainability, and correctness.

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