Automated tools for many-body theory

P. Arthuis*
Technische Universität Darmstadt, Department of Physics, 64289 Darmstadt, Germany,
ExtreMe Matter Institute EMMI and Helmholtz Forschungsakademie Hessen für FAIR (HFHF),
GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany

T. Duguet†
IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France and
KU Leuven, Instituut voor Kern- en Stralingsfysica, 3001 Leuven, Belgium

F. A. Evangelista‡
Department of Chemistry, Emory University, Atlanta, Georgia 30322, USA

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I. SCIENTIFIC ISSUE

The formalism of second quantization, first developed in the context of the quantum field theory, is the natural language for expressing and deriving many-body theories such as perturbation theory, coupled cluster methods, Green's functions approaches, and similarity renormalization group schemes in nuclear physics, condensed matter theory, and quantum chemistry.

Two crucial tools to express, manipulate and simplify algebraic expressions originating from many-body matrix elements of (products of) second-quantized operators are Wick's theorem and diagrammatic methods. For fermions, these matrix elements are typically formulated in terms of quasi-particle operators defined with respect to a many-body vacuum, e.g. a Slater determinant or Bogoliubov product state. Although Wick's theorem and diagrammatic methods have helped accelerate the exploration and implementation of novel many-body methods, the process quickly becomes prone to human error. In certain cases, many-body equations can involve so many contributions that it can become essentially impossible to derive them by hand.

Computer-aided (or automatic) derivation of many-body theories employs sophisticated algorithms to evaluate, simplify, and even automate the implementation of mathematical equations, offering a way to address the challenges mentioned above. In the past three decades, computer-aided derivation of many-body equations has played an ever-increasing role in quantum chemistry [1]. In particular, the early 2000s saw the rapid development of automatic derivation and implementation tools based on algebraic [2, 3], diagrammatic and string or determinant-based methods [4]. Recently, automatic derivation has been extended into many new directions, including arbitrary order response and derivatives, systems with coupled fermionic and bosonic degrees of freedom [5], more general vacua (Hartree-Fock-Bogoliubov, Bardeen-Cooper-Schrieffer, or antisymmetrized geminal power states), and the manipulation of quantum circuits [6].

Another related area is the problem of optimizing tensor operations that arise in many-body methods (factorization, global optimization of the contraction order, the identification of reusable intermediates, and the identification of common factors). In condensed matter physics, computer-aided methods have been used at the interface with Monte Carlo approaches to explore large model spaces and include important contributions at a limited cost [7].

Despite these developments, automatic derivation remains a field with untapped potential and open problems. This is demonstrated in recent works where automatic derivation has been introduced in nuclear structure theory to tackle

* parthuis@theorie.ikp.physik.tu-darmstadt.de
† thomas.duguet@cea.fr
‡ francesco.evangelista@emory.edu

non-standard perturbation theories [8, 9] and the Bogoliubov in-medium similarity renormalization group method [10] as well as in quantum chemistry to deal with arbitrary Fermi vacua [11].

Furthermore, automatic derivation is also crucial to achieve numerical implementations of new many-body theories. For example, internally-contracted multi-reference coupled cluster theory is currently implemented in production-level codes exclusively via automatic derivation tools [12], while computer-generated code has been used to extend perturbation theory calculations to high order for infinite nuclear matter [13]. In nuclear and atomic physics, it is key to take advantage of, e.g., rotational symmetry of the Hamiltonian and the expansion basis to a priori reduce the effective size of the latter and make the numerical scaling tractable. Automated tools are critical to pre-process the algebraic equations accordingly given that it becomes quickly impossible to do it manually [14].

Eventually, automated developments offer opportunities feedback into the theory: what physics insights can be gained from an easier access to a large number of contributions, and can this new theoretical knowledge in turn prove useful for future numerical implementations?

This workshop aims to bring together a group of experts from nuclear physics, condensed matter theory, and quantum chemistry to chart the future of automatic derivation tools in many-body physics. The workshop will aim to stimulate the exchange of ideas among different fields, promote the discussion of common challenges and solutions, and establish standards for code interoperability that will speed up progress in many-body physics.

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II. GOALS

The main goals of the workshop are to

1. introduce attendants to different approaches to computer-aided derivation techniques for many-body theory,

2. exchange ideas regarding state-of-the-art automatic derivation methods between quantum chemists and nuclear physicists,

3. discuss open problems in the field of automatic derivation, including the factorization of tensor contractions and identification of identical terms,

4. identify ways to make current automatic derivation tools interoperable as a way to validate, benchmark, and expand the capabilities of current codes.

III. PROGRAM

Structure

The meeting takes place over 4 days. The first morning is devoted to introductory/pedagogical presentations to inform/educate the local research community on the state of the art approaches developed to tackle the many-body problem. The following talks are focused on specific uses of automated derivation methods.

Introductory Lecture

- *An introduction to the history of computer-aided methods in quantum chemistry*
  Francesco Evangelista (chemistry) Emory University

Scientific talks

- *Automated generation and evaluation of diagrams at play in various many-body methods*
  Pierre Arthuis (nuclear physics) TU Darmstadt
- *Symbolic solution for computational quantum many-body theory development*
  Guo Chen (chemistry) Rice University
- *Bold diagrammatic Monte Carlo*
  Kris van Houcke (condensed matter) Ecole Normale Supérieure
- *Towards an efficient implementation of internally contracted coupled-cluster methods*
  Andreas Köhn (chemistry) University of Stuttgart
- *Symmetry reduction of tensor networks in many-body theory*
  Alexander Tichai (nuclear physics) TU Darmstadt
- *String-based methods for state-selective multi reference coupled cluster*
  Mihály Kállay (chemistry) Budapest University of Technology and Economics
- *Automatic generation of computer codes for correlated wavefunction calculations*
  Anastasios Papadopoulos (chemistry) Max-Planck-Institut für Kohlenforschung
- *Relativistic coupled cluster calculations for atomic spectra*
  Martijn Reitsma and Yuli Chamorro Mena (atomic physics) University of Groningen
- *A quantum computing perspective on many-body methods*
  Nicholas Rubin (quantum computing) Google
- *Automated code generation for many-body perturbation theory diagrams*
  Christian Drischler (nuclear physics) Ohio University
- *Generation of arbitrary order open-shell coupled cluster*
  Michael Hanrath (chemistry) Cologne University
- *Automatic derivation of fermionic many-body theories based on general Fermi vacua*
  Francesco Evangelista (chemistry) Emory University
- *Diagrammatic resummations for the in-medium similarity renormalisation group method*
  Matthias Heinz (nuclear physics) TU Darmstadt
- *Symbolic algebra manipulations for quantum many-body physics*
  Eduard Valeev (chemistry) Virginia Tech

Tentative schedule

	Monday		Tuesday	Wednesday	Thursday
09h15	Welcome				
09h30	**Evangelista**	9h30	**Köhn**	**Rubin**	**Evangelista**
10h45	Break	10h30	Break	Break	Break
11h15	**Arthuis**	11h00	**Tichai**	**Reitsma/Chamorro Mena**	**Heinz**
12h15	Lunch	12h00	Lunch	Lunch	Lunch
14h00	**Chen**	13h30	**Kállay**	**Drischler**	**Valeev**
15h00	Break	14h30	Break	Break	Break
15h30	**van Houcke**	15h00	**Papadopoulos**	**Hanrath**	**End**
16h30	End	16h00	**Discussion session**	**Discussion session**	
		17h00	End	End	