Centre for
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Development of many-body-theory methods for positron-atom interactions

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State of the art and motivations

Atomic physics aims to probe the fundamental nature of universe through high-precision experiment, and develop new technologies through exquisite control of atoms and molecules. Atoms and molecules involve many constituent nuclei and electrons that interact in complicated ways under the laws of quantum mechanics. The theoretical description of such *atomic many-body systems* is extremely challenging. For example, when low-energy positrons (the antiparticles of electrons and the simplest form of antimatter) interact with normal matter, such as atoms, they pull strongly on the electrons and may even cause one of the electrons to 'dance' around the positron, forming so-called positronium (as the positron and electron may annihilate, this may ultimately be a 'dance to the death'). These so called *correlations* have a very strong affect on positron-atom interactions. In particular, they can enhance the rate of positron annihilation by many orders of magnitude. Accurate calculations of positron scattering, binding and annihilation in atoms, crucial for development of fundamental antimatter experiments, positron-based materials diagnostic techniques and PET (Positron Emission Tomography) medical imaging, must fully account for the correlations. Moreover, *precise* calculations require numerical approaches that push scientific computing to its limits.

A powerful method of describing atomic many-body systems, which allows for the study and inclusion of interactions in a natural, transparent and systematic way, is *diagrammatic many-body theory* (see, e.g., [1–3] and the footnote[1]). In this method, instead of computing the complicated many-particle wavefunction, amplitudes for processes of interest — e.g., positron annihilation with an atomic electron — are represented by a series of relatively simple and intuitive diagrams that describe the most physically important contributions to the quantum amplitude of the process [see Fig 1]. The diagrams are constructed systematically according to a strict set of rules governed by the fundamental nature of the underlying interactions. By applying a 'dictionary' to the resulting diagrams, corresponding analytic expressions can be readily generated.

Mathematically, the diagram expansion for an amplitude Q (e.g., positron annihilation with atomic electron) takes the form of a series of integrals over diagrams $\mathcal{D}$ with an ever increasing

[1]The diagrammatic approach to the quantum many-body problem was pioneered by Richard Feynman in 1949 in his famous paper "*The theory of positrons*" [4]. Feynman later shared the 1965 Nobel Prize for his work in the field. Since then, they have "*have revolutionised nearly every aspect of theoretical physics*" [5].

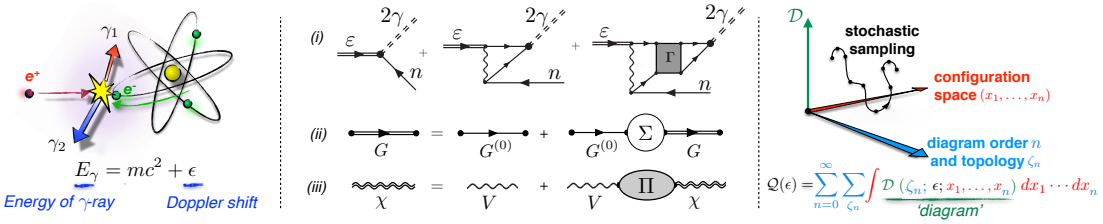

Fig. 1: Left: Positrons *annihilate* with atomic electrons producing Doppler-shifted γ-rays. **Centre:** (i) Amplitude for annihilation of a positron (labelled ε) with an electron in atomic level n, showing independent-particle approximation, first-order and virtual-positronium corrections. Straight lines denote electron or positron Green's functions. The number of wavy lines, which denote two-body Coulomb interactions, specifies the diagram *order*; (ii) Dyson equation for the '*dressed*' Green's functions G, in terms of the non-interacting ones $G^{(0)}$ obtained from atomic structure calculations and the correlation potential Σ, which can also be expressed diagrammatically; (iii) Integral equation for the *screened Coulomb interaction* χ. The 'Γ' (virtual positronium) and 'Π' (polarisation) blocks represent infinite series of electron-positron and electron-electron interactions, respectively. **Right:** In *diagrammatic Monte Carlo*, any quantity $\mathcal{Q}$ that can be written as a sum of diagrams $\mathcal{D}(\zeta_n; x_1 \cdots x_n)$ is calculated to high-precision by stochastically sampling the abstract space of diagram order n, topology ζ_n (i.e., different diagrams of the same order) and configurations $(x_1, \ldots, x_n)$ (i.e., the coordinates of vertices).

number of integration variables

$$Q(y) = \sum_{m=0}^{\infty} \sum_{\zeta_m} \int \underbrace{\mathcal{D}\left(\zeta_m, y; x_1, \ldots, x_m\right)}_{\text{"diagram"}}\, dx_1 \cdots dx_m. \tag{1}$$

Here, y is a set of variables on which $\mathcal{Q}$ depends, m is the diagram *order* (the number of Coulomb interactions), ζ_m labels the *topology* of the diagram (describing differently shaped diagrams of the same order), and $\{x_1, \ldots, x_m\}$ the *configurations* (location of vertices).

The current record number of diagrams calculated for a many-electron atom problem is $\sim$ 2000 (to fourth order in the Coulomb interaction: $m = 4$) [6]. Iterating to higher orders via brute-force is, however, unfeasible, due to the exponentially increasing number of diagrams and integrations that must be computed in Eqn (1). To perform high-precision calculations for general atomic systems, an alternative means of calculating high-order diagrams is required.

Objectives & Methodology

We have had considerable success developing and applying many-body theory of positron interactions with atoms, most notably providing a complete description of the positron interactions with noble-gas atoms [2,3,7–9], and very recently the first-accurate calculations for positronium (an atom consisting of a bound electron-positron pair) interactions with atoms [10]. Those works developed the many-body theory in the bare (undressed) positron-electron Coulomb interaction, i.e., ignoring the modification of the Coulomb interaction caused by the ability of the atomic electrons to respond to presence of the positron, effectively screening it.

This project will revisit the positron-atom problem, with the focus on developing an improved computational implementation of the many-body theory that can provide increased precision for that problem, and also enable the efficient calculation of more general properties and processes involving structured atomic and molecular systems. The first task will be to develop the many-body theory in the *screened* Coulomb interaction, calculating the diagrams in the Feynman formalism [11] as opposed to the basis representation we previously used. We will focus on positron interactions with noble-gas atoms, but can also consider positron interactions with a system of electrons in a harmonic potential, which provides an approximation to the positron

electron-gas [12]. Following this, we will implement Markov Chain Monte Carlo integration routines for the diagram evaluation. We will then focus on developing and implementing the *Diagrammatic Monte Carlo* approach [13, 14], in which, rather than performing explicit integrations, the diagrammatic series is summed to convergence by stochastically sampling the full set of diagrams over the abstract space of diagram order, topology and configuration space (see Fig. 1 right). For condensed matter lattice systems, the method has been used to successfully sum *millions* of diagrams, yielding spectacular agreement with experiment [15]. We will use the positron-atom system as the testbed for the application of this technique to structured atomic and molecular systems. Implementing diagrammatic Monte Carlo may be essential to enable accurate calculations of positron interactions with more complicated systems, including molecules and condensed matter (e.g., by providing a way to calculate the electron-positron ladder series).

Collaborations

We have internationally leading expertise in positron and many-body theory. There is scope to collaborate with the leaders in diagrammatic Monte Carlo in the UK, Germany and USA.

Required skills

The candidate is expected to have good working knowledge of and interest in Quantum Mechanics. It would advantageous (though not essential) to have experience of quantum-field theory/QED/many-body theory (in the context of atomic, nuclear or particle physics). He/she will be expected to learn and master many-body theory methods and their application to many-electron systems. Running, modifying and developing computer codes is an integral and substantial part of the project, but there will be a judicious mix of analytical and numerical work.

Further information

The student will contribute to a vibrant team that is expected to consist of at least two postdoctoral researchers and multiple PhD students delivering the objectives of the European Research Council project ANTI-ATOM: "*Many-body theory of antimatter interactions with atoms, molecules and condensed matter*" led by Dr Green. One postdoctoral researcher is expected to be working on the topic, with whom the student can closely interact.

The project will equip the student with a versatile, broad and transferrable skill set. In particular, the many-body theory methods possess great universality and are used (in slightly different form) in areas ranging from elementary particle theories to condensed matter physics. The experience of handling and writing computer codes, that will be acquired through the work on the project, will be useful in a wide range of future careers.

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