Development of convergent close-coupling approach to hadron interactions with matter

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Abstract. Activities undertaken at Curtin University towards developing a comprehensive approach to all aspects of hadron interactions with matter are reviewed.

1. Introduction
One of the primary benefits of hadron therapy is a large ratio of the radiation dose at the Bragg peak to that in the plateau region before the peak. From the physics point of view three factors must be considered that may potentially enhance or undermine this benefit. (i) In order to reach deep-seated tumour cells therapeutic ion beams should have energies from a hundred up to a few hundreds of MeV per a.m.u. At such high energies, energy losses due to ionisation are small. The main channels of energy losses here are nuclear collisions, which may lead to fragmentation of nuclei of the target, and of the incident beam particles if the latter is a heavy ion like $^{12}$C [1]. These also result in emission of neutrons. In the plateau region, the nuclear fragments and emitted neutrons can cause side effects, including new tumour cells. In addition, the nuclear fragmentation processes may disperse the beam and substantially affect the composition of the beam reaching the Bragg peak region. This complicates radiation dose simulations, which usually assume the initial beam composition. Due to complexity of nuclear interactions, there is no unified theory capable of describing them. Interaction models are generally anchored to experimental data, which in some areas are far from complete [2]. (ii) As the residual beam particles approach the Bragg peak region, their energy reduces significantly. When the energy falls below tens of MeV, energy losses due to excitation and ionisation of the target atoms and molecules become dominant. It is often stated that the theory of these processes is well developed. However, this is not quite correct. Currently available Monte Carlo simulation packages for modelling of biological damage induced by hadrons rely on the Bethe-Bloch (BB) theory of energy losses. However, the BB theory and its numerous improvements cannot meet accuracy requirements. There are a number of reasons for this. First, the BB-type theories do not include electron-capture channels. Second, they are perturbative and their applicability is limited to projectile energies higher than several MeV. Furthermore, they are based on the so-called dipole approximation to the first Born approximation. Third, the BB-type theories do not include coupling between various reaction channels. When hadrons approach the Bragg peak region, their energy diminishes considerably. In this energy region, the probability of electron capture becomes dominant and coupling between the channels – significant. In fact, when the energy falls below 100 keV per a.m.u., further energy losses are purely due to electron capture. Hence, accurate simulations of ion beam passage through matter at the micro- and nanoscale require inclusion of the electron-capture channels in addition to ionization [3]. (iii) In the Bragg peak region, the probability of target ionisation by the incident hadrons reaches
its maximum. This leads to production of a copious number of secondary electrons. These so-called \( \delta \)-rays have energies sufficient to further ionise the target and, as a result of multiple scattering, are capable of causing DNA double-strand breaks. It is estimated that among all the double strand breaks of DNA molecules of tissue treated by ion therapy, about 70% are produced by the \( \delta \)-electrons [3]. Therefore, it is necessary to understand interactions of the produced \( \delta \)-electrons in combination with interactions of the beam ions.

Thus, detailed knowledge of hadron beam interactions with atoms and molecules is paramount for accurate dose simulations in hadron therapy. We have been working on a comprehensive approach to modelling hadron interactions with matter that is capable of addressing all three factors mentioned above. We have developed an approach to hadron collisions with atomic and molecular targets. The approach known as the convergent close-coupling (CCC) [4-6] accounts for all possible reaction channels including ionisation and electron capture and is capable of providing the most detailed and accurate information about the collision process. We have also developed the CCC approach to electron-impact ionisation of atomic and molecular targets [7] applicable to \( \delta \)-electrons. In addition, work is in progress on developing CCC-type approach to nuclear fragmentation, building on our experience in modelling nuclear reactions (see [8-11] and references therein). Further we concentrate on one aspect of these activities. We give a brief account of the CCC approach to hadron scattering in the Bragg peak region.

2. Development of convergent close-coupling approach to hadron-atom collisions

For simplicity we consider hadron collisions with a single-electron target. Generalisation for more complex targets is described in [12-14]. The total scattering wave function is a solution to the fully quantum-mechanical Schrödinger equation

\[
(H - E)\psi_i^+ = 0, \tag{1}
\]

where \( H \) is the three-body Hamiltonian and \( E \) is the total energy. Conventional approaches to ion-atom collisions are based on the approximate time-dependent Schrödinger equation for the electronic part of the wave function that follows from Eq. (1) in a semiclassical approximation [15]. The CCC approach is different and based on expansion of the three-body wave function as

\[
\psi_i^+ \approx \sum_{\alpha=1}^{N} F_\alpha(t, b) e^{i\mathbf{q}_\alpha \cdot \mathbf{p}_\alpha} \psi_\alpha(r_\alpha) + \sum_{\beta=1}^{M} G_\beta(t, b) e^{i\mathbf{q}_\beta \cdot \mathbf{p}_\beta} \psi_\beta(r_\beta), \tag{2}
\]

where \( b \) is the impact parameter. Index \( \alpha \) denotes a quantum state in a channel where the projectile of relative momentum \( \mathbf{q}_\alpha \) is incident on a bound state of the target atom. Index \( \beta \) is reserved for the rearrangement channel, where the atom formed by the projectile after electron capture has momentum \( \mathbf{q}_\beta \) relative to the stripped target nucleus. The position of the projectile with respect to the centre of mass of the target is denoted by \( \mathbf{r}_\alpha \), while \( \mathbf{r}_\beta \) is the position of the projectile-electron pair with respect to the target nucleus. The position of the electron relative to the target proton is \( \mathbf{r}_\alpha \), while \( \mathbf{r}_\beta \) is the electron position relative to the projectile. The basis includes the continuum in a suitably discretized form, where \( \psi_\alpha \) and \( \psi_\beta \) are the target and projectile-centred pseudostates, \( N \) and \( M \) are the numbers of basis functions on the target and projectile centers. The time-dependent expansion coefficients \( F_\alpha(t, b) \) and \( G_\beta(t, b) \) at \( t \to \infty \) represent the transition amplitudes into the target and projectile pseudostates.

We substitute expansion (2) into the Schrödinger equation (1). Then apply the Hamiltonian operator on the wave function and use the semiclassical approximation [15]. Multiplying the result by \( \psi_\alpha^{* \prime}(r_\alpha) e^{-i\mathbf{q}_{\alpha} \cdot \mathbf{p}_{\alpha}} (\alpha' = 1, ..., N) \) and integrating over \( r_\alpha \), and then multiplying by \( \psi_\beta^{* \prime}(r_\beta) e^{-i\mathbf{q}_{\beta} \cdot \mathbf{p}_{\beta}} (\beta' = 1, ..., M) \) and integrating over \( r_\beta \), after some lengthy algebra we get the following set of first-order differential equations for the time-dependent coefficients
\[
\begin{align*}
&\frac{\partial F_\alpha}{\partial t} + i \sum_{\beta=1}^{M} G_\beta R_{\alpha'\beta} = \sum_{\alpha'=1}^{N} F_{\alpha'} D_{\alpha'\alpha} + \sum_{\beta=1}^{M} G_\beta Q_{\beta'\alpha}, \quad \alpha' = 1, 2, \ldots, N, \\
&i \sum_{\alpha=1}^{N} \hat{F}_\alpha K_{\alpha'\alpha} + \hat{G}_{\beta'} = \sum_{\alpha=1}^{N} F_{\alpha} Q_{\beta'\alpha} + \sum_{\beta=1}^{M} G_\beta D_{\beta'\beta}, \quad \beta' = 1, 2, \ldots, M,
\end{align*}
\]

where dots over \( F_\alpha \) and \( G_\beta \) denote time derivative. The system of equations is solved subject to the initial boundary condition specified as

\[
(F_\alpha(-\infty, b) = \delta_{\alpha 1}, \quad \alpha = 1, 2, \ldots, N, \\
(G_\beta(-\infty, b) = 0, \quad \beta = 1, 2, \ldots, M.
\]

Overlap integrals \( K_{\beta'\alpha} \), direct-scattering matrix elements \( D_{\alpha'\alpha} \) and electron-transfer matrix elements \( Q_{\beta'\alpha} \) are given in [6]. Notably, they coincide with the corresponding matrix elements from the conventional close-coupling theory. In addition, the set of equations (3) is also the same. This is despite us starting from the exact Schrödinger equation and using a different ansatz for the total wave function. However, a novel feature of our approach is that it does not use the concept of a so-called electron translation factor, required in the conventional approaches due to an inadequate representation of the electron-capture channels. Some six decades ago Bates and McCarroll [16] realised that the conventional expansion of the electronic part of the wave function does not satisfy the semiclassical time-dependent Schrödinger equation unless an electron translation factor is introduced to remedy the problem. The problem with this artificial electron translation factor is that there are infinitely many ways of choosing it [15]. Our ansatz correctly represents both direct scattering and rearrangement channels, and therefore does not lead to the aforementioned problem. Hence, there is no need to introduce any remedial factor.

3. Results

The CCC approach has been applied to calculate cross sections [4-6, 12-14] and stopping powers [20-23] for hadrons in various atomic and molecular targets in the energy range from 1 keV to 1 MeV. Recently, we have used the wave-packet implementation of the CCC (WP-CCC) to calculate differential cross sections in proton-hydrogen collisions [6]. In particular, doubly differential cross sections for ionisation gave excellent agreement with experimental measurements available at 75 keV. Figure 1 shows the WP-CCC results for angular differential cross sections for elastic scattering, \( n = 2 \) excitation and electron capture in proton-hydrogen collisions at 60 keV. Excellent agreement is observed with experimental measurements [17-19] for every process. See [6] for details of the calculations and more results.

![Figure 1](image-url)

**Figure 1.** Angular differential cross sections for elastic scattering, \( n = 2 \) excitation and electron capture in proton-hydrogen collisions at 60 keV. The experimental data for elastic scattering, excitation and electron capture are from [17], [18] and [19], respectively.
4. Conclusion
We have developed a convergent close-coupling approach to hadron scattering on atomic and molecular targets applicable in the Bragg peak region. The approach starts from the exact fully quantum-mechanical three-body Schrödinger equation for the total scattering wave function. The scattering wave function is expanded using a two-center pseudostate basis that includes the continuum in a suitably discretized form. This allows one to take into account all underlying processes: elastic scattering, excitation, ionisation, and electron capture into bound and continuum states of the projectile. After using the semiclassical approximation we get a system of coupled differential equations for the transition probability amplitudes, well-known in conventional close-coupling methods based on the semiclassical time-dependent Schrödinger equation for the electronic part of the scattering wave function. However, a novel feature of our approach is that it does not use the concept of a so-called electron translation factor, required in other approaches due to an inadequate representation of the electron-capture channels. The convergent close-coupling approach is capable of providing the most detailed and accurate description of the processes taking place in hadron interactions with simple targets.

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6. References
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