Chapter 1

Simulation Pipeline

In this chapter the simulation of a hyperfine spectrum measured at TRIUMF is described in detail. §1 includes little more than a graphical representation of the algorithm followed when the atoms are interacting with the laser. Each subsequent section is dedicated to an individual step in the algorithm, detailing the logic and computations required at that step. The final section of the chapter shows how a hyperfine spectrum is built through the repeated application of the interaction loop.

1.1 Interaction Loop

Fig. 1 shows each step taken an atom as it passes through the simulation. The red rounded rectangles represent preliminary steps in the simulation, where initial properties are imparted to the atom. The first preliminary step selects a velocity and ground state for the atom. The following step is the calculation of the likelihood of excitation for each allowed transition. This prepares the atom for what can be considered the main loop of the algorithm. Here, the atom and laser interact as the atom traverses the IR.

The interaction loop is composed of green ellipses and blue rectangles. Two of the three green ellipses represent regular checks to ensure that the atom is still in the IR. If at any point the atom is found to have moved
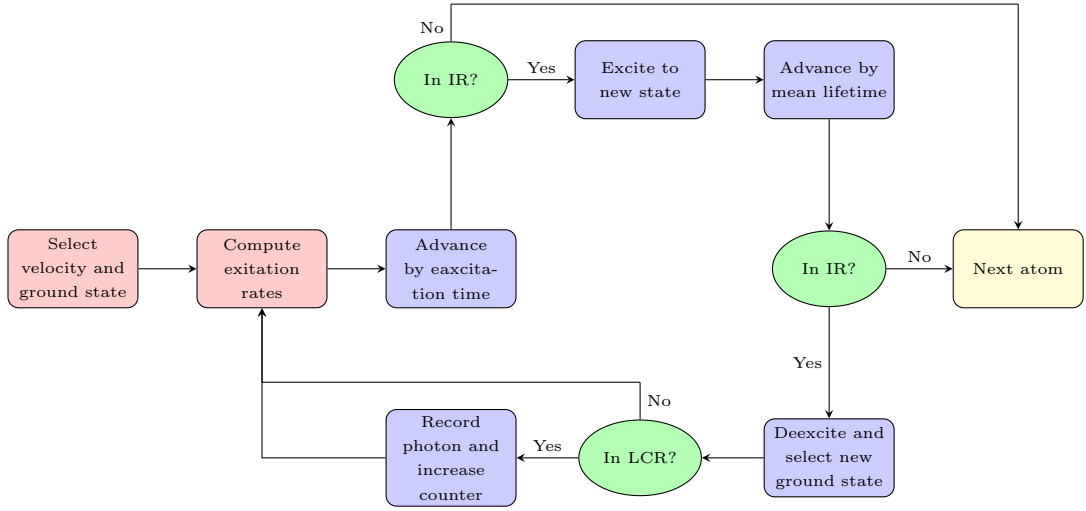
Figure 1.1: Flow chart detailing the steps undertaken by the algorithm to follow the atom as it moves through the IR. The green ellipses and blue rectangles compose the interaction loop of the simulation, where the atom interacts with the laser and goes through excitation/decay cycles. Finally, the yellow rectangle is the end point of the loop, and occurs when then atom has moved beyond the IR.

beyond the IR, then the algorithm moves on to the next atom. The third green ellipse is dedicated to checking if a photon released by the atom would be measured by the PMT. The evolution of the state and position of the atom is described by the blue rectangles.

1.2   Preliminary Steps

The first two steps select the initial properties given to the atom, determining how likely the atom is to interact with the laser. The two most important properties are the velocity and the ground state of the atom. Both are chosen through the sampling of their respective probability distributions.

1.2.1 Velocity Selection

The velocity of the atom v_a can be decomposed in to two elements: the mean velocity of the beam, v_m, and the thermal velocity v_T.

$$v_a = v_m + v_T \tag{1.1}$$

The mean velocity is determined by the energy of the beam and the mass of the atom, i.e.

$$v_m = \sqrt{\frac{2E_b}{m_A}} \tag{1.2}$$

where E_b is the energy of the beam and m_A is the mass of an atom with mass number A.

The thermal velocity is selected by sampling the Maxwell-Boltzmann distribution, described in (INSERT REFERENCE TO THEORY SECTION). This is done using the Box-Muller transform, which samples a uniform distribution twice and converts the results into a sample of a normal distribution. A sample v_T, of a Maxwell-Boltzmann distribution for atoms of mass m_A and temperature T is given by

$$v_T = \sqrt{\frac{KT}{2m_A}}\sqrt{-2\log x_1}\cos(2\pi x_2) \tag{1.3}$$

where $x_1, x_2 \in [0,1]$ are two randomly generated numbers taken from a uniform distribution.

1.2.2 Ground State Selection

For an atom with a coupled angular momentum state F_g as the ground state, the electron can occupy any of the $2F_g + 1$ projections on the axis of quantization. A particular projection, say $F_i \in [-F_g, -F_g + 1, ..., F_g - 1, F_g]$, has a probability of being occupied that is proportional to $2F_i + 1$. Taking the probability space occupied by each projection in to account, the probability that an electron occupies the projection F_i, $P(F_i)$, is given by

$$P(F_i) = \frac{2F_i + 1}{\sum_j 2F_j + 1} \tag{1.4}$$

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Knowing this, the ground state can be chosen through the generation of a random number $x \in [0, 1]$ from a uniform distribution. Each projection is given a range of numbers from 0 to 1, proportional to Eq. 1.4. If x falls in the assigned range, then that ground state is chosen.

1.2.3 Computation of Excitation Rates

With the ground state and the velocity of the atom now selected, the probability that a transition will occur can be calculated. For each allowed transition between the chosen ground state F_g and an excited state $F_{e,i}$, the transition rate γ_i is given by Eq. (REFERENCE THEORY). Note that the laser frequency f_l must be shifted according to the relavistic doppler effect which depends on the velocity of the atom. The frequency observed by the atom, f_o, is given by

$$f_o = f_l \sqrt{\frac{1 + \beta}{1 - \beta}} \tag{1.5}$$

where $\beta = v_a/c.$?

1.3 Interaction Loop

The interaction loop of the algorithm is the place where the atoms undergo several instances of excitation and decay. Also included are regular checks to see in the atom would still be present in the in interaction region, as well as whether or not a released photon would be measured by the light collection system present in the experiment.

1.3.1 Excitation Time

Once all the excitation rates have been computed, the atom can now be advanced by the expected time it takes for a transition to occur. This time is called the excitation time, t_e, and is given by

$$t_e = \sum_i \frac{1}{\gamma_i} \tag{1.6}$$

After time t_e, the atom is advanced a distance $d_e = t_e v_a$. If it is still in the interaction region, then an excited state F_e is chosen by sampling a uniform distribution where each transition is given a region proportional to $1/\gamma_i$, in similar style to the method used to select the ground state. If the atom is no longer in the interaction region after t_e, then it is discarded and the algorithm moves on to the next atom.

1.3.2 Advancing by the Mean Lifetime, Decay and Selection of New Ground State

Once the excited stated of the atom has been selected, then the atom is advanced a distance $d_l = t_l v_a$ where t_l is the mean lifetime of the excited state. The mean lifetimes of each excited state are computed (according to (REFERENCE ENTIRE EMISSION SECTION)) once at the beginning of the simulation, then stored for later use. If the atom is still in the interaction region after having moved d_l, then it decays into one of the allowed ground states. If not, then the simulation moves on to the next atom. As with the selection of the excited state, a uniform distribution is sampled, and each ground state $F_{g,i}$ is given a range of values proportional to the inverse of the lifetime of the transition from the excited state, F_e, to $F_{g,i}$.

Once a ground state is selected, a photon with energy given by (referece theory again) is "released". If the atom is in the light collection region, then this photon is recorded for later analysis. Additionally, a counter that keeps track of the number of photons collected at each beam energy is increased by one. If the atom is not in the LCR, then nothing is recorded, and the excitation-decay process begins again with the computation of excitation rates.

1.4 Simulation of Complete Run

In order to simulate a complete experimental run, a chosen number of atoms, say N, are passed in sequence through the above loop. This is done in turn for each beam energy in a list of energies that are selected such that the doppler shifted laser energies range from the lowest energy to the highest energy transition, with some leeway on either side. This range can be called E_r. The graph of photon counts per beam energy is in fact the hyperfine spectrum.

Result: Simulation of complete hyperfine spectrum

Input all preliminary parameters;

for *Beam energy in E_r* **do**

    for *Each atom* **do**

        Run **interaction loop**;

        Record photon count;

    end

    Sum photon count into counts per beam energy;

end

Plot photon count at each beam energy;

Algorithm 1: Pseudo-code for the simulation of a complete hyperfine spectrum.

The preliminary parameters mentioned in the above pseudo-code refer to all the quantities required to perform a complete simulation of a hyperfine spectrum measured at TRIUMF. A list of these parameters is provided below, for completeness. List of Preliminary Parameters and Their Symbols

- Isotope mass: m_A

- Ground J-state: $\mathbf{J_g}$

- Excited J-state: $\mathbf{J_e}$

- Nuclear spin: $\mathbf{I}$

- Principal quantum number of ground state: n_g

- Principal quantum number of excited state: n_e

- Magnetic dipole hyperfine coefficient of ground state: A_g

- Magnetic dipole hyperfine coefficient of excited state: A_e

- Electric quadrupole hyperfine coefficient of ground state: B_g

- Electric quadrupole hyperfine coefficient of excited state: B_e

- Beam temperature: T_b

- Laser frequency: f_l

- Laser intensity: I_l

- Fine structure transition energy: E_{fs}

- Number of atoms to simulate per beam energy: N_a

- Distance between CEC and LCR: d

- Length of LCR: d_{LCR}