THEORETICAL STUDY OF ATOMIC PROCESSES AND DYNAMICS IN ULTRACOLD RYDBERG PLASMAS

A Thesis
Presented to
The Academic Faculty

by

Gouthaman S Balaraman

In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy in the
School of Physics

Georgia Institute of Technology
December 2008
THEORETICAL STUDY OF ATOMIC PROCESSES AND DYNAMICS IN ULTRACOLD RYDBERG PLASMAS

Approved by:

M. R. Flannery, Advisor
School of Physics
Georgia Institute of Technology

Michael Schatz
School of Physics
Georgia Institute of Technology

Turgay Uzer
School of Physics
Georgia Institute of Technology

Rigoberto Hernandez
School of Chemistry and Biochemistry
Georgia Institute of Technology

John Wood
School of Physics
Georgia Institute of Technology

Date Approved: 10 November 2008
To the prolific minds for their inspiration

To the near and dear ones for their encouragement
I thank my advisor, M. R. Flannery, for introducing me to the field of atomic physics. I still fondly remember his graduate classical mechanics course, where he expounded the intricate connections between classical mechanics and quantum mechanics. His scientific enthusiasm is something I will strive to live up to.

I am grateful to have had the opportunity to work with Daniel Vrinceanu. Daniel has been a friend, mentor, and a scientist to look up to. This thesis wouldn’t be the same without his guidance from numerous discussions I have had with him. Daniel, thanks for everything!

I thank the people on the fifth floor, students in W-503 who have come and gone, for discussions on science, life and beyond. Their company made the long days and weekends little less lonely, and conversations with them have helped put things in perspective.

I am grateful to the School of Physics for giving me a chance to study here. A lot of the lectures that I attended here gave me the background for the work presented in this thesis, and I believe will stand in good stead for years to come.

I thank the hospitality of Los Alamos National Laboratory during the summer I spent there. I thank Jim Cohen, and Lee Collins for making my summer stay possible.

I thank all my friends here in Atlanta, part of RPK, who made my stay in Atlanta for the last five years pleasant and enjoyable. I can’t imagine how it would be without their wonderful company.

I thank my parents, and my sister for nurturing my scientific interest during my formative years. I also thank my cousins, aunts and uncles who have all been a source of constant encouragement.
# TABLE OF CONTENTS

DEDICATION .................................................................................. iii

ACKNOWLEDGEMENTS ................................................................. iv

LIST OF TABLES ........................................................................... viii

LIST OF FIGURES ......................................................................... ix

SUMMARY .................................................................................. xiii

I INTRODUCTION ......................................................................... 1

  1.1 Formation of ultracold plasmas ............................................ 2
  1.2 Rydberg atoms ................................................................. 4
  1.3 Focus of this thesis ............................................................ 6

II QUANTAL-CLASSICAL CORRESPONDENCE IN RADIATIVE CASCADE AND RADIATIVE RECOMBINATION ................................................................. 9

  2.1 Quantal-classical correspondence for emitted power .......... 10
  2.2 Quantal-classical correspondence for dipole matrix elements . 11
  2.3 Symmetrical Heisenberg correspondence ............................ 12
  2.4 Radiative cascade .............................................................. 13
  2.5 Radiative recombination .................................................... 18
  2.6 Discussion ....................................................................... 20

III SYMPLECTIC METHOD FOR THE MODIFIED-KEPLER PROBLEM 22

  3.1 Symplectic propagator ...................................................... 24
    3.1.1 Drift stage .................................................................. 27
    3.1.2 Kick stage .................................................................. 29
    3.1.3 Kepler solver ............................................................ 29
  3.2 Applications ..................................................................... 30
    3.2.1 Kepler atom in uniform electric field .......................... 30
    3.2.2 Kepler atom in monochromatic time dependent field .... 36
  3.3 Discussion ....................................................................... 38
## LIST OF TABLES

1. Properties of Rydberg states ........................................... 4
2. Numerical coefficients used in optimized higher order symplectic schemes. 34
3. Parameters used in the simulation ..................................... 80
# LIST OF FIGURES

1. Schematic of atoms trapped in the magneto-optical trap. ........................................... 2

2. Quantal (dots) and classical (red curve) radial matrix elements as a function of scaled change $s/n = (n - n')/n$ for various initial-state ratios $\ell/n$ from 0.1 to 0.9 in steps of 0.1. The ordinate axis uses a base-10 logarithm. ....................................................... 15

3. Quantal (dots) and classical (blue curve) transition rates $A_{60,\ell\rightarrow n',\ell-1}$ times $\tau_{n,n\rightarrow n-1,n-1} = 3n^5/2A_0$ as a function of $(n - n')/n$ for various initial-state ratios $\ell/n$ from 0.2 to 0.9 in steps of 0.1. ....................................................... 16

4. Quantal (dots) and classical (blue curve) transition rates $A_{60,\ell\rightarrow n',\ell+1}$ times $\tau_{n,n\rightarrow n-1,n-1} = 3n^5/2A_0$ as a function of $(n - n')/n$ for various initial-state ratios $\ell/n$ from 0.1 to 0.9 in steps of 0.1. ....................................................... 16

5. Transition rates $A_{60,\ell\rightarrow n',\ell-1}$ times $\tau_{n,n\rightarrow n-1,n-1} = 3n^5/2A_0$ as a function of $(n - n')/n$. ▲: quantal; —: present classical; ◆: classical model in Ref. [26] ........................................................................................................ 17

6. Plot of quantal (lines) and classical (points) scaled cross sections as a function of $\ell$ for different values of $\eta = 2, 5, 10$ and 20. ....................................................... 19

7. Plot of Kramers (lines) and classical (points) cross sections $\sigma^n_R$ as a function of $n$ for different values of $\eta = 10, 20, 25$ and 30. ....................................................... 20

8. The $\ell$ dependence of quantal (line), classical (dots) and Kramers (dashed line) cross sections for $n = 15$ and $\eta = 20$. ....................................................... 21

9. The relative energy error is compared for long time integration using the step2 integrator and implicit Runge-Kutta of order 4 from GSL. The initial orbit has eccentricity $\epsilon = 0.9$ and energy $w = -0.5$. The electric field is $5.5 \times 10^{-3}$ oriented perpendicularly on the orbit plane. The fixed time step for step2 corresponds to 200 steps per orbit. ....................................................... 32

10. The trajectory when electric field of magnitude $5.5 \times 10^{-3}$ is oriented parallel to the orbit plane. When the eccentricity becomes 1 the traditional integrators fail because the particle comes arbitrarily close to the force center. The symplectic integrator is used to calculate the orbit segment shown here, which goes smoothly from an almost circular shape, to a singular highly eccentric orbit, and back to a circular orbit. .......................... 33

11. Relative error in energy after eight orbits when step2, step4 and step6 are used. Both low eccentricity ($\epsilon = 0.4$) starting orbit, with symbols and dotted lines, and highly eccentric orbit ($\epsilon = 0.9$), with solid lines, are represented. ....................................................... 35
The relative error in energy for an orbit (upper graph) integrated with a time adaptive step (stepA). Eccentricity as shown in the lower graph, goes periodically to unity because the electric field is parallel to the orbital plane.  

Atom energy (upper graph) and the relative error of the $Q$ quantity (lower graph) for the last segment of a long time run.

Plot of Stark transition probabilities $P_{2\rightarrow \ell'}^{(28)}$ as a function of $\ell'$ for values of $\alpha = 3Z/2\tilde{b}\tilde{v} = 0.15$. Histograms are present simulations with $z_0 = 520 \, n^2$ from a sample of 3000 atoms, and curves are from analytical formula [53, 15].

Plot of Stark transition probabilities $P_{2\rightarrow \ell'}^{(28)}$ as a function of $\ell'$ for values of $\alpha = 3Z/2\tilde{b}\tilde{v} = 0.3$. Histograms are present simulations $z_0 = 320 \, n^2$ from a sample of 3000 atoms, and curves are from analytical formula [53, 15].

Plot of Stark transition probabilities $P_{2\rightarrow \ell'}^{(28)}$ as a function of $\ell'$ for values of $\alpha = 3Z/2\tilde{b}\tilde{v} = 0.3$. Histograms are present simulations with full interaction for 3000 atoms and curves are from analytical results using the dipole interaction. (b) Plot of Stark transition probabilities $P_{n\rightarrow \ell'}^{(n)}$ as a function of $\ell'$ for values of $\alpha = 0.6$. Histograms are present simulations with full interaction for 3000 atoms and curves are from analytical formula for the pure dipole case [53, 15].

Contour plots of $<L>$ and $\sigma_L$ as a function of scaled impact parameter and scaled velocity for the (a) ion-dipole and (b) full interaction for transitions from $\ell = 8$ and $n = 10$. Simulation uses 2000 atoms and 100 orbits and the above plot was interpolated using 80 points in the grid.

Contour plots of $<L>$ and $\sigma_L$ as a function of scaled impact parameter and scaled velocity for the (a) ion-dipole and (b) full interaction for transitions from $\ell = 8$ and $n = 10$. Simulation uses 3000 atoms and 150 orbits and 66 point interpolation to render this plot.

Fractional populations for Stark mixing in the excited sodium versus the scaled collisional velocity of the ion for $28d \rightarrow 28\ell'$. The curves with filled symbols are from experiments, and the curve with unfilled symbols are from present calculations. The final angular momentum states are denoted adjacent to the curve.
21 Fractional population for Stark mixing of Na(28d) plotted as a function of the number of atoms in the sample. The various final angular momentum states are denoted next to the curve.

22 Three models with the same ion distribution with $N_i = 24000$ and $\sigma = 100 \, \mu m$, and different electron populations $N_e = 22500, 23000$ and 23500. Parameters are $T = 50$ and $E_0 = -5 \, K$. Upper graph shows the electric potential along the radial direction. The lower graph shows the number density for electrons (color lines) and for the ions (black line). The potential created by the ions only is displayed in the upper graph (black line). The vertical dashed lines indicate the position of cutoff radius $R_0$ for each model, while the horizontal dashed line shows the threshold energy $E_0$.

23 Electron radial distribution for the King distribution, from sampled population (histogram) and theoretical prediction (solid line).

24 Ion radial distribution for the King distribution, from sampled population (histogram) and theoretical prediction (solid line), compared with electron radial distribution (dashed line).

25 Phase space distribution for the King electron distribution. The contour lines are lines of equal density. The run-away ($E = 0$) curve is shown in the right panel. The unit for velocity is $\sqrt{k_B K/m}$, where $k_B$ is the Boltzmann constant and $m$ is the electron mass.

26 The electron velocity for the King distribution from the sample (histogram) and theoretical prediction (solid line), compared with that of a Maxwell-Boltzmann distribution with $T = 50 \, K$ (dashed line).

27 Local temperature variation along the radial direction for the King distribution, for sample (dots) and theoretical prediction (line).

28 Electron energy distribution for the King distribution: from sampled population (histogram) and theoretical prediction (solid line).

29 Schematic of the simulation process.

30 Comparison between the Monte Carlo method (dashed) and exact molecular dynamics (curve), for the electron Lagrange radius for different mass ratios, also denoted on the respective figures, a) 0.1, b) 0.3, c) 0.6, d) 0.9.

31 The evolution of ion size $\sigma$, as a function of time for the Monte Carlo method (dashed) and the molecular dynamics method (curve).

32 The evolution of electron size $\sigma_e = <r_e^2>/3$, as a function of time for the Monte Carlo method (dashed) and the molecular dynamics method (curve).
33 The electron distribution at the end of 9 ns, from the Monte Carlo(dotted) and molecular dynamics(curve) methods. .............................. 81

34 Plasma rms-radius for the ion as a function of time; Vlasov(curve), simulations(dots). ................................................................. 83

35 Plasma expansion velocity parameter as a function of time; Vlasov(curve), simulations(dots). ................................................................. 84

36 The a)ion and b)electron temperature evolution as a function of time; Vlasov(curve), simulations(dots). ......................................................... 85

37 The Lagrange radii of the electrons for mass ratios from 0.1 to 0.9 in steps of 0.1, describing the plasma expansion ............................................ 85

38 Lagrange radii of the electrons for mass ratio from 0.1 to 0.9 in steps of 0.1, for 1000 iterations in stationary state. .............................. 86
In the last decade, ultracold plasmas have been created in the laboratory by photo-ionizing laser-cooled atoms. To understand the overall dynamics of ultracold plasmas, one needs to understand Rydberg collisional processes at ultracold temperatures. The two kinds of problems addressed in this thesis are: study of Rydberg atomic processes at ultracold temperatures, and a study of the overall dynamics of the ultracold plasmas.

Theoretical methods based on quantal-classical correspondence is used to understand Rydberg atomic processes such as radiative cascade, and radiative recombination. A simulation method suitable for ultracold collisions is developed and tested. This method is then applied to study collisional-Stark mixing in Rydberg atoms.

To study the dynamics of the ultracold plasmas, a King model for the electrons in plasmas is proposed. The King model is a stationary, finite sized electron distribution for the electrons in a cloud of fixed ions with a Gaussian distribution. A Monte-Carlo method is developed to simulate the overall dynamics of the King distribution.
CHAPTER I

INTRODUCTION

The last two decades have seen great advances in the field of low temperature physics. The technique of laser-cooling has enabled scientists to cool atoms to temperatures as low as a few nano-Kelvin. The laser-cooling technology led to the creation of Bose-Einstein condensates. Recently ultracold neutral plasmas were created in the laboratory, and they act as a desktop tool to understanding plasma physics.

Plasmas are systems in which sufficient fraction of neutral atoms and molecules have been ionized to form free electrons and ions. Conventional plasmas are formed as a result of collisions between particles at high energies, and hence these are fairly hot. But it is also possible to create ultracold plasmas by using lasers to cool atoms to a few milli-Kelvin temperatures, and then photoionizing electrons to above threshold energies.

In the ultracold plasmas the kinetic energy of the liberated electron can be finely controlled by the manipulating the ionizing laser pulse. The temperature of the electrons can be tuned in the range of 1-1000K, while the ions retain the milli-Kelvin temperatures of the neutral atoms. Experiments on ultracold plasma have revealed surprising dynamics and recombination behaviour, and have allowed us to explore new frontiers of plasma physics.

In another set of very closely related experiments, the cold atoms trapped in the laser are excited just below threshold energies leaving the atoms in highly excited Rydberg states, to form a Rydberg gas. The Rydberg atoms are very sensitive to the environment and exhibit properties different from ground state atoms. The cold Rydberg gas is known to spontaneously evolve form a plasma, and this dynamics is
still not well understood.

There are interesting problems in the field of ultracold plasma physics, that are important to understand and various approaches using a combination of experimental, theoretical and computational methods are used to explore this field.

1.1 **Formation of ultracold plasmas**

The ultracold plasmas are created from laser-cooled neutral atoms. In a configuration of laser beams and magnetic fields known as a magneto-optical trap, as shown in Fig. (fig:mot), the atoms are cooled [25] to about a milli-Kelvin temperatures. As many as $10^9$ atoms can be cooled, with densities in the range of $10^{11}$ $cm^{-3}$. The density of the atoms is largest at the center of the atomic cloud, and the density drops down towards the edges. Typical spatial density profile of the atomic cloud is
that of a spherical Gaussian distribution,

\[ \rho_a(r) = \rho_0 \exp(-r^2/2\sigma^2), \]  

with a width of \( \sigma = 200 - 1500\mu m \).

The ionization step needed to create an ultracold plasma is done using a nanosecond laser pulse. The kinetic of the ionized electron depends on the laser photon energy. The typical electron temperatures achieved in the experiments vary in the range of 1-1000K. It is possible to ionize up to 50% of the trapped atoms, leading to a peak ion density in the range of \(10^6 - 10^9 \text{ cm}^{-3} \). Immediately after ionization, a small fraction of electrons escape the positive ion core. But as a net positive charge develops, the remnant space charge is strong enough to trap the remaining electrons. Depending on the experimental conditions, up to 90% of the electrons can be trapped.

In the first few nano-seconds following the photo-ionization of neutral atoms, the electrons equilibrate among themselves. The ions, because of their heavy mass and low temperatures, are initially frozen in their initial positions. The electrons collide with the ions, transferring a part of its momentum. The ions start to move owing to the pressure exerted by the electrons, and thus the whole plasma begins to expand. The plasma expansion happens in a timescale of few micro-seconds, while it takes a few milli-seconds for the ions and electrons to equilibrate.

In ultracold plasmas, atomic processes can play a major role in the expansion dynamics. An electron in the field of a positive ion collides with another electron, loses enough energy to get captured by the ion, while the other electron takes away the excess energy. This process, known as the three body recombination, becomes increasingly important with increase in electron densities \( \rho_e \), and decrease in electron temperatures \( T_e \) as \( \rho_e^2 T_e^{-9/2} \). In ultracold plasmas, three-body recombination is known to occur substantially, and is a contributing factor to electron heating. The recombined Rydberg atom, with electron binding energy of roughly \( 2k_B T_e \), can then scatter with electrons to excite, de-excite or ionize its valence electron. So, there is a
Table 1: Properties of Rydberg states

<table>
<thead>
<tr>
<th>Physical Value</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ionization potential</td>
<td>$Z^2 \text{Ry} / n^2$</td>
</tr>
<tr>
<td>Characteristic radius</td>
<td>$a_0 n^2 / Z$</td>
</tr>
<tr>
<td>Geometrical area</td>
<td>$\pi a_0^2 n^4 / Z^2$</td>
</tr>
<tr>
<td>Characteristic velocity</td>
<td>$Z v_0 / n$</td>
</tr>
<tr>
<td>Transition frequency between</td>
<td>$\omega_{n,n\pm 1} = 2 \frac{Z^2 \text{Ry}}{\hbar n^3}$</td>
</tr>
<tr>
<td>neighboring states</td>
<td></td>
</tr>
<tr>
<td>Period of classical motion</td>
<td>$T_n = \frac{2\pi}{\omega_{n,n\pm 1}}$</td>
</tr>
<tr>
<td>Average radiative lifetime</td>
<td>$\frac{n^5 [3 \ln(n) - 0.25]}{A_0 Z^4}$</td>
</tr>
</tbody>
</table>

necessity to understand basic collisional processes such as three-body recombination and electron-Rydberg atom scattering at low temperatures.

### 1.2 Rydberg atoms

Rydberg atom is a highly excited atom with a large principal quantum number $n$. In nature, Rydberg atoms are formed in the interstellar space, and in a lab Rybergs are found in ultracold plasmas and can be created by photo-exciting ground state atoms. To understand the kinetics of low temperature plasma, astrophysics, and applications in spectroscopy, it is important to understand collisional processes of Rydberg atoms with ions and neutral atoms. Rydberg atom in a state with principal quantum number $n$, is characterized by very small ionization potential $\text{Ry} / n^2$, very large dimension $a_0 n^2$, and small average velocity of excited atom $v_0 / n$. Here $\text{Ry}$ is the Rydberg unit of energy, $a_0$ is the Bohr radius, and $v_0$ is the atomic unit of velocity. Thus Rydberg atoms are exotic objects exhibiting classical and quantal properties simultaneously. A table of the characteristic properties of a Rydberg atom in excited state $n$, and ion charge $Z$ is shown in Table (1).

Though the experiments on ultracold plasmas are recent, the field of Rydberg atoms itself has a long history. Experiments on collisions involving Rydberg atoms have been carried out since the 1930s, in a number of works on measurement of
spectral-line broadening and shift of Rydberg atomic series induced by collisions with neutral atoms of the buffer gas. Theoretical studies carried out by Fermi [11] laid out some of the basic ideas for describing collisional processes with Rydberg atoms and neutral perturbing atoms.

Progress in the theoretical understanding of impact broadening of spectral lines spurred interest in collisions involving Rydberg atoms during the 1950s and 1960s. Experimental studies focussed on the impact broadening of Rydberg atomic levels arising from collisions with atoms of the buffer gas. Lot of theoretical work was based on both classical and quantal approaches. Classical approach has been used to study inelastic transitions between the excited states and electron impact ionization of atoms. Quantal approaches, on the other hand, were based on perturbation theory with dipole approximation for the interaction potential arising from the colliding charged projectile ($e^-$ or $H^+$).

The 1970s witnessed rapid advances in the laser technique, and it spurred experimental and theoretical works on collisional processes involving Rydberg atoms. Experimentalist were able to selectively excite atoms to a particular Rydberg state and analyze the states using sensitive detection techniques such as selective field ionization. Advances made in the technique of atomic beams enabled experimentalists to measure cross sections and rate coefficients of selectively excited Rydberg states. This also led to significant advances in the collision theory of Rydberg atoms.

Several analytical techniques were developed to study Rydberg collisions with electrons ions and neutrals. Semiclassical methods made use of JWKB approximation to the wavefunction of atomic states and projectile motion. Semi-quantal methods treated the Rydberg electron using quantum mechanics while the projectile motion was treated classically. A good review of the various theoretical methods of Rydberg atom collision can be found in Ref. [12]. In the 1980s and 1990s, simulation techniques based on classical trajectory Monte Carlo (CTMC) simulations became a popular
method to study Rydberg collision.

1.3 Focus of this thesis

The aim of this thesis is the study of atomic collisional and radiative processes of Rydberg atoms at ultracold temperatures, and of the overall dynamics of ultracold plasmas. The problems in ultracold plasma physics addressed in this thesis can be grouped into two categories:

1. Atomic processes at low energies: Rydberg atoms, that are formed during the plasma expansion, collide with ions and electrons in the system. At lower temperatures, the collisional velocities are small, and hence it is important to validate the rates and cross-sections for various atomic processes in the ultracold regime. Some of the recent works include, calculations of electron impact ionization cross-section [50], excitation/de-excitation rates [43], and radiative processes [14]. Chapters 2, 3, and 4 in this thesis address atomic processes at low energies.

   In Chapter 2, a quantal-classical correspondence is used to solve radiative cascade and radiative recombination. Radiative recombination is the process in which the electron recombines with an ion to form a Rydberg atom, by emitting a photon. Radiative cascade is the process in which the electron in the Rydberg atom cascades eventually to the ground state or metastable state by de-excitation accompanied by radiation. A symmetrical version of the Heisenberg correspondence is used to derive radiative recombination cross-sections and transition rates for radiative cascade.

   A lot of collisional processes are very complex, and when pure analytical approaches are not possible CTMC simulations can be used to study Rydberg collisions. CTMC simulations of the slow collision between Rydberg atoms and neutral/charged particles at low temperatures involve stable computation of
trajectories of modified-Kepler systems (i.e.) systems with a potential energy $V(r, t)$ in addition to the long range $1/r$ (Kepler) potential. Computation of these trajectories can be quite challenging when the Rydberg electron travels quite close to its ionic core. Conventional integration routines such as Runge-Kutta method have the deficiency of errors accumulating with increase in simulation time, making them unsuitable for long-timescale simulations. A symplectic integrator suitable for modified-Kepler systems is developed in Chapter 3. The advantages of the symplectic integrator for long timescale simulations are explained, and various examples are discussed.

Stark mixing occurs when a Rydberg atom collides with a slow moving ion, and the Rydberg electron undergoes transitions with change only in angular momentum while its energy remains constant. Simulation of Stark mixing process involves propagating the electron over many Rydberg electron time periods, while the ion passes by slowly. Making use of the symplectic integrator developed in Chapter 3, CTMC simulation of Stark collision process is studied in Chapter 4. Results computed from the simulation are compared with experimental results.

2. **Dynamics of the plasma at low energies**: Cold atoms trapped in a magneto-optical trap are photoionized just above the ionization threshold to create an ultracold plasma (UCP). The dynamics of UCPs have been studied by various experimental groups. Some theoretical groups [38] have used molecular dynamics to study the plasma expansion, but computational costs have limited such studies to a few nanoseconds of plasma dynamics. Other groups [44] have used a fluid model to simplify computation process.

In Chapters 5 and 6, an alternate approach is presented to study the dynamics of the ultracold plasmas. Immediately after the formation of UCPs
in the experiments, a small fraction of the electrons escape from the plasma creating a net positive charge that prevents further escape of electrons. The remaining electrons in the cloud reach a quasi-equilibrium in a few nano-seconds while the ions barely move. Since the most energetic electrons have already left the plasma, the remaining electrons in the quasi-equilibrium state cannot be described by a Maxwell-Boltzmann distribution, which includes electrons with arbitrarily large velocities. In Chapter 5 we propose a King model for the electrons in ultracold plasmas, similar to the distribution found in astrophysics. The King model for ultracold plasmas is a stationary, finite sized distribution for the electrons in a cloud of fixed ions with a Gaussian distribution.

In Chapter 6 the dynamics of the King model are simulated using a Monte Carlo method. The Monte Carlo method is compared with exact molecular dynamics for short timescales, and with the Vlasov equation [30] for long timescales.
In a Rydberg atom, the valence electron is in a high quantum level $n$. A cold Rydberg plasma, which can be attained at sub-milli-Kelvin temperatures, consists of electrons, ions and Rydberg atoms. Such Rydberg states have recently been produced by laser excitation [46] or ionization [29] of atoms initially prepared at sub-milli-Kelvin temperatures. Even for simple atomic systems, like the atomic hydrogen, it is difficult to calculate quantal transition rates and life times involving high $n$ Rydberg levels. Understanding of radiative cascade in Rydberg plasmas is of interest in astrophysics and in recent laboratory experiments to form antihydrogen [17]. The transition rates calculated using the Gordon formula [2] become numerically unstable for $n \geq 50$ and hence there is a need for a more physically transparent approach.

The old quantum theory [5] based on the action-angle formalism of classical mechanics, developed in the 1920s, was fairly successful in explaining the spectra of simple atomic systems. Since the birth of quantum mechanics this classical approach was not vigorously pursued. The difficulty in a full quantal treatment of Rydberg atoms has revived an interest [14, 26] in the old quantum theory, as there is a quantal-classical correspondence as we approach high $n$. Flannery et al. [14] have discussed the quantal-classical correspondence in radiative cascade. The classical version of transition rates presented in Ref. [14], symmetrically included the properties of both initial and final states involved in a transition. This resulted in good agreement with the quantal results. However the treatment was unsatisfactory for large jumps in
low-\(\ell\) Rydberg atoms, i.e. for initial state ratio \(\ell/n \sim 0.1\). Three body recombination, the dominant recombination mechanism in ultracold temperatures, leads to the formation of high \(n\) Rydberg atoms in low \(\ell\) states. The high \(n\) Rydbergs are then brought down to low \(n\) by the radiative cascade. Thus a useful classical treatment should treat the low \(\ell\) Rydberg states correctly. In this Chapter we present a classical treatment of radiative cascade that is a good approximation over a wide array of \(\ell\) values, including the low \(\ell\) states. As an extension, we treat the problem of radiative recombination under the classical approximation, and present the classical radiative recombination cross sections.

The structure of this Chapter is as follow. In Sec. 2.3 we introduce the notion of symmetrical Heisenberg correspondence (SHC) for any general matrix element. In Sec. 2.4 the classical treatment of radiative cascade is done using the principles laid out in Sec. 2.3. A new correspondence is adopted to account for transitions involving large quantum jumps. This treatment is shown to work well even for low \(\ell\) Rydberg states. Radiative recombination is treated classically in Sec. 2.5, where the cross-sections are derived and compared with exact results. Importance of preserving symmetries in correspondence limit is explained by considering the detailed balance of oscillator strengths.

### 2.1 Quantal-classical correspondence for emitted power

The instantaneous classical power of photon emission is given by the Larmor formula [27, 34]

\[
I = \frac{2}{3} \frac{e^2}{c^3} |\hat{r}|^2 \tag{2}
\]

The quantal rate that energy \(E_{if} = \hbar \omega_{if}\) is radiated in the \(i \rightarrow f\) transition is the power [2]

\[
P_{if} = \hbar \omega_{if} A_{if} = \frac{4}{3} \frac{e^2}{c^3} \left( \frac{E_{if}}{\hbar} \right)^4 |\vec{r}_{if}|^2 \tag{3}
\]
where $A_{if}$ is the Einstein transition probability ($s^{-1}$) and $r_{if}$ is the dipole electronic matrix element $\langle \phi_{n_f \ell_f m_f} | r | \phi_{n_i \ell_i m_i} \rangle$. Because $\ddot{r}_{if} = -\omega_{if}^2 r_{if}$ exactly, when exact wave functions $\phi_{i,f}$ are used, the total power radiated into all lower states is

$$P_i = \frac{4}{3} \frac{e^2}{c^3} \sum_{f<i} |\ddot{r}_{if}|^2$$  \hspace{1cm} (4)$$

The sum $\sum_{allf} |\ddot{r}_{if}|^2 = \langle \ddot{r}^2 \rangle_i$ is dominated by a symmetric band of states centered about the highly excited level $i$. Then $\sum_{f<i} |\ddot{r}_{if}|^2 = \frac{1}{2} \langle \ddot{r}^2 \rangle_i$ and

$$P_i = \frac{2}{3} \frac{e^2}{c^3} \langle \ddot{r}^2 \rangle_i,$$  \hspace{1cm} (5)$$

Ignoring the average over state $i$ results in Larmor’s classical expression for the power.

### 2.2 Quantal-classical correspondence for dipole matrix elements

In the equivalent sets $(J, w)$ or $(I \equiv J/2\pi, \theta \equiv 2\pi w)$ of action-angle variables, the position $r$ of a particle with a separable Hamiltonian $H(I)$ and executing bounded periodic motion with an array of the natural angular frequencies $\omega = \partial H / \partial I$ can be Fourier decomposed as

$$r = \sum_s r_s(I) e^{is \theta} = \sum_s r_s(I) e^{is(\omega t + \delta)}$$  \hspace{1cm} (6)$$

This permits the Larmor power formula (2) to be decomposed as $P = \sum_{s \geq 0} P_s$, where each component

$$P_s = \frac{4}{3} \frac{e^2}{c^3} (s \cdot \omega)^4 |r_{i,s}|^2$$  \hspace{1cm} (7)$$

When compared with (3), (7) provides the Bohr-Van Vleck correspondence principle [4, 48] for intensities. This equates the power of line spectra between equally spaced levels $E_{if} = H(n_i) - H(n_f) = \hbar s \cdot \omega$, the Bohr frequency theorem [4], with the power associated with the $s^{th}$ harmonic of the classical motion of state $i$. The correspondence also holds provided $r_{if} = r_{i,s}$, which is the Heisenberg form [21] of a correspondence principle for matrix elements. Since $r$ is real, $r_{i,s} = r_{i,-s}$, as also assumed within the derivation of (5).
2.3 Symmetrical Heisenberg correspondence

Heisenberg Correspondence is useful in that it allows us to equate the matrix element of an operator \( \hat{A} \) with respect to a basis set \( |\phi_n> \) to the Fourier component of the equivalent classical function \( A^C_i(I, \theta) \) expressed in terms of the action-angle variables. That is,

\[
A_{if} = <\phi_f|\hat{A}|\phi_i> \simeq \int A^C(I_i, \theta) \exp(i s \cdot \theta) \, d^3\theta = A^C_i(s) \tag{8}
\]

where the operator \( \hat{A} \) has been replaced by its corresponding classical function \( A^C(I, \theta) \) written in terms of action-angle variables \( I_i = (n_i + \delta)\hbar \) and \( \theta \) respectively, associated with the quantum numbers \( n_i \equiv n_i, \ell_i, m_i \) for the initial state \( i \). The array \( s(s_1, s_2, s_3) \) is the change \( n_f - n_i \) in the quantum numbers, where the quantum numbers of the final state \( f \) are \( n_f \equiv n_f, \ell_f, m_f \). Here \( \delta \) is the Maslov parameter. A formal derivation of this principle from quantum mechanics by considering wave packets is given in Landau and Lifshitz [33]. However, to preserve symmetry of the matrix elements, the Bohr-Sommerfeld quantization rule can be modified [40] to \( I = (n_c + \delta)\hbar \), where \( n_c \) is the arithmetic mean of the initial and final state quantum numbers. It is important that the symmetry of the matrix elements be preserved as it forms the building block of any detailed balance criterion. Often the error in the matrix element increases with increase in the quantum jump \( s_1 \). This can be attributed to the fact that the mean quantum number, \( n_c \), becomes a poor substitute to the initial and final state quantum numbers, especially when the gap between the two states is large. In the literature one finds various \textit{ad hoc} choices for \( n_c \) [39, 40, 7] suited to reduce the error in the matrix elements. In an effort to rigorously overcome this failure at large \( s_1 \), Flannery and Vrinceanu proposed a “symmetrical Heisenberg correspondence” which ensured that the Hermitian character of the dipole matrix element i.e., \( |r_{if}|^2 = |r_{fi}|^2 \) was preserved, without recourse to any average quantum number \( n_c \).

This approach can of course be generalized to any operator \( \hat{A} \) by first comparing
A^{*}_{fi} \simeq \int A^{C*}(I_f, \theta) \exp(is,\theta) \, d^3\theta = A^{C*}_f(s) \tag{9}

which directly shows that the Heisenberg Correspondence does not preserve the Hermitian character $A_{if} = A^{*}_{fi}$ of the operator $\hat{A}$ because the initial and final actions, $I_i$ and $I_f$, used in the classical calculation of $A^C$ in (8) and (9) are not the same. Because $|A_{if}|^2 = A_{if}A^{*}_{if} = A_{if}A_{fi}$ for a Hermitian operator and because $A_{fi} \simeq A_f(-s)$ under Heisenberg Correspondence, then

$$ |A_{if}|^2 \simeq A_i(s)A_f(-s) \tag{10} $$

is our symmetrized version of the correspondence principle for modulus squared of any matrix element. We make use of the symmetrized version to calculate the radial matrix elements, and shall demonstrate its goodness.

### 2.4 Radiative cascade

Radiative cascade is the problem where the electron in the Rydberg atom cascades to the ground state by de-excitation accompanied by radiation. The quantal transition rates for radiative cascade, under the dipole approximation, can be written in terms of the matrix elements of the dipole operator $\mathbf{D} = e\mathbf{r}$. On summing over all the final $m'$ quantum numbers

$$ \sum_{m'} |<n'\ell'm'|n\ell m>|^2 = \frac{\ell}{2\ell + 1} (R_{n\ell}^{n'\ell'})^2 \tag{11} $$

these matrix elements become independent of the initial $m$ quantum number itself. The radial matrix element $R_{n\ell}^{n'\ell'}$ is given as

$$ R_{n\ell}^{n'\ell'} = <n'\ell'|n\ell> = \int_0^\infty \chi_{n'\ell'}(r) \, r \, \chi_{n\ell}(r) \, dr \tag{12} $$

where $<r|n\ell> = \chi_{n\ell}(r)$ satisfies the radial equation

$$ \left[ \frac{d^2}{dr^2} - \frac{\ell(\ell + 1)}{r^2} + \frac{2m}{\hbar^2} \{E_{n\ell} - V(r)\} \right] \chi_{n\ell}(r) = 0 \tag{13} $$
The classical radial matrix elements can be obtained by writing the classical trajectory $r(t)$, periodic in angle variable with angular velocity $\omega$, as a Fourier series

$$r(t) = \sum_s r_s \exp[-i(s_1 \theta + s_2 \psi + s_3 \phi)], \quad (14)$$

where the sum is over all $s = (s_1, s_2, s_3)$. Here $\theta = \omega t + \delta$ is the angular position of the particle in the orbital plane located at $(x, y)$ whose orientation is determined by the Euler angles $\Theta = (\cos^{-1}[m/(l)], \phi, \psi)$. On summing $|r_s|^2$ over $s_3$ yields

$$\sum_{s_3} |r_s|^2 = \frac{1}{2}(R_s)^2 \quad (15)$$

in terms of $R_s$, the Fourier component of $[x + i\Delta \ell y]$, such that $s = -s_1 = n_i - n_f > 0$ and $\Delta \ell = s_2 = \ell_f - \ell_i$. Equation (15) is the classical equivalent of Eq. (11). On comparing Eq. (11) and (15), we realize that the $R_s = [x_s + i\Delta y_s]$ is the classical version of the radial matrix elements. The SHC version of classical radial matrix element is given from Eq. (10) as

$$(R_{n'\ell'}^n) = |R_s(i, n, \ell, \Delta \ell)| |R_s(f, n', \ell', \Delta \ell)| \quad (16)$$

where $i(f)$ stands for initial(final) state and $R_s(j, n_j, \ell_j, \Delta \ell)$ [39, 14], obtained by taking Fourier component of an elliptical path, is given as

$$R_s(j, n_j, \ell_j, \Delta \ell) = \frac{n_j^2 a_0^2}{2s} \left[ \left( 1 - \Delta \ell \frac{\ell_j}{n_j} \right) J_{s-1}(s\epsilon_j) - \left( 1 + \Delta \ell \frac{\ell_j}{n_j} \right) J_{s+1}(s\epsilon_j) \right] \quad (17)$$

Here $\epsilon_j = (1 - (\ell_j + 1/2)^2/n_j^2)^{1/2}$, $s = n_i - n_f > 0$, $\Delta \ell = \ell_f - \ell_i = \pm 1$ and $J_{s\pm1}$ are Bessel functions of order $s \pm 1$. The quantal classical correspondence in Eq. (16) with Eq. (17) has been provided by Flannery and Vrinceanu [14] who showed that this correspondence is extremely accurate for high $\ell$ values but fails for transitions involving large jumps involving low $\ell$ states. This failure can be attributed as follows.

Bohr-Van Vleck correspondence principle Eq. (7) equates the power of line spectra between the equally spaced levels $E_{ii} = \hbar\omega$ with the $s^{th}$ harmonic of the classical motion of state $i$. The energy gap between two nearly spaced levels of hydrogen atom can
be approximated to be equally spaced as $E_{if} \approx s\hbar\omega_i$. Hence Bohr’s correspondence strictly holds only for nearly spaced levels as the equal spacing approximation breaks for transitions involving large jumps. For large jumps we can arrive at a correspondence on replacing $s$ by the nonintegral effective harmonic index $k_j$ for the state $j$, (i.e.) $s \to k_j = E_{if}/\hbar\omega_j$, where $\omega_j$ is the angular frequency of the $j^{th}$ orbit. This replacement is facilitated by the continuity of $R_s(j,n,\ell,\Delta\ell)$ over $s$ for $s \in (0,\infty)$. Hence the new form of radial correspondence using SHC is given as,

\[ (R^{n'\ell'}_n)^2 = |R_{k_i}(i,n,\ell,\Delta\ell)||R_{k_f}(f,n',\ell',\Delta\ell)| \quad (18) \]

such that

\[ R_{k_j}(j,n_j,\ell_j,\Delta\ell) = \frac{n_j^2a_0}{2k_j} \left[ \left( 1 - \Delta\ell\frac{\ell_j}{n_j} \right) J_{k_j-1}(k_j\epsilon_j) - \left( 1 + \Delta\ell\frac{\ell_j}{n_j} \right) J_{k_j+1}(k_j\epsilon_j) \right] \quad (19) \]

The variables $\epsilon_j$, $\Delta\ell$ and $J_{k\pm1}$ retain their original definition. A comparison of the classical radial matrix elements in Eq. (18) with the Gordon formula [2] is shown in Fig. (2). There is excellent agreement between the quantal and classical values for the whole range of $\ell$ values. This a great improvement over the radial correspondence discussed in Ref. [14]. Using this form of radial correspondence the classical version

\[ \text{Figure 2: Quantal}(\text{dots})\text{ and classical}(\text{red curve})\text{ radial matrix elements as a function of scaled change } s/n = (n - n')/n \text{ for various initial-state ratios } \ell/n \text{ from 0.1 to 0.9 in steps of 0.1. The ordinate axis uses a base-10 logarithm.} \]
Figure 3: Quantal (dots) and classical (blue curve) transition rates $A_{60\ell \rightarrow n'\ell +1}$ times $\tau_{n_n=n-1,n-1} = 3n^5/2A_0$ as a function of $(n-n')/n$ for various initial-state ratios $\ell/n$ from 0.2 to 0.9 in steps of 0.1.

Figure 4: Quantal (dots) and classical (blue curve) transition rates $A_{60\ell \rightarrow n'\ell +1}$ times $\tau_{n_n=n-1,n-1} = 3n^5/2A_0$ as a function of $(n-n')/n$ for various initial-state ratios $\ell/n$ from 0.1 to 0.9 in steps of 0.1.

of Einstein $A$ coefficients is given as

$$A_{n_i\ell_i \rightarrow n_f\ell_f} = \frac{4A_0}{3} \frac{\ell_i}{2\ell_i + 1} \left( \frac{n_i^2 - n_f^2}{2n_i^2n_f^2} \right)^3 |R_{ki}(i,n_i,\ell_i,\Delta \ell)||R_{kj}(f,n_f,\ell_f,\Delta \ell)|$$

(20)

Figures 3 and 4 are representative of quantal classical correspondence of Eq. (3) for $\ell \rightarrow \ell \mp 1$ transitions. The agreement is excellent over a wide range of $\ell$ values.

Horbatsch et al. [26] have also arrived at a classical version of $A$ coefficients suitable
Figure 5: Transition rates $A_{60\ell \rightarrow n' \ell' - 1}$ times $\tau_{n,n-1,n-1} = 3n^5/2A_0$ as a function of $(n-n')/n$. ▲ : quantal; — : present classical; ♦ : classical model in Ref. [26]

for low $\ell$ “... directly from the classical properties of the initial orbit, without the need to invoke the properties of the final state.” Before we compare our results with their expression, we would like to make a brief remark on how the approach adopted in Ref. [26] fails to preserve detailed balance criterion. The average oscillator strength for a transition from $n\ell$ to level $n'\ell'$ is given as

$$\bar{f}_{n\ell \rightarrow n'\ell'} = \frac{2}{3} \frac{\ell >}{2\ell + 1} \omega_{n'\ell',n\ell} |< n'\ell'|r|n\ell > |^2, \quad (21)$$

where $\omega_{n'\ell',n\ell} = (E_{n'\ell'} - E_{n\ell})/\hbar$. The average oscillator strength for a transition is proportional to the average oscillator strength of the inverse transition by the following detailed balance criterion

$$\bar{f}_{n\ell \rightarrow n'\ell'} = -\frac{2\ell' + 1}{2\ell + 1} \bar{f}_{n'\ell' \rightarrow n\ell}. \quad (22)$$

On using the radial correspondence Eq. (18) and (19) in Eq. (21), it is easily verified that the detailed balance in Eq. (22) is satisfied. By invoking only the classical properties of the initial state without any reference to that of the final state, the authors in Ref. [26] have been oblivious to the important symmetry in Eq. (22). In
Fig. (5) we compare the present classical transition rate and the one in Ref. [26] with the classical for \( \ell \rightarrow \ell - 1 \) transitions. Our classical estimates are shown to be better even in the low \( \ell \) regime.

2.5 Radiative recombination

Radiative recombination is the process where the electron recombines with an ion to form a Rydberg atom by emitting a photon. The calculation of radiative recombination rates involves calculation of the radial matrix elements for above threshold continuum-bound transitions. Delone et al. [10] find the classical version of matrix elements for the continuum-bound transition as

\[
\langle n\ell + \Delta \ell | r | p\ell \rangle = \frac{\ell p^3}{\sqrt{3\pi}\omega^3} \left[ K_{2/3} \left( \frac{(\ell + 1/2)^3\omega}{3} \right) - \Delta \ell K_{1/3} \left( \frac{(\ell + 1/2)^3\omega}{3} \right) \right]
\]

where the transition frequency \( \omega = 1/2n^2 + p^2/2 \) and \( K_\nu \) is the McDonald functions. This was obtained by analytic continuation of matrix elements for transitions between remote bound states, where \( \ell \ll n, n' \) and \( n \gg \Delta n \gg 1 \), to yield

\[
\langle n'\ell + \Delta \ell | r | n\ell \rangle = \frac{\ell^2}{\sqrt{3\pi}n^3} \left[ K_{2/3} \left( \frac{(\ell + 1/2)^3\omega}{3} \right) - \Delta \ell K_{1/3} \left( \frac{(\ell + 1/2)^3\omega}{3} \right) \right]
\]

We define the SHC version of the modulus squared of the continuum-bound radial matrix element as

\[
| < n\ell + \Delta \ell | r | p\ell > |^2 = R_i(\omega, p, \ell, \Delta \ell) R_f(\omega, n, \ell + \Delta \ell, \Delta \ell)
\] (25)

where \( R_i(\omega, p, \ell, \Delta \ell) \) is the expression given in Eq. (23) and \( R_f(\omega, n, \ell + \Delta \ell, \Delta \ell) \) is the expression given in Eq. (24). The classical version of radiative recombination cross section for the electron to be captured in a state \((n, \ell)\) is given as

\[
\sigma_{RC}^{nl}(E_e) = \frac{4\pi^2\alpha^3\omega^3}{3E_e} \rho(E_e) R_f(p; n\ell)
\]

where \( \alpha \) is the fine structure constant, \( \omega = E_e + 1/2n^2 \) is the energy gap, \( E_e = p^2/2 \) is the energy of the incoming electron and

\[
R_f(p; n\ell) = \ell | < n\ell | r | p\ell - 1 > |^2 + (\ell + 1) | < n\ell | r | p\ell + 1 > |^2
\] (27)
The density of state \( \rho(E) \) depends on the normalization of the continuum wave-function. Here we can arrive at the density of states of the continuum by using an analytic continuation argument and by realizing that \( \rho(E) = 1/(dE/dn) \), which yields \( \rho(E) = 1/(2E)^{3/2} \). This classical expression for cross sections hold good in the range \( \ell \ll n, p^{-1} \) and is fairly accurate for \( \ell/n < 0.7 \) and \( 1/p > 10 \).

A plot comparing the quantal and classical scaled cross sections is shown in Fig. 6 for different energies of the incoming electron. The value for quantal cross sections have been computed by Zerrad et al. [57] for different values of \( \eta = 1/ka_0 \), where \( k \) is the wave number and \( a_0 \) is atomic units. The agreement is very good for low energies \( (\eta > 10) \) but less good for slightly higher energies \( \eta < 10 \). Kramers semiclassical cross section is frequently used to arrive at the radiative recombination cross section to be captured into a bound state \( n \). This is given as

\[
\sigma_n^K(\eta) = \frac{32}{3\sqrt{3}} \alpha_0^3 \frac{\eta^4}{n(n^2 + \eta^2)} \pi a_0^2
\]  

(28)

This formula is fairly accurate [57] for \( \eta > 10 \) and \( n > 10 \). Agreement between the classical and Kramers cross sections is illustrated in Fig. 7. The classical cross section for radiative recombination into level \( n \) has been obtained by summing over all the \( \ell \)
contributions as
\[
\sigma^n_R = \sum_{\ell=0}^{n-1} \sigma^{n\ell}_R
\]
(29)
The \(\ell\) dependence of the Kramers cross section can be written by averaging Kramers cross section by \(n^2\) degenerate \(n\) levels times the degeneracy of \(n\ell\) state.
\[
\sigma^{n\ell}_K = \left[ (2\ell + 1)/n^2 \right] \sigma^n_K
\]
(30)
Figure 8 comapares \(\ell\) dependence of Kramers formula with that of the quantal and classical methods. The classical method is in good agreement with the quantal cross sections. However the averaged Kramers formula underestimates(overestimates) the contribution for low \(\ell\)(high \(\ell\)).

2.6 Discussion

In summary, a symmetrical version of Heisenberg correspondence for the matrix element is introduced in Eq. (10). The SHC naturally accounts for the symmetry of matrix elements and obviates \textit{ad hoc} introduction of mean quantum number in quantizing action. In Section 2.4, the problem of radiative cascade is discussed, and the
Figure 8: The $\ell$ dependence of quantal (line), classical (dots) and Kramers (dashed line) cross sections for $n = 15$ and $\eta = 20$.

classical version for the Einstein transition rate have been derived in Eq. (20). In Section 2.5, radiative recombination is treated classically, and the classical cross-sections for radiative recombination is derived in Eq. (26). The derived classical results are compared with the quantal results, and the results are seen to be in agreement over a range of energy and angular momentum for the Rydberg atoms.
CHAPTER III

SYMPLECTIC METHOD FOR THE MODIFIED-KEPLER PROBLEM

The stable computation of trajectories of modified-Kepler systems – systems with a potential energy \( V(r,t) \) in addition to the long-range \( 1/r \) (Kepler) potential – can be quite challenging for trajectories approaching the origin. The additional potential energy \( V(r,t) \), referred to as the “perturbation” in this chapter, is not necessarily weak.

Given a set of the required initial conditions in the problem, the system of ordinary differential equations for the modified-Kepler problem can be numerically solved by using standard, good-for-all algorithms such as Runge-Kutta or Gear integrators. Such methods only have a good control of the local error, while the global error usually grows exponentially. This is the reason why these methods are unsuitable for treating physical problems which require long-time integrations. In ultracold atomic and molecular physics, the simulation of interaction of a Rydberg atom with an external field or radiation, or collision of a Rydberg atom with a slow projectile, for example, typically involve timescales of hundred of thousands of Kepler orbital time periods. In astrophysics, timescales in solar system simulations are more than \( 10^9 \) years [35]. Thus geometric or symplectic integrators are more suitable for applications involving long-time integration, where the generic integrators are known to be less stable.

Geometric integration is a relatively new branch of Computational Mathematics. It studies algorithms and discretization methods that respect the underlying geometry and qualitative structure of the problems it aims to solve. The principle is that
if more specific information about the problem is explicitly included into the solver, then the solution will be more accurate and stable than those produced by generic methods. For a Hamiltonian system, a numerical method is symplectic if it explicitly preserves the underlying symplectic structure. Many symplectic methods also obey other qualities of the system such as symmetry and time reversal. Although the Hamiltonian itself is in general not conserved (for autonomous systems), it was demonstrated that the error grows only linearly in time. Comprehensive reviews of symplectic methods are presented in references [36] and [20].

Suppose that the Hamiltonian is separable and each term in the separation defines an integrable problem, then a symplectic solution is obtained by propagating the system with each term separately. The traditional way is to split the Hamiltonian into the kinetic energy $T$ plus potential energy $V$. Evolution under the kinetic energy part alone describes the free motion of the system. The potential energy term usually does not depend on momentum coordinates and therefore the position coordinates remain unchanged during the propagation. The system gets a “kick”, a sudden change in momentum. It was proved (see [36], for example) that the leap-frog, or Störmer-Verlet, methods, very popular in Molecular Dynamics simulations, can be derived from a $T + V$ splitting and are therefore symplectic. An essential feature for more general ways of splitting the Hamiltonian is that the terms not only are integrable but also are efficiently computable.

This chapter proposes a symplectic integration method for the modified-Kepler problems by splitting the Hamiltonian into a pure, exactly solvable, Kepler part and a perturbation part. A similar idea was introduced in [55], although a different implementation is proposed, specifically for the n-body simulation of the solar system. The present method has the following advantages:

- the modified Kepler system can be efficiently propagated with a good accuracy using relatively large time steps, thus saving on the computational cost,
• the global error in energy for the problem can be easily estimated, which gives us a good predictor of the accuracy level at any time,

• this is quite stable in handling the Kepler singularity even over long integration timescales,

• extensions to higher order methods and time dependent perturbations are easy to derive.

Three types of symplectic integration implementation done here are \( \text{step2} \), \( \text{stepA} \) and \( \text{stepT} \). Methods \( \text{step2} \) and \( \text{stepA} \) are second-order routines with fixed time step and adaptive time step respectively for time independent problems, and \( \text{stepT} \) is the time dependent version of \( \text{step2} \). We present here two case studies to demonstrate the above mentioned features of this integrator. Interaction of a Rydberg atom with a spatially uniform external field is studied for two cases. One case treats the interaction with a constant field (Stark effect) and the other with that of a monochromatic oscillatory field (laser interaction).

The class of modified-Kepler problems which can take advantage of the method proposed in this chapter includes the interaction of a Rydberg atom with black body radiation, simulation of non-hydrogenic Rydberg atoms by taking into account the quantum defect and solar system simulations.

3.1 Symplectic propagator

The motion of a planet or of a Rydberg electron can be described by the classical equations of motion, derived from the Hamiltonian

\[
H = H_0 + V(r, t)
\]  

(31)

where \( H_0 = p^2/2 - 1/r \) (in an appropriate set of units) is the Kepler Hamiltonian and \( V(r, t) \) is the perturbation potential, not necessarily a weak perturbation but of any
arbitrary strength. The evolution in time of any function $z$ defined over the phase space is given by the general equation

$$\frac{dz}{dt} = \{z, H\} \equiv D_H(z)$$

(32)

where $\{ , \}$ are the Poisson brackets and $D_H$ is an operator defined by the Hamiltonian $H$. Providing the initial condition $z_0$ at $t_0$, the function $z$ is obtained at time $t$ as a solution of the above equation, given as $z(t) = \Phi_{\Delta t}(z_0)$. Formally, the mapping $\Phi$ can written as $\Phi_{\Delta t} = e^{\Delta tD_H}$, in a form reminiscent of the quantum mechanical evolution operator. The mapping $\Phi$ is practical only if the solution to the problem for the Hamiltonian $H$ is explicitly known. However, solutions for the Hamiltonians $H_0$ and $V$ are separately known, and, for any $\Delta t$, the mapping associated with these solutions are $e^{\Delta tD_{H_0}}$ and $e^{\Delta tD_V}$. If the phase space operators $D_{H_0}$ and $D_V$ commute (or their Poisson bracket $\{H_0, V\} = 0$), then the product of exponentials is equal to the exponential of their sum, and the problem has an exact solution: $\Phi_{\Delta t} = e^{\Delta tD_{H_0}}e^{\Delta tD_V}$.

In general this is not true, and the following useful expansion can be derived [56] from the Baker-Campbell-Hausdorff formula

$$\log(e^{\lambda A/2}e^{\lambda B}e^{\lambda A/2}) = \lambda(A + B) - \frac{\lambda^3}{24}[AAB] - \frac{\lambda^3}{12}[BAB]$$

$$+ \frac{7\lambda^5}{5760}[AAAAB] + \frac{\lambda^5}{720}[BBBAB]$$

$$+ \frac{\lambda^5}{480}[AABAB] + \frac{\lambda^5}{3600}[BAAAB]$$

$$- \frac{\lambda^5}{360}[ABBAB] + \frac{\lambda^5}{120}[BABAB] + O(\lambda^7)$$

(33)

where the bracket notation refers to commutators: $[XY] = [X, Y] = AB - BA$, $[XYZ] = [X, [Y, Z]]$, and so on. Operators $A$ and $B$ can be either $D_{H_0}$ or $D_V$.

The Poisson bracket also has the property of being a Lie bracket which means that $[D_X, D_Y] = D_{\{X,Y\}}$.

The meaning of the expansion formula (33) is that the propagator obtained by
successive application of $e^{\lambda A/2}$, $e^{\lambda B}$ and $e^{\lambda A/2}$ is a propagator of an equivalent Hamiltonian $\tilde{H}$ equal to the original $H = A + B$, only in the limit of $\lambda \to 0$. For a small enough time step $\lambda$, the exact solution under $\tilde{H}$ is expected to converge to a solution of $H$. This propagator is symplectic and also preserves the symmetry, time reversibility and first-order invariants of the system. When the perturbation $V$ does not depend on time then both Hamiltonians $H$ and $\tilde{H}$ are conserved. Therefore the global deviation from energy conservation is directly accessible from $\tilde{H} - H$. This is a valuable asset of the symplectic methods, since most good-for-all integration methods cannot easily predict the global behavior of their solutions, in general.

Explicitly, from Eq. (33), on choosing $A = D_V$ and $B = D_{H_0}$, one gets the equivalent Hamiltonian,

$$\tilde{H} = H - \frac{\lambda^2}{24} \{ \{ H_0, V \}, V + 2H_0 \} + O(\lambda^4).$$

(34)

Hence the error in the approximate propagator is second order in the time step $\lambda$. The global error correct up the second order in $\lambda$ is then

$$\Gamma^{(2)} = \tilde{H} - H = -\frac{\lambda^2}{24} \left( F^2 + 2F \cdot F_c + 2p \cdot \frac{\partial}{\partial r} (p \cdot F) \right)$$

(35)

where $F = -\partial V / \partial r$ is the perturbation force and $F_c = -r / r^3$ is the Coulomb force. For small values of $r$, the error is therefore dominated by $\lambda^2 F \cdot r / r^3$. In contrast, the global error for a $T + V$ splitting, obtained from Eq. (33) and using $A = D_{V-1/r}$ and $B = D_T$, is

$$\Gamma^{(2)'} = \Gamma^{(2)} - \frac{\lambda^2}{24} \left( F_c^2 + 2p \cdot \frac{\partial}{\partial r} (p \cdot F_c) \right)$$

(36)

The truncation error for the $T + V$ splitting is still second order in the time step, but is clearly inferior at small distance $r$, where it behaves as $1/r^4$.

Formula (33) suggests a couple of ways to improve the performance of this method. First, if operator $B$ is replaced by $B' = B + \lambda^2/24 \,[A + 2B, [A,B]]$ and providing the evolution under $B'$ is explicitly known, then the $\lambda^3$ term in expansion is removed and
the error is now of the order of $\lambda^5$. The second way of accelerating the convergence is obtained by adapting the time step. Superior order methods are obtained by composing steps with appropriate variable time steps. Examples of such schemes are presented in the next section.

A solution of the perturbed Kepler problem is therefore obtained by evolving the phase space point $(r, p)$ of the system successively, under two elementary operations. The “drift stage” is the evolution under the Kepler Hamiltonian $H_0$, while the evolution under the perturbation Hamiltonian $V$ is called the “kick stage”.

3.1.1 Drift stage

Although a textbook example [19], an explicit solution of the Kepler problem is not entirely trivial. To state the problem, given the position $r_0$, and momentum $p_0$ at time $t_0$, one need to find position $r$ and momentum $p$ at some other time $t_0 + \Delta t$. This mapping denoted by $D(\Delta t)$, gives the position and momentum along a Kepler orbit, from an initial position and momentum, after a time $\Delta t$. A summary of methods for solving this classic initial value problem is given in [9].

The trajectory during the drift stage is a segment of an ellipse, a parabola or a hyperbola, depending whether the “local” energy \( w = H_0 = p^2/2 - 1/r \) is positive, zero or negative, respectively. The geometric size of the ellipse and the orbital period also depend on the local energy. The angular momentum \( L = r \times p \) and the Runge-Lenz \( A = (p^2 - 1/r) r - (rp) p \) vectors, are used to identify the orientation of the orbital plane in space. Although \( w, L \) and \( A \) can be calculated from the initial state vector \((r_0, p_0)\), it is advantageous to keep these quantities in the state vector, alongside with position and momentum. This helps save a number of floating point operations. Besides it can also help avoid the accumulation of round-off errors that might creep up in the calculation. For instance the energy, at the pericenter of the orbit, is the difference of two large numbers: the kinetic and potential energies.
Having as input the thirteen dimensional state vector \((\mathbf{r}, \mathbf{p}, w, \mathbf{L}, \mathbf{A})\), the drift stage proceed as follows:

1. obtain the characteristic parameters of the orbit: semimajor axis \(a = 1/2w\), eccentricity \(\epsilon = \|\mathbf{A}\|\) and orbital angular frequency \(\omega = (2|w|)^{3/2}\),

2. calculate the direction of the pericenter \(\hat{e}_1 = \mathbf{A}/\epsilon\) and the direction in the orbital plane perpendicular to it, \(\hat{e}_2 = \mathbf{L} \times \mathbf{A}/\epsilon L\),

3. find the eccentric anomaly corresponding to the initial position \(u_0 = \arctan(1 - 2|w|r, \sqrt{2|w|rp})\),

4. find the eccentric anomaly \(u\) after time \(\Delta t\) as \(u = \text{Kepler}(\epsilon, u_0 - \epsilon \sin u_0 + \omega \Delta t)\), where \(\text{Kepler}(\epsilon, M)\) is the solution of Kepler’s equation \(u - \epsilon \sin u - M = 0\) as a function of parameters \(\epsilon\) and \(M\),

5. calculate the new position on the orbit corresponding to the new eccentric anomaly \(u\) as

\[
\mathbf{r} = a(\cos u - \epsilon) \hat{e}_1 + a\sqrt{1 - \epsilon^2} \sin u \hat{e}_2 \tag{37}
\]

\[
\mathbf{p} = -\frac{1}{\sqrt{a}} \frac{\sin u}{1 - \epsilon \cos u} \hat{e}_1 + \sqrt{\frac{1 - \epsilon^2}{a}} \frac{\cos u}{1 - \epsilon \cos u} \hat{e}_2 \tag{38}
\]

During steps (1)-(5) mentioned above, energy, angular momentum and Runge-Lenz vectors are not modified. The steps above apply specifically to the case of negative energy (elliptic orbit). It is not difficult to generalize this procedure for the parabolic and hyperbolic motions.

Up to round-off errors, the drift stage integrates exactly the orbit for any time step \(\Delta t\), except for the solution of the transcendental Kepler’s equation which has to be obtained approximately.
3.1.2 Kick stage

In the kick stage the system evolves solely under the perturbation Hamiltonian $V$. This mapping is denoted by $K(\Delta t)$. If $V$ does not depend on momentum, then the position vector is a cyclic coordinate and does not change during this stage. The change in momentum can then be explicitly obtained as

$$p' - p = \Delta p = \int_{t_0}^{t_0 + \Delta t} F dt,$$

where $F$ is the perturbation force derived from the potential $V$. Quantities $w$, $L$ and $A$ in the state vector are updated from $r$, $p$ and $\Delta p$, instead of calculating them directly from $r$ and $p'$. This precludes the accumulation of round-off errors and increases the efficiency of the procedure. Energy, angular momentum and Runge-Lenz vectors are updated during the kick stage as

$$w' = w + p\Delta p + \frac{1}{2}\Delta p^2$$

$$L' = L + r \times \Delta p$$

$$A' = A + (2p\Delta p + \Delta p^2)r - (r\Delta p)(p + \Delta p)$$

3.1.3 Kepler solver

The solution of the transcendental Kepler’s equation is the most time-consuming part in the propagator. The traditional numerical scheme to obtain accurate solutions is to “guess” a good starting approximation and then refine it by using Newton-Raphson iterations until the desired accuracy is obtained. Each iteration involves evaluating trigonometric functions several times. Since each trigonometric function evaluation has a cost of at least several hundreds of microprocessor clocks, regardless if it is done “on-the-chip” or by a library call, the cost of solving the Kepler’s equation can mount easily to thousands of clocks. It is clear that a long time integration, on the order of $10^8$ time steps would require a more refined procedure. A table-driven procedure is proposed here where no trigonometric functions are calculated during iterations.
This method trades memory space in favor of time, the details of which are furnished in the Appendix A.

### 3.2 Applications

#### 3.2.1 Kepler atom in uniform electric field

In the absence of a perturbation, the kick stage reduces to identity and the dynamics is described only by the drift. The propagator was tested and the solution was seen to be practically exact (within the machine precision) even for extremely long time integration. A proper test of this symplectic integrator can only be done in the presence of a perturbation. The simplest perturbation, which is also completely integrable, is the constant and uniform force field.

When a constant force $\mathbf{F}$ acts on the system, the Kepler orbit starts to precess and change its eccentricity. The corresponding potential is $V = -r\mathbf{F}$, such that the energy $E = p^2/2 - 1/r - r\mathbf{F}$ is conserved. For forces $F > (-E/2)^2$ the system can break away and ionize.

The angular momentum and the Runge-Lenz vectors evolve in time according to

$$
\frac{d\mathbf{L}}{dt} = \mathbf{r} \times \mathbf{F} \quad \frac{d}{dt} \left[ \mathbf{A} - \frac{1}{2} \mathbf{r} \times (\mathbf{r} \times \mathbf{F}) \right] = \frac{3}{2} \mathbf{F} \times \mathbf{L}. \tag{43}
$$

Provided the orbit does not change appreciably over one period, then on using the Pauli’s replacement rule $\mathbf{r} \rightarrow -(3/2)\mathbf{A}$ [24], and the fact that $\mathbf{r} \times (\mathbf{r} \times \mathbf{F})|_0^T \approx 0$, the average angular momentum and Runge-Lenz vectors obey equations

$$
\frac{d}{dt} \langle \mathbf{L} \rangle = \frac{3}{2} \mathbf{F} \times \langle \mathbf{A} \rangle \quad \frac{d}{dt} \langle \mathbf{A} \rangle = \frac{3}{2} \mathbf{F} \times \langle \mathbf{L} \rangle. \tag{44}
$$

Within these assumptions, the slow changes in $\mathbf{L}$ and $\mathbf{A}$ are obtained, by solving the above system of equations, as

$$
\langle \mathbf{L} \rangle = \cos(\frac{3}{2}Ft)\mathbf{L}(0) + [1 - \cos(\frac{3}{2}Ft)][\hat{\mathbf{F}} \cdot \mathbf{L}(0)]\hat{\mathbf{F}} + \sin(\frac{3}{2}Ft)[\hat{\mathbf{F}} \times \mathbf{A}(0)] \tag{45}
$$

$$
\langle \mathbf{A} \rangle = \cos(\frac{3}{2}Ft)\mathbf{A}(0) + [1 - \cos(\frac{3}{2}Ft)][\hat{\mathbf{F}} \cdot \mathbf{A}(0)]\hat{\mathbf{F}} + \sin(\frac{3}{2}Ft)[\hat{\mathbf{F}} \times \mathbf{L}(0)] \tag{46}
$$
Both \( \mathbf{L} \) and \( \mathbf{A} \) therefore rotate about each other with a period of \( 4\pi/3F \).

The simplest second order symplectic integrator (\textit{step2}), also called \textit{Strang splitting} [20],

\[
S(\Delta t) = K(\Delta t/2)D(\Delta t)K(\Delta t/2)
\]

(47)

requires only one “drift” stage \( D \) and two “kick” operations \( K \). The “drift” stage involves solving Kepler’s equation and has a higher computational cost than the “kick” stage. An equivalent integrator \( DKD \) is not as efficient, because it uses two “drift” stages.

Figure 9 compares the accuracy and stability of \textit{step2} integrator with a standard implicit Runge-Kutta method of order 4, with adaptive time step (\textit{rk4imp}), from the free GNU Scientific Library (GSL) [18]. The initial orbit has eccentricity 0.9, energy -0.5 and period \( 2\pi \) in the chosen units. An uniform electric field of magnitude \( 5.5 \times 10^{-3} \) is applied along a direction perpendicular to the orbital plane. If the initial orbit represents a ground state hydrogen atom, then the electric field is \( 2.86 \times 10^7 \) V/cm. Because of the scaling of the classical equations of motion, this would also simulate a \( n = 100 \) Rydberg atom in a field of intensity 2.86 kV/cm. The trajectory is simulated for about 4000 orbits, until time 25000. The \textit{step2} subroutine takes \( 8 \times 10^5 \) steps of constant size \( \pi/100 \) and finishes the jobs in 0.7 seconds, while \textit{rk4imp} makes \( 7.6 \times 10^6 \) steps and takes 9.6 seconds to complete. The precision and accuracy parameters are set to \( 10^{-5} \). Although the standard Runge-Kutta integrator runs ten times longer and makes ten times more steps, the relative error for the energy conservation increases. The performance of \textit{step2} are initially worse than \textit{rk4imp}, but the accumulation of errors is much slower. The long time integration advantages of the symplectic method (where the errors remain bounded) are clear.

As shown by Eqs. (45) and (46), when the electric field is oriented parallel to the orbital plane, the trajectory goes to a singular orbit with \( L = 0 \) and unit eccentricity,
Figure 9: The relative energy error is compared for long time integration using the step2 integrator and implicit Runge-Kutta of order 4 from GSL. The initial orbit has eccentricity $\epsilon = 0.9$ and energy $w = -0.5$. The electric field is $5.5 \times 10^{-3}$ oriented perpendicularly on the orbit plane. The fixed time step for step2 corresponds to 200 steps per orbit.

and the particle goes through the Coulomb center. The error for the standard Runge-Kutta integrator accumulates at a much higher rate; every time the singularity is encountered, the error increases by at least one order of magnitude.

A fragment of a trajectory having this kind of singularity is shown in figure 10. Owing to the built-in exact Kepler solution, the symplectic integrator is able to advance through this singularity with no catastrophic consequences. At very small distances, the central Coulomb force is much stronger than the external field and the dynamics is practically governed by the drift stage alone. In order to cope with such extreme situations, the basic step2 integrator can be improved in several ways.

Higher order integrators can be obtained by compounding more stages during one time step. Following [56], a fourth order step4 integrator is obtained using the following symmetric sequence: $K_1D_1K_2D_2K_2D_1K_1$, which uses only three drift stages. Here the following notation is used: $K_{1,2} = K(a_{1,2}\Delta t)$ and $D_{1,2} = D(a_{1,2}\Delta t)$. A sixth order (step6) stepping procedure is obtained by using an appropriate combination of
Figure 10: The trajectory when electric field of magnitude $5.5 \times 10^{-3}$ is oriented parallel to the orbit plane. When the eccentricity becomes 1 the traditional integrators fail because the particle comes arbitrarily close to the force center. The symplectic integrator is used to calculate the orbit segment shown here, which goes smoothly from an almost circular shape, to a singular highly eccentric orbit, and back to a circular orbit.
Table 2: Numerical coefficients used in optimized higher order symplectic schemes.

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_1$</td>
<td>0.6756035959798288</td>
<td>$a_2$</td>
<td>-0.17560359597982883</td>
</tr>
<tr>
<td>$b_1$</td>
<td>1.351207191956578</td>
<td>$b_2$</td>
<td>-1.7024143839193149</td>
</tr>
<tr>
<td>$w_0$</td>
<td>1.3151863206839063</td>
<td>$w_1$</td>
<td>-1.1776798417887</td>
</tr>
<tr>
<td>$w_2$</td>
<td>0.235573213359357</td>
<td>$w_3$</td>
<td>0.784513610477560</td>
</tr>
</tbody>
</table>

elementary step2 steps. For example [56], the following sequence $S_3S_2S_1S_0S_1S_2S_3$ has an error of order 6 in the time step, is symmetric and time reversible. Here $S_{0,1,2,3}$ means step2 steps with time steps $w_{0,1,2,3} \times \Delta t$. The coefficients $w_{0,1,2,3}$ are solutions of a nonlinear order equation which ensure that all errors up to order 6 are canceled. The numerical coefficients used in these higher order integrators are listed in Table 2.

Figure 11 compares the accuracy of step2, step4 and step6 routines as a function of the time step for eight orbits, for low and high eccentricity orbits. Electric field of strength $5.5 \times 10^{-3}$ is oriented parallel to the orbital plane. As expected, higher order integrators have the error decreasing faster with decreasing time steps, but at the cost of a greater workload. For example, step6 method is seven times slower than step2, although it may deliver improvements of several orders of magnitude in precision. However, this behavior is evident only when the time step is smaller than a critical time step, which decreases with increasing eccentricity. For eccentricity 0.9, the advantage of higher orders is manifest only for time steps smaller than $10^{-2}$, for example. In order to understand this feature it is enough to consider the leading terms of expansion (33) in evaluating the global error:

$$\tilde{H} - H \approx -\frac{\lambda^2 F}{12 r^2} + \frac{\lambda^4 F}{720 r^5} + \ldots$$

(48)

The maximum error is obtained when $r$ has a minimum at $r \sim 1 - \epsilon$. The expected convergence is obtained when the $\lambda^4$ correction is smaller than the $\lambda^2$ one, or when $\lambda < \sqrt{6(1-\epsilon)^3}$. Indeed, for $\epsilon = 0.4$ one gets $\lambda < 1.1$, and for $\epsilon = 0.9$ one gets $\lambda < 0.07$, roughly in agreement with the results presented in Fig. 11. The error
Figure 11: Relative error in energy after eight orbits when step2, step4 and step6 are used. Both low eccentricity (\(\epsilon = 0.4\)) starting orbit, with symbols and dotted lines, and highly eccentric orbit (\(\epsilon = 0.9\)), with solid lines, are represented.

saturates around \(10^{-12}\) because of the limited precision imposed by the Kepler solver. A finer grid in the Kepler solver improves this precision.

The error in energy for the basic integrator step2 becomes unbounded in the case of a field parallel to the orbital plane, as the eccentricity becomes unity with a period given by \(4\pi/3F\). Another way of improving the basic integrator step2 is to use an adaptive time step strategy. The singularity is removed from the first term in Eq. (48), and weakened for the second one, if the time step \(\lambda\) is adaptively chosen proportional to distance \(r\) as \(\lambda = \eta r\). Figure 12 shows the improved stability using this strategy (stepA). The electric field has a strength of \(\pi/600\) so that that orbit become singular with a period of 800, as predicted. Eccentricity, as plotted in the lower graph in Fig. 12, is initially 0.2. The energy conservation is bounded, in general, and has spikes whenever eccentricity goes to 1 and the orbit becomes one dimensional,
Figure 12: The relative error in energy for an orbit (upper graph) integrated with a time adaptive step (stepA). Eccentricity as shown in the lower graph, goes periodically to unity because the electric field is parallel to the orbital plane.

because of the $\lambda^4$ (and higher) energy correction which dominates in these cases. In contrast, the implicit Runge-Kutta (rk4imp) shows a catastrophic accumulation of error after the first encounter with singularity, even though the precision and the accuracy parameters are set at $10^{-8}$ and about $10^6$ steps are taken for the segment shown in figure. About the same number of steps are taken by stepA to integrate the orbit over the whole time interval.

3.2.2 Kepler atom in monochromatic time dependent field

Time dependent fields can be taken into account by using a canonical transformation which adds time as a position coordinate to the Hamiltonian (see for example [6]). Therefore, only during the drift stage the time variable is advanced. The time dependent external force does work on the system and the energy is not conserved.
However, when the work is subtracted from energy, the quantity

\[ Q = w - \int_0^t F(s) v \, ds \]  \hspace{1cm} (49)

is conserved, and can be used to quantify the precision level of the integrator.

Figure 13 show the results from a long time integration of Kepler orbit that was started with energy -0.5 and eccentricity 0.9, under a monochromatic uniform field of magnitude 0.1, frequency 2.2 and orientation perpendicular to the orbital plane. During one time step, the trajectory is evolved according to the scheme \((step_T is the time dependent version of \textit{step2}): K(\Delta t/2) F(t) D(\Delta t) K(\Delta t/2)\), where D and K represent the drift and kick stages, while F is the force calculation step at time \(t_0 + \Delta t\). Here \(t_0\) is the time at the beginning of the step. The orbit is advanced for \(3 \times 10^6\) time steps of size \(\pi/100\). Figure 13 shows the variation of energy (upper graph) and the deviation from conservation of the \(Q\) quantity (lower graph) for the last segment of the run.
3.3 Discussion

The integration of the orbit of a particle with a modified Kepler motion can take advantage of the explicit integrability of the Kepler problem. Splitting the Hamiltonian as Kepler part plus a perturbation part, as opposed to the traditional kinetic plus potential energy splitting, has a much lower estimated energy error close to the Kepler singularity, as demonstrated in Eqs. (35) and (36). As shown in Fig. (9), the long time accumulation of energy error in \textit{step2} is slower in comparison to the linear increase in \textit{rk4imp}, even though the number of time steps per orbit for the former is only 10\% of that used by the latter method. The errors in solutions and in angular momentum and Runge-Lenz vectors show qualitatively similar behavior as the energy error.

A time adaptive step \textit{stepA} has been shown here to have excellent energy conservation and stability for long time integration, when the trajectory goes repeatedly through the Coulomb singularity, as in the case of a uniform constant field in the orbital plane. Representative results can be found in Figs. (10) and (12). No evidence of numerical resonances, which appear in multiple time stepping methods for fast-slow systems [36], has been observed for the methods introduced here. Time dependent problems can also be solved using a variant (\textit{stepT}) of the basic step, as demonstrated here in Fig. (13) for a monochromatic field.

The overall efficiency of these methods, \textit{step2}, \textit{stepA} and \textit{stepT}, is limited only by how fast the transcendental Kepler equation can be solved. By using a table of pre-calculated trigonometric and exponential functions, and a fifth order Newton-Raphson refinement, a fast and reasonably accurate Kepler solver is successfully used. The convergence of the second order, basic integrator \textit{step2}, can be improved to obtain fourth order \textit{step4} and sixth order \textit{step6} symplectic schemes. There exist a whole class of problems of topical interest, that can be described as a modified Kepler problem and require long-time integration, and can be efficiently solved by this technique.
CHAPTER IV

STARK MIXING BY ION-RYDBERG ATOM COLLISIONS

In Chapter 3, we developed a numerical method to solve the modified-Kepler problem – systems with a potential energy $V(r, t)$ in addition to the long-range $1/r$ (Kepler) potential. A practical example where this method comes handy is the problem of Stark mixing. In Stark mixing collisions, the Rydberg atom or molecule collides with a slow moving ion inducing transitions within the energy manifold for the Rydberg electron. CTMC simulation of this process would require good energy conservation properties for the integrator of choice, as the electron would have to be integrated over many Rydberg electron time periods. In this Chapter, the Stark mixing process is examined using CTMC method, making use of the Symplectic method discussed in Chapter 3.

4.1 Stark Mixing

The ion-Rydberg atom/molecule collisional process

$$A^{Z+} + Ry(n, \ell) \rightarrow A^{Z+} + Ry(n, \ell')$$

(50)

is called collisional Stark mixing [53, 15, 51, 52, 54] since the $\ell$-changing transitions $\ell \rightarrow \ell'$ occur within the same energy shell $n$ of the Rydberg species and are induced by the time-dependent electric field generated by the passing ion $A^{Z+}$. A Rydberg molecule with its orbiting electron in state $(n, \ell)$ can be considered [13] as a Rydberg atom $Ry(n, \ell)$, particularly for the higher $\ell$ when there is little penetration with the
molecular ionic core. The ion-atom (molecule) electrostatic interaction

\[ V(r, R) = \frac{Ze^2}{R} - \frac{Ze^2}{|R - r|} \quad (51) \]

between the ion, at position \( R \) from the atom whose Rydberg electron is at \( r \), has the long-range \((R \gg r)\) multipole expansion,

\[ V(r, R) \rightarrow -\left( \frac{Ze^2}{R^2} \right) r \cos \theta - \left( \frac{Ze^2}{2R^3} \right) (3 \cos^2 \theta - 1) + ..... \quad (52) \]

where \( \theta \) is the angle between \( R \) and \( r \). At very large ion-atom separations \( R \gg n^2a_0 \), the first term in the RHS of Eq. (52)–the ion-dipole interaction–dominates and induces \( \ell \rightarrow \ell \pm 1 \) transitions at a given time during the collision. When the collision is fast, then there is time only for the dipole \( \ell \Rightarrow \ell \pm 1 \) transitions to occur. For collisions at ultracold energies, there is abundant time during the collision for transitions to occur sequentially, as in the ladder \( \ell \Rightarrow (\ell+1, \ell-1) \Rightarrow (\ell+2, \ell, \ell-2) \Rightarrow (\ell+3, \ell+1, \ell-1, \ell-3) \) and so on, the range of \( \ell' \) depending on the duration of collision. In this sequential \( \ell \Rightarrow \ell \pm 1 \) tree-like way, a distribution of final \( \ell' \) states can occur over a wide range of \( \ell' \) values and this range widens as the collision energy is reduced so that all \( \ell' \) states within the \( n \)-manifold can be eventually populated. This sequence depends on the accuracy/quality of the wave-function taken for the time-dependent perturbed Rydberg atom. For example, when unperturbed Rydberg wavefunctions are used, as in the Born approximation, then the range is confined to only \( \ell \Rightarrow (\ell \pm 1) \) transitions.

For the ion-dipole interaction,

\[ V(r, R) = -\left( \frac{Ze^2}{R^2} \right) r \cos \theta \quad (53) \]

the exact time development operator has been obtained [53, 15, 51, 52, 54] in both classical and quantal formulations. The exact probabilities \( P_{\ell'\ell}^{(n)} \) for the whole array of \( \ell \rightarrow \ell' \) transitions were then extracted. The exact solutions [52] were made possible by the inherent Group Dynamic Symmetry of the Rydberg atom together with the
assumption of the ion-dipole interaction. A universal classical probability was deduced which allowed illustration of rapid convergence of the quantal to the classical results with increasing principal quantum number \( n \). The structure exhibited in the variation of \( P_{\ell'}^{(n)} \) with \( \ell' \) was explained and the Quantal-Classical Correspondence was displayed [53, 15].

Exact solution is, however, not possible when higher-order multipole interactions are included. When the ion-quadrupole term which induces tree-like \( \ell \leftrightarrow \ell \pm 2 \) transitions and higher terms are included in the expansion (52), then only numerical solutions are possible. Rather than adding the higher-order interactions one-by-one within some complicated theoretical formulation, we shall, in this chapter, determine the probabilities \( P_{\ell'}^{(n)} \) for the Stark mixing process (50) from molecular dynamics simulations using the full ion-atom electrostatic interaction (51). In so doing, we shall be able to determine if and where higher multipoles are important to Stark mixing for the ultracold collision energies, of interest. If unimportant, then the exact analytical treatment [53, 15] based on the ion-dipole interaction will be valid over a wide range of ultracold energies. Also, accurate molecular dynamics simulations are of interest here because other competing effects of radiative decay, black-body radiation and inelastic \( n \rightarrow n' \) collisions, which will assume significance as the collision energy is increased, can be easily incorporated, without the need for implementation of complex and difficult theory.

### 4.2 Simulation Methodology

The present study of collisional Stark mixing is based on the Classical Trajectory Monte Carlo (CTMC) method. We start with a distribution of Rydberg atoms in a microcanonical ensemble with a given energy and angular momentum represented by the ‘quantum numbers’ \( n \) and \( \ell \). The orbital radius and velocity are \( a_n = n^2 a_0 \) and \( v_n = v_0 / n \), respectively, where \( a_0 \) and \( v_0 \) are the atomic units of length and
velocity. The collision of the perturber is taken initially to be in the \((Y - Z)\) plane, and the initial condition in Cartesian coordinate system is \(R(X, Y, Z) = (0, b, z_0)\). The initial impact parameter \(b\) is sampled from a distribution uniform in \(b^2\), and the initial condition \(z_0\) was taken to be an arbitrary large number, choice of which is discussed below in Sec. (4.3). With this distribution, we propagate each and every atom under a slowly varying potential due to the slowly passing ion with an initial collisional velocity \(V = (0, 0, v)\). The simulation is stopped when the perturber crosses \(Z = -z_0\). The distribution over the final angular momentum \(\ell'\) of the target Rydberg atoms after the collision is taken and analyzed. We adopt the Symplectic solver described in Chapter 3, and in Ref. [1], as it is custom-made for long time-scale simulations and it has good energy conservation properties. The distribution of angular momentum of the Rydberg atoms after the collision yields the probabilities \(P_{\ell'\ell}^{(n)}\) for \(n\ell \rightarrow n\ell'\) transitions as a function of impact-parameter \(b\).

### 4.2.1 Stark mixing under the ion-dipole interaction

In order to test the accuracy of the molecular dynamics method, we first conduct simulations for the probabilities \(P_{\ell'\ell}^{(n)}\) under the pure ion-dipole interaction (53) and then compare the results with the exact classical analytical probabilities, previously obtained [53, 15]. Once high accuracy is established, the full interaction (51) will then be used. A convenient parameter for this simulation is the dimensionless Stark parameter, defined as the ratio of the Stark to collision frequencies and given by [53, 15]

\[
\alpha = \frac{3Z}{2\bar{b}\bar{v}}
\]

where \(\bar{v} = v/v_n\) and \(\bar{b} = b/a_n\) are the collision velocities and impact-parameters, scaled to the corresponding Rydberg units. The region \(\alpha \leq 1\) of interest is the Orbital adiabatic and Stark sudden region, as explained in Ref. [53].

Some representative graphs comparing the results of the simulation with the exact
Theoretical probabilities are presented in Figs. 14 and 15.

**Figure 14:** Plot of Stark transition probabilities $P_{2 \rightarrow \ell'}^{(28)}$ as a function of $\ell'$ for values of $\alpha = 3Z/2b\tilde{v} = 0.15$. Histograms are present simulations with $z_0 = 520 n^2$ from a sample of 3000 atoms, and curves are from analytical formula [53, 15].

The curves are given by the exact classical formula, Eq. (27) of Ref. [15] and the histograms are the present simulations for a sample of 3000 atoms. The results from the simulations are in excellent agreement with the theoretical results. This procedure will therefore be valuable for the study of Stark collisions under the full interaction (51), in the presence of black-body radiation or other competing processes, as electronic excitation/de-excitation/ionization which will become important as the collision-energy is increased. More refinement can be obtained by taking a larger sample of atoms, though at the cost of greater computational time. Cross sections for Stark mixing can be obtained, if required, from

$$
\sigma_{\ell \ell'}^{(n)}(v) = 2\pi \int_0^{\infty} P_{\ell \ell'}^{(n)}(b) \, db = \pi a_n^2 \left( \frac{9Z^2}{2\tilde{v}^2} \right) \int_0^{\infty} P_{\ell \ell'}^{(n)}(\alpha) \, \alpha^{-3} \, d\alpha
$$

under the proviso that the limit $b \rightarrow 0$ requires special consideration [53].
Figure 15: Plot of Stark transition probabilities $P_{2\rightarrow \ell'}^{(28)}$ as a function of $\ell'$ for values of $\alpha = 3Z/2\bar{b}\bar{v} = 0.3$. Histograms are present simulations $z_0 = 320 \, n^2$ from a sample of 3000 atoms, and curves are from analytical formula [53, 15].

4.3 Sensitivity to simulation parameters

The first factor that we analyze is the dependence on the initial starting condition $z_0$. The two plots in Figs. (14) and (15) are for two different $z_0$ values, $z_0 = 520n^2$ and $z_0 = 320n^2$. The good agreement between the simulations and the theoretical results for the above two cases shows that a modest choice of $z_0 = 320n^2$ will be appropriate for these simulations.

The second factor of importance is the sensitivity to the results, of the number of atoms in the sample. The result produced in Fig. (15) for $\alpha = 0.3$ with a sample of 3000 atoms can be compared with that for a sample of 500 atoms, shown in Fig. (16). The agreement between the simulation and theory in Fig. (16) is not as good as it is in Fig. (15). Thus we see that the results are indeed sensitive to the number of atoms in the sample, and a discussion of convergence with respect to calculation of cross-sections is provided in Sec. (4.5)

Here we have shown that the CTMC method is indeed a valuable computational approach for accurate classical probabilities, and can be a viable tool to investigate
Figure 16: Plot of Stark transition probabilities $P_{2\rightarrow\ell'}^{(28)}$ as a function of $\ell'$ for values of $\alpha = 3Z/2b\bar{v} = 0.3$. Histograms are present simulations $z_0 = 320n^2$ from a sample of 500 atoms, and curves are from analytical formula [53, 15].

Stark mixing under the exact ion-atom (molecule) potential, and other perturbations.

4.4 Stark mixing under the full interaction

So far, we have made a dipole approximation (53) for the interaction between the projectile and the target. However for higher values of $\alpha$ (with smaller impact parameters $b$), this approximation could, in principle, break down. This effect can be investigated by using the exact electrostatic interaction (51) in the code and observing how the higher multipoles affect the transition probabilities. Two representative cases are considered for a sample of 3000 atoms, and $z_0 = 320n^2$ under full interaction: (1) $\alpha = 0.15$; (2) $\alpha = 0.6$.

Fig. 17(a) shows the simulation for $\alpha = 0.15$ under the full interaction potential (51) between the projectile and the target. Here the probabilities are compared with the discretized probabilities for the dipole interaction. The two probabilities are in close agreement, which indicates that the terms quadrupole and higher do not contribute and the dipole interaction is indeed valid at small $\alpha$.

Fig. 17(b) shows the simulation under the full interaction potential (51) and
\(\alpha = 0.6\). The resulting probabilities are compared with the discrete analytical dipole probabilities. The code was run for 3000 atoms, which provides reasonable convergence for \(\alpha = 0.6\). It is noted that the probabilities from our simulation spill over to higher \(\ell'\) values previously inaccessible for the pure dipole case. This is a clear indication of the importance of higher multipoles at higher values of \(\alpha\).

**Figure 17:** (a) Plot of Stark transition probabilities \(P_{\ell \rightarrow \ell'}^n\) as a function of \(\ell'\) for values of \(\alpha = 0.15\). Histograms from the simulation with full interaction for 3000 atoms and curves are from analytical results using the dipole interaction. (b) Plot of Stark transition probabilities \(P_{\ell \rightarrow \ell'}^n\) as a function of \(\ell'\) for values of \(\alpha = 0.6\). Histograms are present simulations with full interaction for 3000 atoms and curves are from analytical formula for the pure dipole case[53, 15].

### 4.4.1 Contour plots

In order to provide a qualitative picture of the collision-induced transitions in the ensemble and to illustrate the difference between the full interaction and dipole interaction, we examine contour plots of the mean \(<L>\) and standard deviation \(\sigma_L\) (not to be confused with the cross-section) in the distribution over angular momentum \(L\). The mean provides the location of the average peak of the distribution, and the standard deviation indicates the width of the distribution about the mean. Contour plots for \(<L>\) and \(\sigma_L\), are shown in scaled impact parameter \(\tilde{b} = b/a_n\) and scaled velocity \(\tilde{v} = v/v_n\) space. Fig. 18(a) is for the ion-dipole interaction and Fig. 18(b) is for the full interaction. The \(<L>\)-plots over the \((4 - 18)\)-range in \(\tilde{b}\) show very clearly where Stark mixing primarily occurs and provides quantitative justification
of the qualitative Fig. 3 of Ref. [53], which illustrates the partitioning of the \((\tilde{b}, \tilde{v})\)-
region into different segments where various processes can occur.

Fig. 18(a) shows that the range of \(\ell'\) widens for smaller \(\tilde{b}\) and \(\tilde{v}\) where \(\alpha\) is larger,
as is evident also from Figs. 17(a,b). This is because large \(\alpha\) imply shorter collision times so that the distribution over final \(\ell'\) is narrow, while the longer collision times associated with smaller \(\alpha\) produce a broader distribution over final \(\ell'\). This is confirmed by the larger \(\sigma_L\) in Fig. 18(a). The full interaction produces a wider range in \(\ell'\) which is reflected in Fig. 18(b). Stark mixing occurs mainly in the Orbital Adiabatic-Stark Sudden region [53], which is the green area of Figs. 18(a,b). The lower portions of Fig. 18(a,b) are now amplified in high-resolution contour plots Figs. 19(a,b) which focus on low impact parameters, the \((5-10)\)-range in \(\tilde{b}\) and low collision velocities \(\tilde{v}\). The green area in Fig. 19(a) for \(< L >\) i.e., where \(< L >\approx 8\) and \(\sigma_L \approx 0\), represents the theoretical demarcation curve between the Stark sudden and Stark adiabatic regions where \(\tilde{b} = 3Z/2\tilde{v}\) (cf., Fig. 3 of Ref. [53]). When the full interaction is adopted, then Fig. 19(b) shows that angular momentum changes do occur in that region, evident also where \(\sigma_L \approx 1.5\).

4.4.2 Comparison with experiments

The cross-sections can be calculated using the expression given in Eq. (55), which can be calculated from the CTMC method as

\[
\sigma_{\ell \rightarrow \ell'} = \pi b_{max}^2 \frac{N_R}{N}
\]

where \(N\) is the total number of trajectories run within a given maximum impact parameter \(b_{max}\), and \(N_R\) is the number of trajectories with angular momentum in the range \((\ell', \ell' + 1)\). The trajectories were initially selected to have a uniform distribution in the square of impact parameter, \(b^2\), in the range \((0, b_{max}^2)\).

For Na(28d) atoms, the quantum defects of the \(s\) and \(p\) states are large, these states are not in the degenerate energy shell and therefore are excluded from the \(\ell\)
mixing process. In the simulation, trajectories with final angular momentum $\ell' < 2$ are excluded from consideration. The choice of $b_{\text{max}}$ depends on the quantum defect $\delta$, and taken in accordance with Ref. [28], as $b_{\text{max}} = \sqrt{3n^5/2\delta}$. The quantum defect value used in the calculations is $\delta = 0.0135$.

In the experiments described in Ref. [47], individual collisions of Na(28d) Rydberg atoms with Na$^+$ were observed for low collisional velocities of the ion. The fractional population

$$f_{\ell'} = \frac{\sigma_{2-\ell'}(v)}{\sum_{\ell'' \neq 2} \sigma_{2-\ell''}(v)}, \quad (57)$$

were measured using selective field ionization corresponding to different final angular
momentum states. The results from the calculation and the experiments shown in Fig. (20), are in good qualitative agreement.

4.5 Discussion

In this chapter, we have shown that Classical Trajectory Monte Carlo simulations, customized for long time-scales, are accurate and do reproduce the Stark mixing probabilities provided by the exact classical analytical solutions based on the ion-dipole interaction alone. The sensitivity of transition probabilities to various parameters – the initial distance of the projectile and the number of atoms used in the simulation – is examined. The fractional population computed for Na(28d → 28ℓ′) is shown for
Figure 20: Fractional populations for Stark mixing in the excited sodium versus the scaled collisional velocity of the ion for $28d \rightarrow 28\ell'$. The curves with filled symbols are from experiments, and the curve with unfilled symbols are from present calculations. The final angular momentum states are denoted adjacent to the curve.

varying atom count in Fig. (21). The convergence is good for more than 4000 atoms in the sample.

The dependence on the initial projectile distance $z_0$ was rather weak, while more atoms were required to get close agreement, particularly for higher values of $\alpha$. Once the accuracy was established, the validity of using only the ion-dipole projectile-target interaction rather than the full interaction was then examined. We demonstrated that the dipole approximation is indeed valid for low values of $\alpha \sim 0.1$ while, at smaller impact-parameters higher multipoles do influence the overall final-state $\ell'$, distribution at the larger $\ell'$, inaccessible to ion-dipole collisions alone. Contour plots illustrate the region of $(\tilde{b}, \tilde{v})$-space important to Stark mixing and confirms the theoretical partitioning previously presented [53]. When the full interaction is used, the transition between the Stark adiabatic and Stark sudden regions become less pronounced than that for the pure dipole interaction.

Practical ways to compute cross-sections using CTMC method is shown, and the
results for fractional population computed from the simulation is compared with the experimental results. The results are in good agreement with experiments. This investigation has also provided a viable and feasible approach wherein effects (e.g., quantum defects, black-body radiation) and other competing processes ($n$-changing collisions, radiative cascade etc.) can now be readily incorporated into a comprehensive treatment of ultracold Rydberg plasmas.
CHAPTER V

KING MODEL FOR ELECTRONS IN A FINITE SIZE
ULTRACOLD PLASMA

5.1 Introduction

Ultracold plasmas (UCP) are obtained from a sample of atoms cooled by standard magneto-optical trap techniques and laser-excited just above the ionization threshold [30]. The excess energy, which can be varied from about 0.1 K to 100 K, is imparted to the free electrons which quickly leave the plasma. However, the trailing slow ions left behind create a net positive space charge that prevents further ejection of electrons. Therefore only a fraction of the electrons effectively leave the cloud; the value of this fraction depends on the number of atoms ionized. The remaining part of electrons reach a local quasi-equilibrium state within a short time, of the order of the electron plasma relaxation time, while the ions barely move, if at all, during this time. Since the most energetic electrons have already left the plasma, the remaining electrons can not be described by a Maxwell-Boltzmann distribution, which includes electrons with arbitrarily large velocities. On a longer time scale, the cloud expands inducing an adiabatic cooling while the three-body recombination and de-excitation collisions tend to warm up the plasma.

Molecular dynamics (MD) simulations can accurately follow the dynamics of a UCP but only for a short time due to extreme computing requirements [38]. It is therefore important to start with a physically plausible configuration and to have the ability to scale the size of the system. Kuzmin and O’Neil [32] started their N-body simulation with a far-from-equilibrium distribution. A hybrid MD approach [30] uses the electronic quasi-equilibrium distribution as a background for the ion motion.
at time steps greater than the electron relaxation time. Recent experiments [16] measure the refilling rate of the Rydberg atom in a UCP at various times during its expansion as an indicator of the instantaneous electron temperature. At these times, a microwave flash re-ionizes the UCP, creating again the conditions for the electronic quasi-equilibrium.

The goal of this chapter is to study the equilibrium distribution of electrons captured by a stationary ion cloud. A practical procedure for sampling the electron position and velocity random distribution is given, which consistently describes the system after the electron equilibration but before the start of expansion. Such distributions can be used as starting point for MD simulations of initial expansion or refilling rates. Following suggestions from [42] and [49], a productive analogy with the dynamics of globular star clusters can be employed to the benefit of UCP simulations. This field of astrophysics has a long history [3] and provides accurate models for the cluster dynamics, which is strikingly similar (evaporation, ejection, soft binaries etc..) with UCP dynamics. However, in contrast to the gravitational case, the attractive forces are counterbalanced by the repulsive forces between like particles, and the mass ratio for the particles in the system is very large. These two simple facts are the basis for important differences between the star clusters and UCP. Evidence that the electron distribution is different from a Maxwell-Boltzmann distribution was also discovered in [44, 45].

The self consistent distribution obtained by solving King’s equation [31] has been proven to provide a very accurate description for many globular clusters. Based on this success, a similar distribution was proposed in the seminal paper [8] to describe the electron distribution in UCP. The present chapter further investigates this direction of research and explores the differences between King’s equation and its solutions as applied in astrophysics and for UCP.
5.2 King electron distribution

We consider a spherically symmetric cloud of $N_i$ heavy ions, clamped on their positions, with the Gaussian density:

$$\rho_i(r) = \frac{N_i}{4\pi\sigma^3} \sqrt{\frac{2}{\pi}} e^{-r^2/2\sigma^2},$$  \hspace{1cm} (58)

where $\sigma$ is the characteristic cloud size. The electric potential created by the ion cloud alone is the regular solution of the Poisson equation $\nabla^2 \Phi_i = -\frac{e}{\epsilon_0} \rho_i$

$$\Phi_i(r) = \frac{N_i e}{4\pi\epsilon_0\sigma} \frac{\text{erf}(r/\sqrt{2\sigma})}{r/\sigma}$$ \hspace{1cm} (59)

A number $N_e \leq N_i$ of electrons move in the potential created by the ion cloud. Their stationary distribution cannot be Maxwell-Boltzmann (MB) since the potential $\Phi_i$ is finite as $r \to \infty$. The problem is that the electrons in the tail of the MB distribution, with large velocities, are able to escape the ionic trap. The King distribution was proposed [31] as a stationary solution for a self-gravitating globular cloud of stars. Electrons with a similar distribution have the phase space density, as defined in [8] and [41]:

$$f(r, v) = \frac{\mathcal{N}}{(4\pi)^2 v_T^3 \sigma^3} \left( e^{-(E-E_0)/kT} - 1 \right) \Theta[-e\Phi(r) \leq E \leq E_0],$$  \hspace{1cm} (60)

where $\mathcal{N}$ is a normalization factor, $v_T = \sqrt{kT/m}$ is a characteristic velocity and $k$ is the Boltzmann constant. Here $T$ is a simple parameter, not the temperature, but related to the electron temperature in a way which will be revealed in Section 5.5. The distribution depends on $r$ and $v$ coordinates only through the energy $E = mv^2/2 - e\Phi(r)$, which ensures that $f$ is a stationary solution of Liouville’s equation. Note that here, $\Phi = \Phi_i + \Phi_e$ is the total electric potential, due to both the ions and electrons. In general, when $N_i > N_e$, the potential $\Phi$ is a positive, monotonically decreasing function of the radial coordinate $r$. The $\Theta$ function is 1 when its argument is true and 0 otherwise, and ensures that only electrons with energy less than the...
threshold energy \( E_0 < 0 \) are trapped. The negative threshold energy \( E_0 \) is related to the maximum spatial extension allowed for electron \( r_0 \), by \( E_0 = -e\Phi(r_0) \). Similar to the globular cluster case, the spatial and energy truncation are necessary to describe systems which are not isolated, but in contact with weak external fields, such as the electric and magnetic fields used to collect charged particles. The limit of the King model for \( r_0 \to \infty \), as discussed in the Section 5.4, has an acceptable solution only for \( N_e = N_i \). This means that an infinite size King model can only model a neutral plasma with the same number of electrons and ions. At a given radial position \( r \), the escape velocity is defined as \( v_e = \sqrt{2e[\Phi(r) - \Phi(r_0)]/m} \).

In order to sample the distribution in Eq. (60), we need to find first the potential \( \Phi \), and the relation between the size \( r_0 \), the threshold energy \( E_0 \), the normalization \( \mathcal{N} \), and the number of electrons \( N_e \). This goal is accomplished by solving the complete Poisson equation \( \nabla^2 \Phi = -\frac{e}{\varepsilon_0} \rho_i + \frac{e}{\varepsilon_0} \rho_e \), where the electron density is obtained by integrating the phase space distribution over the velocity space

\[
\rho_e(r) = \frac{\mathcal{N}}{4\pi v_T^3 \sigma^3} \int_{-e[\Phi(r) - \Phi(r_0)]/kT}^{v_e} (e^{-(E-E_0)/kT} - 1) v^2 dv. \tag{61}
\]

Changing the integration variable from \( v \) to \( x \) according to \( v^2 = 2v_T^2 [x + e\{\Phi(r) - \Phi(r_0)\}/kT] \), we find

\[
\rho_e(r) = \frac{\mathcal{N}\sqrt{2}}{4\pi \sigma^3} \int_{-e[\Phi(r) - \Phi(r_0)]/kT}^{0} \sqrt{x + e\{\Phi(r) - \Phi(r_0)\}/kT} (e^{-x} - 1) \, dx, \tag{62}
\]

which gives an implicit relation between \( \rho_e \) and \( \Phi \). By defining \( W(r) = e[\Phi(r) - \Phi(r_0)]/kT \), the electron density can be calculated by direct integration, as

\[
\rho_e(r) = \frac{\mathcal{N}\sqrt{2}}{4\pi \sigma^3} \int_{-W}^{0} \sqrt{x + W} \left( e^{-x} - 1 \right) \, dx
= \frac{\mathcal{N}\sqrt{2}}{4\pi \sigma^3} \frac{3}{2} \left[ \frac{3\sqrt{\pi}}{4} e^W \text{erf}\sqrt{W} - (W + 3/2)\sqrt{W} \right]. \tag{63}
\]

This expression is valid only for \( 0 \leq r \leq r_0 \), where \( W \geq 0 \), while outside this interval \( \rho_e = 0 \).
The function $W$ is obtained as the solution of the complete Poisson equation when the electron density $\rho_e$ is replaced by expression (63). As a result, the following nonlinear ODE has to be solved

\[
\frac{1}{R} \frac{d^2}{dR^2} RW(R) = -\frac{N_i}{N_0} \sqrt{\frac{2}{\pi}} e^{-R^2/2} + \frac{N}{N_0} \left[ \sqrt{\frac{2}{\pi}} e^W \text{erf}\sqrt{W} - \left( \frac{2}{3} W + 1 \right) \sqrt{2W} \right]
\]  

(64)

where $R = r/\sigma$ is the normalized radial distance and $N_0 = 4\pi \epsilon_0 kT \sigma/e^2$, is the characteristic particle number. The boundary conditions for this equation are: $W'(0) = 0$, $W(R_0) = 0$ and $W(R \to \infty) = -e\Phi(r_0)/kT$, where $R_0 = r_0/\sigma$.

Introducing the notation

\[
\Sigma[W] = \begin{cases} 
\sqrt{\frac{2}{\pi}} e^W \text{erf}\sqrt{W} - \left( \frac{2}{3} W + 1 \right) \sqrt{2W} & , W > 0 \\
0 & , W \leq 0
\end{cases}
\]

(65)

the electron density is simply

\[
\rho_e(r) = \frac{N}{4\pi \sigma^3} \Sigma[W(r/\sigma)]
\]

(66)

and the number of electrons is obtained by integrating Eq. (63) over the coordinate space

\[
N_e = N \int_0^{R_0} R^2 \Sigma[W] \, dR.
\]

(67)

Equation (64) is now written as

\[
\frac{1}{R} \frac{d^2}{dR^2} RW(R) = -\frac{N_i}{N_0} \left( \sqrt{\frac{2}{\pi}} e^{-R^2/2} - \alpha \Sigma[W] \right)
\]

(68)

where parameter $\alpha$ is introduced, such that $N = \alpha N_i$.

This equation is very similar to the equation for the globular clusters, but there are important differences. The right hand side in Eq. (64), unlike in the case of star clusters, is not always negative. The space scale in the plasmas is fixed by $\sigma$, whereas it is a model parameter for globular clusters. There is also no inhomogeneous term equivalent to the ionic contribution in plasmas, for the case of globular clusters.
5.3 Examples

In his seminal paper, King [31] proposed to solve Eq. (64) by starting from the origin and integrating forward until \( W = 0 \). A class of models is therefore obtained for various values of the free parameter \( W(0) \), the value of \( W \) at the origin.

As the right hand side of Eq. (64) is always negative in the gravitational case, this procedure always yields a solution, and the cutoff radius \( R_0 \) for which \( W(R_0) = 0 \) increases with increasing \( W(0) \). The plasma case is more complicated as the RHS of Eq. (64) can in principle be both positive and negative. The solution diverges if the RHS is positive, and hence not all values of \( W(0) \) produce a meaningful model. Since the number of electrons \( N_e \) is related to distribution normalization, the number of electrons cannot be specified from the beginning, which is another serious drawback of this approach.

A better approach is to regard Eq. (64) as a boundary value problem, and to integrate it backwards starting from \( R_0 \). This is facilitated by the observation that the solution to Eq. (64) is fully known outside the sphere of radius \( R_0 \), and has the expression:

\[
W_{\text{out}}(R) = \frac{N_i}{N_0} \frac{\text{erf}(R/\sqrt{2})}{R} - \frac{N_e}{N_0} \frac{1}{R} + \frac{E_0}{kT}, \quad (R \geq R_0)
\]

(69)

If \( N_i, N_e, \) and \( E_0 \) are specified, then the cutoff radius \( R_0 \) is obtained as a solution of \( W_{\text{out}}(R) = 0 \). Since the derivative of \( W \) is also known at \( R_0 \), then Eq. (64) can be integrated backwards for various values of the normalization \( \mathcal{N} \) (or \( \alpha \)), with the goal of canceling the derivative at the origin: \( W'(0) = 0 \). This process is similar to the shooting method to solve boundary value problems.

Figure 22 illustrates three solutions obtained for a cloud of \( N_i = 24000 \) ions, of size \( \sigma = 100 \mu m \), and three different electron populations. The ion density falls down very fast (exponentially), while the electron density extends well outside the ion cloud, decreasing slowly to zero at \( R_0 \).
Figure 22: Three models with the same ion distribution with $N_i = 24000$ and $\sigma = 100 \, \mu m$, and different electron populations $N_e = 22500, 23000$ and 23500. Parameters are $T = 50$ and $E_0 = -5 \, K$. Upper graph shows the electric potential along the radial direction. The lower graph shows the number density for electrons (color lines) and for the ions (black line). The potential created by the ions only is displayed in the upper graph (black line). The vertical dashed lines indicate the position of cutoff radius $R_0$ for each model, while the horizontal dashed line shows the threshold energy $E_0$. 
5.4 The case of no space constrains

This section treats the case $R_0 \to \infty$. An integral equation is obtained from Eq. (64) by using Green’s function for the Poisson equation and regarding the RHS as an inhomogeneous term:

$$ W(R) = \frac{N_i}{N_0} \frac{\text{erf}(R/\sqrt{2})}{R} - \frac{\mathcal{N}}{N_0} \int_0^\infty \frac{x^2}{\max(x, R)} \Sigma\lfloor W \rfloor \, dx $$

(70)

where it is assumed the integral makes sense, or in other words, $N_e = \mathcal{N} \int_0^\infty x^2 \Sigma\lfloor W \rfloor \, dx < \infty$.

The asymptotic behavior of the function $\Sigma$ for small arguments is

$$ \Sigma(x) = \frac{4\sqrt{2}}{15} x^{5/2} + \frac{8\sqrt{2}}{105} x^{7/2} + \mathcal{O}(x^{9/2}) $$

(71)

Therefore, a solution which decays only as $W \sim 1/R$, for $R \to \infty$, which would be obtained if the plasma were not neutral, is not acceptable because in that case $\Sigma$ decrease as $\Sigma\lfloor W \rfloor \sim 1/R^{5/2}$, not fast enough to make the integral convergent.

If one assumes that $W(R) = A/R^\beta$, then the integral equation (70) becomes for large $R$

$$ \frac{A}{R^\beta} = \frac{1}{R} \left( \frac{N_i}{N_0} - \mathcal{N} \int_0^\infty x^2 \Sigma\lfloor W \rfloor \right) - \frac{\mathcal{N}}{N_0} \int_R^\infty x \left( 1 - \frac{x}{R} \right) \Sigma\lfloor W \rfloor \, dx $$

(72)

For $W$ to decay faster than $1/R$ it is required that $\beta > 1$ and that the coefficient in the $1/R$ term, proportional to total charge $N_i - N_e$, vanishes. On equating the LHS with the $1/R^{5/2\beta-2}$ from the second term on RHS, one gets $\beta = 4/3$, which is greater than unity as required.

If $N_e = N_i$, then one obtains the following constraint

$$ \frac{A}{R^{4/3}} = \frac{\mathcal{N}}{N_0} 3\sqrt{2} A^{5/2} $$

(73)

which fixes the value of the normalization constant to

$$ \frac{\mathcal{N}}{N_0} = \frac{5}{3\sqrt{2} A^{3/2}} $$

(74)
A model with electron density going like $\sim R^{-10/3}$ is obtained by starting at some value $R_*$, with initial condition $W = A/R^{4/3}$ and integrating backward eq. (64), toward the origin. The condition of regularity at the origin fixes the value of $A$.

5.5 Results

An ensemble of electrons with statistical properties in the $(r, v)$ plane defined by Eq. (60) can be generated after obtaining the potential $\Phi(r)$ from the solution $W(R)$ of Eq. (64). Because the distribution is isotropic a full three dimensional $(r, v)$ population is obtained by attaching arbitrary directions to electron positions and velocities.

The King distribution in Eq. (60) is generated by first starting with an initial uniform distribution in the $(r, v)$ plane and then performing Metropolis accept/reject steps until convergence. By denoting a point in the $(r, v)$ plane by $x$, a proposed new point $x'$ is obtained by sampling a random distribution which gives $x'$ with probability $P_{x'\rightarrow x}$. A good choice for $P_{x'\rightarrow x}$ is, for example, a normal distribution centered at $x$ and with the standard deviation a fraction of the $(r, v)$ domain sampled. For this distribution $P_{x\rightarrow x'} = P_{x'\rightarrow x}$. The proposed $x \rightarrow x'$ step is accepted with the probability $\Omega_x(x') = \min(\rho(x')/\rho(x), 1)$, by generating a random number in the interval $[0,1]$ and comparing it with the ratio $\rho(x')/\rho(x)$. The proposed step is accepted if the random number is less than $\Omega_x(x')$, or rejected otherwise. Here $\rho$ is the desired distribution function given by Eq. (60). Therefore, the probability of moving point $x$ to $x'$ is $W_{x\rightarrow x'} = P_{x\rightarrow x'}\Omega_x(x')$. Since the detailed balance relation $\rho(x')W_{x'\rightarrow x} = \rho(x)W_{x\rightarrow x'}$ is satisfied, the initial distribution will converge to $\rho$ after sufficient iterations.

The rest of this section will present a detailed analysis for a specific King model. This case has 25,600 ions and 25,088 electrons. The gaussian ion distribution has standard deviation $\sigma = 120 \mu m$. The electron distribution has the parameter $T = 50$ K, threshold energy $E_0 = -5$ K and the cutoff radius $r_0 = 1711 \mu m$. The density in
Figure 23: Electron radial distribution for the King distribution, from sampled population (histogram) and theoretical prediction (solid line).

the center of the cloud for both electrons and ions is about $10^9 \text{ cm}^{-3}$. The electron distribution is obtained after 4000 Metropolis steps.

Figure 23 compares the radial distribution for electrons generated by the Metropolis random walk process with the prediction given by Eq. (63). The good agreement indicates convergence.

In Fig. 24, radial distribution of ions is compared with that of electrons. The electron distribution extends for larger distances and has lower densities at short distances.

The phase space profile of the King distribution is shown in figure 25, where the contour lines indicate constant density. The left figure shows the sampled population while the figure on the right shows the predicted distribution of Eq. 60.

In Fig. 26, the velocity distribution for the sampled electrons can be seen to be in agreement with the theoretical prediction obtained by integrating distribution (60) over spatial coordinates

$$\rho(v) = \mathcal{N} \frac{v^2}{v_T^2} \left[ e^{-v^2/2kT} \int_0^{R^*(v)} e^{W(R)} R^2 dR - \frac{R^*(v)^3}{3} \right], \quad (75)$$

where $R^*(v)$ is the radial position where $E = E_0$ for a given velocity. In contrast, the
Figure 24: Ion radial distribution for the King distribution, from sampled population (histogram) and theoretical prediction (solid line), compared with electron radial distribution (dashed line).

Figure 25: Phase space distribution for the King electron distribution. The contour lines are lines of equal density. The run-away ($E = 0$) curve is shown in the right panel. The unit for velocity is $\sqrt{k_B K/m}$, where $k_B$ is the Boltzmann constant and $m$ is the electron mass.
Figure 26: The electron velocity for the King distribution from the sample (histogram) and theoretical prediction (solid line), compared with that of a Maxwell-Boltzmann distribution with $T = 50$ K (dashed line).

Maxwell-Boltzmann distribution, shown with dashed line, extends for much larger velocities.

Although stationary, the King distribution is not characterized by a unique temperature. The symbol $T$ in Eq. (60) is rather a parameter, and not the temperature. However, it is possible to define a local temperature as a measure of the velocity dispersion: $T_{\text{local}} = m\langle v^2 \rangle / 3$. This results in the following relation:

$$T_{\text{local}}(R) = T \frac{\frac{\pi}{2} e^W \text{erf}\sqrt{W} - \left(\frac{4}{15}W^2 + \frac{2}{3}W + 1\right)\sqrt{2W}}{\frac{\pi}{2} e^W \text{erf}\sqrt{W} - \left(\frac{2}{3}W + 1\right)\sqrt{2W}}, \quad (76)$$

where $W$ is the solution of Eq. (64). Figure 27 compares the predicted position-dependent temperature with the temperatures sampled inside regions separated by a series of spherical shells.

Figure 28 shows the histogram of energies for the sampled King distribution, in good agreement with the theoretical result (solid line) calculated from Eq. (60) as

$$\rho(E) = f(E) g(E) = f(E) \int \int \delta(mv^2/2 - e\Phi(r) - E) \, dr \, dv. \quad (77)$$

Here $g(E)$ is the classical number of states for the given energy – the phase space volume occupied by the energy manifold, and $f$ is the distribution function in Eq. (60).
Figure 27: Local temperature variation along the radial direction for the King distribution, for sample (dots) and theoretical prediction (line).

5.6 Discussion

A stationary, finite size distribution is constructed for the electrons in a cloud of fixed ions with a Gaussian distribution. The model is similar to the King model used in astrophysics, but important differences arise from the fact that in a plasma, in contrast to the gravitational case, there are also repulsive forces, apart from the attractive ones.

The distributions can be used as a starting point in Molecular Dynamics simulations and also in Monte Carlo simulations where working with quasi-equilibrium electron distributions is an essential condition. The King model without space constraints can only exist when the net charge is zero, and for this case the radial density decreases asymptotically as $1/R^{10/3}$.

The electron temperature decreases substantially with increasing distance from the center. One can combine the decrease of density with one in temperature and evaluate the local $r-$dependent rate of TBR using $k_{TBR} \sim \rho_i P_e^2 / T^{9/2}$, as a rough estimate and assuming the validity conditions of the present model.
Figure 28: Electron energy distribution for the King distribution: from sampled population (histogram) and theoretical prediction (solid line).
CHAPTER VI

SIMULATION OF ULTRACOLD PLASMAS

Ultracold plasmas (UCP) are created by photo-ionizing cold atoms in a magneto-optical trap (MOT) using a laser to just above threshold [30]. The UCPs are characterized by: the plasma size $\sigma$, the number of electrons $N_e$, number of ions $N_i$, the electron density $\rho_e$, ion density $\rho_i$, ion temperature $T_i$ and electron temperature $T_e$. The electron number, ion number and their densities can be controlled by varying the intensity of the photo-ionizing laser. Since the ions were created by photoionizing cold atoms, the density profile of the ions is the same as that of the cold atoms, which is a Gaussian distribution characterized by the cloud size of RMS radius $\sigma$. As the ions are created by ionizing cold atoms, their temperature $T_i$ is set by the initial temperature of the cold atoms in the MOT, and is of the order of milli-Kelvin. The average electron temperature $T_e$ on the other hand is determined by the frequency of the ionizing laser beam, and can typically be tuned in the range of $1 - 1000K$. UCPs are good testing beds for our understanding of basic plasma theory, and also provide us a way to understand little tested regimes such as strongly coupled plasmas.

Two parameters that guide the plasma behavior, are the Debye length and the Coulomb coupling parameter. The Debye length $\lambda_D = \sqrt{\varepsilon_0 k_B T_e / \rho_e e^2}$ is the distance over which the charge is screened in a plasma. The Coulomb coupling parameter $\Gamma = e^2/(4\pi\varepsilon_0 a k_B T_e)$ is the ratio of inter-particle potential energy to the kinetic energy. The Wigner-Seitz radius $a = [3 / 4\pi \rho]^{1/3}$ is representative of the separation between the particles at density $\rho$. Strongly coupled plasmas have $\Gamma > 1$ and they depart from our conventional knowledge of plasmas, which are mostly weakly coupled. By tuning the plasma input parameters such as the density and temperature, the coupling
strength can be either weak or strong.

After the creation of the UCP, the system is far from equilibrium, and the dynamics of the plasma system as it progresses towards equilibrium is the subject of this Chapter. The electrons equilibrate amongst themselves and achieve local-thermal equilibrium in a timescale $t_e$ which is of the order of nano-seconds. The ions on the other hand expand radially due to the thermal pressure exerted by the electrons, and the ion relaxation time $t_i$ is of the order of micro-seconds. During the plasma expansion, many atomic-processes influence the dynamics of the system as well. Electrons collide and recombine with an ion by radiative recombination, or three-body recombination (TBR). For electron temperatures of the order of few hundred Kelvin, the radiative recombination is important, and at ultracold temperatures of the order of few Kelvin, the TBR process is more dominant. The TBR rate increases with increase in electron densities and decreases with increase in electron temperatures, and is given as $k_{TBR} \sim \rho_e^2 \rho_i T_e^{-9/2}$. The electron also scatters with the recombined atom, causing excitation, de-excitation or ionization transitions in the Rydberg atom.

Molecular Dynamics (MD) simulation can be used to describe the dynamics of the ultracold plasmas, but they are also computationally expensive. The simulation study done by Mazevet et al. [38] for instance, could describe the dynamics for a few nano-seconds, and the whole micro-second dynamics of the plasma is completely out of scope of MD methods (without approximations). In Chapter 5, the King model for the ultracold plasma was presented, which is the equilibrium distribution of electrons after the electron equilibration but before the start of ion expansion. The King distribution could be used as a starting point for the MD simulation or a Monte Carlo type simulation. The goal of this Chapter is to make use of the King distribution as a starting point to implement a Monte Carlo type simulation for the long timescale expansion dynamics of the ultracold plasma.
6.1 Implementation

In this Chapter, we are interested in understanding the long timescale dynamics of the ultracold plasma. The long timescale in our simulation is of the order of ion expansion timescale $t_i$. We assume that our plasma system has a spherical symmetry, and the number of particles is large (i.e.) $N_t = N_i + N_e \sim 30,000$. The spherical symmetry of the plasma simplifies the potential calculation. An MD simulation keeps track of the trajectories of each and every particle, which is not as useful as their statistics are. In light of this realization, the Monte Carlo method [23] propagates the system at each time-step such that it behaves statistically as the real system.

In the Monte Carlo method, computation is started by assigning to each particle its position $r$, radial velocity $v_r$, transverse velocity $v_t$, and charge $q$ according to King type distribution. The King model is a steady state distribution for the plasma given by the phase space density Eq. (60) in Chapter 5. For large number of particles $N_t$, the electrostatic interaction between the charges can be separated into a smooth mean field contribution, and a small irregular, fluctuating field. The time-step $\Delta t$ in our simulation is such that,

$$t_e \ll \Delta t \ll t_i.$$  

During the interval $\Delta t$, the effect of the fluctuating field can be dropped as a first approximation, and the simulation can be performed using the mean field. This mean field is spherically symmetric, and changes only in the time scale of $t_i$, thus can be treated as time-independent during the time-step $\Delta t$. The electron follows a rosette motion, and their position after time $\Delta t$ is determined by a Monte Carlo step, while the ions are propagated deterministically in the presence of the mean field. The effect of collision in a time $\delta t \ll t_e$ is calculated, and it is multiplied by a scaling factor $\Delta t/\delta t$ to account for its effect in each time-step.

The schematic of the simulation process is outlined in Fig. (29). Three important
steps in the simulation are: 1) potential calculation, 2) collisions, and 3) micro-canonical shuffling of electrons and ion propagation. These three steps will be explained in detail below. Plasma units as defined in Appendix B will be followed, unless mentioned otherwise.

6.1.1 Potential Calculation

We need to evaluate smoothed out potential. The smoothing in the transverse direction is done by considering each particle to be a spherical shell of charge \( q_k \). Let \( r_k \) be the radius of the shells, with charge \( q_k = +1 \) or \(-1\) depending on whether it is an ion or electron. The potential in the interval \( r_k \leq r \leq r_{k+1} \) is given as

\[
U(r) = \frac{1}{4\pi \epsilon_0} \left( \frac{1}{r} \sum_{i=1}^{k} q_i + \sum_{i=k+1}^{N_t} \frac{q_i}{r_i} \right) \\
= \frac{1}{4\pi \epsilon_0} \sum_{i=1}^{N_t} \frac{q_i}{\max(r_i, r)}
\]

(79)
where $N_t = N_i + N_e$. This calculation is done in two steps. Taking $U_k = U(r_k)$, the potential on the shells is calculated first as:

\[
\begin{align*}
U_{N_t+1} &= 0 \\
Q_{N_t} &= \sum_{i=1}^{N_t} q_i \\
U_k &= U_{k+1} + \frac{Q_k}{4\pi\varepsilon_0} \left( \frac{1}{r_k} - \frac{1}{r_{k+1}} \right) \\
Q_{k-1} &= Q_k - q_k
\end{align*}
\]

(80)

Once the potential of the spherical shells have been evaluated, the final step in calculating the potential at a point in the grid for $r_k \leq r \leq r_{k+1}$ is given as

\[
U(r) = U_k + \frac{1/r_k - 1/r}{1/r_k - 1/r_{k+1}}(U_{k+1} - U_k).
\]

(81)

Depending on whether the potential is felt by ions or electrons, the potential well is attractive or repulsive, and an appropriate sign is included. The potential calculation in terms of ‘spheres’ as expressed in Eq. (79) can be rationalized in the following way.

The potential for a charge distribution $\rho(x)$ is defined as

\[
\phi(r) = \frac{e}{4\pi\varepsilon_0} \int \frac{\rho_i(x) - \rho_e(x)}{|x - r|} dx.
\]

(82)

Now, the integral can be evaluated using Monte Carlo sampling, which approximates an integral as

\[
\int f(x)p(x)dx \approx \langle f \rangle \pm \sqrt{\frac{\langle f^2 \rangle - \langle f \rangle^2}{N}}
\]

(83)

for $N$ points $x_i$ distributed according to unit normalized distribution function $p(x)$. Here the mean is denoted as $\langle f \rangle = \sum_{i=1}^{N} f(x_i)/N$. Thus using a Monte Carlo sampling, the potential can be approximated using $N_i$ and $N_e$ points $x_j^{(i,e)}$ having a distribution $\rho_i$ and $\rho_e$ respectively, to yield

\[
\phi(r) \approx \frac{e}{4\pi\varepsilon_0} \left( \sum_{j=1}^{N_i} \frac{1}{|x_j^{(i)} - r|} - \sum_{j=1}^{N_e} \frac{1}{|x_j^{(e)} - r|} \right)
\]

\[
= \frac{e}{4\pi\varepsilon_0} \sum_{L,M} \frac{4\pi}{2L + 1} \left( \sum_{j=1}^{N_i} \frac{r_{j,L}^L}{r_{j,L}^L + 1} Y^*_L,M(\hat{x}_j^{(i)}) - \sum_{j=1}^{N_e} \frac{r_{j,L}^L}{r_{j,L}^L + 1} Y^*_L,M(\hat{x}_j^{(e)}) \right) Y_{L,M}(\hat{r}).
\]

(84)
Here we make use of the expansion

$$\frac{1}{|x - r|} = \sum_{L,M} \frac{4\pi}{2L + 1} r_{r<}^{L} Y_{LM}^*(\hat{x}) Y_{LM}(\hat{r})$$

(85)

in terms of the spherical harmonics $Y_{LM}$, $r_< = \min(r, x)$ and $r_> = \max(r, x)$. For a spherically symmetric distribution for the electrons and ions, such as in our case, only the monopole term in Eq. (84) is non-zero. Thus Eq. (84) reduces to the expression in Eq. (79), hence the ‘sphere’ approximation is nothing but a Monte Carlo estimate of the exact potential for a spherically symmetric distribution.

Once the potential is calculated the energy per unit mass $E$ and angular momentum per unit mass $L$ of the particles are calculated as

$$E_j = \frac{1}{2}(v_r^2 + v_t^2) + \frac{q_j \phi(r)}{M_j}$$

(86)

and

$$L_j = v_r r.$$ 

(87)

Here $q_j$ and $M_j$ are the charge and mass respectively of the particle.

### 6.1.2 Collisions

The electron-electron collisions occur at short timescales, and help electrons equilibrate among themselves. The electrons also collide with ions, and recombine to form Rydbergs. The electron can then scatter with the Rydberg to cause excitation or de-excitation transitions. These are important processes that influence strongly the dynamics of the ultracold plasma. In the simulation, prior to the collision step, the particles are bunched into sectors falling within a grid. The local electron temperature $T_e$, ion density $\rho_i$ and electron density $\rho_e$ are calculated in each of these sectors and is assumed to be constant in that sector. The value of $\rho_e$, $\rho_i$ and $T_e$ are used in calculating the collisional properties. Alternately, the sectors can also be formed by grouping particles into groups of 100 to 150 particles. The results of the simulation
aren't sensitive to this detail. Here we outline the method to incorporate collisions in the code.

6.1.2.1 Electron-electron collision

Electron-electron ($e-e$) collision is elastic, and causes the particles to exchange kinetic energy while the total energy itself is conserved. We simulate the effect of electron-electron collision by perturbing the energy and angular momentum of each electron in a time-step $\Delta t$. The perturbations $\Delta E$ and $\Delta J$ over time $\Delta t$ are calculated for two neighboring electrons, by expressing in the center of mass frame of reference where the magnitude of the velocities remain the same with only the change in direction. The angle of deflection in the center of mass frame is determined from the statistical properties of $e-e$ collision.

Let the coordinates of the two interacting electrons be $(r, v_r, v_t)$ and $(r', v'_{r'}, v'_{t'})$, though the exact orientation of the position and velocity vectors $(r, v)$ and $(r', v')$ are unknown. Missing information will be filled by sampling from random numbers so as to adhere to spherical symmetry. Let us chose the $z-$axis of our coordinate system to be along the position vector $r$ and the velocity $v$ to lie in the $(x,z)-$plane. This choice yields,

$$
\begin{align*}
v &= (v_t, 0, v_r), \\
v' &= (v'_{t'} \cos \phi, v'_{t'} \sin \phi, v'_{r'})
\end{align*}
$$

(88)

where $\phi$ is random selected in the interval $(0, 2\pi)$, since the transverse velocities are isotropic because of spherical symmetry. The relative velocity $w = v' - v$ is given as,

$$
\begin{align*}
w &= (v'_{t'} \cos \phi - v_t, v'_{t'} \sin \phi, v'_{r'} - v_r).
\end{align*}
$$

(89)

The plane of relative motion $(r' - r, v' - v)$ is taken to have an angle $\psi$ with respect to some reference plane. We chose this reference plane to be that defined by $(w, w_1)$,
such that

\[
\mathbf{w}_1 = \left( w_y/w_p, -w_x/w_p, 0 \right)
\]

\[
\mathbf{w}_2 = \left( -w_z/w_p, -w_yw_z/w_p, w_p \right)
\]

are vectors mutually orthogonal to \( \mathbf{w} \) with \( w_p = \sqrt{w_x^2 + w_y^2} \) and \( w = \sqrt{w_x^2 + w_y^2} \). Let the effective angle of deflection in the velocity during the collision be \( \theta_e \), then the relative velocity after encounter will be,

\[
\mathbf{w}' = \mathbf{w} \cos \theta_e + \mathbf{w}_1 \sin \theta_e \cos \psi + \mathbf{w}_2 \sin \theta_e \sin \psi.
\]

The effective angle of deflection \( \theta_e \) is calculated using Rutherford scattering formula. For a test particle having a charge \( q_T \) colliding in a background of field particles of charge \( q_F \), Rutherford formula for the scattering angle is given by

\[
\tan(\theta/2) = \frac{q_T q_F}{4\pi\varepsilon_0 b \mu v_0^2},
\]

where \( \mu^{-1} = m_T^{-1} + m_F^{-1} \) is the reduced mass, \( b \) is the impact parameter, and \( v_0 \) is the initial relative velocity. The contribution from cumulative effect of small angle collisions is more than large-angle scattering events, and the average of \( \theta^2 \) in a given time \( \delta t \) is given as:

\[
<\theta^2> = 8\pi v_0 \rho_e b_0^2 \delta t \ln(\lambda),
\]

where \( b_0 = q_T q_F/(4\pi\varepsilon_0 \mu v_0^2) \), \( \rho_e \) is the electron density per unit volume, \( \lambda = b_{\text{max}}/b_0 \) for a choice of maximum impact parameter \( b_{\text{max}} \). The effective angle of deflection over time \( \Delta t \) is chosen using the Eq. (93) such that

\[
\theta_e = \frac{e^2}{4\pi\varepsilon_0 \mu} \sqrt{\frac{8\pi \rho_e \ln(\lambda) \Delta t}{v_0^2}}.
\]

The choice of \( \ln \lambda \) is less sensitive to \( b_{\text{max}} \) because of the logarithm, and it is of the order of 10 and hence we take \( \ln \lambda = 10 \) in the simulations. Therefore the new
velocities of the two electrons can be transformed back from center of mass frame to
fixed frame of reference to yield:

\[ \mathbf{v}_f = \mathbf{v} - \frac{1}{2}(\mathbf{w}' - \mathbf{w}), \]  

(95)

\[ \mathbf{v}'_f = \mathbf{v}' + \frac{1}{2}(\mathbf{w}' - \mathbf{w}), \]  

(96)

where the subscript \( f \) denotes the final state after collisions. Finally the radial and
transverse velocities of the first electron is computed as:

\[ v_{f,r} = v_{f,z} \quad v_{f,t} = (v_{f,x}^2 + v_{f,y}^2)^{1/2} \]  

(97)

New energy is \( E_f = U(r) + (v_{f,r}^2 + v_{f,t}^2)/2 \) and angular momentum is \( L_f = rv_{f,t} \).
Similar quantities for the second electron can be calculated.

6.1.2.2 Three Body Recombination

The three body recombination and collisional ionization obey detailed balance relation
given as:

\[ k_{tbr}(n) = k_{ion}(n)n^2\lambda_D^3 \epsilon^\epsilon \rho_e \]  

(98)

where \( k_{tbr}(n) \) and \( k_{ion}(n) \) are the three body recombination and ionization rate con-
stants into and out of level \( n \) respectively. The electron density is \( \rho_e \) and the scaled
ionization energy \( \epsilon = \mathcal{R}/n^2k_B T \). From Ref. [37], the ionization rate constant from
level \( n \) is given as

\[ k_{ion}(n) = 11k_0e^{-\epsilon}e^{-\epsilon/3} \]  

(99)

where the natural rate in CGS units, and plasma units is

\[ k_0 = \left( \frac{e^2}{k_B T} \right)^2 \sqrt{\frac{k_B T}{m_e}} [cm^3 s^{-1}] = \frac{279.223504}{T_k^{3/2}} [L_p^3 T_p^{-1}], \]  

(100)
Here $T_K$ is the temperature measured in Kelvin. Thus the three body recombination rate per ion, $\tilde{k}$, into a state $n$ is:

$$\tilde{k}_{tbr}(n) = 11k_0\lambda Dn^2\epsilon^{-7/3}\rho_e^2 = 9.44081 \times 10^{-13}\frac{n^{20/3}}{T_k^{2/3}}\rho_e^2. \ [T_p^{-1}]$$ (101)

On integrating over the quantum states $n$ we get the total recombination rate. We need to set an upper bound for $n$ that we integrate up to to avoid divergence. Here we chose the upper bound to be the Thompson value $n_T = \sqrt{ZR/k_BT}$. This gives the total recombination rate per ion:

$$\tilde{k}_{tbr} = 1.04086 \times 10^7 \frac{\rho_e^2}{T_k^{9/2}} \ [T_p^{-1}]$$ (102)

6.1.2.3 Electron-Rydberg scattering

The rates for energy transfer for a Rydberg atom with energy $E_i$ going to final energy $E_f \pm \Delta E_f/2$, as given in Ref. [37] is

$$R_c(E_i \rightarrow E_f; \Delta E_f) = 11\rho_e k_0 \frac{(-\epsilon_i)^{5/2}\epsilon_i + \epsilon_<}{\epsilon_>} \Delta \epsilon_f$$ (103)

where $\epsilon = E/k_BT$, $\epsilon_< = \min(-\epsilon_i, -\epsilon_f)$, $\epsilon_> = \max(-\epsilon_i, -\epsilon_f)$ and $k_0$ is the expression given in Eq. (100). The rate for all collisional transitions from $E_i$, obtained by integrating over all $E_f$ is

$$R_c(E_i) = \frac{11}{(-\epsilon_i)^{7/3}}(1 + (-\epsilon_i) \times \frac{6}{23})\rho_e k_0$$ (104)

The probability for a collision to occur is proportional to $R_c(E_i)\Delta t$. If a collision event is selected, then the final energy $E_f$, which includes ionization $E_f > 0$, is generated from the probability density function defined over $-\infty < E_f < \infty$

$$P_c(E_f) = \frac{R_c(E_i \rightarrow E_f; \Delta E_f)}{R_c(E_i)} = \left(\frac{-\epsilon_i}{\epsilon_>}\right)^{29/6} \frac{\epsilon_i + \epsilon_<}{1 + \frac{6}{23}(-\epsilon_i)} \Delta \epsilon_f$$ (105)

The recombination and scattering event probabilities are calculated for each sector for a given time $\Delta t$, by taking the product of the rate and time step $\Delta t$. The values
of local electron temperature $T_e$, ion density $\rho_i$, and electron density $\rho_e$ are calculated for each sector and is used in the rate equations. Any residual energy, arising from three body recombination, is distributed among all the electrons in a given sector where recombination occurs. In a similar vein, radiative recombination and radiative cascade processes can be included as well.

### 6.1.3 Electron and Ion Propagation

After the collision step has perturbed the energy and angular momentum of the particles, new realization of the system is obtained by computing new positions and velocities. The ions are heavy and do not move much in a nano-second timescale and they can be propagated deterministically. The electrons, being lighter, gets bounced around, and we use a Monte Carlo treatment in computing positions and velocities.

The deterministic equations of motion for the ion with coordinates $(r, v_r, v_t)$ are

$$\dot{v}_r - \frac{L^2}{r^3} = a_r, \quad L = r v_t = \text{constant},$$  \hspace{1cm} (106)

where the radial acceleration $a_r$ is calculated from Eq. (81) to yield

$$a_r = \frac{q_i}{M_i} \frac{(U_k - U_{k+1})}{1/r_k - 1/r_{k+1}} \frac{1}{r^2} \quad \text{for } r_k \leq r \leq r_{k+1}. \hspace{1cm} (107)$$

The charge and mass of the ion is given as $q_i$ and $M_i$. The equation of motion is integrated using a simple Runge-Kutta integrator for each and every ion.

For the electron, we assume that it moves in the smoothed-out potential $U(r)$ which was computed above in Eq. (81). The electron describes a rosette orbit (quasiperiodic and not closed), with $r$ oscillating between two turning points $r_{\text{min}}$ and $r_{\text{max}}$, which are the roots of

$$Q(r) = 2E + 2\frac{q_e U(r)}{M_e} - \frac{L^2}{r^2} = 0. \hspace{1cm} (108)$$

The probability for the electron to then lie in a interval $dr$ should be equal to the fraction of the time spent by the electron in $dr$, and thus

$$\frac{dt}{\tau} = \frac{dr/|v_r|}{\int_{r_{\text{min}}}^{r_{\text{max}}} dr/|v_r|}. \hspace{1cm} (109)$$
where

\[ |v_r| = \left[ 2E + 2q_eV(r)/M_e - L^2/r^2 \right]^{1/2} = [Q(r)]^{1/2}. \tag{110} \]

Computation of the half-period \( \tau \) can be time consuming. We avoid that by making use of the Von Neumann rejection technique and generate a new position with a distribution proportional to \( 1/|v_r| \). We want a probability distribution proportional to the function \( f(r) = 1/|v_r| \). We take a number \( F \) which is everywhere larger than \( f(r) \) in the interval \( (r_{\text{min}}, r_{\text{max}}) \). We select a point \((r_0, f_0)\) at random in the rectangle \( r_{\text{min}} < r_0 < r_{\text{max}}, 0 < f_0 < F \), with a uniform distribution, i.e. we compute

\[ r_0 = r_{\text{min}} + (r_{\text{max}} - r_{\text{min}})X, \quad f_0 = FX', \tag{111} \]

where \( X \) and \( X' \) are a pair of random numbers in the interval \((0, 1)\). If the point is below the curve, \( f_0 < f(r_0) \), then we take \( r' = r_0 \) as the new position of the electron. If \( f_0 > f(r_0) \), then the value is rejected and a new point in the rectangle is tried with a fresh pair of random numbers until a point below the curve is obtained.

This procedure cannot be directly applied because \( f(r) = 1/|v_r| \) becomes infinite at both ends of the interval. This difficulty is eliminated by the introduction of a new variable \( s \), defined by a relation \( r = r(s) \). The probability to sample a value in \( ds \) should be proportional to:

\[ \frac{1}{|v_r|} \frac{dr}{ds} = g(s) \tag{112} \]

On choosing

\[ r(s) = \frac{1}{2}(r_{\text{min}} + r_{\text{max}}) + \frac{1}{4}(r_{\text{max}} - r_{\text{min}})(3s - s^3), \tag{113} \]

\( r \) varies from \( r_{\text{min}} \) to \( r_{\text{max}} \) as \( s \) varies from \( s_{\text{min}} = -1 \) to \( s_{\text{max}} = 1 \). The probability function at the two extreme intervals is now finite, and takes the value for \( s \rightarrow -1 \)

\[ g(s) \rightarrow g(-1) = [3(r_{\text{max}} - r_{\text{min}})/(dQ/dr)_{r=r_{\text{min}}} ]^{1/2}, \tag{114} \]
and for $s \to +1$

$$g(s) \to g(+1) = [-3(r_{\text{max}} - r_{\text{min}})/(dQ/dr)_{r=r_{\text{max}}}]^{1/2}. \quad (115)$$

Here $dQ/dr$ is computed from Eq. (108).

Once the new position $r'$ is found, the new radial velocity $v_r = [Q(r')]^{1/2}$ and transverse velocity $v_t = L/r'$ are updated. This procedure is repeated for all the electrons in the plasma. The details of electron shuffling is similar to the Monte Carlo method used in the astrophysical community [22], for the planetary dynamics.

At the end of the above three mentioned steps, the energy of electrons is computed. If the electron energy is greater than the threshold energy $E_0$ (part of the King model discussed in Chapter 5), the electrons are allowed to escape. In the simulation, these electrons are removed from the next iteration. The above three steps are repeated for the next time step, and this procedure is repeated until the end of simulations.

### 6.2 Comparison with exact simulations

In Section 6.1, the Monte Carlo method for plasma simulations was explained in detail. In this section, we compare the results of the Monte Carlo method with an exact $N$–body molecular dynamics computation, as a check. The results were compared for a 10 ns simulation of a hydrogenic plasma system (ion mass = 1836 a.u.). The parameters used in the simulations is listed in Table (3). The parameter $E_0$ is the threshold cut-off parameter introduced in Chapter 5. Same set of parameters will be used throughout the chapter, unless mentioned otherwise. The exact computation was done using tree code at LANL, on a 100 processor cluster, and it took about an hour of computation time. The Monte Carlo method was done on a MacBook (laptop), in a matter of few seconds!

In Fig. (30), the Lagrange radius\(^1\) for the electron distribution from the Monte

---

\(^1\)Lagrange radius for a mass ratio $\mu$ is the (spherical) radius of the plasma within which $\mu$ fraction of the total mass is confined.
Figure 30: Comparison between the Monte Carlo method (dashed) and exact molecular dynamics (curve), for the electron Lagrange radius for different mass ratios, also denoted on the respective figures, a) 0.1, b) 0.3, c) 0.6, d) 0.9.
Table 3: Parameters used in the simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_i$</td>
<td>20000</td>
</tr>
<tr>
<td>$N_e$</td>
<td>12000</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>300</td>
</tr>
<tr>
<td>$T$</td>
<td>50</td>
</tr>
<tr>
<td>$T_i$</td>
<td>0.004</td>
</tr>
<tr>
<td>$E_0$</td>
<td>-0.1</td>
</tr>
</tbody>
</table>

Figure 31: The evolution of ion size $\sigma$, as a function of time for the Monte Carlo method (dashed) and the molecular dynamics method (curve).

The Monte Carlo method is compared with the exact computation as the plasma evolves over the 10 $ns$ time scale. The comparison shows that the agreement is satisfactory. The evolution of the average ionic distribution $<r_i^2>/3$ over the 10 $ns$ for the Monte Carlo method is compared with the Molecular Dynamics method in Fig. (31). Similarly, the evolution of the average electron distribution $<r_e^2>/3$ over time is shown in Fig. (32). The agreement between the exact and Monte Carlo method is satisfactory.

Finally in Fig. (33) the electron distribution function is compared for the Monte Carlo and molecular dynamics methods at the end of 9 $ns$. 

80
6.3 Long time scale dynamics

The long time scale dynamics of collisionless plasma is described by the Vlasov equations [30] for the phase-space density $f_\alpha(r_\alpha, v_\alpha)$ as

$$\frac{\partial f_\alpha}{\partial t} + v_\alpha \frac{\partial f_\alpha}{\partial r_\alpha} + m_\alpha^{-1} \frac{\partial f_\alpha}{\partial v_\alpha} q_\alpha \frac{\partial \phi(r_\alpha)}{\partial r_\alpha} = 0.$$  \hspace{1cm} (116)
Here, $\alpha = e, i$ for electrons and ions, respectively, $m_\alpha$ and $q_\alpha$ are the mass and charge of the species $\alpha$ and $\phi$ is the total mean field potential satisfying the Poisson equation,

$$\nabla^2 \phi = \frac{e}{\epsilon_0} (\rho_e - \rho_i), \quad (117)$$

with $\rho_\alpha = \int f_\alpha d\mathbf{v}_\alpha$. The general solution to the Vlasov equation, Eq. (116), doesn’t exist, however approximate solutions under certain assumptions and simplifications is possible. In ultracold plasmas, the initial shape of the plasma created in a magneto-optical-trap has a Gaussian phase space density

$$f_i \propto \exp \left( -\sum_k \frac{r_k^2}{2\sigma_k^2} \right) \exp \left( -\sum_k \frac{m_i(v_k - \gamma_k r_k)^2}{2k_B T_i} \right), \quad (118)$$

which under quasi-neutrality condition ($\rho_e(r) \approx \rho_i(r)$) can be solved. The summation in Eq. (118) runs over $k = x, y, z$; the rms-radius of the Gaussian spatial distribution $\sigma$, local expansion velocity parameter $\gamma$ and ionic temperature $T_i$ are time dependent. Under quasi-neutrality approximation, the mean-field potential can be expressed in terms of the ion density as

$$\frac{e}{\epsilon_0} \frac{\partial \phi}{\partial r} \approx k_B T_e \rho_e^{-1} \frac{\partial \rho_e}{\partial r} \approx k_B T_i \rho_i^{-1} \frac{\partial \rho_i}{\partial r}. \quad (119)$$

Plugging the Gaussian form of solution as given by Eq. (118) in the Vlasov equation (116) and solving yields

$$\sigma^2(t) = \sigma^2(0) \left( 1 + \frac{t^2}{\tau_{\text{exp}}^2} \right),$$

$$\gamma(t) = \frac{t/\tau_{\text{exp}}}{1 + t^2/\tau_{\text{exp}}^2},$$

$$T_i(t) = \frac{T_i(0)}{1 + t^2/\tau_{\text{exp}}^2},$$

$$T_e(t) = \frac{T_e(0)}{1 + t^2/\tau_{\text{exp}}^2}, \quad (120)$$

where the characteristic plasma expansion time is given by

$$\tau_{\text{exp}} = \sqrt{\frac{m_i \sigma(0)^2}{k_B[T_e(0) + T_i(0)]}}. \quad (121)$$
The plasma dynamics for higher electron temperatures behaves as a collisionless plasma, and we will validate our long timescale simulation by comparing with the solution to the Vlasov equation.

The characteristic plasma expansion time $\tau_{\text{exp}}$ given in Eq. (121) depends on the equilibrium electron temperature. But in the King model for the plasma, the electrons are only locally in thermal equilibrium, and the expression in the form of Eq. (121) per se is not meaningful. Hence, we fit our results to the characteristic plasma expansion time of the form

$$
\tau_{\text{exp}} = \xi \sqrt{\frac{\sigma^2 M_i}{T}},
$$

(122)

where $T$ is the temperature parameter in the King model, and $\xi$ is a fitting parameter that is determined empirically. To compare with the Vlasov results, the parameters in Eq. (120) should be evaluated from the simulations, which is done by calculating the following averages:

$$
\sigma^2(t) = \langle r_i^2 \rangle / 3
$$

$$
\gamma(t) = \langle \frac{v_{i,r}}{r} \rangle
$$
\( t_{\text{exp}} = 0.9 \, \text{s}^2 \)

\( M_{i} \langle v_{i,t}^2 \rangle \)

\( M_{e} \langle v_{e,t}^2 \rangle \)

\( \langle \rangle \)

Here, the subscript \( i \) and \( e \) stand for ion and electron respectively, and subscript \( r \) and \( t \) correspond to radial and transverse components respectively. The \( \langle \rangle \) denotes an average over the distribution.

In Figs. (34) and (35), the results from the simulation are compared with the Vlasov solution given in Eq. (120). The plot in Fig. (34) is compares time evolution of the plasma size \( \sigma^2 \) for the simulations and the plot in Fig. (35) compares the velocity expansion parameter in the simulation. The characteristic plasma expansion time in the simulations is fitted with a fitting parameter \( \xi = 0.9 \) in Eq. (122).

The ion and electron temperatures are shown in Figs. (36) where the temperatures of the ion and electron species from the simulations are compared with the Vlasov solutions. The ions are created from the atoms which were in thermal equilibrium, so the ion temperatures are uniform. On the other hand, in the King model, the electron only has a local thermal equilibrium, and hence reference to electron temperature only has meaning in an average sense as defined in Eq. (123). That explains the agreement.
Figure 36: The a)ion and b)electron temperature evolution as a function of time; Vlasov(curve), simulations(dots).

in Fig. 36(a) being better than in Fig. 36(b).

6.4 Technical limitations

The Monte Carlo method makes use of the mean potential to compute the orbital motion of the electrons and ions, but the computed mean potential is not completely smooth as it contains random fluctuations in the radial direction. These fluctuations are also time dependent as the potential is computed for every time-step. The accumulation of these fluctuations can cause spurious expansion of the plasma. To test

Figure 37: The Lagrange radii of the electrons for mass ratios from 0.1 to 0.9 in steps of 0.1, describing the plasma expansion
the extent of spurious expansion in our simulations, we switch off collisions, keep the ions fixed, and perform only the electron shuffling step. If the spurious expansion is minimal, then we expect the Lagrange radii of the electrons to be approximately a constant straight line. The result of this test is demonstrated in Fig. (38). Here we see that the Lagrange radii is almost constant for mass ratio $\mu < 0.7$, but the outer core starts to show a little drift. Increasing the number of ions and electrons in the plasma can help improve the statistics, and reduce spurious expansion. In contrast, Fig. (37) shows the Lagrange radii of the electrons with the ion expansion obtained from the same number of iterations as in Fig. (38). This shows that in our system, spurious expansion has only had a negligible effect to the overall plasma dynamics.

The second limitation that we have witnessed is that Monte Carlo method is not stable enough at high electron and ion densities, or when $N_i$ is approximately equal to $N_e$. In this case, once again the potential estimation is not smooth, as the electrons and ions alternate frequently, and the mean potential thus estimated is not smooth or slowly varying. This has been a drawback to the code, and has prevented us from witnessing the importance of recombination and Rydberg scattering.
6.5 Discussions

A Monte Carlo method for plasma dynamics is developed and implemented. The simulation is started from a King type distribution discussed in Chapter 5. For short timescales, results from the Monte Carlo method is compared with exact molecular dynamics simulation. A snapshot of the electron distribution over 9ns shown in Fig. 30, and the time evolution of ion rms-radius shown in Fig 31 agree well for the two approaches. Electron distribution shown in Fig. 33 after 9ns simulation for the two methods agree well within numerical errors.

For long timescales, the results from the simulation of King model is compared with Vlasov solution for a quasi-neutral plasma. The results from the simulation and the Vlasov equation for time evolution of: ion rms-radius in Fig. 34, velocity expansion parameter in Fig. 35, and electron and ion temperatures in Fig. (36), are in good agreement for a characteristic expansion time given in Eq. (122). This method is however unstable for electron densities $\approx 10^9\text{cm}^{-3}$, $N_i \approx N_e$ and $T < 30$. Effort is underway to fix this issue.
CHAPTER VII

SUMMARY AND CONCLUSION

This thesis is a theoretical study of collisional and radiative processes in Rydberg atoms at ultracold temperatures, and of the dynamics of ultracold plasmas. Chapters 2, 3 and 4 deal with the study of atomic processes involving Rydberg atoms. Chapter 5 introduces the King model for ultracold plasmas, and the dynamics of the King model is studied in Chapter 6.

In Chapter 2, a symmetrical form of Heisenberg correspondence is presented. This correspondence is used to address radiative cascade of Rydberg atoms and radiative recombination at cold temperatures. Results based on quantal-classical correspondence agree very well with quantal theory.

In Chapter 3, a Symplectic integrator for a system in a modified-Kepler systems, (i.e.) systems with a potential energy $V(r, t)$ and $1/r$ (Kepler) potential – is developed and implemented. The Symplectic integrator splits the Hamiltonian into an exactly solvable Kepler part, and a perturbation part. The energy error in Symplectic integrator remains bounded over time, and is suitable for long timescale atomic simulations. The Symplectic integrator is extended to handle time-dependent (perturbation) potentials. Examples from long timescale atomic simulations are discussed, where the Symplectic integrator performs much better than conventional integrators such as the implicit Runge-Kutta method.

In Chapter 4, the Symplectic integrator developed in Chapter 3 is used to study Stark mixing. Simulations from Stark mixing under the dipole approximation for the ion-Rydberg atom interaction, is shown to be in good agreement with previous theory. Stark mixing under the full ion-Rydberg atom interaction is discussed, and is seen to
be important at low impact parameters. Fractional population for Stark mixing of Na(28d) calculated from simulations is in good agreement with experimental results.

The King model for ultracold plasmas is introduced in Chapter 5. The King model for ultracold plasmas is a stationary, finite sized distribution for the electrons in a cloud of fixed ions with a Gaussian distribution. The King model is implemented, and the properties of the generated distribution are compared with theoretical prediction. As an extension, the King model with no space constraints is discussed.

In Chapter 6, a Monte Carlo based method for the simulating plasma dynamics is discussed and implemented. The results from the Monte Carlo method are compared with exact Molecular Dynamics for short timescales, and there is good agreement between the two methods. While the Molecular Dynamics takes about an hour of computation time on a 100 processor cluster, the Monte Carlo method reproduces the same results on a laptop in a matter of few seconds. Long time scale simulations from the Monte Carlo method are compared with the Vlasov method, and the overall agreement is good.

The form of quantal-classical correspondence presented in this thesis has shown very good agreement with the quantal results for radiative transition rates in Rydberg atoms, and cross-sections for radiative recombination. This has given us a transparent picture of the underlying quantal processes. The symplectic method developed in Chapter 3 is very robust for numerical simulations of collisional processes involving Rydberg atoms. This approach can now be used to simulate more complicated collisional processes. This we hope will enable one to understand the physics of the collision processes in an ultracold plasma better.

This thesis presents a simple yet computable model for the electrons trapped in the ultracold plasmas. This is the first model to describe the equilibrium state of electrons trapped in the ultracold plasma experiments. This model can be used as a starting point for simulation of the plasma system. A Monte-Carlo based method
for simulation of the ultracold plasma presented in Chapter 6 reproduces the plasma expansion in great detail. It is also extremely fast compared to a full molecular dynamics simulation. The method presented here also is transparent enough, and is amenable to test the importance of various collisional processes.

In conclusion, we have presented new theoretical treatments of the both the collisional processes and the overall dynamics relevant to the physics of ultracold Rydberg plasmas. The theory has been advanced to such a degree so as to render feasible future studies of various characteristics of Rydberg atomic processes such as, collision of Rydberg atoms in the presence of two competing influences like radiation and Stark mixing. The computational methods presented here are sufficiently sophisticated to describe the complicated plasma dynamics with reasonable computational resources.
APPENDIX A

KEPLER SOLVER

The Kepler solver takes two branches, depending whether the orbit is elliptic or hyperbolic. For negative energy, or when $0 \leq \epsilon \leq 1$, the equation to solve is

$$u - \epsilon \sin u - M = 0. \quad (124)$$

In the hyperbolic case, for positive energy, or for $1 \leq \epsilon \leq \infty$, Kepler’s equation has the form

$$\epsilon \sinh u - u - M = 0. \quad (125)$$

Equation (124) is solved as follows:

1. using the fact that Eq. (124) is invariant to $(M \rightarrow M + n\pi, \ u \rightarrow u + n\pi, \ \epsilon \rightarrow (-1)^n\epsilon)$ and $(M \rightarrow \pi - M, \ u \rightarrow \pi - u)$ transformations, the argument $M$ of the equation can be mapped to the $[0, \pi)$ interval. The equation needs to be solved only for $0 \leq \epsilon \leq 1$ and $0 \leq M \leq \pi$. The solution for arbitrary $M$ is obtained by adding $n\pi$.

2. for large eccentricity ($\epsilon \rightarrow 1$) and low $M$ the solution of Eq. (124) has an essential singularity. This can be seen by seeking a solution as power series in $M$. Equating the coefficients, order by order, one gets $u(\epsilon, M) = M/(1 - \epsilon) - M^4\epsilon/6(1 - \epsilon)^4 + \mathcal{O}(M^5)$. This series does not converge uniformly when $\epsilon \rightarrow 1$. On the other hand when $\epsilon = 1$ and the Taylor expansion of sin is used one gets

$$u(\epsilon = 1, M) = (6M)^{1/3} + \mathcal{O}(M).$$

A direct Newton-Raphson approach is started for the extreme cases when $\epsilon - 1 \approx M \approx 0$, using $(6M)^{1/3}$ as initial guess.

3. for the “regular” cases, a grid is set up for the $[0, \pi]$ interval with points $u_k = k\pi/n_g, \ k = 0, \ldots, n_g$ and a table of sine and cosine at the grid points is stored.
at the start of the program. From an initial grid index guess $u = M$, a Newton-Raphson iteration for indices is started using the following mapping: $k \rightarrow k' = k + \Xi[(M + \epsilon s_k - u_k)/(1 - \epsilon c_k)]$, where $\Xi$ is a function returning the integer truncation of a real number, and $s_k$ and $c_k$ are the sine and cosine values at the grid point $k$. At the end of this process the solution is localized between two grid points with an accuracy no greater than the grid spacing $\pi/n_g$. In this way, the process has both the quadratic convergence of Newton-Raphson’s method and the stability of bisection method.

4. A last fifth-order Newton-Raphson refinement is obtained using the grid point closest to the solution obtained at the previous step. However, instead of searching for a $u$ value which satisfies Eq. (124), it is more efficient to look for a solution in the unknown $\tan(u/2)$. This procedure delivers then directly the pair $(\sin u, \cos u)$ corresponding to the solution, and hence no trigonometric function need to be explicitly calculated during the procedure call! Assuming that the values of the function $f_0$ and of the first four derivatives $f_1, f_2, f_3$ and $f_4$ are known at the grid point, then the following corrections are obtained

\[
\delta_2 = \frac{f_0}{f_1}, \quad \delta_3 = \frac{f_0}{f_1 + \frac{\delta_2}{2} f_2}, \quad \delta_4 = \frac{f_0}{f_1 + \frac{\delta_2}{2} f_2 + \frac{\delta_3}{6} f_3}, \quad \delta_5 = \frac{f_0}{f_1 + \frac{\delta_2}{2} f_2 + \frac{\delta_3}{6} f_3 + \frac{\delta_4}{24} f_4},
\]

to give the approximate solution $\tan u/2 \approx \sqrt{(1 - c_k)/(1 + c_k)} + \delta_5$.

The accuracy of this procedure is expected to be of the order $(\pi/n_g)^5$. Indeed, in tests using $n_g = 1024$, the error in finding both $\sin u$ and $\cos u$ were $10^{-14} - 10^{-15}$ except for the range of $\epsilon \rightarrow 1$ and $M \rightarrow 0$ where the error is no greater than $10^{-12}$.

A similar approach is taken to solve Eq. (125). Although Kepler’s equation for positive energy is not manifestly periodic, a mapping to the standard interval is
obtained by observing that Eq. (125) can be written as $\epsilon_1 e^u - \epsilon_2 e^{-u} - u - M = 0$ and that the following set of transformations

$$u \rightarrow u + nD \quad M \rightarrow M + nD \quad \epsilon_{1,2} \rightarrow \epsilon_{1,2} e^{\pm nD}$$

leave this form invariant. In this way, the equation needs to be solved only in the standard interval $[0, D)$ where $D$ is arbitrary. For convenience, $D$ is chosen $D = 2.0$. This interval is gridded and the exponential $e_k = \exp u_k$ is calculated at each grid point $k$. The Newton-Raphson grid iteration

$$k \rightarrow k' = k + \Xi[(M + u_k - \epsilon_1 e_k - \epsilon_2 e^{-1}_k)/(\epsilon_1 e_k + \epsilon_2 e^{-1}_k - 1)]$$

ends by identifying the grid point closest to the solution. The solution for $e^u$ is obtained from this grid point after a fifth order Newton-Raphson refinement. This subroutine returns an approximation for the $(\sinh u, \cosh u)$. Precision levels similar to the elliptic case are obtained.

When tables of sine, cosine and exponential are build at the set up of the program, the drift stage can then be performed without evaluation of any transcendental function, which brings significant improvements to the efficiency of the integrator.
APPENDIX B

PLASMA UNITS

The plasma units are denoted with a subscript $p$. Following set of units are used in our simulation:

Length: $L_p = 10^{-6} m$

Mass: $M_p = M_e = \text{Electron Mass} = 9.1093897 \times 10^{-31} kg$

Energy: $E_p = k_B(1K) = \text{Energy at } 1K = 1.380658 \times 10^{-23} JK^{-1}$

Charge: $Q_p = q_e = \text{Electron Charge} = 1.60217733 \times 10^{-19} C$

From the above definitions, unit of time has the derived units:

Time: $T_p = \left( \frac{M_p L_p^2}{E_p} \right)^{1/2} = 2.568629095131044 \times 10^{-10} s$

Some constants in Plasma Units

Coulomb Constant: $\frac{1}{4\pi \epsilon_0} = 16.709982167195587 \frac{E_p L_p}{Q_p^2}$

1 Rydberg: $\mathcal{R} = 157886.54604 \ E_p$

Debye Length: $\lambda_D = \frac{\hbar}{\sqrt{2\pi m_e k_B T}} = \frac{0.0745382}{T_K^{1/2}} \ L_p$

$T_K$ is temperature measured in Kelvin.
REFERENCES


