

***Improvements to the Finite
Temperature Average-Atom
Model:
The RPA equations –
A progress report***

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Outline of talk

- Motivation and background to this work
- The average-atom model/equations
- The RPA equations
- Some preliminary results
- Conclusions

Motivation

- At low/intermediate densities it is possible to calculate, at some level of detail, the radiative properties which are needed to describe the atomic processes in a plasma (e.g. current LANL ATOMIC code)
- At high densities more approximate methods must be used. Plasma effects (e.g. pressure ionization) often dominate and must be taken into account in a consistent manner which must also treat the correlations between the bound and free electrons [Blenski, ApJ **127**, 239 (2000)]
- Recent and planned intense laser pulse experiments expect to reach these very high (approaching solid) densities
- Only viable way forward are average-atom type approaches

Background: Average-Atom approach

- The AA approximation is where the charge and excited-state distributions inside a plasma are replaced by a single fictitious ionic species which has the average charge of the ions in the plasma and the average population distribution of the ions among the various excited states
- Fundamental assumption that the plasma can be modeled by a finite temperature electron system in a central potential
- This central potential has contributions from the nucleus, the bound and free electrons, and from the other ions and electrons within the plasma

Background

- The work of Csanak and Kilcrease [JQSRT **58**, 537 (1997)] discussed the AA model and the fact that the orbitals calculated by a standard average atom (AA) approach cannot represent the “excited orbitals” of an atom in a plasma [this was also pointed out by F. Perrot]
- Basically because these “excited orbitals” are calculated in the incorrect potential (V^N , not the correct V^{N-n_j}), due to the non-removal of the self interaction term in the H-F equation for these orbitals
 - [For the ground state, the self interaction term is removed, as pointed out by H. Kelly, but not for the excited states]

Background

- This may not make a significant difference for thermodynamic quantities (such as EOS properties), but for spectral properties, such as photoabsorption, more accurate schemes are necessary
- A promising approach to computing the correct AA excited orbitals is the temperature-dependent Hartree-Fock approximation, or Random Phase Approximation (RPA)
 - This introduces important channel-coupling between excited states into the problem
 - This also removes the self-interaction term from the excited orbitals and so properly describes the “excited states” of an average atom.
- This can be considered a solution to the Latter-tail correction problem as discussed by, e.g. Salzmann et al in their work on photoexcitation and photoionization of hot dense Al plasmas
- In the $T=0$ limit this approach is identical to that pioneered by Amusia for photoionization

Background

- Subsequently, Csanak and Meneses [JQSRT **71**, 281 (2001)] developed these RPA equations and constructed them in a coupled integro-differential form
- They then solved these in the *single-channel approximation*.
- They used the AA orbitals and occupation numbers from the INFERNO code to compute oscillator strengths for a He plasma
- This includes the ion-ion correlations in a fairly crude way, where the ion density is presumed to be zero within the ion (AA) sphere, and constant outside it

Background

- Recently, Csanak and Daughton [JQSRT **83**, 83 (2004)] solved the same *single-channel* RPA equations for He and Li plasmas.
- In this case they used an AA model which included ion correlation, in which the ion density is computed from hypernetted chain (HNC) theory
- They compared oscillator strengths and transition energies with previous calculations of Rozsnyai, where fairly good agreement was found over a range of densities

Background

- In this work, we solve the RPA equations using an improved AA model based on the APATHY code of Bill Daughton. This incorporates a pseudo-atom approach which allows a clear definition of the internal energy of the system.
- We solve the RPA equations using a Linear Algebra (LA) technique pioneered by Lee Collins
- This allows us to solve the coupled-channel equations in a fairly straightforward manner
- Preliminary results are presented

Finite temperature RPA

- Will not derive the RPA equations here!
- Suffice to say for now that the derivation is based on the work of Csanak and Kilcrease using the AA orbitals.
- The RPA approach produces the appropriate potential for the excited electron of the “average-atom” and can incorporate channel-coupling effects

Average-atom eigen-functions

- The AA orbitals $[P_{\nu l}(r)]$ are eigenfunctions of the AA one-electron problem written in the form

$$H_{l_i}^{AA} P_{\nu_i l_i}(r) = \varepsilon_{\nu_i l_i} P_{\nu_i l_i}(r)$$

- where H^{AA} is the AA radial Hamiltonian with:

$$H_{l_i}^{AA} = -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l_i(l_i + 1)}{2r^2} - \frac{Z}{r} + V^{AA}(r)$$

- Z the nuclear charge
- $V^{AA}(r)$ includes the *electrostatic* plus *local exchange* potential of the AA model. It is temperature and density dependent and depends on the Fermi factor

$$n_i = \frac{1}{1 + e^{\beta(\varepsilon_i - \mu)}}$$

- $\varepsilon_{\nu l}$ is the eigen-energy of the AA orbital $P_{\nu l}(r)$

- In differential form the *coupled-channel* RPA equations look like:

$$\begin{aligned}
 & (H_{l_i}^{AA} - \varepsilon_{v_j} - \omega_n) P_{(v_j l_j) n l_i}^L(r_1) = \\
 & - n_{v_j l_j} \frac{\sqrt{(2l_i + 1)(2l_j + 1)}}{4\pi} \sum_{l'} \sqrt{(2l + 1)(2l' + 1)} \sum_{v'} \left\{ \right. \\
 & \beta_{l_i l_j}^L \int_0^\infty dr_4 V_L(r_1, r_4) P_{(v' l') n l}^L(r_4) P_{v' l'}(r_4) P_{v_j l_j}(r_1) \\
 & \left. - \sum_\lambda \alpha_{l_i l_j L}^\lambda \int_0^\infty dr_4 P_{v_j l_j}(r_4) V_\lambda(r_1, r_4) P_{(v' l') n l}^L(r_1) P_{v' l'}(r_4) \right\} \\
 & + \sum_{v_i} n_{v_i l_i} P_{v_i l_i}(r_1) \mathfrak{S}_{v_i l_i, v_j l_j}^{n l_i}
 \end{aligned}$$

Exchange term

Contribution to the electrostatic potential

Orthogonality term:
Given by

$$\begin{aligned}
 \mathfrak{S}_{v_i l_i, v_j l_j}^{n l_i} &= \beta_{l_i l_j}^L \int_0^\infty dr_3 \int_0^\infty dr_4 P_{v_i l_i}(r_3) P_{v_j l_j}(r_3) V_L(r_3, r_4) P_{(v' l') n l}^L(r_4) P_{v' l'}(r_4) \\
 &- \sum_\lambda \alpha_{l_i l_j L}^\lambda \int_0^\infty dr_3 \int_0^\infty dr_4 P_{v_i l_i}(r_3) P_{v_j l_j}(r_4) V_\lambda(r_3, r_4) P_{(v' l') n l}^L(r_3) P_{v' l'}(r_4)
 \end{aligned}$$

α and β are angular factors

Finite temperature RPA

- These RPA equations are the proper one-electron equations for the orbitals of an “excited electron” in the plasma
- ω_n is the transition energy of interest
- The 1st and 2nd terms on the RHS remove exactly the electrostatic and exchange pieces of the potential necessary to remove the self-interaction.
- The amount of charge removed is controlled by n_j ; the fractional occupation number of the AA orbital.
- The final orthogonality term controls the overlap between the true excited-states and the AA “excited states”. Again, its importance depends on the occupation number of these AA “excited-states”.
- Finally, $V_L(r_1, r_2)$ is the multipole component in the expansion of the Coulomb potential

Average-Atom approach: APATHY

- To solve the AA equations and to generate a self-consistent set of AA orbitals and potentials we use the *APATHY* code
- Developed by Bill Daughton and collaborators at LANL
- Solves non-relativistic Schrödinger equation for bound/continuum wavefunctions for electron density
- Sophisticated treatment of the ion-ion correlations using a “pseudo-atom” approach along with hypernetted-chain theory
- Has been compared in detail with SESAME database for Al and Si for a range of EOS quantities

Solution of the RPA equations

- Use the Linear Algebra (LA) method [eg: Collins & Schneider, PRA **24**, 2387 (1981)] to solve the RPA equations
- This has previously been used in many other scattering problems and has found to be a robust, reliable method
- Extension of the LA method to treat bound-state problems also made by Lee Collins
- Problem is recast into an integral equation and solved using numerical quadrature
- Equation is converted into integral form by using Green's functions
- Extension to a coupled-channel problem has been made and is currently being tested

Results

- Preliminary calculations so far
- Compare a He plasma at 10 eV at various densities with previous work of Csanak and Daughton, as well as older AA results of Rozsnyai
- Good agreement is found for the single-channel case using the LA method
- Found that inclusion of the orthogonality term makes little difference for these conditions

He plasma oscillator strengths – SCRPA calculations

T=10 eV, $\rho=1.5 \times 10^{19}/\text{cm}^3$

All quantities in atomic units

We compare with the previous
calculations of Csanak & Daughton

		w_{2p}	OS	w_{3p}	OS	w_{4p}	OS	w_{5p}	OS
C & D		1.58	2.70e-2	1.84	5.30e-3	1.94	1.93e-3	1.98	9.00e-4
LA code		1.58	2.70e-2	1.85	5.33e-3	1.94	1.93e-3	1.98	9.01e-4

T=10 eV, $\rho=1.5 \times$

$10^{20}/\text{cm}^3$

		w_{2p}	OS	w_{3p}	OS	w_{4p}	OS	w_{5p}	OS
C & D		1.51	0.109	1.75	2.13e-2	1.82	7.01e-3	1.85	2.57e-3
LA code		1.51	0.109	1.75	2.15e-2	1.82	7.08e-3	1.85	2.64e-3

He plasma oscillator strengths – SCRPA calculations

T=10 eV, $\rho=1.5 \times 10^{20}/\text{cm}^3$
All quantities in atomic units

Convergence of calculations with respect
to the number of points in the LA calculation

		w_{2p}	OS	w_{3p}	OS	w_{4p}	OS	w_{5p}	OS
LA code (60)		1.51	0.109	1.75	2.15e-2	1.82	7.08e-3	1.85	2.64e-3
LA code (80)		1.51	0.109	1.75	2.15e-2	1.82	7.08e-3	1.85	2.64e-3
LA code (90)		1.51	0.109	1.75	2.15e-2	1.82	7.08e-3	1.85	2.64e-3

He plasma oscillator strengths – SCRPA calculations

T=10 eV, $\rho=1.5 \times 10^{19}/\text{cm}^3$

Comparing OS divided by
initial occupation number

We compare our calculations with
previous AA calculations of Rozsnyai

		w_{2p}	OS	w_{3p}	OS	w_{4p}	OS	w_{5p}	OS
Rozsnyai		1.56	3.50e-1	1.83	7.49e-2	1.93	2.72e-2	1.97	1.20e-2
LA code		1.58	3.82e-1	1.85	7.54e-2	1.94	2.74e-2	1.98	1.28e-2

T=10 eV, $\rho=1.5 \times 10^{20}/\text{cm}^3$

		w_{2p}	OS	w_{3p}	OS	w_{4p}	OS	w_{5p}	OS
Rozsnyai		1.73	0.288	1.93	6.00e-2	1.99	2.14e-2	-	-
LA code		1.51	0.337	1.75	6.64e-2	1.82	2.18e-2	1.85	8.12e-3

He plasma oscillator strengths – SCRPA calculations

T=10 eV, $\rho=1.5 \times 10^{20}/\text{cm}^3$
All quantities in atomic units

Effect of including orthogonality term in RPA
equations

	w_{2p}	OS	w_{3p}	OS	w_{4p}	OS	w_{5p}	OS
LA code (no orthogonality)	1.51	0.109	1.75	2.15e-2	1.82	7.08e-3	1.85	2.64e-3
LA code (orthogonality to 3 orbitals)	1.51	0.109	1.75	2.16e-2	1.82	7.12e-3	1.85	2.65e-3

Orthogonality term has a small effect for this system

Conclusions & future directions

- Formulated an RPA approach to properly describe spectral properties of atoms in dense plasmas
- Used the APATHY code to solve the AA equations
- Used the Linear Algebra code to solve the RPA equations
- We are now in a position to solve the coupled-channel RPA equations and apply them to systems of interest

- In differential form the *single-channel* RPA equations look like:

$$\begin{aligned}
 & (H_{l_i}^{AA} - \varepsilon_{v_j} - \omega_n) P_{(v_j l_j) n l_i}^L(r_1) = \\
 & - n_{v_j l_j} \beta_{l_i l_j}^L \int_0^\infty dr_4 v_L(r_1, r_4) P_{(v_j l_j) n l_i}^L(r_4) P_{v_j l_j}(r_4) P_{v_j l_j}(r_1) \\
 & - n_{v_j l_j} \sum_{\lambda=\text{even}} \alpha_{l_i l_j L}^\lambda \int_0^\infty dr_4 [P_{v_j l_j}(r_4)]^2 v_\lambda(r_1, r_4) P_{(v_j l_j) n l_i}^L(r_1) \\
 & + \sum_{v_i} n_{v_i l_i} P_{v_i l_i}(r_1) \mathfrak{S}_{v_i l_i, v_j l_j}^{n l_i}
 \end{aligned}$$

Exchange term



Contribution to the electrostatic potential



Orthogonality term:
Given by



$$\begin{aligned}
 \mathfrak{S}_{v_i l_i, v_j l_j}^{n l_i} &= \beta_{l_i l_j}^L \int_0^\infty dr_3 \int_0^\infty dr_4 P_{v_i l_i}(r_3) P_{v_j l_j}(r_3) v_L(r_3, r_4) P_{(v_j l_j) n l_i}^L(r_4) P_{v_j l_j}(r_4) \\
 &- \sum_{\lambda=\text{even}} \alpha_{l_i l_j L}^\lambda \int_0^\infty dr_3 \int_0^\infty dr_4 P_{v_i l_i}(r_3) P_{v_j l_j}(r_4) v_\lambda(r_3, r_4) P_{(v_j l_j) n l_i}^L(r_3) P_{v_j l_j}(r_4)
 \end{aligned}$$

α and β are angular factors

APATHY: outline

- The AA approximation is where the charge and excited-state distributions inside a plasma are replaced by a single fictitious ionic species which has the average charge of the ions in the plasma and the average population distribution of the ions among the various excited states
- Fundamental assumption that the plasma can be modeled by a finite temperature electron system in a central potential
- This central potential has contributions from the nucleus, the bound and free electrons, and from the other ions and electrons within the plasma
- A local exchange potential is used which is a function of the electron density [we use a finite-temperature exchange-correlation potential of Perdew and Dharmawardana]

- Several different AA approaches have been used
- Standard approach is “ion cell” model:
 - Confine each ion to a cell
 - Each cell contains Z electrons and is neutral
 - One solves for a self-consistent potential (for the electrons):

$$\nabla^2 V(r) = 4\pi Ze\delta(r) - 4\pi en_e(r)$$

- More recent approach is ion correlation model
- Statistical distributions of both ions and electrons are computed around the test ion

$$\nabla^2 V(r) = 4\pi Ze\delta(r) - 4\pi e[Z^* n_i(r) - n_e(r)]$$

- Properly adding up the various energy terms is still ambiguous

APATHY: AA model

- Decompose plasma into N identical charge clouds
- One has a central “pseudo-atom” with a statistical distribution of other pseudo-atoms
- Energy of a single pseudo-atom is clearly defined, as is the interaction energy between the pseudo-atom and the rest of the plasma
- Allows the total internal energy of the system to be easily written
- Results in a self-consistent potential for system of the form

$$V(r) = V_{atom}(r) + n_i \int g(r') V_{atom}(r - r') dr' + V_{exc}(r)$$

APATHY: AA model

- In this equation V_{atom} is defined as

$$V_{atom}(r) = -\frac{Z}{r} + \int \frac{n_e(r')}{|r-r'|} dr'$$

- Where the bound and free electron densities are given as

$$n_{eb}(r) = \sum_{n,l} f(\varepsilon_{nl}, \mu) \frac{2(2l+1)}{4\pi} \frac{u_{nl}^2(r)}{r^2}$$

$$n_{ef}(r) = \int_0^\infty d\varepsilon f(\varepsilon_{nl}, \mu) \sum_{l=0}^\infty \frac{2(2l+1)}{4\pi} \frac{u_{el}^2(r)}{r^2}$$

- Where f is the usual Fermi factor and $u(r)$ are the radial atomic wavefunctions for a given state
- A local exchange potential is used which is a function of the electron density [we use a finite-temperature exchange-correlation potential of Perrot and Dharma-wardana]

APATHY: Ion-ion correlation

- Hypernetted Chain Theory (HNC) to compute ion density
- Non-perturbative method, well suited to modeling the long-range interactions
- Uses the Ornstein-Zernike relation to compute the pair correlation function $h(r)$:

$$h(r) = c(r) + n_{i_0} \int c(|r - r'|) h(r') d^3 r'$$

- The radial distribution function $g(r)$ is then simply given from the closure relation:

$$g(r) = 1 + h(r) = \exp[-\beta u(r) + h(r) - c(r) + B(r)]$$

- The ion density is then given as $n_i(r) = n_{i_0} g(r)$ with n_{i_0} the macroscopic ion density for a given canonical ensemble.