1 Atomic Resonances in Plasmas

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2 FINAL REPORT

The long-term goal of the project has been **the extension of the theory of atomic processes in plasmas** with emphasis on various resonance phenomena. This encompasses the inclusion of stochastic plasma fluctuations into atomic structure calculations as well as the extension of standard electron propagator techniques to multichannel propagator methods for resonant and direct scattering calculations. Conventional atomic structure programs require substantial modifications if they are to be linked with high temperature and/or high density plasma research. The development and testing of these modifications has been an important part of the research project which also has provided new insights into the theory of atomic processes in plasmas to be discussed below.

2.0.1 Screening of the Electron Interaction (Debye Model).

The studies of **electron correlation in the Debye model** have produced a number of unexpected and important results which would not have been feasible using a more sophisticated plasma model. This warrants to continue the studies of Debye screening. The Debye model is simple enough to evaluate screened electron correlation with the same accuracy as this is possible in standard atomic calculations. The results, however, are very different. Among the unexpected findings are the unusually **high degree of stability** of bound ionic systems, **noticeable line shifts** in dense plasmas and the **possibility of bound excited states of the negative hydrogen ion**. In particular, shifted emission lines have have recently been measured in dense plasmas (K. Eidmann, private communication. Such measurements in combination with a careful theoretical analysis constitute a **new tool for**

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plasma diagnostics. Now the relevance of electron correlation has been reckognized, it is no longer appropriate to neglect electron correlation in the diagnostic process.

The initial screening calculations have been augmented by including also the screening of the electron-electron interaction. A stabilizing effect of this extension has been expected, its magnitude, however, is a surprise. While more detailed studies are needed, it appears likely that the abundance of negative ions in certain astrophysical plasmas will find a natural explanation. Phenomena connected with positively charged ions in high density plasmas are also effected. Above all, the **very recently observed red shift of optical transitions of helium-like argon in dense plasmas** may not only qualitatively but also quantitatively reproduced. **The Debye model delivers very different predictions when the electron-electron interaction is screened as opposed to an unscreened interaction**. This has been established by very accurate calculations for helium-like ions. We expect to find the massive line shifts needed to reproduce the recent experimental data. **A new and powerful tool for plasma diagnostics in future research is developing.**

For plasma diagnostic purposes it is necessary to relate experimental quantities to relevant plasma parameters, such as particle density n and temperature T. Assuming local thermal equilibrium (LTE), this is done with a Saha-Boltzmann population analysis and has been reported for a hydrogen plasma. The radiation due to transitions between low-lying electronic states is an important tool in the diagnostic process. For this purpose the knowledge of accurate transition energies, oscillator strengths and line profiles is required. The previously reported variational calculations with highly accurate integral transform wave functions containing the interelectronic distance explicitly as a dynamical variable have been extended to total P and D states. A brief report has been published before, an explicit one is in preparation. Total S states of screened two-electron systems had been published previously. The higher angular momentum states of screened potentials exhibit shape resonances as a new feature. This is the topic of a finishing master's thesis (A. Solovyova).

The **possibility of electronically excited states of the negative hydrogen ion in particular plasma environments has been one of the most exciting findings**: A simplifying assumption of the Debye theory is spatial uniformity of the screening environment. In general, one encounters spatial fluctuations of the screening potential. In such an environment electron pairs, being two light particles, will preferentially move toward regions with stronger screening power since, by doing so, the overall energy of the system is lowered. Electron-ion pairs, on the other hand, being less mobile, cannot take as easily advantage of the local fluctuations as the light particles but, within the given limitations, will move toward regions of weaker screening thus lowering the energy of the system. To simulate the effects of such a disparity in the average screening, several scenarios have been assumed in which the repulsive e-e interaction has been screened more than the attractive e-ion force. Our results point toward the **possibility** of excited states without being conclusive. **Gradients of the density of the required magnitude can be found near solid surfaces.**

In order to study more-electron systems in plasmas **we have modified existing atomic and molecular computer codes to include the Debye interaction.** The difficulty with these attempts in the past used to be an expansion to replace the standard expansion of the Coulomb interaction for two-electron matrix elements. The analytic procedure to do this is quite straight forward. The analytic form of the coefficients, however, turned out complicated. Recently we developed a method to calculate screened two-electron integrals which sidesteps a modification of the von-Neumann expansion altogether. The further development of this method, together with representative computations is part of the master's thesis mentioned above. An earlier study which emphasizes the need for screened interactions in scattering was given by Weisheit.

2.0.2 Stochastic Time Fluctuations (Extended Debye Model).

In order to deal with time dependent features, it is usually preferable to use Green function techniques. In the present study, however, the time-dependent Schrődinger equation has been used, thus taking advantage of the high accuracy provided by the linear and non-linear variational techniques developed previously for the Coulomb potential. **Stochastic time fluctuations have been introduced by assuming a randomly fluctuating function** for the electron-ion and electron-electron potentials. The fluctuations are represented by a time dependent Debye parameter. These studies of a fluctuating hydrogen Debye-plasma reproduce experimentally observed line widths well and incorporate the so-called lowering of the continuum threshold at the same time. In that respect the model has some advantage over more conventional methods for microfields. Initially, the fluctuations had been introduced assuming no rapid changes of the electric fields. When this assumption was finally dropped, the line shapes started to resemble Voigt profiles as has been shown in Li Zhang's master's thesis.

A final remark justifying our extensive use of the Debye model may be in place: We are, of course, aware of the limitations of this approach and try to attach warning flags whenever the danger of overextending occurs. There is, however, no way to study the effect of the screened electron correlation as precisely with non-analytic interactions and potentials. In the end, one will have to represent "realistic" interactions as a superposition of Yukawa type functions. There is no reason to believe that the results will be very different from what the simple Debye model is capable to deliver. But this will have to be shown.

2.0.3 A Dynamic Approach to Atomic Processes in Plasmas.

It is appropriate to mention here also an extension of our work which has only begun last summer, since it is related to ongoing research on the multichannel propagator method as an intermediate step and has been assigned to a new Ph.D. student (Preston Jones).

The work with the static Debye potential has provided new insights into the spectroscopy of atomic systems in a screening environment (such as reduced binding energies, modified transition energies and strengths). It is not the final answer, though. The reason is simple: The Debye parameter is proportional to the square root of the plasma temperature. Hence, the Debye potential is temperature dependendent. **Temperature dependent theories have to be set up in the framework of quantum statistics.** The use of just Schrődinger's equation is not sufficiently general. Such a theory is aimed at here as a natural extension of our past research on Debye plasmas. A natural choice to accomplish this is the use of temperature-dependent Green functions. The strong effects of the plasma environment as a heat bath induce not only the well-known screening effects of the Debye model but lead also to statistical occupancies of excited electron orbitals. This again affects the strengths of optical transitions and thus the opacity of the plasma. As a first step, we have started to **implement a temperature-dependent version of the random phase approximation** (henceforth called TRPA) to evaluate spectroscopic atomic data when it is modified by the plasma. This work has been started last summer together with G. Csanak from Los Alamos National Laboratory who proposed the idea of using temperature dependent

Green functions in the first place. The theory has been outlined, the angular momentum analysis of the working equations has been completed, but no calculations have been completed so far. Although the collaboration with Dr. Csanak provides access to several computer codes used at LANL which we probably could not obtain otherwise, a sizeable amount of work needs to be done before the actual computing can begin.

2.0.4 Multichannel Propagator Method

The ramifications of the introduction of quantum statistics are wide and will carry over to the subsequent step of the project, the multichannel propagator theory, which has actually been a research project of ours for some time, restricted so far to the zero temperature situation. This approach will have to be reformulated, with the plasma environment included.

In Green function treatments of many-electron systems one solves effective one-particle equations as opposed to solving many-particle Schrődinger equations. The potentials to be employed in such computations, the so-called optical potentials, account for the correlation effects, in principle, accurately. Ordinarily, one transforms into energy space and then solves energy-dependent pseudo-eigenvalue equations. In hot and dense plasmas many of the atomic properties can no longer be assessed with conventional atomic structure calculations because some or all of the electronic states disintegrate into the continuum. **The concept of propagators provides a useful tool in situations like this because it is closer to scattering methods** than to stucture studies. In view of the particular considerations mandated by the temperature dependence the further extension of the multichannel propagator method to plasmas at finite values of T is planned, but only after the TRPA is fully implemented.

At the moment there is still analytical research required to generalize the multichannel propagator approach beyond the second order version which, in the past, we have successfully applied to compound states of a helium target plus projectile ($1s,ns^2$) each with several decay channels. The results for energies and widths compare well with other calculations and with experimental results.have not yet been fully implemented. We expect noticeable improvements once the non-linear optimizations needed in resonance calculations are in place. This work has suffered some delay when the student who worked on it left the program prematurely, as explained in a note at the end of this section. **The analytic work, on the other hand, has made**

substantial progress and will be reported in a lengthy publication which is being written up right now.

Note: This past research period was unusual in that the two PhD students who had been funded by the contract decided suddenly to accept industrial job offers and left the program with only an MS degree. Unfortunately, this left parts of the planned Ph.D. research unfinished or not even started. The problem here is unfinished work which is buried in two master's theses - not quite complete enough for publication yet interesting enough not to be abandoned altogether. Fortunately, after some delay, we could find sufficiently qualified new students to fill the vacancies in the project, pick up the unfinished work and, hopefully, incorporate it into their new Ph.D. research projects. DOE graciously agreed to a no-cost extension of the original two-year funding period.

The award supported recently two graduate students working on their dissertations (Alina Solovyova and Song-Tao Dai). Recently, a third PhD student, Preston Jones, joined the group. He has not yet been supported by the contract.