T-4
Atomic & Optical Theory

The Development and Implementation of the Time-Dependent Hartree-Fock Approximation for an Atom (Ion) in a Finite Temperature and Finite Density Plasma

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The time-dependent Hartree-Fock (TDHF) approximation was introduced in *Atomic and Molecular Physics* for the description of the linear response of atomic and molecular systems to an externally applied field, as well as of their excited states, both discrete and continuum.[1] As such, the method proved to be very successfull for obtaining good approximations for atomic polarizabilities and generalized oscillator strengths, as well as for photoionization cross sections. In the TDHF approximation, the wavefunction of the atomic (molecular) electrons is assumed to have a Slater determinant form in the presence of an external, time-dependent potential which is treated as fully coupled in. After obtaining the linear response function from this assumption, a model for the atomic (molecular) excited states emerges. The TDHF approximation description of excited states can be characterized in a coupled-channel formulation, with each channel defined by removing an electron from a given orbital occupied in the ground state. Thus, for the excited electron in each channel, a physically meaningful potential is created. In the case of *finite temperature systems*, the use of the wavefunction description is not convenient, and the more appropriate techniques of density matrices or propagators must be used. For the description of finite temperature inhomogeneous electron systems, the analogue of the Hartree-Fock approximation was introduced, which was called the average atom (AA) model.[2] The AA model was defined via a factorization of the two-electron density matrix or the two-electron propagator in terms of one-electron density matrices and propagators, respectively. This assumption constitutes the generalization of the Slater determinant form for finite temperature case. In the AA model, various orbitals are fractionally occupied according to the Fermi-Dirac distribution function, and a self-consistency is required between the potential and the one-electron orbitals that are the eigenfunctions of the one-electron Hamiltonian with the self-consistent potential.

The time-dependent Hartree-Fock (TDHF) approximation for *finite temperature inhomogeneous fermion systems* was discussed by de Cloizeaux[3] and Csanak and Kilcrease,[4] via the use of density matrix formalism and the temperature dependent propagator technique, respectively. The fundamental assumption is, here again, that the factorization of the two-electron density matrix and propagator is made in the fundamental equations which include an external potential as fully coupled in. This assumption leads to an equation for the linear response function and an interpretation of the "excited states" of the atom in the finite temperature plasma emerges.[4] The fundamental equations of the TDHF approximation in the finite temperature case also can be written in a coupled-channel form.[4] The advantage of the propagator technique is that the various terms can be interpreted physically via the help of Feynman-type diagrams,

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and it also lends itself easily to an extension to incorporate physically meaningful higher order terms, e.g., the plasma-screening of the interelectronic interaction and polarization effects. The purpose of the present work is the implementation of the TDHF approximation for atoms (ions) in finite temperature and finite density plasmas. We have performed angular momentum and spin analyses on the general equations. We obtained a coupled channel formulation of the problem where both energetic and angular-momentum channels are coupled. In the coupled channel formulation, it can be clearly seen that a channel-potential is obtained from the AA potential by subtracting from the AA potential the contribution associated with one of the fractionally occupied AA orbital for all AA orbitals with non-negligible occupation numbers. The channel-potentials and the coupling potentials depend on the temperature thus providing a pseudo-potential description of the atomic system in the plasma. (See figure.) We also obtained terms that are generalizations of the orthogonality constants that enter the zero temperature TDHF approximation.[1] As a first step, we introduced the

approximation scheme, which decouples both the angular momentum and the energy channels, and obtained solutions for these equations. We solve the coupled equations using a linear algebraic technique that has had considerable success in treating electron scattering from atoms and molecules.[5] The technique allows a natural progression in complexity from single to highly coupled multichannel cases.

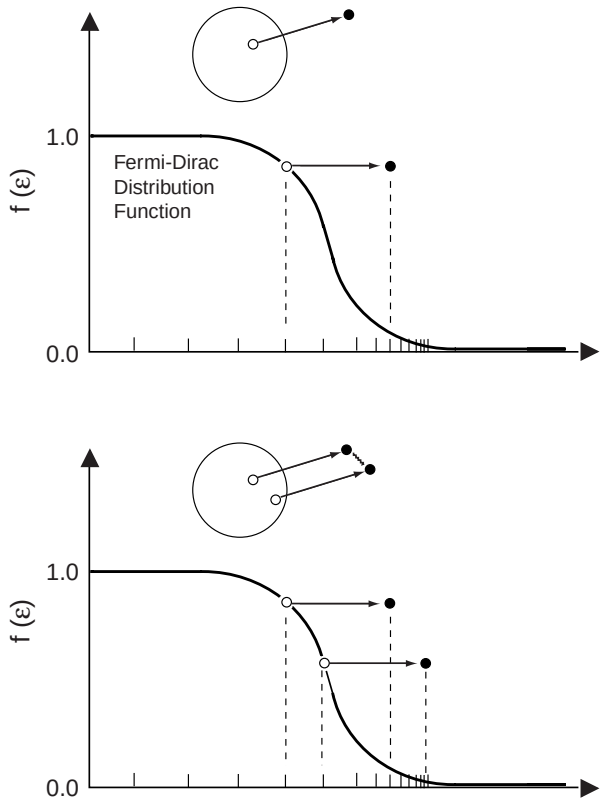

Figure: ***Upper panel****–by removing an electron from a fractionally-occupied orbital (○) in the AA model, a physically meaningful* ***channel-potential*** *is created for the excited electron (●).*
Lower panel*–two electrons "excited" from AA model orbitals interact (●〰●) via* ***coupling-potential*** *in the TDHF approximation.*

1. M. Ya. Amusia, *Atomic Photoeffect*, Plenum Press, New York (1990) and references therein.

2. R. M. More, *Adv. in At. Molec. Phys*. **21**, 305 (1985) and references therein.

3. J. de Cloizeaux, in *'Many-Body Physics,'* eds. C. de Witt and R. Balian, Gordon and Breach, New York (1968).

4. G. Csanak and D. P. Kilcrease, *JQSRT* **58**, 537 (1997).

5. L. A. Collins, B. I. Schneider, D. L. Lynch, and C. J. Noble, *Phys. Rev. A* **52**, 1310 (1995) and references therein.

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