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Efficient calculation of degenerate atomic rates by numerical quadrature on GPUs

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ABSTRACT

The rates of atomic processes in cold, dense plasma are governed strongly by effects of quantum degeneracy. The electrons follow Fermi–Dirac statistics and their high density limits the number of quantum states available for occupation after a collision. These factors preclude a direct solution to the usual rate coefficient integrals. We summarize the formulation of this problem and present a simple, but efficient method of evaluating collisional rate coefficients via direct numerical integration. Numerical quadrature has an intrinsically high level of parallelism, ideally suited for graphics processor units. GPUs are particularly suited to this problem because of the large number of integrals which must be carried out simultaneously for a given atomic model. A CUDA code to calculate the rates of significant atomic processes as part of a collisional-radiative model is presented and discussed. This approach may be readily extended to other applications where rapid and repeated evaluation of many integrals is required.

1. Introduction

Fermi–Dirac statistics have long been used to describe the distribution of electrons in metallically bonded solids, but plasmas of comparable electron densities have only recently become experimentally accessible. Recent advances in short wavelength lasers have allowed the creation of warm dense plasmas at solid or greater densities, due to their correspondingly high critical densities. These advances have spurred investigations into the effects of degeneracy on the atomic rates and hence on macroscopic plasma properties [1–3].

Fermi–Dirac statistics complicate the calculation of quantities in dense plasmas because many of the integrals in the calculations of basic plasma properties and atomic rates, which are discussed below, do not have closed-form solutions. Collisional-radiative models typically require >100 rates to be assembled into the rate matrix and may in turn be evaluated at a large number of spatial or temporal points in line with a hydrodynamic solver. We therefore require a large degree of parallelism to make this problem tractable. The Compute Unified Device Architecture is a programming tool to enable large scale parallel computation on Nvidia GPUs, which are emerging as a computational asset for physicists.

In Section 2 we review the Fermi–Dirac distribution and its use in the integrals for atomic rates in degenerate plasmas. In Section 3 we discuss quadrature on GPUs, which may be of general interest. In Section 4 we present the results of a simple collisional-radiative model of a degenerate plasma, which is greatly sped up by carrying out integrals on a GPU. Example code for generic 1- and 2-dimensional quadrature on GPUs, as well as the collisional-radiative model are available for download [4].

2. Definition of atomic rate coefficients

2.1. The Fermi–Dirac distribution and chemical potential

For a given electron kinetic energy ϵ, density n_e and temperature T_e, the Fermi probability of occupation is given by [5]

$$F(\epsilon, T_e) = \frac{1}{\exp\left(\frac{\epsilon-\mu}{T_e}\right) + 1}, \tag{1}$$

where $\mu(T_e, n_e)$ is the chemical potential. It is convenient to use the familiar units of electronvolts (1 eV $=$ q_e J, where q_e is the elementary charge) for energies; temperatures are implicitly multiplied by the Boltzmann constant, $k_B = 8.617$ eV K^{-1}. The energy distribution function is given by

$$f_{FD}(\epsilon, T_e) = \frac{G}{n_e}\sqrt{\epsilon}F(\epsilon, T_e) \tag{2}$$

with $G = 4\pi\left(2m_e/h^2\right)^{3/2}$ the degeneracy of a free electron. The chemical potential is defined so as to normalize this distribution, but it is computationally convenient to use a direct formula; for example, see the Padé approximation given here [6]. A collision

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in a degenerate plasma may only occur if there are sufficient unoccupied quantum states for all the resultant fermions and we take account of this by using Pauli blocking factors,

$$\tilde{F}(\epsilon, T_e) = 1 - F(\epsilon, T_e). \tag{3}$$

Finally, the Fermi–Dirac distribution has a corresponding heat capacity defined through

$$C_V(T_e, n_e) = \frac{G}{n_e}\int_0^\infty \frac{\epsilon^{3/2}}{1+\exp(\frac{\epsilon-\mu}{T})}d\epsilon. \tag{4}$$

The total electron kinetic energy density $\varepsilon = n_e C_V$ allows the electron temperature to be determined. We do this by inverting the heat capacity through a Padé approximation.

2.2. Definition of atomic rate coefficients

The rate coefficients of atomic or nuclear processes are typically given by an integral over the cross-section weighted by the distribution function, typically denoted $\langle\sigma v\rangle$. The usual approach to define such integrals is usually *ad hoc*; a more rigorous approach [7] is generalized for degenerate rates in Appendix A.

The total collisional excitation rate follows directly from the treatment in Appendix A, given by

$$J^\uparrow(E_j, T_e, \mu) = N_i G\sqrt{\frac{2}{m_e}}\int_{E_j}^\infty \Omega\left(\frac{\epsilon_0}{E_j}\right)F(\epsilon_0, T_e)\tilde{F}(\epsilon_0 - E_j, T_e)d\epsilon_0, \tag{5}$$

where E_j is the excitation energy and the collision strength is related to the total cross-section by $\Omega(\epsilon_0) = \sigma(\epsilon_0)/\epsilon_0$. We consider a collision strength typical of optically allowed transitions,

$$\Omega\left(\frac{\epsilon_0}{E_j}\right) = B_0 \ln\left(\frac{\epsilon_0}{E_j}\right) + \sum_{k=1}^{5} B_k\left(\frac{\epsilon_0}{E_j}\right)^{-(k-1)}. \tag{6}$$

The methods presented here can be extended to optically forbidden transitions straightforwardly.

The collisional ionization rate is given by

$$K^\uparrow = N_i G\sqrt{\frac{2}{m_e}}\int_{E_i}^\infty\int_0^{\epsilon_0-E_i}\epsilon_0\frac{d\sigma^\uparrow}{d\epsilon_1}F(\epsilon_0, T_e)\tilde{F}(\epsilon_1, T_e) \times \tilde{F}(\epsilon_0-\epsilon_1-E_i, T_e)d\epsilon_1 d\epsilon_0, \tag{7}$$

where E_i is the ionization potential and $\frac{d\sigma^\uparrow}{d\epsilon_1}$ is the differential cross-section. This differential cross-section gives the distribution of outgoing electrons and is necessary to account for both blocking factors in this case. The experimental uncertainty in differential cross-sections is typically much higher than that for the total collisional ionization cross-sections. We have proposed [3] a differential cross-section similar to that by Mott, modified to be consistent with the well-known BELI [8] formula,

$$\frac{d\sigma^\uparrow}{d\epsilon_1} = \frac{1}{2E_i\epsilon_0}\left[\frac{C_0E_i}{(\epsilon_1+a)(\epsilon_1+b)} + \frac{C_0E_i}{(\epsilon_0-\epsilon_1-E_i+a)(\epsilon_0-\epsilon_1-E_i+b)} + \sum_{k=1} kC_k\frac{\epsilon_1^{k-1}+(\epsilon_0-\epsilon_1-E_i)^{k-1}}{\epsilon_0^k}\right], \tag{8}$$

with the quantities

$$a = \frac{1}{2}\left(\sqrt{\epsilon_0^2+4E_i^2}-\epsilon_0\right)$$
$$b = a + E_i.$$

In the calculations below, we consider for simplicity that the outer electrons are ionized preferentially, as the effect of Pauli blocking is severe for inner-shell electrons.

These atomic rates may be related to their inverse through simple algebraic formulas, which can be derived using the approach in Appendix A together with appropriate micro-reversibility relations [7], noting in particular that $\tilde{F}(\epsilon, T_e) = \exp((\epsilon-\mu)/T_e)F(\epsilon, T_e)$. In particular, we have for the rate of collisional deexcitation

$$J^\downarrow = \frac{g_j}{g_{j'}}\exp(E_j/T_e)J^\uparrow, \tag{9}$$

where the g factors correspond to the degeneracies of the upper and lower level respectively. For three body recombination, we have

$$K^\downarrow = \frac{g_i}{g_{i+1}}\exp(\mu/T_e)\exp\left(\frac{E_i}{T_e}\right)K^\uparrow. \tag{10}$$

The total rate of photoionization, for radiation with a photon of energy ϵ_γ and spectral intensity $I(\epsilon_\gamma)$, is given by

$$L^\uparrow = N_i\int_{E_i}^\infty \sigma_\gamma(\epsilon_\gamma)I(\epsilon_\gamma)\tilde{F}(\epsilon_\gamma - E_i, T_e)d\epsilon_\gamma. \tag{11}$$

The photoionization cross-section typically falls off above threshold as some negative power of the photon energy; for example, the cross-section for hydrogen-like ions scales as $\sigma(\epsilon_\gamma)\propto\epsilon_\gamma^{-3}Z^{-2}$. We parameterize the photoionization cross-section above threshold by

$$\sigma_\gamma = D_0\left(\frac{\epsilon_\gamma}{E_i}\right)^{-2} + D_1\left(\frac{\epsilon_\gamma}{E_i}\right)^{-3}. \tag{12}$$

Aside from including the Fermi–Dirac energy distribution, the effects of degeneracy do not alter the rate of radiative recombination from its classical form, because the outgoing photons are bosons and not subject to Pauli blocking. Furthermore, radiative recombination is likely to be insignificant compared to photoionization for the large radiation fluxes in high energy density physics experiments.

Radiative processes have an effect not only on the ionization of the plasma, but also the temperature. Photoionization also heats the plasma, because the remainder of the photon energy is carried away mostly by the ionized electron. The corresponding rate of change in the electron kinetic energy is

$$\left(\frac{d\varepsilon}{dt}\right)_L = N_i\int_{E_i}^\infty(\epsilon_\gamma - E_i)\sigma_\gamma(\epsilon_\gamma)I(\epsilon_\gamma)\tilde{F}(\epsilon_\gamma - E_i, T_e)d\epsilon_\gamma. \tag{13}$$

Photons are captured by free electrons in the presence of ions by inverse bremsstrahlung, with a corresponding rate of change of kinetic energy

$$\left(\frac{d\varepsilon}{dt}\right)_{\mathrm{IB}} = \int_{\epsilon_c}^\infty\int_0^\infty \kappa_{IB}(\epsilon_\gamma)I(\epsilon_\gamma)F(\epsilon_0, T_e) \times \tilde{F}(\epsilon_\gamma+\epsilon_0, T_e)d\epsilon_0 d\epsilon_\gamma, \tag{14}$$

where the inverse bremsstrahlung absorption coefficient is given by

$$\kappa_{IB} = \frac{1}{6\sqrt{6}\pi^{5/2}}\frac{e^6(hc)^2}{\varepsilon_0^3(m_ec^2)^{3/2}}\epsilon_\gamma^{-3}\left[1-\exp\left(-\frac{\epsilon_\gamma}{T_e}\right)\right]\sum_{i=1}^{Z} i^2 N_{i,j}. \tag{15}$$

Radiation with frequencies below the resonant electron frequency is reflected and we therefore take the corresponding critical photon energy $\epsilon_c = \hbar c \times \sqrt{n_e e^2/m_e c^2\varepsilon_0}$ as the lower limit for the inverse bremsstrahlung integral. The integral over the electron energy ϵ_0 can be carried out analytically, leaving the integral over the photon energy to be done numerically.