An explicit numerical scheme for Milne's phase-amplitude equations

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Models used in atomic physics of plasma should in principle account for continuum electrons in the atomic structure. This can lead to rather intensive computation and memory storage, because accounting for the continuum requires sampling of the radial wavefunctions in both the radius and momentum spaces (see, for instance, [1, 2, 3]).

Alternative formalisms for the one-electron basis may bring a more efficient numerical representation of the continuum. For instance, an average-atom numerical algorithm resorting to the basis of Siegert states was recently proposed and studied [4], using the method of solution of [5].

Milne's phase-amplitude (MPA) representation [6] is based on a slowly varying amplitude function. It has a direct link with the Wentzel-Kramers-Brillouin approximation. It also has a strong numerical interest, for it resorts to slowly varying, nonperiodic functions, and thus allows one to circumvent the Shannon sampling limit. This interest has long been recognized in the literature, and MPA representation was used for Bessel functions calculations [7] and atomic-physics computations [8, 9].

In this poster, we first discuss the limitations of some known methods for solving the MPA equations [8, 9]. We then propose a new explicit method of solution, which addresses these limitations. Such a method may prove itself useful in dense-plasma modeling and in the calculation of atomic-processes cross-sections. Examples of such applications are given.

References

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