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The use of B-splines for calculating the electronic properties of atoms in plasmas

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Abstract

Standard quantum-mechanical calculations are currently used in the framework of atomic physics for plasma applications. Recently, atomic physicists working on computational techniques have come to use B-spline bases. The aim of this paper is to show how B-splines basis sets are also well adapted for the representation of bound as well as continuum electronic wavefunctions of atoms in plasmas. Some implementation details and the advantages of this approach are discussed for two typical applications, namely, the LTE confined average atom (AA) and the AA immersed in a jellium. Details concerning opacity calculations using B-splines are also given.

Keywords: Atomic physics; Numerical methods; Radiative opacity

1. Introduction

The calculation of electronic properties of atoms for arbitrary matter density and temperature is required for the calculation of radiative opacity and equations of state, not to mention the more complex treatment of non-LTE plasmas. A cornerstone of the (non-relativistic) calculations is the solution of the Schrödinger equation for arbitrary radial potential and for different boundary conditions, which includes both bound and free orbital calculations. For this the traditional approaches invoke finite-difference methods such as the Numerov scheme [1].

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The aim of this paper is to explore an alternative approach which belongs to the class of *spectral* methods where the functions of the radial variable r are expanded on a basis set. In the context of atomic and molecular physics, B-spline basis sets have recently become quite popular (see Refs. [2,3] for a broad review). The reason for this success is derived from the capability of B-spline functions to be specifically designed to suit a particular problem, which gives B-splines an advantage over other functions like Gaussian, Slater-type orbital and Sturmian. We shall show how this method can be used and implemented in the context of plasma applications. Three related topics will be used to illustrate this approach: the computation of electronic levels inside an ion cell, the determination of the displaced electron density when a positive charge is introduced into jellium and the calculation of radiative opacities.

2. A quick survey of B-spline functions

A mathematical definition of B-spline functions does not give an immediate feeling of the utility of these functions. However, for completeness we include a simple introduction to B-splines with the problem of interpolating a set of data. Consider for instance a few points as in Fig. 1 and suppose we want to interpolate between these points. The simplest way of doing this consists in drawing straight lines between the data and then build an interpolating function f as a *piecewise straight line function*. More precisely, between two data points i and $i+1$, the polynomial of order 2 (and degree 1), $f(t) = at + b$, can be written as $f(t) = ((t_{i+1} - t)/(t_{i+1} - t_i))f_i + ((t - t_i)/(t_{i+1} - t_i))f_{i+1}$. This gives rise to the idea of introducing a set of functions H_i such that

$$
\begin{aligned}
H_i(t) &= \frac{t_{i+1} - t}{t_{i+1} - t_i} \quad \text{for } t_i \leqslant t < t_{i+1}, \\
&= \frac{t - t_{i-1}}{t_i - t_{i-1}} \quad \text{for } t_{i-1} \leqslant t \leqslant t_i, \\
&= 0 \quad \text{otherwise.}
\end{aligned}
$$

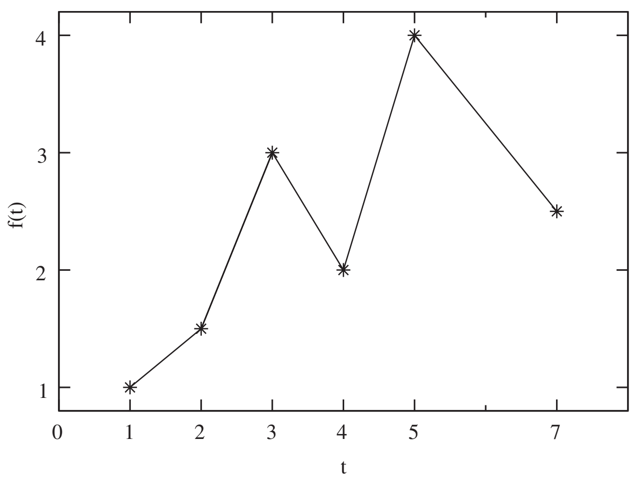

Fig. 1. A set of data interpolated by straight lines.