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An Improved Integration Scheme for Mode-Coupling-Theory Equations

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Abstract. Within the mode-coupling theory (MCT) of the glass transition, we reconsider the numerical schemes to evaluate the MCT functional. Here we propose nonuniform discretizations of the wave number, in contrast to the standard equidistant grid, in order to decrease the number of grid points without losing accuracy. We discuss in detail how the integration scheme on the new grids has to be modified from standard Riemann integration. We benchmark our approach by solving the MCT equations numerically for mono-disperse hard disks and hard spheres and by computing the critical packing fraction and the nonergodicity parameters. Our results show that significant improvements in performance can be obtained employing a nonuniform grid.

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1 Introduction

When a liquid is cooled or compressed towards structural arrest, its particles experience a slowing down of transport because they remain "captured" in transient "cages" formed by neighboring particles. This phenomenon is known as the "cage effect" and is the underlying microscopic picture behind the glass transition [1]. The approach to structural arrest is connected with the appearance of several fascinating dynamical processes that manifest themselves in the low-frequency spectra or in the long-time behavior of time-correlation functions of the system [1]. Among these features, in particular, we recall the stretching of the response functions over time intervals extending over several orders of magnitude, a two-step relaxation process of the density-correlation function,

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and the aforementioned drastic slowing down of transport coefficients such as viscosity or diffusion. All of these features have been observed both in experiments [2–12] and molecular-dynamics simulations [13–21].

In parallel to experiments and simulations, various theoretical frameworks provided different interpretations of the glass transition [22]. Among them, the mode-coupling theory (MCT) of the glass transition was originally developed to account for the cage effect in simple fluids by calculating explicitly the dynamics of density fluctuations. The theory is based on closed nonlinear integro-differential equations for a set of correlation functions where the coupling coefficients are determined by the equilibrium structural properties only. In particular, the dependence on system parameters such as temperature and density is smooth and no assumptions on anomalous exponents, transitions or slow relaxations are built into the starting equations of the theory. The success of MCT derives from the many detailed predictions of striking features associated with the structural arrest [1,23–30].

For numerical solutions of MCT equations, one has to discretize the wave-number dependence of the interesting functions such as the intermediate scattering functions and the structure factors. Usually, this is done by taking a uniform grid of wave numbers. The limiting factor in solving MCT equations is the evaluation of the MCT kernels (one for each wave number of the grid) which appear in the equations of motion of the correlation functions. This evaluation has a computational cost that in principle scales as the third power of the grid size.

Nowadays, with modern CPUs, MCT equations for simple fluids in bulk can be solved in relatively short times. However, some recent extensions of MCT require the introduction of matrix-valued correlation functions. The consequence is that the computational effort required to solve the relative MCT dynamics becomes by orders of magnitude more demanding and, even more crucial, that the limits of computer allocation memory are easily exhausted. This is the case, for example, of a generalization of MCT to multi-component fluids obtained through equations of motion that have to couple the different particle species [31–34]. As a matter of fact, numerical solutions of multi-component MCT are up-to-date limited to 5 different species at most in the three-dimensional case [35] and, due to the fact that the structure of the MCT equations is more complex, to 2 species only in the two-dimensional case [36–38]. Other examples, in which tensorial correlation functions appear, are advanced extensions of MCT apt to study the glassy behavior of molecular liquids [39–46], or active Brownian particles [47], or probe particles driven by a constant force through a colloidal glass [48]. Finally, matrix-valued correlation functions also appear in an extension of MCT describing simple fluids in confinement by introducing symmetry-adapted fluctuating density modes mirroring the broken translational symmetry [49–55]. Intuitively, in the latter case the structure of MCT equations is more similar to the two-dimensional case than to the three-dimensional one and only recently a numerical solution for the full-time dependence of MCT equations in a confined system has been presented [56].

In this paper we show that a uniform grid for the wave numbers may not be the most