

1. Record Nr.	UNINA9910457244703321
Autore	Snook Ian
Titolo	The Langevin and generalised Langevin approach to the dynamics of atomic, polymeric and colloidal systems [[electronic resource] /] / Ian Snook
Pubbl/distr/stampa	Boston, : Elsevier, 2006
ISBN	1-280-74716-1 9786610747160 0-08-046792-X
Descrizione fisica	1 online resource (321 p.)
Disciplina	530.14/4
Soggetti	Langevin equations Brownian movements Random dynamical systems Physics Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Cover; The Langevin and Generalised Langevin Approach to the Dynamics of Atomic, Polymeric and Colloidal Systems; Copyright page; Contents; Preface; Notation; A. Potential Energy Functions; B. Symbols Used; C. Operations; Chapter 1. Background, Mechanics and Statistical Mechanics; 1.1 Background; 1.2 The Mechanical Description of a System of Particles; 1.3 Summary; 1.4. Conclusions; References; Chapter 2. The Equation of Motion for a Typical Particle at Equilibrium: The Mori-Zwanzig Approach; 2.1 The Projection Operator; 2.2 The Generalised Langevin Equation 2.3 The Generalised Langevin Equation in Terms of the Velocity 2.4 Equation of Motion for the Velocity Autocorrelation Function; 2.5 The Langevin Equation Derived from the Mori Approach: The Brownian Limit; 2.6 Generalisation to any Set of Dynamical Variables; 2.7 Memory Functions Derivation of Expressions for Linear Transport Coefficients; 2.8 Correlation Function Expression for the Coefficient of Newtonian Viscosity; 2.9 Summary; 2.10 Conclusions; References; Chapter 3.

Approximate Methods to Calculate Correlation Functions and Mori-Zwanzig Memory Functions; 3.1 Taylor Series Expansion
3.2 Spectra 3.3 Mori's Continued Fraction Method; 3.4 Use of Information Theory; 3.5 Perturbation Theories; 3.6 Mode Coupling Theory; 3.7 Macroscopic Hydrodynamic Theory; 3.8 Memory Functions Calculated by the Molecular-Dynamics Method; 3.9 Conclusions; References; Chapter 4. The Generalised Langevin Equation in Non-Equilibrium; 4.1 Derivation of Generalised Langevin Equation in Non-Equilibrium; 4.2 Langevin Equation for a Single Brownian Particle in a Shearing Fluid; 4.3 Conclusions; References; Chapter 5. The Langevin Equation and the Brownian Limit
5.1 A Dilute Suspension - One Large Particle in a Background 5.2 Many-Body Langevin Equation; 5.3 Generalisation to Non-Equilibrium; 5.4 The Fokker-Planck Equation and the Diffusive Limit; 5.5 Approach to the Brownian Limit and Limitations; 5.6 Summary; 5.7 Conclusions; References; Chapter 6. Langevin and Generalised Langevin Dynamics; 6.1 Extensions of the GLE to Collections of Particles; 6.2 Numerical Solution of the Langevin Equation; 6.3 Higher-Order BD Schemes for the Langevin Equation; 6.4 Generalised Langevin Equation; 6.5 Systems in an External Field
6.6 Boundary Conditions in Simulations 6.7 Conclusions; References; Chapter 7. Brownian Dynamics; 7.1 Fundamentals; 7.2 Calculation of Hydrodynamic Interactions; 7.3 Alternative Approaches to Treat Hydrodynamic Interactions; 7.4 Brownian Dynamics Algorithms; 7.5 Brownian Dynamics in a Shear Field; 7.6 Limitations of the BD Method; 7.7 Alternatives to BD Simulations; 7.8 Conclusions; References; Chapter 8. Polymer Dynamics; 8.1 Toxvaerd Approach; 8.2 Direct Use of Brownian Dynamics; 8.3 Rigid Systems; 8.4 Conclusions; References Chapter 9. Theories Based on Distribution Functions, Master Equations and Stochastic Equations

Sommario/riassunto

The Langevin and Generalised Langevin Approach To The Dynamics Of Atomic, Polymeric And Colloidal Systems is concerned with the description of aspects of the theory and use of so-called random processes to describe the properties of atomic, polymeric and colloidal systems in terms of the dynamics of the particles in the system. It provides derivations of the basic equations, the development of numerical schemes to solve them on computers and gives illustrations of application to typical systems. Extensive appendices are given to enable the reader to carry out computations to illustrate
