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A Resource Letter CSSMD-1
Computer Sirnulation Studies by the Method of Molecular Dynamics

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In this letter we present a comprehensive bibliography on computer simulation studies by the method of Molecular Dynamics. The bibliography includes references to relevant literature published up to mid 1973, starting from the first paper of Alder and Wainwright, published in 1957. The procedure of the method of Molecular Dynamics, the main fields of study in which it has been used, its limitations and how these have been overcome in some cases are also discussed. We hope this resource letter would be of help to research workers, particularly to students and others who might wish to start computer simulation studies by using the Molecular Dynamics method.

Apresentamos, neste trabalho, extensa bibliografia sobre estudos de simulação em computador pelo método da Dinâmica Molecular. A bibliografia inclue referências a literatura relevante publicada até meados de 1973, começando pelo primeiro trabalho de Adler e Wainwright, publicado em 1957. O desenvolvimento do método da Dinâmica Molecular, os principais campos de trabalho em que tem sido empregado, as suas limitações e como têm elas sido superadas, são aqui discutidos. Esperamos que este trabalho seja de valia aos pesquisadores e, particularmente, aos estudantes e outros que pretendam trabalhar em estudos de simulação em computador, empregando o método da Dinâmica Molecular.

The Molecular Dynamics Method

The first paper on the Molecular Dynamics method was written by Alder and Wainwright'. The method was designed to study molecular dynamic motion (hence the name Molecular Dynamics (MD)) by solving exactly the simultaneous classical equations of motion of severa1 hundred particles by means of fast electronic computers. The method has been used to study non-equilibrium as well as equilibrium properties of a system. It may be mentioned that the Monte Carlo method of computer simulation studies provides information only on equilibrium properties.

The MD method owes its origin to the advent of electronic computers which could be used to study the many-body which cannot be solved

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analytically. To follow in detail the motion of a limited number of molecules, one must equate the instantaneous force on a molecule, due to all the others located at known positions, to its mass times its acceleration, and then solve all the simultaneous equations so obtained to find the trajectories of the molecules. However, it is a formidable task to obtain an analytic solution even for a three body system. Since all real physical systems are many body systems consisting of a very large number of particles, one has to study the mutual interactions of a large number of molecules, in order to obtain information on the thermodynamic. transport and structural behaviour of the system. An exception might be extremely rarified gases which could, perhapas, be treated as ideal gases whose molecules may be regarded as non-interacting with one another. It is in this context that the relevanc. and utility of the MD method should be evaluated. Given a law of intermolecular force, it is possible to trace out, with the aid of a computer, the molecular trajectories for a limited number of molecules and thus by-pass the insurmountable difficulties of finding an analytical solution.

The main features of MD computer simulation studies (or 'experiments') are:

(a) The systems are finite, the numbers of particles (N) usually being ≤ 1000;

fb) The interaction potential is assumed to be known and treated pairwise additive, i.e.

$$\phi(1,\ldots,N) = \sum_{i>j=1}^{N} \phi(r_{ij}); \tag{1}$$

(c) The range r, of the pair potential $\phi(r)$ is assumed to be finite. i.e., $r > r_c$, $\phi(r) = 0$;

(d) The classical equations of motion,

$$m\boldsymbol{a}_i = m\,\frac{d\boldsymbol{V}_i}{dt} = -\sum_{\substack{j=1 \\ i\neq j}}^{N} \frac{\partial}{\partial \boldsymbol{r}_i}\,\phi(r_{ij}), \tag{2}$$

with

$$\mathbf{V}_i = \frac{d\mathbf{r}_i}{dt}, \tag{3}$$

are solved by finite difference techniques with time steps Δt between 10^{-14} and 10^{-15} secs. This means that knowing the force on the i'" molecule

at a given instant of time. the new position of this molecule after a time increment At is computed. Severa1 different algorithms have been used. The simplest which is in common use is

$$\mathbf{r}_i(t + \mathrm{At}) = -\mathbf{r}_i(t - \mathrm{At}) + 2\mathbf{r}_i(t) + a_i(t)\mathrm{At}^2. \quad (4)$$

The method in which the force summation on the right hand side of equation (2) is evaluated directly – requiring (N – 1) additions – will be called the original MD method, since a new method has recently been proposed (Ref. 388) which avoids this summation for the long range forces.

(e) From the new positions and velocities of molecules, the potential acceleration and force experienced by each molecule, in the new configuration, are again found and the entire process repeated, timestep by timestep, to study the evolution of the system in time as well as space;

(f) The positions, velocities, accelerations and other relevant informations are stored on tapes for subsequent analysis of the results.

The Main Fields of Study

The literature on MD computer simulation studies, already very large, is increasing rapidly and the trend is bound to continue in view of the availability of bigger and faster computers and techniques to overcome the limitations (to be discussed later) from which the MD method suffers. Some of the major fields of studies investigated by this method are*:

(I) Structural and thermodynamic properties of mostly simple monatomic liquids which obey the Lennard-Jones (LJ) potential

$$\phi(r_{ij}) = \varepsilon\left[(\sigma/r_{ij})^{12} - (\sigma/r_{ij})^{6}\right], \quad (5)$$

where o has dimensions of distance and c those of energy (Refs. 36, 88, 121, 123, 159, 193, 197, 198, 202, 207, 238, 239, 243, 246, 249, 253, 254, 259, 262, 301, 303 and 364).

(II) Diatomic liquids (Refs. 120, 368), ionic liquids (Refs. 245, 256, 305, 325), liquid metals (Refs. 67, 127, 165, 369), and water (Refs. 242, 309, 310, 353 – 361).

(III) Velocity autocorrelation function, diffusion coefficients and liquid structures (Refs. 36, 37, 93, 176, 195, 205, 249, 259, 261, 301, 302, 303, 370).

*Some references included in the bibliography are given here for each field of study.

(IV) Time correlation functions (Refs. 199, 204, 221, 265).

(V) Free-path distributions (Refs. 51, 122).

(VI) Binary mixtures (Refs. 34, 210, 240 253, 254, 291).

(VII) Studies of gases (Refs. 130, 247, 304, 320, 363).

(VIII) Liquid-solid phase transition (Refs. 161, 299, 312, 318).

(IX) Solid-liquid phase transition (Refs. 95, 129, 206, 237, 241, 251, 298, 317, 367, 372, 390).

(X) Surface properties of crystals (Ref. 164); lattice dynamics of solids (Ref. 167).

(XI) Radiation damage in crystals (Refs. 12, 30, 371).

(XII) Point defects and vacancy motion (Refs. 153, 196, 200, 263, 300).

(XIII) Solids under shockwave compression (Refs. 78, 319, 365).

(XIV) Neutron scattering (Ref. 6, 68); X-ray scattering (Ref. 124).

(XV) Properties and phase transitions of elastic spheres (Refs. 1, 5, 11, 34, 35, 51, 128, 163, 195, 236, 260, 263, 264, 266), discs (Refs. 19, 26, 90, 128), squares (Refs. 308, 311, 314, 373).

(XVI) Ground-state properties of quantum systems (Ref. 94).

(XVII) Magnetic systems (Ref. 188).

(XVIII) Electric dipoles (Refs. 91, 113, 160, 244).

(XIX) Time behaviour of harmonic and anharmonic oscillators (Refs. 189, 190).

(XX) Liquid structure and light scattering (Refs. 198, 366, 374).

(XXI) Molecular dynamics as a test for intermolecular potentials (Ref. 316).

The Limitations

The core capacity and speed of computers inevitably limited the application of the MD method to finite systems usually consisting of, as already mentioned, $N \leq 1000$ molecules.

The bottleneck in the original MD method is the calculation of the forces on all the particles. To find the force on each particle requires the summation of contributions from each of the other $(N-1)$ particles in the system, thus a total of $\sim N^2$ computer operations is required to find the force on all N particles. This work may be reduced if the potential of interaction is only of short range by limiting the force contributions to nearby particles ($r < r_c$). Even so the largest system reported using the original MD method is that of Schofield (Ref. 370) on the study of the liquid state obtained with a system of 4,000 particles.

The finiteness of the system also influenced the choice of the substances and the problems which have been investigated by the MD method. The choice of the substances whose interaction can be described in terms of the LJ potential is made partly because the interaction of a molecule with other molecules beyond a certain region can be ignored and, therefore, in effect, a molecule interacts only with a limited number of molecules in a given region surrounding it. Thus, the finiteness of the system is not too restrictive in the study of such substances. However, the original MD method has been used to study ionic substances also, see e.g., Woodcock (Ref. 245), Woodcock et al. (Ref. 325) and Rahman et al. (Ref. 305). The number of particles included in the simulations of such substances is typically only 64 or 216. Since to study the phase transition and the coexistence of both the phase of a substance, a relatively large number of particles, $N \approx 10^4$ is considered desirable (Ref. 7), systems having $N \leq 10^3$ are obviously not suitable to study phase transitions in three dimensions. Thus, the finite size of the system in the MD method is restrictive of the choice of problems also.

The Modified Method

The MD method has recently been modified by Hockney *et* al. (Ref. 388) to make it applicable even to those systems in which long range interactions must be studied. In the modified method, the long range electrostatic potential in, e.g., an ionic system is found by solving Poisson's equation for the given charge configuration on a spatial finite-difference mesh.

Short range force contributions, from riearby particles only, are then added in the usual way. This new Particle-Particle/Particle-Mesh (PPPM) method avoids the need to sum force conti-ibutions from all other particles in the system. The number of computer operations required to calculate the long range forces is proportional to N (as compared with N^2 for the original method) and consequently large systems with 10,000 particles can be simulated. Although the initial work has been done in two-dimensions the method generalises to three dimensions and is potentially capable of handling larger systems with long range forces that are of arbitrary shape.

The Bibliography

The references in the bibliography are arranged in the chronologicai order to appreciate how the use of the MD method for computer simulation studies has been increasing during the last fifteen years or so. All relevant references that came to our notice have been included in the bibliography. However, it is possible that some references might have been omitted. We would very much appreciate if any such references are brought to our notice. To make the bibliography more useful. we have included in it some references whose results are akin to or have a bearing on those of the MD method. The MD references can be easily distinguished by the letters MD which generaily accompany their serial numbers in the bibliography.

References

MD 1. Phase transition for a hard sphere system. B.J. Alder and T E Wainwright, J. Chem. Phys. 27, 1208 (1957), also see Proc. Intern Union of Pure and Applied Physics on "Statistical mechanical theory of transport properties", Brussels (1956). and Symposium on the "Many body problem", New York (1957).

For periodic boundary conditions used in the MD method. see B.J. Alder. S.P. Frankel and V.A. Levinson, J. Chem. Phys. 23. 417 (1955): for the evaluation of pressure from the radial distribution function. see J. G. Kirkwood, E. K. Maun and B. J. Alder. J. Chem. Phys. 18. 1040 (1950).

For the initial choice of the values of LJ parameters ε and σ for argon. see A. Mitchels, Hub Wijker and H.K. Wijker, Physica 15. 627 (1949).

2. Density expansions of distribution functions I, I. Oppenheimer and P. Masur, Physica 23, 197 (1957).

3. Radial distribution function of fluids I, K. Hiroiki, J. Phys. Soc. Japan 12, 326 (1957).

4. Correlation factors for diffusion in solids, K. Compaan and Y. Haven, Trans. Faraday Soc. 52, 786 (1956).

MD 5. Molecular dynamics computations for the hard sphere system, T.E. Wainwright and B.J. Alder, Nuovo Cimento, Suppl 9, 116 (1958); also see B. J. Alder and T. E. Wainwright in Proc. Intern. Symp. 'Transp processes in statistical mechanics', edited by I. Prigogine (Interscience, New York, 1958), p. 97.

MD 6. Scattering of slow neutrons by a liquid, G. Vineyard, Phys. Rev. 110, 999 (1958).

7. Studies in molecular dynamics. I. General method, B.J. Alder and T.E. Wainwright, J. Chem. Phys. 31, 459 (1959). In this paper, details of the MD method are given.

MD 8. Molecular motions, B.J. Alder and T.E. Wainwright. Scientific American, October 1959.

MD 9. Perturbation calculations in equilibrium Statistical Mechanics I. Hard sphere basis potential, E.B. Smith and B.J. Alder, J. Chem. Phys. **30,** 1191 (1959).

10. Statistical mechanics of rigid spheres, H. Reiss, H.L. Frisch and J.L. Lebowitz, J. Chem. Phys. 31, 369 (1959).

MD 11. Studies in molecular dynamics II. Behaviour of a small number of elastic spheres, B. J. Alder and T. E. Wainwright, J. Chem. Phys. 33, 1439 (1960).

MD 12. Dynamics of radiation damage, J.B. Gibson, A.N. Goland, M. Milgram and G.H. Vineyard, Phys. Rev. 120, 1229 (1960).

13. Transport coefficients from dissipation in a canonical ensemble, E. Helfand, Phys. Rev. 119, 1 (1960); also see I.Z. Fisher, Sovt. Phys. Uspekhi 2, 783 (1960).

14. The heat of fusion of the alkali metal halides, A.S. Dworkin and M.A. Bredig, J. Phys. Chem. 64, 269 (1960).

15. Formulation of a cell model using periodic boundary conditions, D.R. Squire and Z.W. Salsburg, J. Chem. Phys. 35, 486 (1961).

16. Thermodynamic properties of small systems, J.L. Lebowitz and J. K. Percus, Phys. Rev. 124, 1673 (1961).

17. Theory of the two and one dimensional rigid sphere fluids, E. Helfand, H.L. Frisch, J.L. Lebowitz, J. Chem. Phys. 34, 1037 (1961).

18. Distributions of interstitials and vacsncies produced by an incident fast neutron, M. Yoshida, J. Phys. Soc. Japan 16, 44 (1961).

MD 19. Phase transitions in elastic discs, B.J. Alder and T.E. Wainwright Phys. Rev. 127, 359 (1962).

MD 20. The application of Mont Carlo methods to physico chemical problems, M.A.D. Fluendy and E.B. Smith, Quarter Review 16. 241 (1962).

21. Sixth and seventh Virial coefficients for the parallel hard-cube model. W.G. Hoover and A.G. DeRocco, J. Chem. Phys. 36, 3141 (1962)

22. Equation of state of classical hard spheres at high density. Z.W. Salsburg and W.W. Wood, J. Chem. Phys. **37,** 798 (1962).

23. Point defects in copper, R.A. Johnsor. and E. Brown, Phys. Rev. 127. 446 (1962).

24. The density of liquid $NaCl$ and KCl and an estimate of their critical constants together with those of the alkali halides, A.D. Kirschembaum. J.A. Cahill, P.J. McGonigal and A.V. Grosse, J. Inorg. Nucl. Chem. 24. 1287 (1962).

MD 25. Lattice theories of the liquid state, J.A. Barker (Pergamon Press. London, 1963).

MD 26. Cooperative motion of hard disks leading to melting, B.J. Alder. W.G. Hoover and T.E. Wainwright, Phys Rev. Leti. 11, 241 (1963): also see, B.J. Alder, Proc. Symp. Maths 15, 335 (1963) and B.J. Alder and T.E. Wainwright in 'The many Body Problem', ed. J. Percus (Wiley — Interscience, New York, 1963), p. 511.

27. First order phase transition in a gas of long thin rods, R. Zwanzig, J. Chem. Phys. **39,** 1714 (1963).

28. The virial expansion in two dimensions. S. Rowlinson, Mol. Phys. 7, 593 (1964).

29. Cohesive energy of the alkali halide crystals, MP. Tosi, J. Phys. Chem. Solids 24, 965 (1963).

MD 30. Range and damage effects of tunnel trajectories in a wurtzite structure, J.R. Beeler and D.G. Besco, J. Appl. Phys **34,** 2873 (1963).

31. Defect configurations in heavy-atom bombarded BeO, J.R. Beeler and D.G. Besco, J. Phys. Soc. Japan **18,** Suppi. 111, 159 (1963); also see Proc. Symp. Radiation Damage in Solids (IAEA, Vienna, 1962) V.l, p.43 and Bull. Am. Phys. Soc. 7, 437 (1962).

32. The channelling of energetic atoms in crystal lattices, M.T. Robinson and O.S. Oen, Appl. Phys. Lett. **2,** 30 (1963); also see J. Appl. Phys. **34,** 302 (1963) and Bull. Am. Phys. Soc. 7, 171 (1962).

33. Comparison of the classical theories of unimolecular reactions II. A model calculation, E. J. Thiele, J. Chem. Phys. 39, 474 (1963).

MD 34. Studies in molecular dynamics III. A mixture of hard spheres, B.J. Alder, J. Chem. Phys. 40, 2724 (1964).

MD 35. Triplet correlations in hard spheres, B.J. Alder, Phys. Rev. Lett. **12,** 317 (1964).

MD 36. Correlations in the motions of atoms in liquid Argon, A. Rahman, Phys. Rev. **136,** A405 (1964).

MD 37. Triplet correlations in liquids, A. Rahman, Phys. Rev. Lett. **12,** 575 (1964).

MD 38. 'The Techniques of High Speed Computer Experiments', J.R. Beeler, Jr., in 'Physics of Many Particle Systems', ed. E. Meeron (Gordon and Breach, New York, 1964).

39. High density equation of state for hard parallel squares and cubes, W. G. Hoover, J. Chem. Phys. 40, 937 (1964).

40. Fifth and Sixth virial coefficients foi hard spheres and hard disks. F.H. Ree and W.G. Hoover J. Chem. Phys 40. 939 (1964): for third and fourth virial coefficients, see, e.g., Phys. Rev. 85, 777 (1952).

41. Intermolecular potential functions and the second and third virial coefficients, A. E. Sherwood and J. M. Prausnitz, J. Chem. Phys. 41.429 (1964).

42. The equation of state of the classical hard sphere liquid, H.L. Frisch, Adv. Chem. Phys. 6, 229 (1964).

43. Calculation of the hard sphere viscosity by means of correlated functions, T.E. Wainwright, J. Chem. Phys. 40. 2932 (1964).

44. The solid state of rare gases, G. Pollack Rev. Mod. Phys. 36. 748 (1964).

45. Dynamics of radiation in a body centred cubic lattice. C. Erginsoy, G.H. Vineyard and A. Englert, Phys. Rev. 133, A595 (1964).

46. Interstitials and vacancies in a-iron, R.A. Johnson. Phys. Rev. 134A. 1329 (1964).

47. Systematic approach to explanation of the rigid disk phase transition. F.H. Stillinger, E.A. Dimarzio and R.L. Kornegay. J. Chem Phys 40. 1564 (1964).

48. Approximations to the pair correlation function for a hard-sphere fluid, M. Klein, Phys. Fluids 7, 391 (1964).

49. Radial distribution functions of fluid argon. A A. Khan. Phys. Rev. A134, 367 (1964).

50. On the theory of classical fluids, L. Verlet. Physica 30. 95 (1964)

MD 51. Free path distributions for hard spheres, B.J. Alder and T. Einwohner, J. Chem. Phys. 43, 3399 (1965).

52. Hard sphere fluid, W.L. Frisch, Science 150, 1249 (1965)

53. Bounds on the configurational integral for hard parallel squares and cubes, W.G. Hoover, J. Chem. Phys. 43, 371 (1965).

54. Hard sphere lattice gases I. Plane square lattice, D S. Gaunt and M.E. Fisher, J. Chem. Phys. 43, 2840 (1965).

55. Rigid disks at high densities, F.H. Stillinger, Z.W. Salsburg and R.L. Kornegay, J. Chem. Phys. **43,** 932 (1965).

56. Time correlation functions and transport coefficients in statistical mechanics, R. Zwanzig, Ann. Rev. Phys. Chem. 16, 67 (1965).

57. The statistical mechanics of simple liquids, S.A. Gray and P. Gray (Wiley-Interscience, New York, 1965).

58. A continued fraction representation of the time correlation functions, H. Mori, Prog. Theo. Phys. (Kyoto) **34,** 399 (1965).

59. High temperature expansion of thermal transport coefficients, H.L. Frisch and B. Berne, J. Chem. Phys. **43,** 250 (1965).

60. Interfacial tension effects in finite, periodic, two dimensional systems, J.E. Mayer and W.W. Wood, J. Chem. Phys. 42, 4268 (1965).

61. High frequency elastic moduli of simple fluids, R. Zwanzig and R.D. Mountain, J. Chem. Phys **43,** 4464 (1965).

62. Virial coefficients for the hard-core gas in two dimensions, P.C. Hemmer, J. Chem. Phys. **42,** 1116 (1965).

63. Self-diffusion and structure in molten group II chlorides J. O'M. Bockris, R.S. Richards and L. Nanis, J. Phys. Chem. 64, 1627 (1965).

64. Time correlation functions and transport coefficients in statistical mechanics, R. Zwanzig, Ann. Rev. Phys. Chem. 16, 67 (1965).

65. Self-consistent approximations for molecular distribution functions, J.S. Rowiinson, Mol. Phys **9,** 217 (1965).

MD 66. Liquid structures and self-diffusion, A. Rahman, J. Chem. Phys. **45,** 2585 (1966).

MD 67. Effects of a long range oscillatory potential on the radial distribution function and the constant of self-diffusion in iiquid Na, **A.** Paskin and A. Rahman, Phys. Rev. Lett. 16, 300 (1966).

MD 68. The expansion of correlation functions and the theory of slow neutron scattering, B.R. Nijboer and A. Rahman. Physica **32,** 415 (1966).

MD 69. The liquid state, J.A. Pryde (Hutchinson and Co., London 1966).

70. Existence of two phases in one dimensional classical fluids. M. Ross and B.J. Alder, Phys. Rev. Lett. 16, 1077 (1966).

71. Pressure and entropy for hard particles at high density, W.G. Hoover. J. Chem. Phys. 44, 221 (1966).

72. Cell theories for hard particles, W.G. Hoover and B.J. Alder. J. Chem. Phys. 45, 2361 (1966).

73. Van der Waals theory of transport n dense fluids. J.H. Dymond and B.J. Alder, J. Chem. Phys. 45, 2061 (1966).

74. Phase transition of a hard core lattice gas. The square lattice with nearest-neighbour exclusion. F.H. Ree and D.A. Chesnut. J. Chem. Phys. 45, 3983 (1966).

75. Numerical investigations of a simple model of a one-dimensional fluid, J.L. Anderson and J.K. Percus, J. Comput. Phys. 1. *68* (1966).

76. Statistical mechanical properties of small systems in the isothermal-isobaric ensemble, Z. W. Salsburg, J. Chem. Phys 44. 3090 (1966).

77. Point defect calculations for an fcc lattice. R.A. Johnson. Phys. Rev. 145, 423 (1966).

MD 78. Shockwave propagation in cubic lattices. D.H. Tsai and C.W. Beckett, J. Geophys. Res. 71, 2601 (1966).

79. On the calculation of autocorrelation functions of dynamical variables. B.J. Berne, J.P. Boon and S.A. Rice, J. C'hem. Phys. 45. 1086 (1966).

80. Structure and resistivity of liquid metals, N.W. Ashcroft and J. Lekner. Phys. Rev. 145. 83 (1966).

81. Etude des equations de Percus et Yevick, D'Hyperchaine et de Born et Green dans le cas des fluides classiques, D. Levesque. Physica 32. 1985 (1966).

82. Fifth Virial Coefficients. J.A. Barker. P.J. Leonard and A. Pornpe. J. Chem. Phys. 44, 4206 (1966).

83. Momentum autocorrelation function for systems with finite spatial boundaries, R. Nossal, J. Chem. Phys. **45,** 1097 (1966).

84. Computer simulation of vacancy migration, J.H. Weiner and W.F. Alder, Phys. Rev. **144,** 511 (1966).

85. On the rotational diffusion of molecules, R.G. Gordon, J. Chem. Phys. **44,** 1830 (1966).

86. Accurate numerical method for calculating frequency — distribution functions in solids, G. Gilat and L.J. Raubenhaumer, Phys. Rev. 144, 390 (1966).

87. Monte Carlo study of a one-component plasma I, S.G. Brush, H.L. Shalin, E. Teller, J. Chem. Phys. **45,** 2102 (1966).

MD 88. Computer experiments on classical fluids I. Thermodynamic properties of L.J. molecules, L. Verlet, Phys. Rev. 159, 98 (1967).

MD 89. Collective coordinates in classical systems, A. Rahman, Phys. Rev. Lett. 19, 420 (1967).

MD 90. Studies in molecular dynamics IV. The pressure, collision rate and their number dependence for hard disks, W.G. Hoover and B.J. Alder, J. Chem. Phys. **46,** 686 (1967).

MD 91. Molecular dynamics of weakly coupled electric dipoles on a rigid lattice I. The approach to equilibrium, M. Kohler and A. Bellemans, J. Chem. Phys. **47,** 1261 (1967).

MD 92. Ensemble dependence of fluctuations with application to machine calculations, J.L. Lebowitz, J.K. Percus and L. Verlet, Phys. Rev. **153,** 250 (1967).

MD 93. Velocity autocorrelations for hard spheres, B.J. Alder and T.E. Wainwright, Phys. Rev. Lett. **18,** 988 (1967).

MD 94. Ground state of liquid He-4 and He-3, D. Schiff and L. Verlet, Phys. Rev. 160, 208 (1967).

MD 95. Use of computer experiments to locate the melting transition and calculate the entropy in the solid phase, W.G. Hoover and F.H. Ree, J. Chem. Phys. 47, 4873 (1967).

96. On the theory of classical fluids VI, L. Verlet and D. Levesque. Physica ***36.*** 254 (1967).

97. Phase transitions in two dimensional lattice gases of hard square molecules, A. Bellemans and R.K. Nigam, J. Chem. Phys. **46.** 2922 (1967).

98. Rigid disks at high density II. Z.W. Salsburg, W.G. Rudd and F.H. Stillinger, Jr.. J. Chem. Phys. **47,** 4534 (1967).

99. Statistical mechanical calculations of linear molecules I. Potential energy functions, J.R. Sweet and W.A. Steele, J. Chem. Phys. **47.** 3022 (1967); **11.** Correlation functions and second virial coefficients J. Chem. Phys. 47, 3029 (1967).

100. Semi empirical potential and the bound state of the helium-4 diatom. L.W. Bruch and I. McGee. J. Chem. Phys. **46.** 2959 (1967).

101. Velocity inversion and irreversibility in a dilute gas of hard disks. J. Orban and A. Bellemans, Phys. Lett. ,924, 620 (1967).

102. Velocity inversion in statistical mechanics, R. Balescu. Physica 36. 433 (1967).

103. Square well fluid at low densities, J.A. Barker and D. Henderson. Can. J. Phys. **45,** 3959 (1967); see also J. Chem. Phys. 47. 2856 (1967). and J. Chem. Phys **47,** 4714 (1967).

104. Velocity auto-correlation in classical fluids. K. Singwi and M.P. Tosi, Phys. Rev. **157,** 153 (1967).

105. Elementary excitations in classical liquids, R. Zwanzig. Phys. Rev. **156,** 190 (1967).

106. Shock compression of argon III. The Thomas-Fermi Dirac theory, M. Ross and B.J. Alder, J. Chem. Phys. 47, 4129 (1967).

107. Shock compression of argon II. Non-additive repulsive potential. M. Ross and B.J. Alder, J. Chem. Phys. 46, 4203 (1967); for pt. I. see M. Van Thiel and B.J. Alder, J. Chem. Phys. 44, 1056 (1966).

108. Introduction to the liquid state, P. Egelstaff (Academic Press. New York, 1967).

109. Lattice defects and their interactions. M. Doyama and R.M.J. Cotterill, ed. Hasiguti (Gordon and Breach, New York. 1967).

110. Lattice thermal conductivity in disordered harmonic and anharmonic crystal modes, D.N. Payton, III, M. Rich and W.M. Visschar. Phys. Rev. 160, 706 (1967).

111. Screw dislocation core structure in body-centred cubic iron. R. Chang, Phil. Magazine 16, 1021 (1967).

112. Dimensional methods in the statistical mechanics of ionic systems. M. Blander, Adv. Chem. Phys. 11. 83 (1967).

MD 113. Molecuiar dynamics of electric dipoles on a rigid lattice. The dielectric response function, A. Bellemans, M. Gancberg and M. Kohler, Phys. Rev. Lett. 18, 1192 (1967).

114. Time-reversible difference procedures, **O.** Buneman. J. Comput. Phys. 1, 517 (1967).

115. Seventh virial coetficients for hard spheres and hard disks. F.H. Ree and W.G. Hoover J. Chem. Phys. **46,** 4181 (1967).

116. Systematic approximations to the partition function for crystalline solids, **A.** Beyerlin, Z.W. Salsburg, J. Chem. Phys. **47,** 3763 (1967).

117. Pressure-consistent integral equation for classical fluids: hard sphere solution, F. Lado, J. Chem. Phys. 47, 4828 (1967).

118. Vibrational relaxation of diatomic molecules in gases and liquids, B.J. Berne, J. Portner and R.G. Gordon, J. Chem. Phys **47,** 1600 (1967).

119. Determination of molecular quadrupole moments from viscosities and second virial coefficients, T. Spurling and E. Mason, J. Chem. Phys. **46,** 322 (1967).

MD 120. Linear and angular momentum autocorrelation functions in diatomic liquid, G.D. Harp and B.J. Berne, J. Chem. Phys. **49,** 1249 (1968).

MD 121. Computer experiments on classical fluids II. Equilibrium correlation functions, L. Verlet, Phys. Rev. **165,** 201 (1968).

MD 122. Molecular dynamics VI. Free path distributions and collision rates for hard sphere and square-well molecules, T. Einwohner and B.J. Alder, J. Chem. Phys. **49,** 1458 (1968).

MD 123. Current fluctuations in classical liquids, A. Rahman, Fourth IAEA Symposium on Neutron Elastic scattering Vol. I (IAEA, 1968).

MD 124. Note on X-ray scattering by argon, D. Levesque and L. Verlet, Phys. Rev. Lett. 20, 905 (1968).

MD 125. Computer experiments on liquids and solids: A comparative study of atomic motions in liquid and solid argon, A. Rahman. unpublished.

MD 126. Numerical statistical mechanics, B.J. Alder and W.G. Hoover in Physics of Simple liquids, ed. H.N.V. 'Temperley, J.S. Rowlinson and G.S. Rushbrooke (North Holland, Amsterdam, 1968).

MD 127. Effective ion-ion interactions in liquid metals, N.H. March in Physics of Simple liquids, ed. H.N.V. 'Temperley. J.S. Rowlinson and G.S. Rushbrooke (North Holland, Amsterdam, 1968).

MD 128. Studies in molecular dynamics V. High-density equation of state and entropy for hard disks and spheres, B.J. Alder, W.G. Hoover and D.A. Young, J. Chem. Phys. 49, 3688 (1968).

MD 129. Instability modes prior to melting, B.J. Alder, W.R. Gardner. J.K. Hoffer, N.E. Phillips and D.A. Young, Phys. Rev. Lett. 21, 732 (1968).

MD 130. Molecular reorientation in liquids and gases, B.J. Berne. P. Pechukas and G. Harp, J. Chem. Phys. 49, 3125 (1968).

MD 131. Phonon spectrum changes in small particles and their implications for superconductivity, J.M. Dickey and A. Paskin, Phys. Rev. Lett. 21, 1441 (1968).

132. Phase transitions in two dimensional lattice gases of hard core molecules. The triangular lattice, J. Orban and A. Bellemans, J. Chem. Phys. 49, 363 (1968).

133. Excess free energy of a two component mixture of hard spheres slightly different in size, A. Bellemans and J. Orban, Chem. Phys. Lett. 2. 253 (1968).

134. Lattice models of hardcore molecules with attractions: The phase diagram, J. Orban, J. Van Craen, and A. Bellemans, J. Chem. Phys. 49, 1778 (1968).

135. The dynamic three dimensional structure of liquid sodium, A. Paskin and A. Rahman, Acta Cryst. (International) 21, pt. 7, Suppl. A, 237 (1968).

136. Equation of state of the disc fluid from approximate integral equations, F. Lado, J. Chem. Phys. 49, 3092 (1968).

137. Rigid disks and spheres at high densities III, W.G. Rudd, Z.W. Salsburg, A.P. Yu and F.H. Stillinger, J. Chem. Phys. 49, 4857 (1968); for pt II, see J. Chem. Phys. 46,3962 (1967), and for pt I, J. Chem. Phys. 40,1564 (1964); also see J. Chem. Phys. 47, 4534 (1967).

138. Shock compression of argon and xenon IV. Conversion of xenon to a metal-like state, M. Ross, Phys. Rev. 171, 777 (1968).

139. Melting transition and communal entropy for hard spheres, W.G. Hoover and F.H. Ree, J. Chem. Phys 49, 3609 (1968).

140. Simple dense fluids, H.L. Frisch and Z.W. Salsburg (Academic Press, New York, 1968).

141. Corrections to the kinetic theory of fluid diffusion, J.H. Dymond and B.J. Alder, J. Chem. Phys. 48, 343 (1968).

142. Statistical mechanical calculation of surface properties of simple liquids and liquid mixtures I. Pure Liquids, LW. Plesner and O. Platz, J. Chem. Phys. 48, 5361 (1968).

143. Frequency dependent friction friction constant analysis of diffusion in simple liquids, P. Martin and S. Yip, Phys. Rev. 170, 151 (1968).

144. Dynamical correlations in simple liquids and cold neutron scattering by argon, R. Desai and S. Yip, Phys. Rev. 166, 129 (1968).

145. Moments of the momentum density correlation functions in simple liquids, D. Forster, P.C. Martin and S. Yip, Phys. Rev. 170, 155 (1968); see also Phys. Rev. 170, 160 (1968).

146. Dense-gas formulation of self-diffusion in liquid metals, P. Ascareli and A. Paskin, Phys. Rev. 165, 222 (1968).

147. Statistical-mechanical calculation of surface properties of simple liquids and liquid mixtures II. Mixtures, I.W. Plesner, O. Platz and S.E. Christiansen, J. Chem. Phys. 48, 5364 (1968).

148. Physical properties of molecular crystals, liquids and glasses, A. Bondi (John Wiley and Sons, New York, 1968).

149. Self-diffusion in solid krypton, A.V. Chadwick and J.A. Morrison. Phys. Rev. Lett. 21, 1803 (1968).

150. Melting in argon at high temperature, R.K. Crawford and W.B. Daniels, Phys. Rev. Lett. 21, 367 (1968).

151. Theories of atomic motions in simple classical liquids, K.S. Singuri and A. Sjolander, Phys. Rev. 167, 152 (1968).

152. The morphology of interstitial aggregates in iron, R. Bullough and R.C. Perrin, Proc. Ray. Soc. A. 305, 541 (1968).

MD 153. Persistence of vacancy motions, C.H. Bennett and B.J. Alder, Solid State Commun. 6, 785 (1968).

154. Mechanism of vibrational relaxation, B.J. Berne, R.G. Gordon, and V.F. Sears, J. Chem. Phys. 49, 475 (1968).

155. Atomic interactions in argon, J.A. Barker and A. Pompe. Aust. J. Chem. 21, 1683 (1968).

156. Density measurements of compressed solid and liquid argon. W. Van Witzenburg and J.C. Stryland, Canad. J. Phys. 46, 811 (1968).

157. Direct correlation function and equation of state of fluid argon, J. Woodhead-Galloway, T. Gaskell and N.H. March, J. Phys. C1, 271 (1968).

MD 158. 'Computer Studies of condensed matter, A. Rahman, Revista del Nuovo Cimento 1, 315 (1969).

MD 159. Computer studies of phase transitions of classical fluids, L. Verlet, Proc. Culham Conf. on Computational Physics, UKAEA, Culham Lab. and IPPS, Vol. I (1969).

MD 160. Molecular dynamics of weakly coupled electric dipoles on a rigid lattice II. The dielectric response function, A. Bellemans, M. Kohler and M. Ganceberg, J. Chem. Phys. 51, 2578 (1969).

MD 161. Crystallization with a Lennard-Jones potential: A computer experiment, F.W. de Wette, R.E. Allen, D.S. Hughes and A. Rahman, Phys. Lett. 29A, 548 (1969).

MD 162. Theories of liquids, G.A. Neece and B. Widom, Ann. Rev. Phys. Chem. V. 20, ed. H. Eyring, C.J. Christensen and H.S. Johnston (Annual Reviews Inc., California 1969).

MD 163. Studies in molecular dynamics VII. Hard sphere distribution functions and an augmented Van der Waals theory, B.J. Alder and C.E. Hecht, J. Chem. Phys. 50, 2032 (1969).

MD 164. Calculation of dynamical surface properties of noble-gas crystals II. Molecular dynamics, R.E. Allen, F.W. de Wette and A. Rahman, Phys. Rev. 179, 887 (1969); also see Phys. Rev. 179, 873 (1969).

MD 165. Computer experiments on liquid metals, D. Schiff, Phys. Rev. 186, 151 (1969).

MD 166. Molecular dynamics studies of the microscopic properties of dense fluids, P. Fehder, J. Chem. Phys. 50, 2617 (1969).

MD 167. Computer simulation of the lattice dynamics of solids, J.M. Dickey and A. Paskin, Phys. Rev. 188, 1407 (1969).

168. Pair potential for argon, J.H. Dymond and B.J. Alder, J. Chem. Phys. 51, 309 (1969).

169. The structure of soiid chiorine in relation to Van der Waals forces, P. Weyland and O. Dideberg, Bull. Soc. Roy. Sci. Liège (Belgium) 38, 533 (1969). in French.

170. Crystal transformation for hard spheres, B.J. Alder, B.P. Carter and D.A. Young, Phys. Rev. 183, 831 (1969).

171 Highly anharmoniccrystals, M. Fixman, J. Chem. Phys. 51,3270 (1969).

172. Calculation of dynamical surface properties of noble-gas crystals I. The quasi-harmonic approximation, R.E. Allen and F.W. de Wette, Phys. Rev. 179, 873 (1969).

173. Pair distribution function for fluid hard spheres, R.O. Watts and D. Henderson, Mol. Phys. 16, 217 (1969).

174. Statistical error due to finite time averaging in computer experiments R.W. Zwanzig and N.K. Ailawadi, Phys. Rev. 182, 280 (1969).

175. Comparison of interatomic potentials for argon, D. Levesque, J. Vieillard-Baron, Physica 44, 345 (1969).

MD 176. Transport coefficients from molecular dynamics for a very small system, C. Bruin, Phys. Lett. A28, 777 (1969).

177. Viscosity and density in molten BeF2-LiF solutions, S. Cantor, W.T. Ward and C.T. Maynihan, J. Chem. Phys. 50, 2874 (1969).

178. Generalized Lindemann melting law, M. Ross, Phys. Rev. 184, 233 (1969).

179. Generalized hydrodynamics and time correlation functions, S. Chung and S. Yip, Phys. Rev. 182, 323 (1969).

180. Kinetic equation approach to time-clependent correlation functions, J.K. Percus, J. Lebowitz and J. Sykes, Phys. Rev. 188, 487 (1969).

181. Relation between local structure and thermodynamic properties in aqueous liquids, F.H. Stillinger and A. Ben-Naim, J. Phys. Chem. 73, 900 (1969).

182. Variational approach to the equilibrium thermodynamic properties of simple liquids I., G.A. Mansoori and F.B. Canfield, J. Chem. Phys. 51, 4958 (1969); II variational approach to melting II., J. Chem. Phys. 51, 4967 (1969).

183. Perturbation theory and the equation of state for fluids, D. Levesque and L. Verlet, Phys. Rev. 182, 307 (1969).

184. Equation of state for non-attracting rigid-spheres, N.G. Carnahan and K.E. Starling, J. Chem. Phys 51, 635 (1969).

185. Asymptotic decay of the pair correlation function in one dimensional fluids, B. Widom, J. Phys. Soc. Japan 26, Suppl. 283 (1969).

186. Structure and dynamics of very thin films, F.W. de Wette and R.E. Allen, Phys. Rev. 187, 878 (1969).

187. On the formation and migration eritropies of vacancies in metals, P. Wynblatt, J. Phys. Chem. Solids 30, 2201 (1969); also see, Entropies of lattice defects, H.B. Huntington, G.A. Shirn and E.S. Wajda, Phys. Rev. 99, 1085 (1955).

MD 188. Self-motion in a classical ferromagnet, R. E. Watson, M. Blume and G. Vineyard, Phys. Rev. 181, 811 (1969).

MD 189. Computer Studies on the approach to equilibrium in coupled anharmonic oscillators I. Two dimensional case, H. Hirooka and N. Saito, J. Phys. Soc. Japan 26,624 (1969).

MD 190. Computer Studies on the approach to equilibrium in coupled anharmonic oscillators II, one-dimensional case, N. Oogama, H. Hirooka and N. Saito, J. Phys. Soc. Japan 27, 815 (1969).

191. The density of random close packing of spheres, G.D. Scott and D.M. Kilgour, Brit. J. Appl. Phys. (J. Phys. D) 2, 863 (1969).

192. The optimization of particle calculations in 2 and 3 dimensions, J.P. Boris and K.V. Roberts, J. Comput. Phys. 4, 552 (1969).

MD 193. Statistical mechanics of fluids: enhancement of diffusion by vortex-like motion of classical hard particles, B.J. Alder and T.E. Wainwright, J. Phys. Soc. Japan (Supplement) 26, 267 (1969).

194. Phase transition of the Lennard-Jones system, J.P. Hansen and L. Verlet, Phys. Rev. 184, 151 (1969).

MD 195. Studies in molecular dynamics VIII. The transport coefficients for a hard-sphere fluid, B.J. Alder, D.M. Gass and T.E. Wainwright, J. Chem. Phys. 53, 3813 (1970).

MD 196. Molecular dynamical studies of the motion of point defects in a crystalline lattice, D. Tsai, R. Bullough and R.C. Perrin, J. Phys. C3, 2022 (1970).

MD 197. Computer experiments on classical fluids III. Time-dependent self-correlation functions, D. Levesque and L. Verlet, Phys. Rev. A2, 2514 (1970).

MD 198. A molecular dynamics investigation of the coherent scattering functions of simple fluids, J. Kurkijarvi, Ann. Acad. Sci. Fennicae AVI (Finland) no. 346, 3 (1970).

MD 199. Time correlation functions, memory functions and molecular dynamics, G.D. Harp and B.J. Berne, Phys. Rev. A2, 975 (1970).

MD 200. Molecular dynamics studies of iattice defects, R.M.J. Cotterill. Fourth Nordic Solid State Conf. Turku, Finland (1970).

201. Computer Rechnungen und Frequenzspektrum von festem Blei bei 300K, von E. Stoll, Helvetica Physica Acta **43,** 456 (1970).

202. The study of simple liquids by computer simulation, I.R. McDonald and K. Singer, Quarterly Reviews of the Chem. Soc. 24, 238 (1970).

203. The role of computer experiments in materials research, J.R. Beeler in Adv. in Materials Research V.4, ed. H. Herman (Interscience 1970).

204. On the calculation of time correlation functions, B.J. Beme and G.D. Harp, Adv. Chem. Phys. 17, 63 (1970).

205. Decay of the velocity autocorrelation function, B.J. Alder and T.E. Wainwright, Phys. Rev. 1, 18 (1970).

206. Melting and the softening of the transverse phonon modes in solids, J.M. Dickey and A. Paskin, Phys. Rev. B1, 851 (1970).

MD 207. 'Anomalies' in the radial distr bution functions for simple liquids, P. Fehder, J. Chem. Phys. 52, 791 (1970)

208. Molecular dynamics of photo-dissoc ation-quasi-diatomic model for ICN, K.E. Holdy, Lynn C. Klotz and K.R. Wilson, J. Chem. Phys. 52, 4588 (1970).

209. Molecular dynamics in hydrogenous liquids during the transmission of slow neutrons, N. Iliescu and S. Rapeanu, Rev. Roumaine Phys. 15, 121 (1970).

MD 210. Corrections to the kinetic theory of fluid diffusion II. Binary mixtures, J.H. Dymond and B.J. Alder, J. Chem. Phys. 52, 923 (1970).

211. I am curious (transport coefficients), E.A. Mason, J.R. Dorfman, R. Zwanzig, Am. J. Phys. **38,** 435 (1970).

212. Augmented Van der Waals theory for mixtures, M. Rigby and B.J. Alder, J. Chem. Phys. 52, 3665 (1970).

213. Triplet-dipole dispersion forces in dense fluids, I.R. McDonald and L.V. Woodcock, J. Phys. **C3,** 722 (1970).

214. Asymptotic time behaviour of correlation functions, M.H. Ernst, E.H. Hauge and J.M.J. van Leeuwen, Phys. Rev. Lett. 25, 1254 (1970).

215. Temperature dependence of the atomic self-motion in liquid argon, P. Zandveld, C.D. Andriesse, J.D. Bregman, A. Hasman and J.J. Van Loef, Physica 50, 511 (1970).

216. Dynamics of liquid-solid transition, T. Schneider, R. Brout, H. Thomes and J. Feder, Phys. Rev. Lett. 25, 1423 (1970).

217. Theory of dielectric relaxation in polar liquids, T.W. Nee and R.W. Zwanzig, J. Chem. Phys. 52, 6353 (1970).

218. Melting of argon at high temperatures, S.M. Stishov, I.N. Makarenko, V.I. Ivanov., V.I. Fedosimov, J.E.T.P. Letters 11, 13 (1970).

219. On the correlation functions for hard sphere fluids, D. Henderson and R.O. Watts, Mol. Phys. 18, 429 (1970).

220. Melting of sodium at high pressures. V.A. Ivanov, I.N. Makarenko and S.M. Stishov, Zh. Eksper. Teor. Fiz. Pisma (USSR) p. 12; JETP Lett. (USA) 12, 7 (1970).

MD 221. On the calculation of time correlation functions, B.J. Berne and G.D. Harp in Advances in Chemical Phys. V. 17, ed. Prigogine and S. Rice (Wiley-Interscience, New York, 1970).

222. Statistical mechanics of single-occupancy systems of spheres, disks and rods, F.H. Ree, J. Chem. Phys. 53, 920 (1970).

223. Cooperative phenomena and the decay of the angular momentum correlation function at long times, N.K. Ailawadi and B.J. Berne, J. Chem. Phys. 54, 3569 (1970).

224. Hydrodynamics and coliective angular momentum fluctuations in molecular fluids, N.K. Ailawadi, B.J. Berne and D. Forster, Phys. Rev. **A3,** 1462 (1970).

225. Hydrodynamic theory of the velocity correlation function, R. Zwanzig and M. Bixon, Phys. Rev. **A2,** 2005 (1970).

226. The fluctuation-dissipation theorem, R. Kubo, Report Prog. Phys. 29, 255 (1966).

227. Therrnodynamics of binary systems near the Iiquid-gas critical point, W.F. Saam, Phys. Rev. **A2,** 1461 (1970).

228. M-6-8 potential function, M. Klein and H.J.M. Hanley, J. Chern. Phys. **53,** 4722 (1970).

229. Hard-square solids at high densities, A.L. Beyerlin, W.G. Rudd, Z.W. Salsburg and M. Buynoski, J. Chem. Phys. **53,** 1532 (1970).

230. Soft-sphere equation of state, W.G. Hoover, M. Ross, K.W. Johnson, D. Henderson, J. Barker and B.C. Brown J. Chem. Phys. 52, 4931 (1970).

231. New rnodel for the study of liquid-vapour phase transition, B. Widom and J.S. Rowlinson, J. Chem. Phys 52, 1670 (1970).

232. The viscosity of liquid argon and liquid rnethane along isotherms as a function of pressure, J. Hellemans, H. Zink and O. Van Paemel, Physica 46, 395 (1970).

233. Lattice dynarnics with three-body forces: argon, M.V. Bobetic and J.A. Barker, Phys. Rev. **32,** 4169 (1970).

234. Phase transition of the Lennard-Jones II. High-temp. limit, J.P. Hansen, Phys. Rev. **A2,** 221 (1970).

MD 235.. Size and surface effects on the phonon properties of srnall particles, J.M. Dickey and A. Paskin, Phys. Rev. B1, 851 (1970).

MD 236. Computer simulation of phase changes (especially the hard--sphere Bose gas), L. Verlet, First European Conf. on condensed matter, Florence, Italy, 14-17 Sept. (1971).

MD 237. Molecular dynamics study of melting and related phenornena, R.M.J. Cotterill, P.O. Esbjon, W. Damgard Kristensen, E.J. Jensen, J.W. Martin and L.B. Pedersen, First European Conf. on Condensed Matter, Florence, Italy, 14-17 Sep. (1971).

MD 238. Investigation of critical phenomena in a Lennard-Jones System by means of molecular dynamics, E. Stoll and T. Schneider, First European Conf. on Condensed Matter, Florence, Italy, 14-17 Sept., 1971.

MD 239. Statistical mechanical calculation of surface properties of simple liquids IV. Molecular dynamics, C.A. Croxton and R.P. Ferrier, J. Phys. C4, 2247 (1971).

MD 240. Molecular dynamics study of CO in liquid argon, B. Borstnik and A. Azman, Chem. Phys. Lett. 11, 374 (1971).

MD 241. Molecular dynamical studies of the phase transformation of iron under pressure, D.H. Tsai and R.A. MacDonald, Trans. Am. Crystallogr. Ass. (USA) Vol. 7 (1971); Symposium on mechanisms of phase transitions.

MD 242. Molecular dynamics study of liquid water, A. Rahman and F.H. Stillinger, J. Chem. Phys. 55, 3336 (1971).

MD 243. Liquid argon-Monte Carlo and molecular dynamics calculations, J.A. Barker, R.A. Fisher and R.O. Watts, Mol. Phys. 21, 657 (1971).

MD 244. Molecular dynamics of rough disks assemblies and dielectric relaxation, E. Kestemont and A. Bellemans, J. Comput. Phys. 7,515 (1971).

MD 245. Isotliermal molecular dynamics calculations for liquid salts, L.V. Woodcock, Chem. Phys. Lett. 10, 257 (1971).

MD 246. A molecular dynamics investigation of the surface correlations in liquid argon, C.A. Croxton, Phys. Lett. A35, 330 (1971).

MD 247. Molecular dynamics of two dimensional gases with realistic potentials, H.W. Harrison and W.C. Shieve, J. Stat. Phys. 3, 35 (1971).

MD 248. Atom-atom potential in molecular dynamics computations of orientational motion, B. Quentric and C. Brot, J. Chem. Phys. 54, 3655 (1971).

MD 249. The self-diffusion coefficient in argon at liquid densities, J.J. Van Loef, Phys. Lett. A35, 169 (1971).

MD 250. Time reversal symmetry violation and the H-theorem, A. Aharony, Phys. Lett. 37A, 45 (1971).

MD 251. Statistical theories of melting, W.G. Hoover and M. Ross, Contemporary Phys. 12, 339 (1971).

MD 252. Molecular dynamics studies of liquids, A. Rahman in Interatomic Potentials and Simulation of Lattice Defects, ed. P.C. Gehlen and J.R. Beeler, Jr.

MD 253. Molecular dynamics study of L.J. Liquid mixtures, B. Borstnik and **A.** Azman, Berichte der Bunsengessellschaft fuer Physikalische Chemie, 75, 392 (1971).

MD 254. Study of diffusion coefficients in mixtures of Lennard-Jones molecules in the liquid range, B. Borstnik and A. Azman, J. Chem. Phys. 55, 1988 (1971).

MD 255. Topics in Time Dependent Statistical Mechanics, B.J. Berne and D. Forster in Annual Review of Physical Chemistry V. 22, ed. H. Eyring, C.J. Christensen, and H.S. Johnston (Annual Reviews Inc., California 1971).

MD 256. Fused salts, C.A. Angell in Annual Review of Phys. Chem. V. 22, ed. H. Eyring, C.J. Christensen and H.S. Johnston (Annual Reviews Inc., California 1971).

MD 257. Computer calculations for model systems, F.H. Ree in Physical Chemistry-An Advanced Treatise, VIII A, ed. H. Eyring, D. Henderson and W. Jost (Academic Press, 1971).

MD 258. Time-dependent properties of condensed media, B.J. Berne in Physical Chemistry-An Advanced Treatise VIII B, ed. H. Eyring, D. Henderson and W. Jost (Academic Press, 1971).

MD 259. Microscopic mechanism for self-diffusion and relative diffusion in simple liquids, P. Fehder and R. Futrell, J. Chem. Phys. 54,4921 (1971).

MD 260. The equation of state for parallel hard spheres, W.G. Rudd and H.L. Frisch, J. Comput. Phys. 7, 394 (1971).

MD 261. Diffusion coefficients for the inverse twelfth power repulsive potentials, M. Ross and P. Schofield, J. Phys. C4, L 305 (1971).

MD 262. Computer experiments on classical fluids III. Time-dependent self-correlation functions. D. Levesque and L. Verlet. Phys. Rev. A2, 2514 (1971).

MD 263. Studies in molecular dynamics IX, Vacancies in hard sphere crystals, B.J. Alder and C.H. Bennett J. Chem. Phys. 54, 4796 (1971).

MD 264. Hard sphere equation of state in the close packed limit, B.J. Alder, D.A. Young, M.R. Mansingh and Z.W. Salsburg, J. Comput. Phys. 7, 361 (1971).

MD 265. Decay of time correlations in two dimensions, T.E. Wainwright, B.J. Alder and D.M. Gass Phys. Rev. A4, 233 (1971).

MD 266. The thermal conductivity of a hard sphere solid, D.M. Gass, B.J. Alder and T.E. Wainwright J. Phys. and Chem. Soiids 32, 1797 (1971).

267. Critica1 point of metals from the Van der Waals model, D.A. Young and B.J. Alder, Phys. Rev. A3, 364 (1971).

268. Fluid order and freezing, P. Hutchinson, M. Ross, P. Schofield and W.R. Conkie, J. Phys. **A4,** 1114 (1971).

269. Triplet potential for argon, J.H. Dymond and B.J. Alder, J. Chem. Phys. 54, 3472 (1971); also see Ber. Bunsenges Phys. Chem. 75,394 (1971).

270. On the equation of state of small systems, J. Hubbard, J. Chem. Phys. 55, 1382 (1971).

271. Fluid-solid phase transition of a hard sphere Bose system, J.P. Hansen, D. Levesque and D. Schiff, Phys. Rev. A3, 776 (1971).

272. Three body interactions in liquid and solid helium, R.D. Murphy and J.A. Barker, Phys. Rev. A3, 1037 (1971).

273. A functional derivative approach to thermodynamicaily self-consistent radial distribution functions, P. Hutchinson and W.R. Conkie, Mol. Phys. 21, 881 (1971).

274. Cooperative phenomena and the decay of the angular momentum correlation functions at long times, N.K. Ailawadi and B.J. Berne J. Chem. Phys. 54, 3569 (1971).

275. Existence of a phase transition in a continuous ciassical system, D. Ruelie, Phys. Rev. Lett. **27,** 1040 (1971).

276. Velocity auto-correlation function and diffusion coefficient in a liquid, T. Gaskell, J. Phys. C4, 1466 (1971).

277. Pair distribution in the classicai rigid disk and sphere systems, F.H. Stillinger, J. Comput. Phys. 7, 367 (1971).

278. Approximate equation of state for soft spheres, R.O. Watts, Aust. J. Phys. **24,** 53 (1971).

279. High temperature transport coefficients for rare gases from neon to xenon, J.H. Dymond. J. Phys. **B4,** 621 (1971).

280. Diffusion in dense fluids, J.H. Dymond, Diffusion Processes. Strathclyde, Scotland (Gordon and Breach, 1971).

281. Effective pair potentials in fluids in the presence of three body forces II, R.J. Dulla, J.S. Rowlinson and W.R. Smith, Mol. Phys. **21,** 299 (1971).

282. Entropy and molecular correlation functions in open systems II. Two and three body correlations, R.D. Mountain and H.J. Raveche J. Chem. Phys. **55,** 2250 (1971); also see J. Chem. Phys. **55,** 2242 (1971).

283. Hydrodynamics and collective angular momentum fluctuations in molecular fluids, N.K. Ailawadi, B.J. Berrie and D. Forster, Phys. Rev. **A3,** 1462 (1971).

284. Light scattering from shear waves: the role of angular momentum fluctuations in light scattering, N.K. Ailawadi, B.J. Berne and D. Forster, Phys. Rev. **A3,** 1472 (1971).

285. Lattice dynamics of fcc argon with three body forces, M.L. Klein, J.A. Barker and T.R. Koehler Phys. Rev. **B4,** 1983 (1971).

286. Statistical mechanics of small systems, J.B. Hubbard, J. Comput. Phys. **7,** 502 (1971).

287. Radial distribution functions and superficial quantities for rigid--sphere fluids; method of 'point' chemical potential using scaled particle theory, S.J. Harris, D.M. Tully-Smith, J. Chem. Phys. **55.** 1104 (1971).

288. Determination of models for collision-induced polarizability by the method of moments, H.B. Levine and G. Birnbaum, J. Chem. Phys. **55,** 2914 (1971).

289. Thermodynamic properties of the fluid and solid phases for inverse power potentials, W. G. Hoover, S. G. Gray and K. W. Johnson, J. Chem. Phys. 55, 1128 (1971).

290. Particle method for the numerical solution of the time-dependent Schroedinger equation. J.H. Weiner and A. Askar. J. Chem. Phys. 54. 3534 (1971).

MD 291. Computer simulation of the system N2 in fluid argon-correlation functions and relaxation times, E.F. O'Brien and G. Wilse Robinson. Chem. Phys. Lett. 8. 79 (1971).

292. Numerical Fourier transforms in one. two and three dimensions for liquid state calculations. F. Lado. J. Comput. Phys. 8, 417 (1971).

293. Non-additive interactions. C.D. Present. Contemp. Phys. 12. 595 (1971).

294. High density hard square particles approaching a close-packed brickwall configuration. A. Beyerlein. J. Comput. Phys. 7. 403 (1971).

295. Radial correlation functions of metallic melts calculated from structural models of the liquid state. I.A. Kotze and D. Kuhlmann-Wilsdorf. Phil. Mag. **23.** 1133 (1971).

296. Density and temperature dependence of intermolecular light scattering in simple fluids. P.A. Fleury. W.B. Daniels and J.M. Worlock. Phys. Rev. Lett. **27,** 1493 (1971).

297. Computer simulation of phase changes (especially the hard sphere Bose gas). L. Verlet. First European Conf. on Condensed matter. Florence, Italy. 14-17 Sept. 1971 (Geneva. Switzerland: European Phys. Soc. 1971). p. 34.

MD 298. Recent contributions to the understanding of the melting phenomena. R.M.J. Cotterill. High Temp. – High Press. (GB) 4. 236 (1972): also presented at the Third Nordic High-Temp. Symposium 7-9 June, 1972.

MD 299. Molecular dynamics studies of freezing in monoatomic systems, C.H. Bennett. Presented at the Second National Conf. Crystal Growth. Princeton. N.J.. U.S.A.

MD 300. Interstitial migration in FCC lattice: a molecular dynamics study. L.B. Pedersen. J.W. Martin and R.M.J. Cotterill. J. Phys. C (GB) 5. 3296 (1972).

MD 301. Temperature and density dependence of the self-diffusion coefficient in simple liquids, J.J. van Loef, Physica **62,** 345 (1972).

MD 302. Correlation in a rubidium system of some hundred atoms, W. Schommers Z. Phys. (Germany) 257, 78 (1972) (in German).

MD 303. Calculated self-diffusion coefficients for liquid argon, R.A. Fisher and R.O. Watts, Australian J. Phys. **25,** 529 (1972).

MD 304. A computer programme for molecular dynamics of dilute gases, A. Aharony, J. Comput. Phys. 10, 341 (1972).

MD 305. Structure and motion in liquid BeF_2, $LiBeF_3$ and LiF from molecular dynamics calculations, A. Rahman, R.H. Fowler and A.H. Narten, J. Chem. Phys. 57, 3010 (1972).

MD 306. Studies in molecular dynamics XI. Correlation functions of a hard-sphere test particle, P.T. Herman and B.J. Alder, J. Chem. Phys. **56,** 987 (1972).

MD 307. Studies in molecular dynamics X. Corrections to the Augmented Van der Waals theory for the square-well fluid, B.J. Alder, D.A. Young and M.A. Mark, J. Chem. Phys. 56, 3013 (1972).

MD 308. Molecular dynamics of hard parallel squares, C. Carlier and H.L. Frisch, Phys. Rev. **A6,** 1153 (1972).

MD 309. Molecular dynamics study of temperature effects on water structure and kinetics, F.H. Stillinger and A. Rahman, J. Chem. Phys. 57, 1281 (1972).

MD 310. Proton distribution in ice and the Kirkwood correlation factor, A. Rahman and F.H. Stillinger J. Chem. Phys. 57, 4009 (1972).

MD 311. Comparison of two simple theories with molecular dynamics results for parallel hard squares, M.A. Cotter and H.L. Frisch, J. Chem. Phys. 57, 1011 (1972).

MD 312. Molecular dynamics simulation of liquid-solid transition-microdynamics of condensation nucleus growth, B. Borstnik, and A. Azman, Chem. Phys. Lett. 14, 451 (1972).

MD 313. Numerical experiments in statistical mechanics, B.J. Alder, Comput. Phys. Commun. **3,** Suppl. 86 (1972).

MD 314. Molecular dynamics of the Widom-Rowlinson parallel hard--square model, H.L. Frisch and C. Carlier, Phys. Rev. Lett. 28,1019 (1972).

MD 315. Computer simulation of molecular dynamics, M.L. Prueitt, Ph.D. thesis, Univ. New Mexico, Albuquerque, USA., Univ. Mich. Ann Arbor, Mich., USA. Order no. 72-4012.

MD 316. Molecular dynamics as a test for intermolecular potentials, V.M. Jansoone and O.B. Verbeke, Ber. Bunsenges Phys. Chem (Germany) 76, 157 (1972).

MD 317. A molecular dynamics study of the melting of a two-dimensional crystal, R.M.J. Cotterill and L.B. Pedersen, Solid State Commun. (USA) **10,** 439 (1972).

MD 318. Molecular dynamics simulation of liquid-solid transition I. Response function model, B. Borstonik and A. Azman, Chem. Phys. Lett. 12, 620 (1972).

MD 319. Molecular dynamics simulation of shock waves in a three dimensional solid, A. Paskin and G.J. Dienes, J. Appl. Phys. **43,** 1605 (1972).

MD 320. Molecular dynamics of two-dimensional gases and the formation of bound states, H.W. Harrison, W.C. Schieve and J.S. Turner, J. Chem. Phys. 56, 710 (1972).

321. Numerical Calculation of the density auto correlation function for liquid argon, F. Lado, Phys. Rev. A5, 2238 (1972).

322. Extension of scaled particle theory for rigid disks, M. Cotter and F.H. Stillinger, J. Chem. Phys. 57, 3356 (1972).

323. Thermodynamically self-consistent radial distribution functions for inverse power potentials, P. Hutchinson and W.R. Conkie, Mol. Phys. 24, 567 (1972).

324. Motion and clustering of vacancies with pressure, B.J. Alder Third International Conf. on High Pressure-Engineering solids under pressure,

Aviemore. Scotland. 10-15 May, 1972 (London England: Inst. Mech. Engineers. 1972), p. 181.

MD325. Ion clusters in molten K_2 Mg Cl, (Raman Spectrum), B. R. Sundheim and L.V. Woodcock. Chem. Phys. Lett. 15, 191 (1972).

326. The computer study of transport processes under extreme conditions, A.W. Lees and S.F. Edwards, J. Phys. **C5,** 1921 (1972).

327. Optimized cluster expansions for classical fluids 111, Applications to ionic solutions and simple liquids, J.C. Henderson, D. Chandler and J.D. Weeks. J. Chem Phys. **57,** 2626 (1972).

328. Intermolecular forces in liquids: comparison of the analytic effective potential with computer calculations of the many-body effects, T. Halicioglu and **O.** Sinanoglu, Phys. Rev. **A5,** 2223 (1972).

329. Equilibrium theory of simple liquids. L. Verlet and J.J. Weis Phys. Rev. **A5.** 939 (1972).

330. Perturbation theory for repulsive forces in classical fluids. Selected applications. S. Chung and D. Chandler. J Chem. Phys. **56,** 4989 (1972).

331. Perturbation theory of thermal transport coefficients. R.O. Watts, J. Chem. Phys. **56,** 3731 (1972).

332. Virial expansions for a binary mixture model and for a related one component model, J.P. Straley. M.A. Cotter. T.J. Lie and B. Widom, J. Chem. Phys. 57. 4484 (1972).

333. Interpretation of the crystal structure of Li, Be F_4 in terms of the Born Mayer-Huggins model. W.R. Busing. J. Chein. Phys. **57.** 3008 (1972).

334. Serially deposited amorphous aggregatss ofhard spheres. C.H. Bennett. J. Appl. Phys. **43,** 2727 (1972).

335. Triplet correlations in liquid argon. M.P. Tosi and M.C. Abramo. Lett. Nuovo Cimento 5, 1044 (1972).

336. A simplified theory of liquid-solid transitions III. Hard Core transitions. H. Mori, S. Isa. H. Okamoto and H. Furukawa. Prog. Theo. Phys (Japan) 48, 1474 (1972).

337. Numerical solution of the eigenvalue problem in infinite matrices in molecular dynarnics. E. Mathier. A. Attanassio. J. Keller. P. Nosberger. A. Bauder and H.H. Gunthard. Comput. Phys. Coinmun. 4. 20 (1972).

338. Solution of the Percus-Yevick equation using the Dymond Alder potential for argon. R.L. Kerber J. Chem. Phys. 56. 2488 (1972).

339. Velocity autocorrelation function and diffusion coefficient in a liquid 11. M.I. Barker and T. Gaskell. J. Phys. C5. 253 (1972).

340. Molecular dynamics: dissociation of H, by He. N.J. Brown and N.J. Munn. J. Chem. Phys. 56. 1983 (1972).

341. R.M.J. Cotterill and L.B. Pedersen, in Interatornic Potentials and Simulation of Lattice Defects, eds. P.C. Gehlen. J.R. Beeler and R.1. Jaffee (Plenum, New York. 1972), p. 439.

342. G.H. Vineyard. in Interatomic Potentials and Simulation of Lattice Defects. eds. P.C. Gehlen. J.R. Beeler and R.I. Jaffee (Plenum. New York. 1972). p. XV.

343. Mean spherical model for the 6.12 potential, R.O. Watts. D. Henderson and J. Barker. J. Chem. Phys. 57. 5391 (1972).

344. R. Collins. in Phase Transitions and Critical Phenomena. V.2. eds. C. Domb and M.S. Green (Academic Press. London. 1972). p. 271.

345 J.A Barker and D. Henderson. in Annual Review of Physical Chemistry. V. 23. eds. H. Eyring. C.J. Christensen and H.S. Johnston. (Annual Reviews Inc.. Palo Alto. California. 1972). p. 439..

346. Some quantitative aspects of ionic melt microstructure, L.V. Woodcock, Proc. Roy. Soc. A (GB) **328,** 83 (1972).

347. Light scattering from ionic liquids. J.H.R. Clarke and L.V. Woodcock. J. Chem. Phys. 57. 1006 (1972).

348. Mean spherical model for the 6:12 potential. R.O. Watts. D. Henderson and J. Barker. J. Chem. Phys. 57. 5391 (1972).

349. Energies. volumes and entropies of forrnation of point defects in fcc Lennard-Jones systems. L. Borstnig Pedersen. Cryst. Lattice Defects (GB) **3.** 145 (1972).

350. Computer Simulation of Phase Trznsition. T. Schneider. Second General Conf. European Phys. Soc. on Trends in Phys.. Wiesbaden. Germany. 3-6 October 1972 (Petit-Lancy. Switzerland European Phys. Soc. 1972). p. 30.

351. Perturbation theory for the thermodynamical properties of simple liquids. L. Verlet and J.J. Weis. Mol. Phys. (GB) 24. 1013 (1972).

352. Hydrodynamic theory of the angular velocity auto-correlation function. B.J. Berne. J. Chem. Phys. 56. 2164 (1972).

M D 353. Molecular dynamics of a droplet of 475 moiecules. A. Rahman. Report of a CECAM Workshop on Molecular Dynamics and Monte Carlo Calculations on water (Orsay. 1972). p. 40.

M D 354. Molecular dynamics with the Ben-Naim Stillinger model. A. Rahman. Report of a CECAM Workshop on Molecular Dynamics and Monte Carlo Calculations on Water (Orsay. 1972). p. 56.

M D 355. Molecular dynainics with the Boi potential. A. Rahman. Report of a CECAM Workshop on Molecular Dynamics and Monte Carlo calculations on Water (Orsay. 1972). p. 58.

M D 356. Molecular dynamics on 216 polarisable water molecules. H.J.C. Berendsen and G.A. van der Velde. Report of a CECAM Workshop on Molecular Dynamics and Monte Carlo Calculations on Water (Orsay. 1972). p. 63.

M D 357. Polarisability and quantum calculations. P. Barnes. Report of a CECAM Workshop on Molecular Dynarnics and Monte Carlo Calculations on Water (Orsay. 1972). p. 77.

M D 358. Polarizability effects in ice. J. Orban and A. Bellemans. Report of a CECAM Workshop on Molecular Dynamics and Monte Carlo Calculations on Water (Orsay. 1972). p. 90.

M D 359. Molecular dynamics with a first-order quantuin correction. K. Singer. Report of a CECAM Workshop on Molecular Dynamics and Monte Carlo calculations on water (Orsay. 1972). p. 94.

M D 360. A direct approach to quantum – niechanical molecular dynamics. H.J.C. Berendsen. Report of a CECAM Workshop on Molecular Dynamics and Monte Carlo calculations on Water (Orsay. 1972). p. 98.

MD 361. The Kirkwood correlation factor in a model ice. J. Orban. Report of a CECAM Workshop on Molecular Dynamics and Monte Carlo Calculations on Water (Orsay. 1972). p. 11.

MD 362 Molecular dynamics studies of the properties of small clusters of argon atoms. D.J. McGinty, J. Chem. Phys. **58.** 4733 (1973).

MD 363. Molecular dynamics study of dimer formation. Herman W. Harrison and William C. Shieve. J. Chem. Phys. **58.** 3634 (1973).

MD 364. Computer experiments on classical fluids IV. Transport properties and time correlation functions of the Lennard-Jones liquid near its triple point. D. Levesque. L. Verlet and J. Kurkijarvi. Phys. Rev. **A7.** 1690 (1973).

MD 365. Second sound in a solid under shock compression. D.H. Tsai and R.A. MacDonald. J. Phys. C (GB) **6.** p. L 171 (1973).

MD 366. Depolarized light scattering froin monatomic fluids. Bruce J. Berne. Marvin Bishop and A. Rahman. J. Chem. Phys **58**. 2696 (1973).

MD 367. Molecular dynamics studies of inelting 1. Dislocation density and pair distribution function. E.J. Jensen. W.D. Kristensen and R.M.J. Cotterili Phil. Mag. (GB) **27.** 623 (1973).

MD 368. Simulation of diatomic homonuclear liquids. J. Barojas. D. Levesque and B. Quentrec. Phvs. Rev. A7. 1092 (1973).

MD 369. A pair potentiai for liquid rubidiuin from the pair correlation function. W. Schommers. Phys. Lett. **A43.** 157 (1973).

MD 370. Computer siinulation studies of the liquid state. P. Schofield. Coinput. Phvs. Commun (Netherlands) **5.** 17 (1973).

MD 371. Coinputer siinulation in radiation damage studies. 1.M. Torrens. Comput. Phys. Commun (Netherlands) **5**. 32 (1973)

MD 372. Melting of microcrystals in two dimensions: A molecular dynamics simulation. R.M.J. Cotterill. Comput. Phvs. Commun. (Netherlands) **5**. 28 (1973).

MD 373. Molecuiar dynamics studv of clustering in hard parallel squares. C. Carlier and H.L. Frisch. Phvs. Rev. A7. 348 (1973).

MD 374. Depolarization of light in atomic fluids, B.J. Alder. J.J. Weis and M.L. Strauss, Phys. Rev. **A7,** 281 (1973).

375. Collective motions in classical liquids III., Liquid sodium. K.N. Pathak. K.S. Sicgwi. Nuovo Cimento 1313. 185 (1973).

376. Equations for the correlation function in the Bijl-Dingle-Jastrow description of liquid ^{4}He at absolute zero, Deok Kyo Lee and F.H. Ree Phys. Rev. **A7.** 730 (1973).

377. Studies in molecular dynamics by collision induced infra-red absorption in H, – rare gas mixture i. Profile analysis and the intercollisional interference effect. J.W. MacTaggart and H.L. Welsh. Can. J. Phys. 51. 158 (1973).

378. Frequency moments and viscosities of liquid sodium, R. Bansal, J. Phys. G6, 1204 (1973).

379. Ordering metastability and phase transitions in two dimensional systems, J.M. Kosterlitz and D.J. Thouless, J. Phys. ***C6,*** 1181 (1973).

380. Correlation functions of classical fluids I. The radial distribution functions of mixtures of Kihara molecules in the Percus-Yevick approximation and their thermodynamic functions, L.L. Lec, H.M. Hulburt J. Chem. Phys. 58, 44 (1973).

381. Correlation functions of classical fluids II, The direct correlation functions of Kihara molecules in the Percus-Yevick theory and the integral cornpressibility equation of state. L.L. Lec and H.M. Hulburt, J. Chem. Phys. 58, 61 (1973).

382. Free molecule flow in a right circular cylinder. E. Garelis and T.E. Wainwright, Phys. Fluids 16, 476 (1973).

383. Limiting behaviour of fluid distributions: functions for small distances, D. Henderson, Mol. Phys. (GB) 25, 603 (1973).

384. Statistical mechanical calcuiation of the surface properties of a strongly interacting boson fluid, **C.A.** Croxton, J. Phys. C (GB) 6, 411 (1973).

385. General theory of elastic light scattering, L. Blum and H.L. Frisch J. Chem. Phys. 58, 135 (1973).

386. Phase transitions in two dimensional lattice gases of hardcore molecules with long-range attractions, C.K. Hall and G. Stell, Phys. Rev. **A7,** 1679 (1973).

387. Evaluation of boundary effects in monomerdimer mixtures by the method of lattice constants II. Extension to the simple cubic lattice and general discussion, **A.** Bellemans, Physica 65, 89 (1973).

MD 388. **A** 10,000 particle molecular dynamics model with long range forces, R.W. Hockney, S.P. Goel, J.W. Eastwood, Chem. Phys. Lett. (in press 1973).

MD 389. **A** quiet high-resolution computer model of a plasma, R.W. Hockney, S.P. Goel, J.W. Eastwood, J. Computational Physics (to appear).

MD 390. **A** molecular dynamics study of the melting of a three-dimensional crystal, R.M.J. Cotterill, E.J. Jensen, W. Damgaard Kristensen (in press 1973).

391. Statistical mechanics of dense ionized matter I. Equilibrium properties of the classical one-component plasma, J. P. Hansen, LPTHE 73/9 (Orsay, March 1973).

392. Statistical mechanics of dense ionized matter 11. Equilibrium properties and melting transition of the crystallized one-component plasma, E.L. Pollock and J.P. Hansen, LPTHE 73 12 (Orsay, March 1973).