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Theoretical models for fluid thermodynamics based on the quasi-Gaussian entropy theory

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**Theoretical models for fluid
thermodynamics based on the
quasi-Gaussian entropy theory**

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door

Andrea Amadei

geboren op 14 januari 1966
te Rome, Italië

Promotor: Prof. dr. H.J.C. Berendsen

*Wat mij 's nachts bezighoudt
is het geritsel van oorzaken,
geritsel als van kleine dieren
scharrelend onder herfstbladeren
onvermoeibaar op zoek naar mijn ontwaken.¹*

To Paola, Spartaco and Francesca

Beoordelingscommissie:

Prof. dr. M. Winnink

Prof. dr. D. Frenkel

Prof. dr. D. Bedeaux

This Thesis is based on the following publications:

1. A. Amadei, M.E.F. Apol and H.J.C. Berendsen. *Extensions of the quasi-Gaussian entropy theory*. J. Chem. Phys. **106**, 1893-1912 (1997). [Chapter 2]
2. A. Amadei, M.E.F. Apol and H.J.C. Berendsen. *On the use of the quasi-Gaussian entropy theory in non-canonical ensembles. I. Temperature dependence of thermodynamic properties*. J. Chem. Phys. **109**, 3004-3016 (1998). [Chapter 3]
3. M.E.F. Apol, A. Amadei and H.J.C. Berendsen. *On the use of the quasi-Gaussian entropy theory in non-canonical ensembles. II. Density dependence of thermodynamic properties*. J. Chem. Phys. **109**, 3017-3027 (1998). [Chapter 4]
4. D. Roccatano, A. Amadei, M.E.F. Apol, A. Di Nola and H.J.C. Berendsen. *Application of the quasi-Gaussian entropy theory to molecular dynamics simulations of Lennard-Jones fluids*. J. Chem. Phys., in press. [Chapter 5]
5. A. Amadei, M.E.F. Apol, G. Chillemi, H.J.C. Berendsen and A. Di Nola. *Derivation of a general fluid equation of state based on the quasi-Gaussian entropy theory: application to the Lennard-Jones fluid*. Submitted. [Chapter 6]
6. M.E.F. Apol, A. Amadei, H.J.C. Berendsen and A. Di Nola. *An equation of state for sub- and supercritical water based on the quasi-Gaussian entropy theory*. Manuscript in preparation. [Chapter 7]

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