



Advanced methods for atomic scale spin simulations and application to localized magnetic states

Gideon Philipp Müller

Schlüsseltechnologien / Key Technologies

Band / Volume 205

ISBN 978-3-95806-432-4

Forschungszentrum Jülich GmbH
Peter Grünberg Institut (PGI)
Quanten-Theorie der Materialien (PGI-1/IAS-1)

Advanced methods for atomic scale spin simulations and application to localized magnetic states

Gideon Philipp Müller

Schriften des Forschungszentrums Jülich
Reihe Schlüsseltechnologien / Key Technologies

Band / Volume 205

ISSN 1866-1807

ISBN 978-3-95806-432-4

CONTENTS

INTRODUCTION	1
1.1 General	1
1.2 Model	8
1.2.1 The extended Heisenberg Hamiltonian	9
1.2.2 The micromagnetic Hamiltonian	11
1.2.3 Derivatives of the energy	13
1.3 Monte Carlo	16
1.4 Landau Lifshitz Gilbert dynamics	22
1.4.1 Precession dynamics	24
1.4.2 Stochastic LLG	27
1.4.3 Current-driven dynamics	28
1.4.4 Energy minimisation	30
1 RATE THEORY AND MINIMUM ENERGY PATHS	33
1.1 Introduction	33
1.2 Calculating minimum energy paths	35
1.2.1 The nudged elastic band method	35
1.2.2 Adaptation to spin systems	37
1.2.3 Improvements on the regular NEB method	40
1.2.4 Test: Gaussian potentials	42
1.2.5 Application to a 2D skyrmion texture	45
1.2.6 Nontrivial 2D textures: skyrmion "sacks"	46
1.3 Transition rate calculations	57
1.3.1 Transition state theory	58
1.3.2 HTST: harmonic approximation	59
1.3.3 Entropy contributions	64
1.3.4 Zero mode contributions	65
1.4 The dynamical matrix	67
1.5 Eigenmodes of the dynamical matrix	69
1.5.1 Simplification in the precession-only case	70
1.6 Transition rate test case: 2D skyrmions	72
1.6.1 Simple cubic lattice	73
1.6.2 Hexagonal lattice	75
1.6.3 Arrhenius plot of the radial collapse	76
1.7 Rate theory applied to a skyrmion on a racetrack	77

2	SADDLE POINT SEARCHES	81
2.1	Minimum mode following method	81
2.2	Considering constraints	84
2.2.1	Eigenmodes of the Hessian matrix	87
2.3	MMF applied to a single spin	87
2.4	Novel skyrmion transition revealed by the MMF method	91
3	IMPLEMENTATION: SPIRIT - A SPIN SIMULATION FRAMEWORK	99
3.1	Code Structure	100
3.1.1	Considerations for the variety of methods	105
3.1.2	Considerations for parallelisation	106
3.1.3	Considerations for simplicity	109
3.2	Hamiltonians	110
3.3	Solvers	113
3.3.1	Heun	113
3.3.2	Depondt	114
3.3.3	4 th order Runge-Kutta	114
3.3.4	Semi-implicit midpoint	115
3.3.5	Velocity projection	116
3.3.6	Nonlinear conjugate gradients	117
3.3.7	Comparison of dynamics solvers	118
3.4	Graphical user interface	120
3.5	Application Programming Interface	127
3.5.1	C API layer	127
3.5.2	Python API	127
4	3D MAGNETIC TEXTURES	129
4.1	The chiral bobber	130
4.2	In search of new localised states	133
5	CONCLUSION	145
	APPENDIX	149
A	Energy data interpolation	150
B	Gaussian Hamiltonian	152
B.1	Derivatives	152
B.2	GNEB test script	153
B.3	MMF test script	155
C	Derivations of the Hessian matrix on Riemannian manifolds	157
C.1	The spin manifold	157
C.2	Projection	157
C.3	Transformation	158
C.4	Constrained Hessian approach	158

C.5	Projector-based approach	159
C.6	Spherical coordinate approach	161
C.7	Covariant approach	161
D	MMF mode and force fields	163
E	Contributors to Spirit	166
F	Used software packages	170
BIBLIOGRAPHY		171

Schlüsseltechnologien / Key Technologies
Band / Volume 205
ISBN 978-3-95806-432-4

Mitglied der Helmholtz-Gemeinschaft

