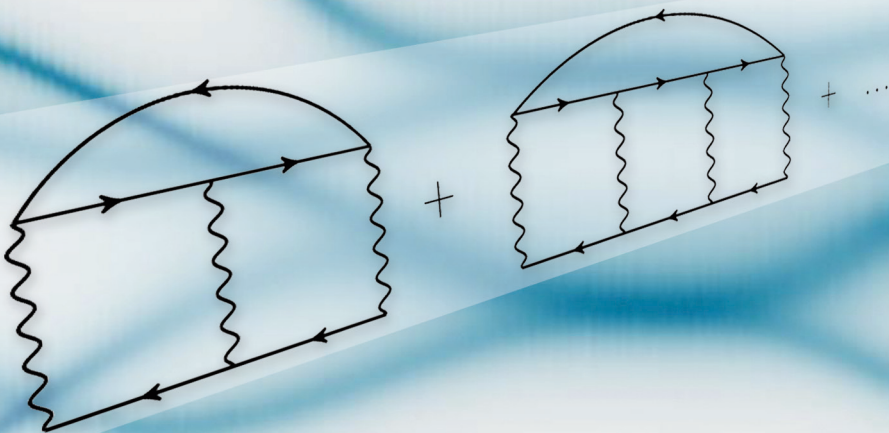


Spin-wave excitations and electron-magnon scattering in elementary ferromagnets from *ab initio* many-body perturbation theory

Mathias Christian Thomas David Müller



Schlüsseltechnologien /
Key Technologies
Band/ Volume 146
ISBN 978-3-95806-242-9

Forschungszentrum Jülich GmbH
Peter Grünberg Institute (PGI)
Quantum Theory of Materials (PGI-1 / IAS-1)

Spin-wave excitations and electron-magnon scattering in elementary ferromagnets from *ab initio* many-body perturbation theory

Mathias Christian Thomas David Müller

Schriften des Forschungszentrums Jülich
Reihe Schlüsseltechnologien / Key Technologies

Band / Volume 146

ISSN 1866-1807

ISBN 978-3-95806-242-9

Contents

1	Introduction	1
2	Theoretical Foundations	7
2.1	Many-Body Perturbation Theory	8
2.1.1	Green Function	11
2.1.2	Hedin Equations	13
2.2	Density-Functional Theory	16
2.2.1	Kohn-Sham Formalism	17
2.3	Full-Potential Linearized Augmented-Plane-Wave Method	19
3	Spin-Wave Excitations	23
3.1	Introduction	23
3.2	Theory	28
3.3	Implementation	32
3.3.1	Formulation in a Wannier Basis	34
3.3.2	Sum Rules	37
3.4	Formal Discussion of the Goldstone-Mode Condition	41
3.4.1	One-Band Hubbard Model	44
3.4.2	Local-Spin-Density Approximation	46
3.4.3	Coulomb Hole and Screened Exchange Approximation	48
3.5	Results	50
3.5.1	Computational Details	50
3.5.2	Coulomb Hole and Screened Exchange Approximation	51
3.5.3	Spin-Wave Dispersions	55
3.6	Summary	61
4	Electron-Magnon Scattering	63
4.1	Introduction	63
4.2	Theory	67

4.3	Implementation	75
4.3.1	Formulation in a Wannier Basis	76
4.3.2	Frequency Integration	77
4.4	Quasiparticle Concept	81
4.4.1	Quasiparticle Equation	81
4.4.2	Spectral Function	82
4.4.3	Effective Mass	83
4.4.4	Satellites	85
4.5	Formal Discussion of the Electron-Magnon Self-Energy	87
4.6	Computational Details	92
4.6.1	Frequency Integration	93
4.6.2	Starting-Point Dependence	97
4.7	Results	100
4.7.1	Iron	103
4.7.2	Cobalt	111
4.7.3	Nickel	116
4.8	Summary	122
5	Conclusions	127
 Appendix		
A	Padé Approximation	133
B	Coulomb Hole and Screened Exchange Self-Energy	139
	List of Abbreviations	141
	Bibliography	143
	List of Publications	171
	Acknowledgment	173

Schlüsseltechnologien /
Key Technologies
Band / Volume 146
ISBN 978-3-95806-242-9

