Implementation of a relativistic full-potential KKR method and a numerical discussion for the Mathieu potential

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For the implementation of a fully-relativistic full-potential Korringa-Kohn-Rostoker Green function method, an accurate solution of the single-site scattering problem is necessary. Within this talk an implementation of a solver for the single-site scattering problem will be discussed, first, by means of the direct solution of the underlying differential equations and, second, by means of the solution of the Lippmann-Schwinger equation. Furthermore the numerical accuracy for the Mathieu potential [1] will be compared. Instead of using the Lippmann-Schwinger equation like in previous implementations [2,3], it will be shown, that the solution via linear multi-step methods is a reasonable choice. In particular, an Adams-Bashforth-Moulton predictor-corrector method was implemented within the KKR code Hutsepot and it will be used to compare analytical and numerical band structure calculations.

References

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