A 19: Atomic systems in external fields II

Time: Tuesday 14:00–15:15 Location: V57.05

A 19.1 Tue 14:00 V57.05

Spectra of harmonium in a magnetic field using the Herman-Kluk propagator — •Frank Grossmann[1] and Tobias Kramer[2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden — [2]Institut für Thoeretische Physik, Universität Regensburg, 93053 Regensburg

For two interacting electrons in a harmonic quantum dot and a constant magnetic field, we show that time-dependent semiclassical calculations using the Herman-Kluk initial value representation of the propagator [1] lead to eigenvalues of the same accuracy as WKB calculations with Langer correction [2]. The latter are restricted to integrable systems, however, whereas the time-dependent initial value approach allows for applications to high-dimensional, possibly chaotic dynamics and can be extended to arbitrary shapes of the potential. The Langer correction is not needed due to the fact that we are using Cartesian coordinates [3].

[1] M. Herman and E. Kluk, Chem. Phys. **91**, 27 (1984)
[2] F. Grossmann and T. Kramer, J. Phys. A **44**, 445309 (2011)
[3] G. van de Sand and J.-M. Rost, Phys. Rev. A **59**, R1723 (1999)

This work was supported by the DFG through grants GR 1210/4-2 as well as KR 2889/2.

A 19.2 Tue 14:15 V57.05

Moving neutral atoms in neutron star magnetic fields — •Thorsten Kersting and Günter Wunner — 1. Institut für Theoretische Physik, Universtität Stuttgart

In the past years, significant improvements in numerical calculations of atoms in neutron star magnetic fields have lead to the possibility of producing a huge amount of atomic data, which can serve as a basis for modeling neutron star atmospheres. To calculate the quantity of interest, i.e. the opacity, from cross sections and dipole strengths, it is necessary to consider broadening effects due to influences of the hot plasma in the neutron star atmosphere. The largest broadening effect for atoms in neutron star magnetic fields is likely to be the influence of the motional stark effect induced by the magnetic field. We present a method for calculating energies and wave functions which not only works for hydrogen and hydrogen-like helium, as in previous work, but also for any neutral atom.

A 19.3 Tue 14:30 V57.05

Hartree-Fock calculations for the photoionisation of light to medium-heavy atoms and ions in neutron star magnetic fields — •Peter Diemand, Thorsten Kersting, Damir Zajec, and Günter Wunner — 1. Institut für Theoretische Physik, Universität Stuttgart

We derive the photoionisation cross section in dipole approximation for many-electron atoms and ions in neutron star magnetic field strengths in the range of 10^7 to 10^9 T. Both bound and continuum states are treated in adiabatic approximation in a self-consistent way. Bound states are calculated by solving the Hartree-Fock-Roothaan equations using finite element and B-spline techniques. We have taken into account mass and photon density in the neutron star's atmosphere as well as thermal occupation. The data are of importance for the quantitative interpretation of observed x-ray spectra that originate from the thermal emission of isolated neutron stars. They can serve as input for modeling neutron star atmospheres as regards chemical composition, magnetic field strength, temperature, and redshift. Our main focus in this talk lies on helium, since it is simple enough to calculate all possible transitions when limiting the quantum numbers, while still being sufficiently complicated to show all the basic structures and behaviour of heavier elements up to iron.

A 19.4 Tue 14:45 V57.05

Advanced Landau expansion of atoms in neutron star magnetic fields — •Christoph Schimeczek and Günter Wunner — 1. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart

Chasing the origin of still unexplained absorption features in the spectra of neutron stars with intense magnetic fields of 10^8 T, we have developed efficient tools to describe atomic states under such conditions. By enhancing our Hartree-Fock method to a full 2D variation and introducing approximations for the electron interaction terms we can reduce the absolute error for the binding energies to below one per cent and increase the range of validity of our code towards the regime of intermediate magnetic field strengths. Furthermore, the increase in calculation time compared to simpler methods is kept very low, resulting in an extraordinary program efficiency.

A 19.5 Tue 15:00 V57.05

Correlation function quantum Monte Carlo calculations for ground and excited states of helium and lithium in neutron star magnetic fields — •Sebastian Boblest, Dirk Meyer, and Günter Wunner — Universität Stuttgart

We present results of the application of the correlation function quantum Monte Carlo method to the calculation of atomic data of helium and lithium in neutron star magnetic fields, using symmetry adapted basis sets computed with a Hartree-Fock-Roothaan method. These results include energy levels for ground and excited states at different magnetic field strengths with unprecedented accuracy. The atomic data obtained in these and future calculations for medium-heavy atoms are of relevance to the analysis of features discovered in the thermal emission spectra of isolated neutron stars.