

# **University of Stuttgart** Institute for Theoretical Physics I

### Introduction

Excitons in cuprous oxide are described by the Hamiltonian

$$\mathcal{H} = \frac{\boldsymbol{p}_{e}^{2}}{2\boldsymbol{m}_{e}} + \mathcal{T}_{h}(\boldsymbol{p}_{h}, \boldsymbol{I}, \boldsymbol{S}_{h}) - \frac{\boldsymbol{e}^{2}}{4\pi\boldsymbol{\varepsilon}_{0}\boldsymbol{\varepsilon}|\boldsymbol{r}_{e} - \boldsymbol{r}_{h}|}, \qquad (1)$$

where the kinetic energy of the hole includes band structure terms and the spin-orbit interaction depending on the quasispin I = 1 and the hole spin  $S_h = 1/2$ . In the bulk the Hamiltonian can be reduced to three-dimensional relative coordinates, which is the basis for quantum mechanical and semiclassical investigations.



# Classical exciton dynamics, quantum wells, and EIT in cuprous oxide

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#### **Excitons in quantum wells**

In a hydrogenlike model for excitons in quantum wells the Hamiltonian (1) can be reduced to three degrees of freedom in the coordinates ( $\rho$ ,  $z_{\rm e}$ ,  $z_{\rm h}$ ). Spectra (here for m = 1) are obtained using B-spline basis functions with a highly optimized version (CPU time and memory reduced to 1.2% and 16%) of a program written by Pavel Belov. The ground state energy of the quantum wells without Coulomb interaction  $E_{N_{\rm e},N_{\rm h}} = \frac{\pi^2 \hbar^2}{2d^2} \left( \frac{N_{\rm e}^2}{m_{\rm e}} + \frac{N_{\rm h}^2}{m_{\rm h}} \right)$  has been subtracted.

F. Schweiner, J. Main, M. Feldmaier, et al., PRB **93**, 195203 (2016) J. Ertl, M. Marquardt, M. Schumacher, et al., PRL **129**, 067401 (2022)

# Chaos in the classical exciton dynamics

For the investigation of the classical exciton dynamics we apply an adiabatic approach by assuming that the dynamics in coordinate space is slow compared to the spin dynamics. This yields energy surfaces  $W_{y,g}(\mathbf{p})$  for the computation of yellow and green exciton orbits using the classical Hamiltonian

$$H = \frac{\boldsymbol{p}^2}{2\boldsymbol{\mu}} + \boldsymbol{W}_{y,g}(\boldsymbol{p}) - \frac{\boldsymbol{e}^2}{4\pi\boldsymbol{\varepsilon}_0\boldsymbol{\varepsilon}\boldsymbol{r}}.$$
 (2)

The classical exciton dynamics of both yellow and green excitons with principal quantum number n = 5 in two-dimensional symmetry planes of the crystal are



analyzed with Poincaré surfaces of section (PSOS).

Top: The PSOS for the yellow exciton series in the symmetry plane perpendicular to the [001] axis consists of mostly regular tori.



#### P. A. Belov, PRB **105**, 155417 (2022) N. Scheuler, Bachelor thesis, Univ. Stuttgart, in preparation (2023)



When the band structure terms are considered, symmetries are further broken resulting in a four-dimensional coordinate space. Using relative and center of mass coordinates in the *xy*plane and a further transformation to cylindrical coordinates we have derived the complete Hamiltonian

Bottom: The PSOS for the green exciton series in the symmetry plane perpendicular to [001] (left) shows a mixed regular-chaotic phase space. The dynamics for the green series in the symmetry plane perpendicular to  $[1\overline{1}0]$  (right) is completly chaotic.



$$\mathcal{H} = \mathcal{T}(\rho, \rho_{\rho}, \varphi, L_{z}, \rho_{z_{e}}, \rho_{z_{h}}, \mathbf{I}, \mathbf{S}_{h}) + \mathcal{V}(z_{e}, z_{h}) - \frac{e^{2}}{4\pi\varepsilon_{0}\varepsilon\sqrt{\rho^{2} + (z_{e} - z_{h})^{2}}},$$

which will be the basis for future exact quantum computations of excitons in quantum wells including the valence band structure.

F. Pfeiffer, Bachelor thesis, Univ. Stuttgart, in preparation (2023)

# **Electromagnetically induced transparency (EIT) in Cu<sub>2</sub>O**

EIT is a well established phenomenon in atomic physics. We have investigated possible interseries transitions between exciton states of the green and yellow series to realize EIT in cuprous oxide. For a three-level system consisting of a green 2*P*-state and a yellow 1*S*-state it is possible to achieve EIT using a laser field of ~ 100 kV/cm. The decay rates are given as  $\Gamma_{2P}^{g} = 2.14$  THz,  $\Gamma_{1S}^{y} = 50$  GHz and the Rabi frequencies are  $\Omega_{p} \ll \Omega_{c} = 249$  GHz. Similar results have been found for intraseries transitions in the yellow series.

green 2P

1.0 -

#### J. Ertl, P. Rommel, M. Mom, et al., PRB **101**, 241201(R) (2020) S. Rentschler, Bachelor thesis, Univ. Stuttgart, in preparation (2023)

February 28, 2023—https://itp1.uni-stuttgart.de/



P. Rommel, J. Main, S. O. Krüger, and S. Scheel, PRB **104**, 085204 (2021) J. Zeitler, Bachelor thesis, Univ. Stuttgart, in preparation (2023)



