SEARCHFOR EXCEPTIONAL POINTS IN CUPROUS OXIDE

P. Egenlauf, P. Rommel, J. Main

Institut für Theoretische Physik, Universität Stuttgart, Germany



University of Stuttgart Germany

INTRODUCTION

For non-hermitian operators eigenvalues as well as eigenstates can degenerate. This is referred to as exceptional point. For excitons in cuprous oxide in external electric and magnetic fields they appear for specific combinations of electric and magnetic field strengths and have already been calculated in a hydrogenlike model in parallel fields [1]. Theory and calculations are now extended by considering the band structure [2].

RESONANCES

- Coulomb potential can carry bound states
- Coulomb-Stark potential with external electric field f: bound states become resonances with a finite lifetime described by a complex eigenvalue $E \Rightarrow E - i\frac{\Gamma}{2}$

SEARCHING FOR EXCEPTIONAL POINTS

- Cover search area with ellipses
- Look for exchange behavior to find the ellipses which surround the EP

• Tunneling through potential barrier



COMPLEX COORDINATE ROTATION



- Eigenvalues of resonances solve Schrödinger equation
- Wave functions of resonances are non-normalizable

• Cover limited area with smaller ellipses and repeat the procedure



CONSIDERING THE BAND STRUCTURE

- Start with known EP for hydrogenlike model in parallel fields [1]
- Band stucture parameter *s* is multiplicated with the second and third Luttinger parameter as well as the η -values to controll the band structure
- Took steps of $\Delta s = 0.1$ to follow the trajectory of the EP in field plane \rightarrow extrapolate to s = 1 after finding the EP for s = 0.5
- coordinate rotation • Complex $S_{\theta}\Psi\left(\boldsymbol{r}\right)=\Psi\left(\boldsymbol{r}e^{\mathrm{i}\theta}\right)$
- Solve rotated Schrödinger equation $S_{\theta}\mathcal{H}S_{\theta}^{-1}S_{\theta}\Psi = ES_{\theta}\Psi$
- Wave functions of resonances are independent of complex rotation angle

EXCEPTIONAL POINTS

- Exceptional points are found for specific values of electric and magnetic field strengths
- Eigenvalues and eigenvectors degenerate at the EP
- Orbiting the EP in field plane \rightarrow exchange behavior of the two eigenvalues belonging to the EP

• EP moves along a straight line \rightarrow compared to hydrogenlike model (s = 0) the magnetic and electric field strengths for considered band structure (s = 1) were reduced by 4%



EXCITONS IN CUPROUS OXIDE

- Different stimulated states only yellow excitons (J = 1/2) were contemplated 0.484eV in the calculations
- Band structure is considered in the Hamiltonian
 - \rightarrow described by Luttinger parameters

green blue 2.172eV $|=E_{o}$ viole 0.131eV 1

- $\mathcal{H} = \mathcal{H}_{\text{hydrogenlike}} + s \cdot \mathcal{H}_{\text{bandstructure}}$ with $s \in [0, 1]$
- Diagonalization in a complete basis [2]

FUTURE WORK

- So far, basis functions have been restricted to yellow states with J = 1/2
- Future work: Consideration of the full basis including the green states with J = 3/2
- Comparisons with experimental results

REFERENCES

[1] M. Feldmaier et al., JPB 49, 144002 (2016). [2] P. Egenlauf, Bachelorarbeit, Universität Stuttgart (2020), DOI: 10.18419/opus-11120.