A quantum treatment of the anisotropic diamagnet Kepler problem in a silicon crystal with low concentration of phosphorus impurities

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Abstract

In this work we study the anisotropic diamagnetic Kepler problem which is related with the behavior of electron interaction with low densities of phosphorus impurities in a silicon crystal focusing on the case of a magnetic field along the [111] direction of the crystal. Here we propose a full quantum description to this problem by choosing an appropriate basis and implementing the complex rotation method to study the resonance states. With this approach we reproduce and improve reported results on the bound spectrum and resolve for the first time resonances above the first Landau ionization threshold.

Introduction

The study of classical chaotic systems and the properties of the corresponding quantum system have been of great interest along last years. Here, we study artificial atoms realized experimentally on silicon crystal with phosphorus impurities which are a useful analogue to study hydrogen-like atoms in presence of high magnetic fields such as the ones found in white dwarfs [1]. There is also evidence that suggests that the intensity and direction of the magnetic field can be tuned to control the transition from a regular to a chaotic regime. This opens the possibility of using chaos in future applications in semiconductor devices [2].

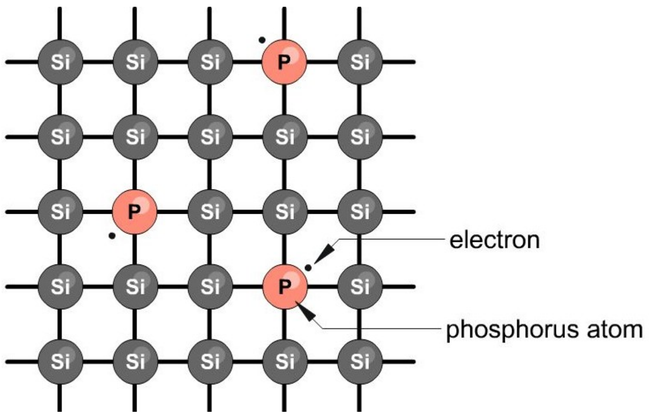

Figure 1. Graphic representation of the phosphorus impurities acting as artificial atoms inside the silicon crystal.

The effective mass in the silicon crystal displays an anisotropy giving rise to a give rise to a second-rank tensor for the effective mass which made this system more complicated than the one found with usual atoms, this problem is called the anisotropic diamagnetic Kepler problem (ADKP).

In this work we propose an ab-initio quantum approach for the description of the ADKP which combines a representation in a Sturmian basis representation [3] with the method of complex rotation [4] for the description of the resonances to reproduce photothermal ionization spectrum measurements.

Model

The effective mass theory in a silicon crystal with low concentration of phosphorus impurities leads to the Hamiltonian of the envelope function as

$$H = \frac{1}{2}(\boldsymbol{p} - q\boldsymbol{A})m^{*-1}(\boldsymbol{p} - q\boldsymbol{A}) - \frac{q^2}{4\pi\epsilon r}$$

Choosing our coordinate system such that the z direction corresponds to the [111] direction in the crystal, the mass tensor takes the form

$$m^* = \begin{pmatrix} m_\perp & 0 & 0 \\ 0 & m_\perp & 0 \\ 0 & 0 & m_\parallel \end{pmatrix}$$

Where $m_{||} = 0.9163m_0$ and $m_\perp = 0.1905m_0$, and m_0 is the bare electron mass.

Choosing the symmetric gauge, $\boldsymbol{A}=-1/2(\boldsymbol{r}\times\boldsymbol{B})$, our Hamiltonian can be written as $H = H_1 + H_2$,

$$\hat{H}_1 = \underbrace{-\frac{1}{2}\nabla^2 - \frac{1}{2}B_z\hat{L}_z - \frac{1}{r} + \frac{1}{8}B_z^2(x^2+y^2)}_{\text{Hydrogen atom}} - \frac{1}{2}(\gamma-1)\frac{\partial^2}{\partial z^2}.$$

$$\hat{H}_2 = \frac{1}{8}((x^2+y^2)B_z^2 + z^2B_x^2 - 2zxB_zB_x + \gamma y^2B_x^2) \\ i\frac{1}{2}\gamma B_x y\frac{\partial}{\partial z} - i\frac{1}{2}zB_x\frac{\partial}{\partial y}.$$

Here H_1 corresponds to the Hamiltonian for a magnetic field on the z direction, this term contains the Hamiltonian for an hydrogen atom plus a term with derivatives respect to z which gives us information about the effect of the anisotropy of the system [3]. H_2 give us information about the further effects of the anisotropy in the presence of the magnetic field.

In this work we focus on the case of a magnetic field in the z direction ([111] crystal direction) for which only the term H_1 is importan. We use the complex rotation method which provides the energies and autoionization rates [4,5]. Then we choose the Sturmian basis representation for the Coulomb potential to solve the Schrödinger equation and use the Lanczos algorithm [6] to solve the eigenvalue problem..

Results

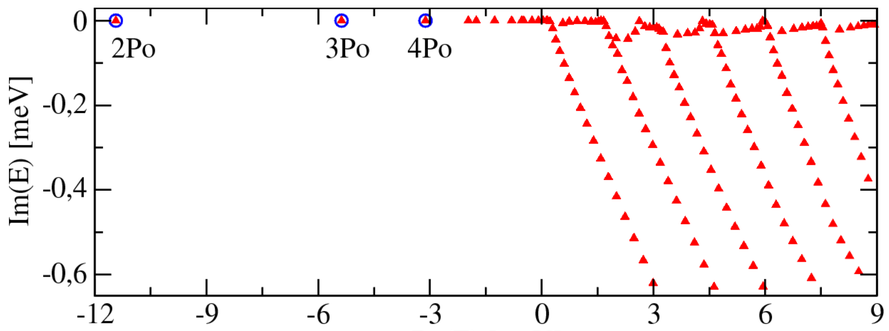

Figure 2. Odd parity spectrum of the rotated Hamiltonian for B_z = 2.4 T. The basis size is 20000. The blue dots indicates the states for which the quadratic Zeeman splitting is shown in Figure 3.

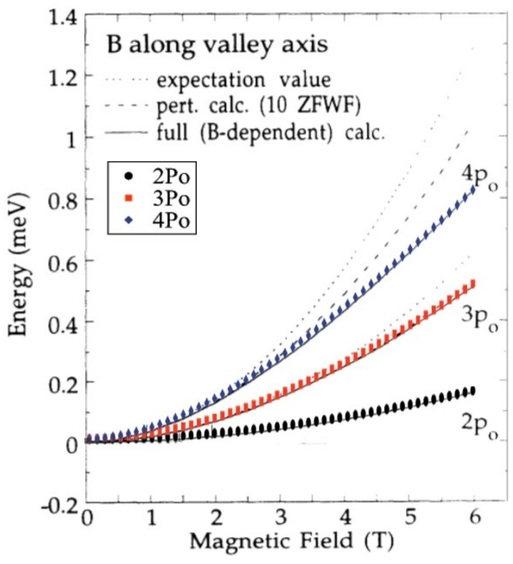

Figure 3. Comparative graph between the quadratic Zeeman shifts of the three lowest energy states with odd parity Zeeman (circles, squares and diamonds) and the ones found by Thilderkvist [7]

Conclusions

Within this approach we were able to reproduce and improve reported results on the bound spectrum of the field free and the diamagnetic anisotropic Kepler problem. Furthermore, we report here for the first time an spectrum above the first Landau ionization threshold.

References

[1] Murdin B.N *et al.* "Si:P as a laboratory analogue for hydrogen on high magnetic field white dwarf stars," Nature Communications, vol. 4, p. 1469, feb 2013.

[2] W. Zhou, Z. Chen, *et al.* "Magnetic Field Control of the Quantum Chaotic Dynamics of Hydrogen Analogs in an Anisotropic Crystal Field". Phys.Rev. Lett. 105, 024101 (2010).

[3] D. Wintgen, H. Marxer, and J. S. Briggs. "Efficient quantisation scheme for the anisotropic Kepler problem." J.Phys. A 20(15), L965 (1987).

[4] E. Balslev and J. M. Combes. "Spectral properties of many-body Schrödinger operators with dilatation-analytic interactions." Comm. Math. Phys. 22(4), 280–294 (1971).

[5] J. Madroñero. "Spectral properties of planar helium under periodic driving." Phd thesis,ludwig-maximilians-universität münchen (2004).

[6] Lanczos, "An iteration method for the solution of the eigenvalue problem of linear differential and integral operators," J. Res. Natl. Bur. Stand., vol. 45, p. 225, 1950.

[7] A. Thilderkvist *et al.* "Quadratic Zeeman effect of shallow donors in silicon." Phys. Rev. B 49 (1994).