The Spin-Orbit Interaction of an Electron in a Cylindrical Potential

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The effect of the spin-orbit interaction on the wave function of a low energy electron traveling through a cylindrical potential was explored using perturbation theory. The equations of the first order corrections to the wave functions $|n\, m\, \sigma\rangle$ and wave propagation constants $\beta_{n\,|m|}$ due to the the spin-orbit interaction were determined for the electron. The form of the unperturbed solution was found to fit that of the Bessel equation. Non-degenerate perturbation theory was successfully used to calculate the first order perturbations $|n\, m\, \sigma\rangle^1$ to the wave functions due to the spin-orbit interaction.

I. INTRODUCTION

The solutions for the wave function of an electron in a spherically symmetric potential (or known by some as the hydrogen atom), have been known for a good part of the twentieth century. Surprisingly, the solutions corresponding to an electron in a cylindrically symmetric potential are not as well known. An example of a cylindrically symmetric potential for an electron could be a very thin wire or a carbon nanotube such as rolled up graphene. One problem with this system is that its complexity hampers our ability to solve for exact solutions, which is why an approximation method such as perturbation theory can be used to calculate the final solution. Perturbation theory can be thought of as a tool similar to spectral decomposition in linear algebra or Taylor series in introductory calculus – it approximates solutions to a system to an arbitrary order of precision k, which in this paper is one.

One pitfall of the Schrödinger-Pauli equation is that it ignores the small changes or "corrections" to the wave function due to relativistic mass increase, the *zitterbwegung*, and the spin-orbit interaction. The first of these effects is well understood as the relativistic mass increase of the electron as it approaches the speed of light [1]. The second term, *zitterbewegung*, first proposed by Schrödinger [2] and first computed by Darwin [3], is German for "trembling motion" on the order of the reduced Compton wavelength λ_c. The third and final term represents the interplay between the electron spin angular momentum and orbital angular momentum [4], which is what we will focus on in this paper.

II. THEORY

The overarching goal of this paper is to calculate the allowed perturbed wave propagation constants β' due to spin-orbit interaction and to determine the perturbed wave functions Ψ' that result from these constants. The Schrödinger-Pauli equation in cylindrical coordinates is

$$\hat{H}^0 \Psi^0_{\omega\, n\, |m|\, \sigma}(\rho, \phi, z, t) = E_\omega \Psi^0_{\omega\, n\, |m|\, \sigma}(\rho, \phi, z, t), \qquad (1)$$

where $\Psi^0_{n\,|m|\,\sigma}(\rho, \phi, z, t)$ is the unperturbed wave function in cylindrical coordinates and $E_{n\,|m|}$ is the energy associated with the angular frequency ω by $E_\omega = \hbar\omega_{n\,|m|}$ where $\hbar$ is reduced Planck's constant. "Unperturbed" in this case means that the wave function does not yet account for the relativistic/*zitterbewegung*/spin-orbit corrections. It is important to note that, throughout this paper, the superscripts 0 and 1 are not powers but are orders. In this system, the eigenvalues are the wave propagation constants $\beta^0_{n\,|m|}$, given by $\beta^0_{n\,|m|} = \hbar/\hat{p}_z$, where $\hat{p}_z$ is the azimuthal component of the momentum. The nature of $\beta^0_{n\,|m|}$ is the same as that of k (spring constant), or any other wave propagation constant. The nth energy state is n, the azimuthal orbital angular momentum quantum number is m, and the spin angular momentum quantum number (or "spin") is σ. In this project, the main contributions to the perturbation come from m and σ, hence the name "spin-orbit interaction." The angular component is ϕ and the azimuthal component is z. The operator $\hat{H}^0$ of the unperturbed state can be written

$$\hat{H}^0 = mc^2 + \frac{\hat{p}^2}{2m} - eV(\rho), \qquad (2)$$

where $\hat{p} = -i\hbar\nabla$ is the momentum operator, $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$ is the gradient/Laplacian, m is the mass of the electron, e is the charge of the electron, and $V(\rho)$ is the potential at a normalized radius $\rho = r/a$. Here, r is the radial distance and a is the radius of the wave-guide (or the "cylinder"). This non-dimensionalizes the radial direction such that ρ is between zero and one within the cylinder and greater than one outside, which is something that proves to be useful throughout the calculations.

Since energy is given by $E^0 = \hbar\omega$, we can set ω as an experimental parameter. This means that for a given electron, we have a known ω because we chose it. Thus, ω can be eliminated from the subscript of Ψ^0. Using separation of variables, the unperturbed wave function can be rewritten as

$$\Psi^0_{n\, m\, \sigma}(\rho, \phi, z, t) = \psi^0_{n\, m}(\rho, \phi) e^{i(\beta^0_{n\,|m|} z - \omega t)} \hat{e}_\sigma, \qquad (3)$$

where $\beta^0_{n\,|m|}$ is the wave propagation constant. Noting that the Laplacian is comprised of a sum of squares of derivatives (which are hidden in $\hat{H}^0$), taking the z derivative of the wave function twice pulls down a factor of $-(\beta^0_{n\,|m|})^2$ times the same wave function, making $\beta^0_{n\,|m|}$ a handy parameter of the wave function's behavior as it travels through the potential. To make the notation more convenient, we set $(\beta^0_{n\,|m|})^2 = B^0_{n\,|m|}$. Furthermore, since this quantity is proportional to the wave function's azimuthal momentum, it is a good indicator of the wave front's speed down the tube. The function of the spin is simply to an add a two-ness to the system.

Multiplying both sides of Eq. 1 by $-2m/\hbar^2$ produces eigenvalues $B^0_{n\,|m|}$, making the equation fit the form of a Bessel equation [Appendix A]. The two solutions to this equation are called Bessel functions, Bessel J and Bessel K. This imposes a boundary condition equation,

$$\frac{U_{n\,|m|}J_{|m|+1}(U_{n\,|m|})}{J_{|m|}(U_{n\,|m|})} = \frac{\sqrt{R^2 - U^2_{n\,|m|}}K_{|m|+1}(\sqrt{R^2 - U^2_{n\,|m|}})}{K_{|m|}(\sqrt{R^2 - U^2_{n\,|m|}})}, \tag{4}$$

where $U_{n\,|m|} = a\sqrt{k^2(0) - B^0_{n\,|m|}}$ and the experimental parameter $R = (a/\lambda_c)\sqrt{2\Delta}$, and $\lambda_c = \hbar/(mc)$ is the reduced Compton wavelength. The constant $k(0)$ is given by

$$k(0) = \frac{2}{\lambda_c^2}\frac{\hbar\omega}{mc^2}. \tag{5}$$

The unperturbed wave function can now be expressed as

$$\Psi^0_{n\,m\,\sigma}(\rho, \phi, z, t) = \frac{N}{a}Z_{|m|}(U_{n\,|m|}\rho)e^{im\phi}e^{i(\beta^0_{n\,|m|}z - \omega t)}\hat{e}_\sigma, \tag{6}$$

where $Z_{|m|}(U_{n\,|m|}\rho)$ is the general form of the Bessel J and Bessel K functions, since we do not yet know what ρ the function will be evaluated at.

Now that we have a workable form of the unperturbed wave function, we can focus on the bigger picture of the paper. The actual perturbed Hamiltonian for the system is given,

$$\hat{H} = \hat{H}^0 + \hat{H}_{Rel} + \hat{H}_{Dar} + \hat{H}_{SO}, \tag{7}$$

where $\hat{H}^0$ is the original unperturbed Hamiltonian, $\hat{H}_{Rel}$ is the perturbation to the Hamiltonian due to relativistic effects, $\hat{H}_{Dar}$ is the perturbation to the Hamiltonian due to *zitterbewegung*, and $\hat{H}_{SO}$ is the perturbation to the Hamiltonian due to the spin-orbit interaction. The last of these perturbations is given by

$$\hat{H}_{SO} = \frac{e}{2m^2c^2}\hat{\mathbf{S}}\cdot(\mathbf{E}\times\hat{\mathbf{p}}), \tag{8}$$

where $\hat{\mathbf{S}} \equiv (\hbar/2)\hat{\vec{\sigma}}$ is the spin vector operator of 2×2 Pauli spin matrices, $\vec{E}$ is the vector representing the electric field of the electron, and $\hat{\mathbf{p}} \equiv -i\hbar\nabla$ is the momentum operator. Multiplying by $-2m/\hbar^2$ and doing some manipulation (shown in Appendix B), we get

$$\hat{H}_{SO} = \frac{-\Delta\chi'(\rho)}{2a^2\rho}(\hat{\sigma_z}\hat{l_z} + \rho\hat{\mathbf{N}}\partial_z), \tag{9}$$

where Δ is a constant representing the normalized height of the potential, $\chi(\rho)$ is a dimensionless function that increases monotonically from 0 to 1. The number operator is given by $\hat{\mathbf{N}} \equiv \hat{\sigma_+}\hat{l_-} - \hat{\sigma_-}\hat{l_+}$, where $\hat{\sigma_\pm}$ and $\hat{l_\pm}$ are the raising and lowering operators of the z components of spin and orbital angular momentum respectively.

From non-degenrate perturbation theory, we know that perturbed energies E^1_n and wave functions $\left|n^1\right\rangle$ are given by

$$E^1_n = \left\langle n^0\right|\hat{H'}_{SO}\left|n^0\right\rangle, \tag{10}$$

and

$$\left|n^1\right\rangle = \sum_{n'\neq n}\frac{\left\langle n'\right|\hat{H'}_{SO}\left|n\right\rangle}{E^0_n - E^0_{n'}}\left|n'\right\rangle, \tag{11}$$

where the primed quantum numbers represent all possible arbitrary quantum numbers up to $n_{\max}$. It is important to note that these equations are for non-degenerate perturbation theory, which does not work for our purposes because unperturbed states with differing quantum numbers that can have the same $B^0_{n\,|m|}$ and the equation would end up being divided by zero. Thus, we must use degenerate perturbation theory, which generates a perturbation $B^1_{n\,|m|}$ as opposed to $E^1_{n\,|m|}$. Because of this, we get

$$B^1_{n\,|m|} = {}^0\langle n\,m\,\sigma|\,\hat{H}_{SO}\,|n\,m\,\sigma\rangle^0, \tag{12}$$

and

$$|n\,m\,\sigma\rangle^1 = \sum_{n'\neq n}^{n_{max}}\sum_{m'_n\neq m_n}^{m_{max}}\sum_{\sigma'_n\neq\sigma_n}^{\sigma_{max}}\frac{{}^0\langle n'\,m'\,\sigma'|\,\hat{H}_{SO}\,|n\,m\,\sigma\rangle^0}{B^0_{n\,|m|} - B^0_{n'\,|m'|}}\,|n'\,m'\,\sigma'\rangle, \tag{13}$$

where the inner product is

$${}^0\langle n'\,m'\,\sigma'|\,\hat{H}'\,|n\,m\,\sigma\rangle^0 = \int_0^{2\pi}\int_0^\infty \Psi^0_{n'\,m'\,\sigma'}{}^\dagger\hat{H}_{SO}\Psi^0_{n\,m\,\sigma}\,rdrd\phi. \tag{14}$$

Evaluating the inner product in Eq. 12 yields the result

$$B^1_{n\,|m|} = \frac{-2\Delta\pi}{a^2} N^2_{n\,|m|} J^2_{|m|}(U_{n\,|m|}1), \tag{15}$$

which can be solved by inserting the calculated values of $U_{n\,|m|}$. The first order correction to $\beta_{n\,m}$ is approximated by

$$\beta^1_{n\,|m|} \approx \frac{1}{2}\frac{B^1_{n\,|m|}}{\beta^0_{n\,|m|}},$$

for $v<<c$ [6]. Knowing $\beta^1_{n\,|m|}$ allows us to determine the perturbed allowed wave propagation constants corrected to the first order, which are given by

$$\beta'_{n\,|m|} = \beta^0_{n\,|m|} + \beta^1_{n\,|m|}.$$

In its most abstract form, the inner product from Eq. 14 can be written as

$$\langle n'\,m'\,\sigma'|\,\hat{H}_{SO}\,|n\,m\,\sigma\rangle = \Big\langle n'\,m'\,\sigma'\Big|\Big[-\frac{\Delta\chi'}{2a^2\rho}\Big(2\sigma\,m\Big|n\,m\,\sigma\Big\rangle^0 +\rho\partial_z\Big(\Big|n,\,m{-}1,\,\sigma{+}1\Big\rangle^0\delta_{\sigma,\,-\frac{1}{2}}+\Big|n,\,m{+}1,\,\sigma{-}1\Big\rangle^0\delta_{\sigma,\,+\frac{1}{2}}\Big)\Big)\Big],$$

which evaluates to

$$\begin{aligned}\langle n'\,m'\,\sigma'|\,\hat{H}_{SO}\,|n\,m\,\sigma\rangle = \int_0^{2\pi}\int_0^{\infty} &\frac{N_{n'\,|m'|}}{a} Z_{n'\,|m'|}(U_{n'\,|m'|}\rho)e^{-im'\phi}e^{-i(\beta^0_{n'\,|m'|}z-\omega t)}\hat{e}^{\dagger}_{\sigma'}\\ &\Big[-\frac{\Delta\chi'}{2a^2\rho}\Big(2\sigma m\frac{N_{n\,|m|}}{a}Z_{n\,|m|}(U_{n\,|m|}\rho)e^{im\phi}e^{i(\beta^0_{n\,|m|}z-\omega t)}\hat{e}_{\sigma}\\ &+\rho\partial_z\Big(\frac{N_{n\,|m-1|}}{a}Z_{n\,|m-1|}(U_{n\,|m-1|}\rho)e^{i(m-1)\phi}e^{i(\beta^0_{n\,|m-1|}z-\omega t)}\hat{e}_{\sigma+1}\delta_{\sigma,-\frac{1}{2}}\\ &+\frac{N_{n\,|m+1|}}{a}Z_{n\,|m+1|}(U_{n\,|m+1|}\rho)e^{i(m+1)\phi}e^{i(\beta^0_{n\,|m+1|}z-\omega t)}\hat{e}_{\sigma-1}\delta_{\sigma,+\frac{1}{2}}\Big)\Big)\Big]\,rdrd\phi,\end{aligned} \tag{16}$$

After extensive manipulation, Eq. 16 is found to be equal to

$$\begin{aligned}\langle n'\,m'\,\sigma'|\,\hat{H}_{SO}\,|n\,m\,\sigma\rangle = &\frac{-\Delta\pi}{a^2}N_{n'\,|m'|}J_{|m'|}(U_{n'\,|m'|}1)\\ &\Big[2N_{n\,|m|}\delta_{m\,m'}\delta_{\sigma\,\sigma'}J_{|m|}(U_{n\,|m|}1)\\ &+iN_{n\,|m-1|}\delta_{(m-1),m'}\delta_{+\frac{1}{2}\,\sigma'}\beta^0_{n\,|m-1|}J_{|m-1|}(U_{n\,|m-1|}1)\\ &+iN_{n\,|m+1|}\delta_{|m+1|,m'}\delta_{-\frac{1}{2}\,\sigma'}\beta^0_{n\,|m+1|}J_{|m+1|}(U_{n\,|m+1|)}1)\Big].\end{aligned}$$

Inserting this into Eq. 13 cancels the m and σ sums making the new equation for the first order perturbation to the wave function,

$$\begin{aligned}|n\,m\,\sigma\rangle^1 = -\frac{\Delta\pi}{a^2}\sum_{n'\neq n}^{n_{max}}\Bigg[&\frac{2\,N_{n'\,|m|}N_{n\,|m|}J_{|m|}(U_{n'\,|m|}1)J_{|m|}(U_{n\,|m|}1)}{B^0_{n\,|m|}-B^0_{n'\,|m|}}\Big|n'\,m\,\sigma\Big\rangle\\ &+\frac{i\delta_{\sigma,+\frac{1}{2}}\beta^0_{n\,|m-1|}N_{n'\,|m-1|}N_{n\,|m-1|}J_{|m-1|}(U_{n'\,|m-1|}1)J_{|m-1|}(U_{n\,|m-1|}1)}{B^0_{n\,|m|}-B^0_{n'\,|m-1|}}\Big|n,'\,m-1,\,+\frac{1}{2}\Big\rangle\\ &+\frac{i\delta_{\sigma,-\frac{1}{2}}\beta^0_{n\,|m+1|}N_{n'\,|m+1|}N_{n\,|m+1|}J_{|m+1|}(U_{n'\,|m+1|}1)J_{|m+1|}(U_{n\,|m+1|}1)}{B^0_{n\,|m|}-B^0_{n'\,|m+1|}}\Big|n,'\,m+1,\,-\frac{1}{2}\Big\rangle\Bigg].\end{aligned} \tag{17}$$

Thus, we get a first order perturbation $|n\,m\,\sigma\rangle^1$ by adding to the unperturbed wave function $|n\,m\,\sigma\rangle^0$,

$$|n\,m\,\sigma\rangle' = |n\,m\,\sigma\rangle^0 + |n\,m\,\sigma\rangle^1. \tag{18}$$

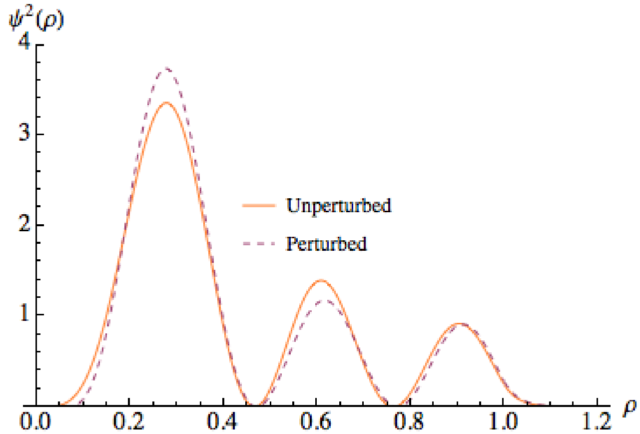

FIG. 1: Perturbed and unperturbed wave functions - The plot represents the probability of finding an electron along the radial direction ρ from the center of the waveguide for unperturbed and perturbed $\left|3,\, 2,\, -\frac{1}{2}\right\rangle$ eigenstates.

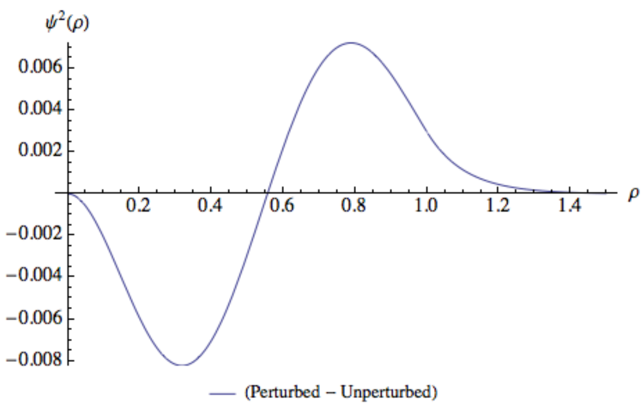

FIG. 2: Difference of the perturbed and unperturbed wave functions - The plot represents the difference of the perturbed and unperturbed wave functions along the radial direction ρ from the center of the waveguide for unperturbed and perturbed $\left|6,\, 2,\, -\frac{1}{2}\right\rangle$ eigenstates.

III. APPLICATION AND RESULTS

The electron waveguide parameter was chosen to be $R = 20$ and $\omega = 3.88172 \times 10^{16}$ Hz. The new perturbed wave functions were generated by adding the small perturbations due to spin-orbit to the unperturbed wave functions, as shown in Fig. 1. The plot is based on $\left|3,\, 2,\, -\frac{1}{2}\right\rangle$ perturbed and unperturbed eigenstates. The perturbed eigenstate is just slightly different from the unperturbed one, as expected. The initial downward curve in Fig. 2 indicates that the perturbed wave function is just slightly larger than the unperturbed one. The second part of the curve indicates exactly the opposite. This can be thought of as a "breathing" change, where the expectation expands or contracts. In this particular case, it means the the energy is pulled more towards the center of the waveguide. For different values of n, the probabilities of finding the electron at the origin were different.

IV. CONCLUSION

The effect of the spin-orbit interaction on the wave function of a low energy electron traveling through a cylindrical potential calculated successfully. The form of the unperturbed solution was found to fit that of the Bessel equation. Unfortunately, not enough plots were obtained due to bugs in the Mathematica code that modeled the system. We hope to obtain more plots once the code is fixed.

V. ACKNOWLEDGEMENTS

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Appendix A: Unperturbed Solutions

Substituting Eq. 2 into Eq. 1 and multiplying both sides of the resulting equation by $-2m/\hbar^2$ produces

$$\left(\frac{-\hat{p}^2}{\hbar^2}+\frac{2m}{\hbar^2}eV(\rho)\right)\Psi^0_{n\,|m|\,\sigma}(\rho,\phi,z,t) = \frac{-2m}{\hbar^2}E_0\,\psi^0_{n\,|m|\,\sigma}(\rho,\phi,z,t). \quad \text{(A1)}$$

Here, we define the zero-point energy to be mc^2 and $\Delta\chi(\rho)\equiv -eV(\rho)/mc^2$ where Δ is the dimensionless normalized difference in potential at the radius and at the center of the potential. Since $\hat{p}=-i\hbar\nabla$, we can rewrite this to be $\hat{p}^2=-\hbar^2(\partial_x^2+\partial_y^2+\partial_z^2)=-\hbar^2(\nabla_T^2+\partial_z^2)$ where ∇_T^2 is the transverse Laplacian. Using this and rearranging the equation produces

$$\left(\nabla_T^2+\frac{2m}{\hbar^2}E_0-\frac{2m^2c^2}{\hbar^2}\Delta\chi(\rho)\right)\Psi^0_{n\,|m|\,\sigma}(\rho,\phi,z,t) = -\partial_z^2\,\psi^0_n(\rho,\phi)\,e^{i(\beta^0_{n\,|m|}z-\omega t)}, \quad \text{(A2)}$$

where the partial derivative brings down a factor of $-(\beta^0_{n\,|m|})^2$ and makes a more condensed eigenvalue equation

$$\left[\nabla_T^2+k^2(\rho)\right]\Psi^0_{n\,|m|\,\sigma}(\rho,\phi,z,t)=B^0_{n\,|m|}\Psi^0_{n\,|m|\,\sigma}(\rho,\phi,z,t), \quad \text{(A3)}$$

making $B^0_{n\,|m|}$ the new eigenvalue of the equation with

$$k^2(\rho)\equiv\frac{2}{\lambda_c^2}\left(\frac{\hbar\omega}{mc^2}-\Delta\chi(\rho)\right). \quad \text{(A4)}$$

where λ is the reduced Compton wavelength. We define $\chi(\rho)$ such that it is 0 at $\rho=0$ and 1 at $\rho=1$ so that, after converting the transverse Laplacian to cylindrical Laplacian and a good deal of manipulation, we can rewrite Eq. A3 as

$$\left(\partial_\rho^2+\frac{1}{\rho}\partial_\rho+U^2_{n\,|m|}(\rho)-\frac{m^2}{\rho^2}\right)\Psi_{n|m|}(\rho)=0, \quad \text{(A5)}$$

where $U^2_{n\,|m|}(\rho)=a^2[k^2(\rho)-B^0_{n\,|m|}]$ is found numerically and the equation fits the form of the Bessel equation, which has known solutions [10].

The physical boundary conditions limit these Bessel functions to those that go to 0 at infinity, are continuous and have a continuous derivative at $\rho=1$. These conditions impose the following equation that must be satisfied

$$\frac{UJ_{|m|+1}(U)}{J_{|m|}(U)}=\frac{\sqrt{R^2-U^2}K_{|m|+1}(\sqrt{R^2-U^2})}{K_{|m|}(\sqrt{R^2-U^2})}, \quad \text{(A6)}$$

where $U\equiv a\sqrt{k^2(0)-B^0_{n\,|m|}}$ and $R\equiv(a/\lambda)\sqrt{2\Delta}$. This equation can be solved numerically using Mathematica by picking values for ω, a, and Δ, and generating a set of values of $U_{n\,|m|}$. After this, each $B^0_{n\,|m|}$ can be computed by using the definition of $U_{n\,|m|}$.

Appendix B: First-Order Perturbed Spin-Orbit Hamiltonian

The perturbation to the Hamiltonian corresponding to energy of an electron in a cylindrically symmetric potential is

$$\hat{H}'=-\left(\frac{1}{2mc^2}\left(\frac{\hat{p}^2}{2m}\right)^2+\frac{e\hbar^2}{8m^2c^2}\nabla\cdot\mathbf{E}-\frac{e}{2m^2c^2}\hat{\mathbf{S}}\cdot(\mathbf{E}\times\hat{\mathbf{p}})\right), \quad \text{(B1)}$$

which makes the expression for the spin-orbit Hamiltonian

$$\hat{H}_{SO}=\frac{e}{2m^2c^2}\hat{\mathbf{S}}\cdot(\mathbf{E}\times\hat{\mathbf{p}}). \quad \text{(B2)}$$

Multiplying both sides of Eq. B2 by $-2m/\hbar^2$ and defining the zero point energy $eV(0)=mc^2$ forces the Hamiltonian to have the same units as $B^1_{n\,|m|}$. This yields

$$\hat{H}_{SO}=-\partial_r\Delta\chi(\rho)\,\frac{\hat{\boldsymbol{\sigma}}}{2}\cdot\left[\hat{\mathbf{r}}\times\frac{\hat{\mathbf{p}}}{\hbar}\right], \quad \text{(B3)}$$

given that the momentum operator $\hat{\mathbf{p}}\equiv-i\hbar\nabla$, $\mathbf{E}=-\partial_r V(\rho)\hat{\mathbf{r}}$, and $\rho=r/a$, where $\hat{\mathbf{S}}$ is comprised of Pauli spin matrices

$$\hat{\boldsymbol{\sigma}}=\begin{bmatrix}\hat{\boldsymbol{\sigma}}_x\\ \hat{\boldsymbol{\sigma}}_y\\ \hat{\boldsymbol{\sigma}}_z\end{bmatrix}$$

where

$$\hat{\boldsymbol{\sigma}}_x=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},\ \hat{\boldsymbol{\sigma}}_y=\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix},\ \text{and}\ \hat{\boldsymbol{\sigma}}_z=\begin{bmatrix}1 & -0\\ 0 & -1\end{bmatrix},$$

such that $\hat{\mathbf{S}}=\hbar\hat{\boldsymbol{\sigma}}/2$. Using these matrices and evaluating the dot and cross products in Eq. B3 gives the final form of the spin-orbit Hamiltonian

$$\hat{H}_{SO}=\frac{\Delta\chi'(\rho)}{2a^2\rho}\left(\hat{\sigma}_z\hat{\ell}_z+\rho\hat{\mathbf{N}}\partial_z\right), \quad \text{(B4)}$$

where $\hat{\mathbf{N}}\equiv\hat{\sigma}_+\hat{l}_--\hat{\sigma}_-\hat{l}_+$ is the number operator, $\hat{\sigma}_\pm$ and $\hat{l}_\pm$ are the raising and lowering operators of the z components of spin and orbital angular momentum respectively.

Appendix C: Evaluation of the Inner Product

Substituting in $\hat{H}_{SO}$ for $\hat{H}'$ yields

$$\langle n'\,m'\,\sigma'|\,\hat{H}_{SO}\,|n\,m\,\sigma\rangle = \Big\langle n'\,m'\,\sigma'\Big|\Big[-\frac{\Delta\chi'}{2a^2\rho}\Big(2\sigma\,m\Big|n\,m\,\sigma\Big\rangle^0 +\rho\partial_z\Big(\Big|n,\,m{-}1,\,\sigma{+}1\Big\rangle^0\delta_{\sigma,\,-\frac{1}{2}}+\Big|n,\,m{+}1,\,\sigma{-}1\Big\rangle^0\delta_{\sigma,\,+\frac{1}{2}}\Big)\Big)\Big],$$

Substituting in the explicit wave function for $|n\,m\,\sigma\rangle^0$ as written in Eq. 6, and the transpose of this is ${}^0\langle n\,m\,\sigma|$, and pulling out constants yields a product of integrals of the form

$$\begin{aligned}\langle n'\,m'\,\sigma'|\,\hat{H}_{SO}\,|n\,m\,\sigma\rangle = \int_0^{2\pi}\int_0^{\infty}\frac{N_{n'\,|m'|}}{a}Z_{n'\,|m'|}(U_{n'\,|m'|}\rho)e^{-im'\phi}e^{-i(\beta^0_{n'\,|m'|}z-\omega t)}\hat{e}^\dagger_{\sigma'}\\ \Big[-\frac{\Delta\chi'}{2a^2\rho}\Big(2\sigma m\frac{N_{n\,|m|}}{a}Z_{n\,|m|}(U_{n\,|m|}\rho)e^{im\phi}e^{i(\beta^0_{n\,|m|}z-\omega t)}\hat{e}_\sigma\\ +\rho\partial_z\Big(\frac{N_{n\,|m-1|}}{a}Z_{n\,|m-1|}(U_{n\,|m-1|}\rho)e^{i(m-1)\phi}e^{i(\beta^0_{n\,|m-1|}z-\omega t)}\hat{e}_{\sigma+1}\delta_{\sigma,-\frac{1}{2}}\\ +\frac{N_{n\,|m+1|}}{a}Z_{n\,|m+1|}(U_{n\,|m+1|}\rho)e^{i(m+1)\phi}e^{i(\beta^0_{n\,|m+1|}z-\omega t)}\hat{e}_{\sigma-1}\delta_{\sigma,+\frac{1}{2}}\Big)\Big)\Big]\,rdrd\phi,\end{aligned} \tag{C1}$$

It is much easier to tackle this equation if it is broken up into three parts. After some simplification, the first part becomes

$$\begin{aligned}A\equiv\\ -\frac{\Delta}{a^2}\int_0^{2\pi}\int_0^{\infty}\delta_{\sigma\,\sigma'}\,\delta_{m\,m'}N_{n'\,|m'|}N_{n\,|m|}Z_{n'\,|m'|}Z_{n\,|m|}\chi' d\rho\,d\phi,\\ =-\frac{\Delta 2\pi}{a^2}\delta_{\sigma\,\sigma'}\,\delta_{m\,m'}N_{n'\,|m'|}N_{n\,|m|}J_{|m'|}(U_{n'\,|m'|}1)J_{|m|}(U_{n\,|m|}1),\end{aligned}$$

with the help of $\chi'(\rho)$ turning into a Dirac delta for a Heaviside Step Potential. The Dirac delta, $\delta(\rho-1)$, simplifies all the ρ terms in the infinite integral to unity. A factor of 2π was pulled out from the definite ϕ integral since the variable itself was not present.

The second part,

$$\begin{aligned}B\equiv-\frac{\Delta i}{2a^2}\delta_{\sigma\,-}\hat{e}^\dagger_{\sigma'}\,\hat{e}_{\sigma+1}N_{n'\,|m'|}N_{n\,|m-1|}\beta^0_{n\,|m-1|}\\ \int_0^{2\pi}e^{i(-m'+m-1)\phi}\,d\phi\int_0^{\infty}Z_{n'\,|m'|}Z_{n\,|m-1|}\chi'\rho d\rho.\end{aligned} \tag{C2}$$

This part of the equation can be simplified by realizing that the definite ϕ integral evaluates to 2π when $m'=(m-1)$ and 0 when $m'\neq(m-1)$, collapsing the integral into $2\pi\delta_{(m-1)\,m'}$. Likewise, $\hat{e}_{\sigma+1}$ and $\hat{e}^\dagger_\sigma$ can be replaced with $\delta_{(\sigma+1)\,\sigma'}$. As with part A, the $\chi'(\rho)$ becomes a Dirac delta that further simplifies Eq. C2 to,

$$\begin{aligned}B=-\frac{\Delta\pi i}{a^2}\delta_{+\frac{1}{2},\,\sigma'}\delta_{(m-1),\,m'}N_{n'\,|m'|}N_{n\,|m-1|}\beta^0_{n\,|m-1|}\\ J_{|m'|}(U_{n'\,|m'|}1)J_{|m-1|}(U_{n\,|m-1|}1).\end{aligned} \tag{C3}$$

Similarly, the third part,

$$\begin{aligned}C\equiv-\frac{\Delta i}{2a^2}\delta_{\sigma\,+}\hat{e}^\dagger_{\sigma'}\,\hat{e}_{\sigma-1}N_{n'\,|m'|}N_{n\,|m+1|}\beta^0_{n\,|m+1|}\\ \int_0^{2\pi}e^{i(-m'+m+1)\phi}\,d\phi\int_0^{\infty}Z_{n'\,|m'|}Z_{n\,|m+1|}\chi'\rho d\rho\end{aligned}$$

evaluates to

$$\begin{aligned}C=-\frac{\Delta\pi i}{a^2}\delta_{-\frac{1}{2},\,\sigma'}\delta_{(m+1),\,m'}N_{n'\,|m'|}N_{n\,|m+1|}\beta^0_{n\,|m+1|}\\ J_{|m'|}(U_{n'\,|m'|}1)J_{|m+1|}(U_{n\,|m+1|}1).\end{aligned} \tag{C4}$$

Thus, adding up parts A, B, and C, we get

$$
{}^{0}\langle n'\,m'\,\sigma'|\,\hat{H}_{SO}\,|n\,m\,\sigma\rangle^{0} = -\frac{\Delta 2\pi}{a^2}\delta_{\sigma\,\sigma'}\,\delta_{m\,m'}N_{n'\,|m'|}N_{n\,|m|}J_{|m'|}(U_{n'\,|m'|}1)J_{|m|}(U_{n\,|m|}1)
- \frac{\Delta\pi i}{a^2}\delta_{+\frac{1}{2},\,\sigma'}\delta_{(m-1),\,m'}N_{n'\,|m'|}N_{n\,|m-1|}\beta^{0}_{n\,|m-1|}J_{|m'|}(U_{n'\,|m'|}1)J_{|m-1|}(U_{n\,|m-1|}1)
- \frac{\Delta\pi i}{a^2}\delta_{-\frac{1}{2},\,\sigma'}\delta_{(m+1),\,m'}N_{n'\,|m'|}N_{n\,|m+1|}\beta^{0}_{n\,|m+1|}J_{|m'|}(U_{n'\,|m'|}1)J_{|m+1|}(U_{n\,|m+1|}1). \quad \text{(C5)}
$$

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