Ex5666: A particle in a two dimensional box with a potential step

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The problem:

An electron with mass $\boldsymbol{M}$ is in a two dimensional box $|x| < a$, $|y| < b$. Inside the box there is a step potential $V(x) = \frac{1}{2}V_0 \cdot sgn(x)$.
In this question you need to consider spin-orbit interaction. Units: $c = 1$, $e = 1$, $g \approx 2$.

1. Write the Hamiltonian using the position and momentum operators and the spin operator σ_z.
2. Write the unperturbed eigenstates $|n, m\rangle$ in the standard basis.
3. Write an expression for the matrix elements $\langle n, m|V(x)|1, 1\rangle$.
4. Calculate the second order correction of the ground state energy which arise from the electrostatic interaction.
5. Which states are not effected by the spin-orbit interaction?
6. Repeat section 3 for spin-orbit interaction.
7. Repeat section 4 for spin-orbit interaction.

TIP: Use the following symbols:
$\text{SIN}_\nu(\theta) = cos(\nu\theta)$ for $\nu = 1, 3, \ldots$
$\text{SIN}_\nu(\theta) = sin(\nu\theta)$ for $\nu = 2, 4, \ldots$
$c_\nu = \int_0^{\pi\backslash 2} sin(\nu\theta)cos(\theta)d\theta$

The spin state σ_z is a "good quantum number"- you should only address it in your answer to section 6.
The answers to sections 4 and 7 are series, clearly state the summation index.

The solution:

1.

$$\mathcal{H} = \frac{1}{2M}\hat{p}^2 + V(\hat{x}) - \frac{1}{2M^2}(g-1)(\vec{\mathcal{E}} \times \vec{p})\vec{S} = \frac{1}{2M}\hat{p}^2 + \frac{1}{2}V_0 \cdot \text{sgn}(\hat{x}) + \frac{V_0}{4M^2}\hat{p_y} \cdot \delta(\hat{x}) \cdot \hat{\sigma_z}$$

2. Boundary conditions:

$$\Psi(x = \pm a) = \Psi(y = \pm b) = 0$$

$$| \, n, m\rangle = \frac{1}{\sqrt{ab}} \cdot \text{SIN}_n\left(\frac{\pi x}{2a}\right) \cdot \text{SIN}_m\left(\frac{\pi y}{2b}\right)$$

eigenvalues:

$$\mathcal{E}_{n,m} = \frac{1}{2M}\left[\left(\frac{\pi n}{2a}\right)^2 + \left(\frac{\pi m}{2b}\right)^2\right], \quad \text{for} \quad V_0 = 0$$

3.

$$\langle n,m|V(x)|1,1\rangle = \frac{V_0}{2ab}\int_{-a}^{a}\mathrm{SIN}_n\left(\frac{\pi x}{2a}\right)cos\left(\frac{\pi x}{2a}\right)\mathrm{sgn}(x)dx\cdot\int_{-b}^{b}\mathrm{SIN}_m\left(\frac{\pi y}{2b}\right)cos\left(\frac{\pi y}{2b}\right)dy =$$

$$= \frac{2\delta_{1,m}\cdot V_0\cdot c_n}{\pi}, \quad \text{for} \quad n = 2,4,\ldots$$

4.

$$E_{11}^{[2]} = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{(|\langle n,m\mid V\mid 1,1\rangle|)^2}{E_{11}-E_{n,m}} = -\frac{32MV_0^2a^2}{\pi^4}\sum_{n=1}^{\infty}\frac{c_{2n}^2}{4n^2-1}$$

5. The spin-orbit term of the Hamiltonian is:

$$\mathcal{H}_{SO} = \frac{V_0}{4M^2}\hat{p_y}\cdot\delta(\hat{x})\cdot\hat{\sigma_z}$$

Thus the eigenstates for which $\Psi(x=0)=0$ are unaffected by the delta function. This condition applies only to even n.

6.

$$\langle n,m|\mathcal{H}_{SO}|1,1\rangle = \frac{-iV_0\cdot\sigma_z}{4M^2ab}\int_{-a}^{a}\mathrm{SIN}_n\left(\frac{\pi x}{2a}\right)cos\left(\frac{\pi x}{2a}\right)\delta(x)dx\cdot\int_{-b}^{b}\mathrm{SIN}_m\left(\frac{\pi y}{2b}\right)\frac{\partial}{\partial y}cos\left(\frac{\pi y}{2b}\right)dy =$$

$$= \frac{iV_0\cdot\sigma_z\cdot c_m}{2M^2ab} \quad \text{for} \quad m = 2,4,\ldots\ ;\ n = 1,3,\ldots$$

7.

$$E_{11}^{[2]} = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{(|\langle n,m\mid\mathcal{H}_{SO}\mid 1,1\rangle|)^2}{E_{11}-E_{n,m}} = -\frac{2V_0^2}{M^3\pi^2a^2b^2}\sum_{n=1,3,\ldots}^{\infty}\sum_{n=2,4,\ldots}^{\infty}\frac{c_m^2}{\frac{n^2-1}{a^2}+\frac{m^2-1}{b^2}}$$