Degenerate levels in a rotating box

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In this problem we are interested in the two first excited levels of a square potential well. Let us take the potential in the form

$$V(x,y) = \begin{cases} \infty & \text{if } |x| > \frac{a}{2} \text{ or} |y| > \frac{a}{2} \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

The normalized wavefunctions of these states are

$$\begin{aligned} \psi_1 &= \frac{2}{a} \cos \frac{\pi x}{a} \sin \frac{2\pi y}{a} \\ \psi_2 &= \frac{2}{a} \sin \frac{2\pi x}{a} \cos \frac{\pi y}{a} \end{aligned} \tag{2}$$

Now let us apply the concept of Berry phase to degenerate levels. Assume that the potential well is slowly rotating around the z axis. That means that the eigenfunctions also become angle–dependent.

Let us search for a solution of the Schrodinger equation in the form

$$\psi(t) = (\alpha(t)\psi_1^\theta + \beta(t)\psi_2^\theta)e^{-iEt} \tag{3}$$

Here θ is the rotation angle and E is the energy of the states. After substituting this ψ into Schrodinger equation, we get

$$\dot\alpha\psi_1 + \dot\beta\psi_2 + \alpha\partial_\theta\psi_1\dot\theta + \beta\partial_\theta\psi_2\dot\theta = 0 \tag{4}$$

Taking the scalar product with ψ_1^θ, ψ_2^θ we get

$$i\frac{d}{d\theta}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = -i\begin{pmatrix}\langle\psi_1\partial_\theta\psi_1\rangle & \langle\psi_1\partial_\theta\psi_2\rangle \\ \langle\psi_2\partial_\theta\psi_1\rangle & \langle\psi_2\partial_\theta\psi_2\rangle\end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} \tag{5}$$

The matrix elements can be easily calculated after the following observation:

$$\psi^\theta = e^{-i\hat{l}_z\theta}\psi^0 \tag{6}$$

and

$$\partial_\theta\psi = -i\hat{l}_z\psi \tag{7}$$

So,

$$i\frac{d}{d\theta}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = -\begin{pmatrix}0 & \langle\psi_1\hat{l}_z\psi_2\rangle \\ \langle\psi_2\hat{l}_z\psi_1\rangle & 0\end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} \tag{8}$$

The diagonal elements vanish because of the mirror symmetry.

The last step is to compute the matrix element of l_z. This is quite straightforward:

$$\begin{aligned}\langle\psi_1 \hat{l}_z \psi_2\rangle &= -\frac{4i}{a^2}\int dx\, dy \cos\frac{\pi x}{a}\sin\frac{2\pi y}{a}(x\partial_y - y\partial_x)\sin\frac{2\pi x}{a}\cos\frac{\pi y}{a} \\ &= \frac{8\pi i}{a^3}\int dx\, x\cos\frac{\pi x}{a}\sin\frac{2\pi x}{a}\int dy \sin\frac{\pi y}{a}\sin\frac{2\pi y}{a} = \\ &= \frac{8i}{\pi^2}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} dx\, x\cos x\sin 2x\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} dy \sin y \sin 2y = \frac{256i}{27\pi^2}\end{aligned} \tag{9}$$

Finally,

$$i\frac{d}{d\theta}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \frac{256}{27\pi^2}\sigma_y\begin{pmatrix}\alpha\\ \beta\end{pmatrix} \tag{10}$$

$$\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \exp\left\{-\frac{256i}{27\pi^2}\sigma_y\theta\right\}\begin{pmatrix}\alpha_0\\ \beta_0\end{pmatrix} = \begin{pmatrix}\cos\frac{256}{27\pi^2}\theta & -\sin\frac{256}{27\pi^2}\theta\\ \sin\frac{256}{27\pi^2}\theta & \cos\frac{256}{27\pi^2}\theta\end{pmatrix}\begin{pmatrix}\alpha_0\\ \beta_0\end{pmatrix} \tag{11}$$