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6 Exercise - Introduction to Group Theory

6.1 (No crossing rule)

ψ_1 and ψ_2 shall be eigenfunctions of a hamiltonian H_0 with different eigenvalues. They transform as the same 1-dimensional irreducible representation. We assume the same symmetry for the perturbation operator V as that of the hamiltonian H_0. We then have:

$$\begin{aligned} H_{11} &= \langle\psi_1|H_0+V|\psi_1\rangle \\ H_{22} &= \langle\psi_2|H_0+V|\psi_2\rangle \\ H_{12} &= \langle\psi_2|H_0+V|\psi_1\rangle = H_{21} \end{aligned}$$

We will now set up the secular equation for this problem and solve it for the energy. The Hamiltonian can be written as:

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$

therefore we can find the eigenvalues (energies) using $\det\left(H - E\,I\right) = 0$, with I the unit matrix. We therefore get:

$$\begin{vmatrix} H_{11}-E & H_{12} \\ H_{21} & H_{22}-E \end{vmatrix} = 0$$

leading to the equation:

$$\begin{aligned} \left(H_{11}-E\right)\left(H_{22}-E\right) - H_{21}H_{12} &= 0 \\ H_{11}H_{22} - H_{11}E - EH_{22} + E^2 - H_{12}^2 &= 0 \\ E^2 - \left(H_{11}+H_{22}\right)E + H_{11}H_{22} - H_{12}^2 &= 0 \end{aligned}$$

which leads to the eigenvalues:

$$E_{1,2} = \frac{\left(H_{11}+H_{22}\right)}{2} \pm \sqrt{\frac{\left(H_{11}+H_{22}\right)^2}{4} - H_{11}H_{22} + H_{12}^2}$$

or rewritten:

$$E_{1,2} = \frac{\left(H_{11}+H_{22}\right)}{2} \pm \frac{1}{2}\sqrt{\left(H_{11}-H_{22}\right)^2 + 4H_{12}^2}$$

this immediately shows, that the eigenvalues will never be degenerate, if $H_{12} \neq 0$, while $\Delta E = |E_1 - E_2| \neq 0$. We can now use the approximation $H_{12} \ll H_{11} - H_{22}$ to simplify our energy values, but first we rewrite:

$$E_{1,2} = \frac{\left(H_{11}+H_{22}\right)}{2} \pm \frac{\left(H_{11}-H_{22}\right)}{2}\sqrt{1 + \frac{4H_{12}^2}{\left(H_{11}-H_{22}\right)^2}}$$

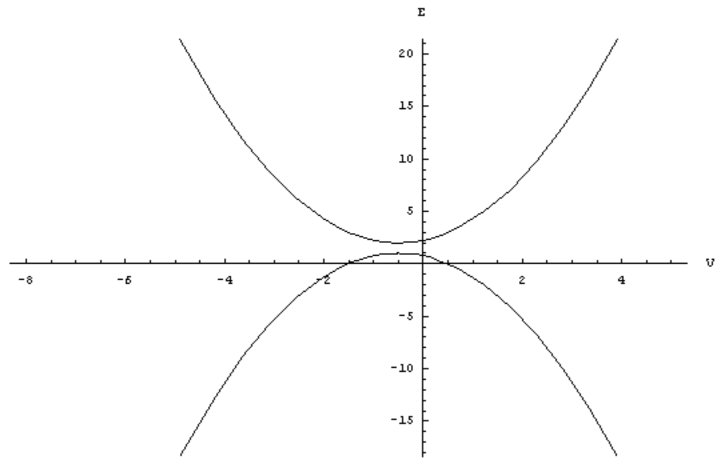

Abbildung 1: diagram of energies as function of V, while E_1 represents the lower line and E_2 the upper line.

now we see, that we can use the Taylorexpansion for the root, while $H_{12} \ll H_{11} - H_{22}$ holds and therefore $\frac{4H_{12}^2}{(H_{11}-H_{22})^2} \ll 1$:

$$\sqrt{1+x}\Big|_{x=0} = \sqrt{1} + \frac{1}{2}x + \ldots \approx 1 + \frac{1}{2}x$$

we get:

$$E_{1,2} = \frac{(H_{11}+H_{22})}{2} \pm \frac{(H_{11}-H_{22})}{2}\left(1 + \frac{4H_{12}^2}{2\,(H_{11}-H_{22})^2}\right)$$

this leads to the energies:

$$\begin{aligned} E_1 &= H_{11} + \frac{H_{12}^2}{(H_{11}-H_{22})} \\ E_2 &= H_{22} - \frac{H_{12}^2}{(H_{11}-H_{22})} \end{aligned}$$

From this we can say, that interacting states ($H_{12} \neq 0$) want to seperate from each other. This means, that energy states want to seperate, if they transform as the same irreducible representation and the eigenfunctions have different eigenvalues for the same hamiltonian. The behaviour of the energies can be seen in the diagram. The diagram of the energies in dependance of V can be found in figure 1. We see that the smallest distance between the two eigenvalue parabola seems to be $2\,|H_{12}|$. Also we see that there is no intersect of the energy parabola.

6.2 (centrosymmetric groups)

We are going to find out which state combinations of the irreducible representations in the means of g and u (gerade or ungerade parity) are allowed for the centrosymmetric groups. A group is called centrosymmetric, if the inversion is one of it's symmetry elements. For sure if the total product of the irr. reps is u there will be no transition.

The transitions are defined by

$$\int \varphi_f \vec{O} \varphi_i d\tau \rightarrow \varphi_f \otimes \vec{O} \otimes \varphi_i$$

should be g for a transition to occur.

a) electric dipole transitions

The electric dipole operator is defined by $\vec{O} = e\vec{r}$. While it transforms like an odd representation (u) the transitions between states of the same parity are forbidden, meaning:

$$\begin{aligned} g \otimes g &= g \\ u \otimes u &= g \end{aligned}$$

will lead to a total product of u meaning no transition:

$$\begin{aligned} g \otimes u \otimes g &= u \\ u \otimes u \otimes u &= u \end{aligned}$$

This means, only transitions with different parity are allowed:

$$\begin{aligned} g \otimes u \otimes u &= g \\ u \otimes u \otimes g &= g \end{aligned}$$

b) magnetic dipole transitions

The magnetic dipole operator $\vec{O} = \frac{e}{2m}\left(\vec{l} + 2\vec{s}\right)$ transforms like an even representation (g), therefore the transitions are forbidden for states of different parity, meaning

$$\begin{aligned} g \otimes u &= u \\ u \otimes g &= u \end{aligned}$$

and for the total product:

$$\begin{aligned} g \otimes g \otimes u &= u \\ u \otimes g \otimes g &= u \end{aligned}$$

therefore, only state combinations with the same parity are allowed:

$$\begin{aligned} g \otimes g \otimes g &= g \\ u \otimes g \otimes u &= g \end{aligned}$$