Clarification of Expectation Values

Expectation value is the ensemble average over many identical systems. Does not have to correspond to an actual measured value.

Ex: Spin-1/2 particles can have spin-up $\frac{\hbar}{2}|\uparrow\rangle$ or spin-down $\frac{\hbar}{2}|\downarrow\rangle$.

Expectation value $\Rightarrow 0$, but not a possible measurement

*This was assuming
$$\hat{S}_z|\uparrow\rangle_z = +\frac{\hbar}{2}|\downarrow\rangle_z$$
$$\hat{S}_z|\downarrow\rangle_z = -\frac{\hbar}{2}|\downarrow\rangle_z$$

We are going to prove that in the basis of an operator $\hat{Q}$, a state $|\psi\rangle$ has expectation value $\langle\psi|\hat{Q}|\psi\rangle = \sum_n q_n|c_n|^2$.

q_n are eigenvalues of $\hat{Q}$, c_n are coefficients.

Q1. Show $|\psi\rangle = \sum_n c_n|q_n\rangle$ using bra-ket notation.

A1: $|\psi\rangle = \sum_n |q_n\rangle\langle q_n|\psi\rangle = \sum_n c_n|q_n\rangle$ where $c_n \equiv \langle q_n|\psi\rangle$

$\hat{Q}|q_n\rangle = q_n|q_n\rangle$

Q2: Use Q1 to show $\langle\psi|\hat{Q}|\psi\rangle = \sum_n q_n|c_n|^2$

A2:
$$\langle\psi|\hat{Q}|\psi\rangle = \langle\psi|\hat{Q}\sum_n c_n|q_n\rangle = \sum_n \langle\psi|\hat{Q}|q_n\rangle$$
$$= \sum_n c_n\langle\psi|q_n|q_n\rangle = \sum_n q_n c_n\langle\psi|q_n\rangle$$
$$= \sum_n q_n c_n c_n^* = \sum_n q_n|c_n|^2 \quad \text{since } c_n^* = \langle\psi|q_n\rangle$$

Q3: Use the identity $\mathbb{1}$ expressed in terms of the eigenstates of $\hat{Q}$ to show $\langle\psi|\hat{Q}|\psi\rangle = \sum_n q_n|c_n|^2$.

A3:
$$\langle\psi|\hat{Q}|\psi\rangle = \langle\psi|\hat{Q}\,\mathbb{1}|\psi\rangle = \langle\psi|\hat{Q}\sum_n|q_n\rangle\langle q_n|\psi\rangle$$
$$= \sum_n\langle\psi|q_n|q_n\rangle c_n = \sum_n q_n c_n^* c_n = \sum_n q_n|c_n|^2$$

Q4: What if $\hat{Q}$ has a continuous spectrum? $\hat{Q}|q\rangle = q|q\rangle$? Use the identity $\mathbb{I}$ in continuous form w.r.t. q to find the expectation value $\langle\psi|\hat{Q}|\psi\rangle$.

A4: $\mathbb{I} = \int_{-\infty}^{\infty} |q\rangle\langle q|\, dq$

$$\langle\psi|\hat{Q}|\psi\rangle = \langle\psi|\hat{Q}\,\mathbb{I}|\psi\rangle = \langle\psi|Q\int_{-\infty}^{\infty}|q\rangle\langle q|\,dq\,|\psi\rangle$$

$$= \int_{-\infty}^{\infty} \langle\psi|Q|q\rangle\langle q|\psi\rangle\, dq$$

$$= \int_{-\infty}^{\infty} \langle\psi|q|q\rangle\langle q|\psi\rangle\, dq = \int_{-\infty}^{\infty} q\, \underbrace{\langle\psi|q\rangle\langle q|\psi\rangle}_{|\psi|^2}\, dq$$

$$\Rightarrow \langle\psi|\hat{Q}|\psi\rangle = \int_{-\infty}^{\infty} q\,|\psi|^2\, dq$$

Q5: What if $|\psi\rangle$ isn't expanded in the basis of $\hat{Q}$? Show $\langle\psi|\hat{Q}|\psi\rangle = \sum_{n,m,i,j} C_m^* C_n Q_{ij}\, \delta_{mj}\, \delta_{in}$.

A5: $\langle\psi|\hat{Q}|\psi\rangle = \langle\psi|Q\sum_n |q_n\rangle\langle q_n|\psi\rangle$ $\qquad C_n \equiv \langle q_n|\psi\rangle$

$= \sum_n \langle\psi|\hat{Q}|q_n\rangle\langle q_n|\psi\rangle$ $\qquad C_m^* \equiv \langle\psi|q_m\rangle$

$$= \sum_{n,m} \langle\psi|q_m\rangle\langle q_m|\hat{Q}|q_n\rangle\langle q_n|\psi\rangle$$

$$= \sum_{n,m} C_m^* C_n \underbrace{\langle q_m|\hat{Q}|q_n\rangle}_{\text{still a sum}}$$

$$= \sum_{n,m} C_m^* C_n \langle q_m|\hat{Q}\sum_i |q_i\rangle\langle q_i|q_n\rangle$$

$$= \sum_{n,m,i} C_m^* C_n \sum_j \langle q_m|q_j\rangle\langle q_j|\hat{Q}|q_i\rangle\langle q_i|q_n\rangle$$

$$= \sum_{n,m,i,j} C_m^* C_n \langle q_m|q_j\rangle\, Q_{ij}\, \langle q_i|q_n\rangle$$

$$= \sum_{n,m,i,j} C_m^* C_n Q_{ij}\, \delta_{mj}\, \delta_{in}$$

Q6: What if $\hat{Q}$ has a continuous spectrum?
Use $\mathbb{I} = \int |q\rangle\langle q| \, dq$ to show $\langle\psi|\hat{Q}|\psi\rangle = \iint \langle\psi|q'\rangle\langle q'|\hat{Q}|q\rangle\langle q|\psi\rangle \, dq \, dq'$

A6: $\langle\psi|\hat{Q}|\psi\rangle = \langle\psi|\hat{Q}\int|q\rangle\langle q|\psi\rangle \, dq = \int \langle\psi|\hat{Q}|q\rangle \langle q|\psi\rangle dq$

$$= \int\left(\int\langle\psi|q'\rangle\langle q'|\hat{Q} \, dq'\right)|q\rangle\langle q|\psi\rangle \, dq$$

$$= \iint \langle\psi|q'\rangle\langle q'|\hat{Q}|q\rangle\langle q|\psi\rangle \quad dq \, dq'$$

Q7: Show A6 reduces to $\langle\psi|\hat{x}|\psi\rangle = \int \psi^*(x) \, x \, \psi(x) \, dx$
if $\hat{Q} = \hat{x}$.

A7: $\langle\psi|\hat{Q}|\psi\rangle = \iint \langle\psi|q'\rangle\langle q'|\hat{Q}|q\rangle\langle q|\psi\rangle \, dq \, dq'$

Let $\hat{Q} = \hat{x}$

$\langle\psi|x'\rangle = \psi^*(x')$

$\langle x|\psi\rangle = \psi(x)$

$$\Rightarrow \langle\psi|\hat{x}|\psi\rangle = \iint \langle\psi|x'\rangle\langle x'|\hat{x}|x\rangle\langle x|\psi\rangle \, dx \, dx'$$

$$= \iint \langle\psi|x'\rangle\langle x'|x|x\rangle\langle x|\psi\rangle \, dx \, dx'$$

$$= \iint \langle\psi|x'\rangle \, x \, \langle x'|x\rangle\langle x|\psi\rangle \, dx \, dx'$$

$$= \iint \langle\psi|x'\rangle \, x \, \delta(x'-x)\langle x|\psi\rangle \, dx \, dx'$$

$$= \iint \psi^*(x') \, x \, \delta(x'-x) \, \psi(x) \, dx \, dx'$$

$$\langle\psi|\hat{x}|\psi\rangle = \int \psi^*(x) \, x \, \psi(x) \, dx$$