Thomas-Reiche-Kuhn sum rules

Abstract

Derivation of Thomas-Reiche-Kuhn sum rules for position operator.

Index Terms

operator algebra , perturbation theory

In perturbation theory, one frequently encounters the following summation:

$$S \equiv \sum_m (E_m - E_n)|\langle m|X|n\rangle|^2 \tag{1}$$

where $|m\rangle$ and $|n\rangle$ are eigenstates of $H = P^2/2m + V(X)$, and we want to prove that the summation is equal to $\frac{\hbar^2}{2m}$.

We first convert $E_m - E_n$ term into a commutation as follows.

$$(E_m - E_n)\langle m|X|n\rangle = \langle m|[H, X]|n\rangle = \langle m|[\frac{P^2}{2\mu}, X]|n\rangle = \frac{-i}{\mu}\langle m|P|n\rangle \tag{2}$$

So we have,

$$\begin{aligned} S &= \frac{-i}{\mu}\sum_m \langle m|P|n\rangle\langle n|X|m\rangle = \frac{-i}{m}\langle n|X|\sum_m |m\rangle\langle m|P|n\rangle \\ &= \frac{-i\hbar}{m}\langle n|XP|n\rangle \end{aligned} \tag{3}$$

Note that S is manifestly real from its definition, so we can add up its complex conjugate which will simply double it.

$$\begin{aligned} S &= \frac{S + S^*}{2} = \frac{-i\hbar}{2m}\langle n|XP|n\rangle + \frac{i\hbar}{2m}\langle n|PX|n\rangle \\ &= \frac{\hbar^2}{2m}\langle n|[X, P]|n\rangle = \frac{1}{2m} \end{aligned} \tag{4}$$

Let's test the sum rule on the nth state of the oscillator. For the harmonic oscillator,

$$\begin{aligned} S &= w\sum_m (m + 1/2 - n - 1/2)|\langle m|X|n\rangle|^2 \\ &= w\sum_m (m - n)\frac{\hbar^2}{2mw}\left(\sqrt{n+1}\delta_{m,n+1} + \sqrt{n}\delta_{m,n-1}\right)^2 \\ &= \frac{\hbar^2}{2m}(n + 1 - n) = \frac{\hbar^2}{2m}, \end{aligned} \tag{5}$$

which agrees with the sum rule.

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