

Error estimation for truncating Hamiltonian

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Start with the appropriately scaled Hamiltonian

$$H = H_0 + \lambda \sum_{n=2}^{\infty} \ell^{-2n+2} (\lambda_{1,n} p^{2n} + \lambda_{2,n} x^{2n})$$

where $H_0 = \frac{p^2 + x^2}{2}$ has eigenvalues

$$E_n = n + \frac{1}{2}.$$

As a warmup, we'll consider the most straightforward case

$$H = H_0 + \lambda_4 \ell^{-2} (p^4 + x^4)$$

The question we'd like to answer is, given an error tolerance T and a value of λ_4 , how small does ℓ need to be before we can't detect the quartic term within our tolerance?

Define $\lambda = \lambda_4 \ell^{-2}$ and write

$$E_n(\lambda) = E_n(0) + R(\lambda).$$

We just want $|R(\lambda)| < T$ for all λ . If $\frac{dE}{d\lambda} \leq Q$ on $[0, \lambda]$, then $R(\lambda) \leq Q\lambda$. [1] Since

$$\begin{aligned} \frac{dE_n}{d\lambda} &= \langle n | \frac{dH}{d\lambda} | n \rangle \\ &= \langle n^{(0)} | (p^4 + x^4) | n^{(0)} \rangle \\ &= 3n^2 + 3n + \frac{3}{2} \end{aligned}$$

is constant,

$$R(\lambda) \leq \lambda \left(3n^2 + 3n + \frac{3}{2} \right).$$

To get what we want, we just need

$$\lambda \left(3n^2 + 3n + \frac{3}{2} \right) < T$$

or

$$\ell > \sqrt{\frac{\lambda \left(3n^2 + 3n + \frac{3}{2} \right)}{T}}$$

For the states, write

$$|n(\lambda)\rangle = \sum_m c_{n,m}(\lambda) |m\rangle.$$

Then $c_{n,m}(\lambda) = \delta_{n,m} + R(\lambda)$. Now

$$\begin{aligned} \frac{d}{d\lambda} c_{n,m}(\lambda) &= \langle m | \frac{d}{d\lambda} | n(\lambda) \rangle \\ &= \frac{\langle m | p^4 + x^4 | n \rangle}{E_m(0) - E_n(0)} \\ &= \frac{1}{8} \left(\sqrt{n(n-1)(n-2)(n-3)} \delta_{m,n-4} - \sqrt{(n+1)(n+2)(n+3)(n+4)} \delta_{m,n+4} \right) \end{aligned}$$

REFERENCES

- [1] https://en.wikipedia.org/wiki/Taylor%27s_theorem#Estimates_for_the_remainder