ARDB-327

The Feynman-Hellmann Theorem

Ben Cowan

1 Statement of the theorem

The Feynamn-Hellmann theorem [1] demonstrates the relationship between perturbations in an operator on a complex inner product space and the corresponding perturbations in the operator's eigenvalue. It shows that to compute the derivative of an eigenvalue with respect to a parameter of the operator, we need only know an eigenvector and the derivative of the operator. This technique can be useful for instance in computing dispersion relations; we provide an example of this in the next section.

The Feynman-Hellmann theorem can be stated precisely as follows:

The Feynman-Hellmann theorem. Suppose H is a complex inner product space with inner product denoted $\langle , \rangle$, and let $\alpha_0 \in \mathbb{R}$ and U be a neighborhood of α_0. Suppose that for each $\alpha \in U$, there is a Hermitian operator $T(\alpha)$ on H and a $\psi(\alpha) \in H$ such that the functions T and ψ are both differentiable at α_0 and for each $\alpha \in U$, $\langle \psi(\alpha), \psi(\alpha) \rangle = 1$ and there is a $\lambda(\alpha) \in \mathbb{C}$ with $T(\alpha)\psi(\alpha) = \lambda(\alpha)\psi(\alpha)$. Then the function $\lambda : U \to \mathbb{C}$ is differentiable at α_0 and

$$\lambda'(\alpha_0) = \left\langle \psi(\alpha_0), T'(\alpha_0)\psi(\alpha_0) \right\rangle .$$

Proof. We assume as fact two basic results from linear algebra:

> *Lemma 1.* With T and ψ defined as above, the function $\phi : U \to H$ given by $\phi(\alpha) = T(\alpha)\psi(\alpha)$ is differentiable at α_0 with $\phi'(\alpha_0) = T'(\alpha_0)\psi(\alpha_0) + T(\alpha_0)\psi'(\alpha_0)$.
>
> *Lemma 2.* For $v, w : U \to H$ differentiable at α_0, the function $f : U \to \mathbb{C}$ given by $f(\alpha) = \langle v(\alpha), w(\alpha) \rangle$ is differentiable at α_0 with $f'(\alpha_0) = \langle v'(\alpha_0), w(\alpha_0) \rangle + \langle v(\alpha_0), w'(\alpha_0) \rangle$.

With these lemmas we have first of all that for each $\alpha \in U$,

$$\lambda(\alpha) = \lambda(\alpha) \langle \psi(\alpha), \psi(\alpha) \rangle = \langle \psi(\alpha), \lambda(\alpha)\psi(\alpha) \rangle = \langle \psi(\alpha), T(\alpha)\psi(\alpha) \rangle .$$

Then

$$\begin{aligned} \lambda'(\alpha_0) &= \left\langle \psi'(\alpha_0), T(\alpha_0)\psi(\alpha_0) \right\rangle + \left\langle \psi(\alpha_0), (T\psi)'(\alpha_0) \right\rangle \\ &= \left\langle \psi'(\alpha_0), T(\alpha_0)\psi(\alpha_0) \right\rangle + \left\langle \psi(\alpha_0), T'(\alpha_0)\psi(\alpha_0) \right\rangle + \left\langle \psi(\alpha_0), T(\alpha_0)\psi'(\alpha_0) \right\rangle . \end{aligned}$$

Now since each $T(\alpha)$ is Hermitian, $T'(\alpha_0)$ is Hermitian and $\lambda(\alpha_0) \in \mathbb{R}$, so

$$\begin{aligned} \left\langle \psi(\alpha_0), T(\alpha_0)\psi'(\alpha_0) \right\rangle &= \left\langle T(\alpha_0)\psi(\alpha_0), \psi'(\alpha_0) \right\rangle \\ &= \lambda(\alpha_0)^* \left\langle \psi(\alpha_0), \psi'(\alpha_0) \right\rangle \\ &= \lambda(\alpha_0) \left\langle \psi(\alpha_0), \psi'(\alpha_0) \right\rangle . \end{aligned}$$

We then have

$$\begin{aligned}\lambda'(\alpha_0) &= \lambda(\alpha_0)\left(\big\langle\psi'(\alpha_0),\psi(\alpha_0)\big\rangle + \big\langle\psi(\alpha_0),\psi'(\alpha_0)\big\rangle\right) + \big\langle\psi(\alpha_0),T'(\alpha_0)\psi(\alpha_0)\big\rangle \\ &= \lambda(\alpha_0)\,\frac{d}{d\alpha}\left.\langle\psi(\alpha),\psi(\alpha)\rangle\right|_{\alpha_0} + \big\langle\psi(\alpha_0),T'(\alpha_0)\psi(\alpha_0)\big\rangle \\ &= \big\langle\psi(\alpha_0),T'(\alpha_0)\psi(\alpha_0)\big\rangle\end{aligned}$$

since each $\psi(\alpha)$ has unit norm. ■

2 An example application

We can readily apply the Feynman-Hellmann theorem to Photonic Crystal [2] computations. Let V be a unit cell of the crystal. Then the inner product space consists of differentiable vector fields on V which are periodic in the crystal lattice, with inner product given by

$$\langle\mathbf{F},\mathbf{G}\rangle = \int_V \mathbf{F}(\mathbf{x})^*\cdot\mathbf{G}(\mathbf{x})\,d^3\mathbf{x}.$$

For each $\mathbf{k}$ in the first Brillouin zone there is an eigenvalue relation

$$T\mathbf{u} = \frac{\omega^2}{c^2}\mathbf{u},$$

where the operator T is given by

$$T\mathbf{u} = (\boldsymbol{\nabla}+i\mathbf{k})\times\left[\frac{1}{\epsilon_r}(\boldsymbol{\nabla}+i\mathbf{k})\times\mathbf{u}\right],$$

with ϵ_r being the relative permittivity of the medium. Then T is Hermitian, as is proved in [2].

Suppose we wish to compute the group velocity v_g in the z-direction for a given mode of the crystal. We can consider T to be a function of $\mathbf{k}$. Then the Feynman-Hellmann theorem gives

$$\begin{aligned}\left\langle\mathbf{u},\frac{\partial T}{\partial k_z}\mathbf{u}\right\rangle &= \frac{\partial}{\partial k_z}\left(\frac{\omega^2}{c^2}\right) \\ &= \frac{2\omega}{c^2}\frac{\partial\omega}{\partial k_z} = \frac{2\omega}{c^2}v_g,\end{aligned}$$

so the group velocity is simply

$$v_g = \frac{c^2}{2\omega}\left\langle\mathbf{u},\frac{\partial T}{\partial k_z}\mathbf{u}\right\rangle.$$

Since $\partial T/\partial k_z$ can be computed analytically, finding the group velocity once a mode has been found is a computationally easy task.

References

[1] The Feynman-Hellmann theorem is often presented in the context of Quantum Mechanics; see for instance D. J. Griffiths, *Introduction to Quantum Mechanics* (Prentice Hall, Englewood Cliffs, NJ, 1995), Problem 6.27.

[2] J. D. Joannopoulos, R. D. Meade, J. N. Winn, *Photonic Crystals: Molding the Flow of Light* (Princeton Univ. Press, Princeton, NJ, 1995)