

Derivative Issues With Wavefunctions Written as Infinite Fourier Series

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In (1) an in depth study is presented of the wavefunction $W(x)=C x (L-x)$ in the interval $[0,L]$. This wavefunction is normalized and one may calculate the average energy using $H=-1/2m \hbar^2 d^2/dx^2$ using $W(x)$. The problem which arises is that $\langle W | H | W \rangle = 0$. If one uses $W(x) = \sum_n a(n) \sin(n\pi x/L)$ no issues appear. (1) resolves the situation by suggesting that $\langle W | H | W \rangle$ be replaced with $\langle HW | HW \rangle$. In such a case, using $W(x)$ or the infinite Fourier series yields the same result.

Here we suggest that the Fourier series is the physical representation because $\sin(n\pi x/L)$ are measurable eigenstates. An infinite series of such eigenstates is a little unusual in that one has a situation similar to the canonical or grand canonical case in statistical mechanics, i.e. any energy is allowed. As a result, calculations using the infinite Fourier series yield dependable results. From (2) it is possible to have a Fourier series represent a function $W(x)$, but have dW/dx not be represented by d/dx of the Fourier series. This may happen when the dW/dx does not have the same endpoints values as d/dx Fourier series as is the case here. Furthermore, quantum mechanics uses $\langle HW | HW \rangle$ for the Hermitian operator H , and this holds for a Fourier series, but not for $W(x)=C x (L-x)$. In this note we show that $\langle W(\text{Fourier}) | H | W(\text{Fourier}) \rangle$ leads to a Fourier representation of a constant squared which shows why $\langle HW | HW \rangle$ with $W= Cx(L-x)$ yields the same result.

Wavefunction and Fourier Series

The time-independent Schrodinger equation yields a complete basis of functions. For the case of a particle in a box with infinite walls at $x=0$ and $x=L$:

$$E_n = 1/2m (n\pi\hbar/L)^2 \quad ((1a)) \quad \text{and} \quad W_n(x) = \sqrt{2/L} \sin(n\pi x/L) \quad ((1b))$$

The states $W_n(x)$ are physical states which are measurable. As a result, a linear superposition of such states is a physical OR situation in probability. If the superposition is infinite, one has an infinite Fourier series which is a little unusual as it allows for any energy. This seems to be similar to the canonical or grand canonical partition functions in statistical mechanics.

The point we wish to make is that in the case of a Fourier series representing a function such as:

$$W(x)= C x(L-x) \quad \text{with} \quad C= \sqrt{30 / L^5} \quad ((2))$$

there is no guarantee that dW/dx is equivalent to d/dx Fourier series according to (2) because d/dx Fourier series is 0 at $x=0$ and $x=L$, but $dW/dx = C(L-2x)$ and $d/dx dW/dx = -2C$ are not. Thus calculations using derivatives of $W(x)$ must be taken with care. In some cases, they may match the result using the Fourier series and in other cases, they may not.

As shown in (1), a case where the two approaches coincide is:

$$\langle W(\text{Fourier}) | H | W(\text{Fourier}) \rangle = \langle W(x) | H | W(x) \rangle \quad ((3))$$

A case where they don't coincide is:

$$\langle W(\text{Fourier}) | H | W(\text{Fourier}) \rangle \neq \langle W | H | W \rangle \quad ((4)) \text{ because } \langle W | H | W \rangle = 0 \text{ which is unphysical.}$$

Furthermore, in quantum mechanics H , the Hamiltonian, is Hermitian and one has the important result:

$$\langle W | H | W \rangle = \langle H W | W \rangle \quad ((5))$$

This result holds for $W(\text{Fourier})$ because:

$$\frac{d}{dx} \left\{ \frac{dW}{dx} \frac{d}{dx} \frac{dW}{dx} \right\} = \frac{d}{dx} \frac{dW}{dx} \frac{d}{dx} \frac{dW}{dx} + \frac{d}{dx} \frac{dW}{dx} \frac{d}{dx} \frac{dW}{dx}$$

The integral on the LHS is 0 because $\frac{d}{dx} \frac{dW}{dx}$ is 0 at the endpoints 0, L for all $\sin(n\pi x/L)$ functions. Thus:

$$\langle H W(\text{Fourier}) | W(\text{Fourier}) \rangle = - \int dx \frac{dW}{dx} \frac{d}{dx} \frac{dW}{dx}$$

$$\text{Using: } \frac{d}{dx} \left\{ W \frac{d}{dx} \frac{dW}{dx} \right\} = \frac{dW}{dx} \frac{d}{dx} \frac{dW}{dx} + W \frac{d}{dx} \frac{d}{dx} \frac{dW}{dx}$$

gives 0 on the LHS because W vanishes at the endpoints and so ((5)) holds.

For $W = C x(L-x)$, however, ((5)) does not hold. $\langle W | H | W \rangle = 0$, but $\langle H W | W \rangle = (-1/2m) C C$ (4).

Thus, it seems that one may not necessarily use derivatives of a wavefunction in all cases, but may use the derivatives of the Fourier representation.

Link Between the Fourier Case and $W(x)$

In (1) it is shown that if one uses $\langle H W | W \rangle$ then one obtains the same result for both $W(\text{Fourier})$ and $W(x)$. (1) considers domains of operators and provides a lengthy discussion. Here we try to show that $H W = \text{constant}$ which may be written as a Fourier series. Thus:

$$\text{constant} * \text{constant} = \{ \text{Fourier series of a constant} \} \{ \text{Fourier series of constant} \} \quad ((6))$$

We argue that $\langle W(\text{Fourier}) | H | W(\text{Fourier}) \rangle$ has the same form as ((6)).

In (1), one has:

$$\langle W(\text{Fourier}) | H | W(\text{Fourier}) \rangle = \sum_n E_n E_n \langle W_n | W \rangle \langle W | W_n \rangle$$

where $W_n = C \sin(n\pi x/L)$ and $W = Cx(L-x)$. This in turn is equivalent to:

$$C \sum_{n=1}^{\infty} \frac{1 - (-1)^n}{n} \sin(n\pi x/L) \quad ((7))$$

$\{ \}$ vanishes for n even.

Next consider the Fourier series for a constant from (3):

$$1 = \sum_{n=1}^{\infty} \frac{1 - (-1)^n}{n} \sin(n\pi x/L) \quad ((8))$$

Note that this Fourier series is odd about $x=0$, but one is concerned with a positive constant for $x=0$ to $x=L$. One may note that the constant 1 and the series are not the same at $x=0$.

Thus:

$$1 \cdot 1 = \left\{ \sum_{n=1}^{\infty} \frac{1 - (-1)^n}{n} \sin(n\pi x/L) \right\} \sum_{n=1}^{\infty} \frac{1 - (-1)^n}{n} \sin(n\pi x/L)$$

If one integrates over dx and notes that $\sin(n\pi x/L)$'s are orthogonal, one has the form:

$$\sum_{n=1}^{\infty} \frac{1}{n^2} \{1 - (-1)^n\}^2 \quad ((9))$$

This, however, is exactly the form of ((7)), thus $\langle W(\text{Fourier}) | H | W(\text{Fourier}) \rangle$ is equivalent to:

$$\text{constant} \cdot \text{constant} \text{ or } \langle -1/2m \frac{d}{dx} \frac{d}{dx} Cx(L-x) | -1/2m \frac{d}{dx} \frac{d}{dx} Cx(L-x) \rangle$$

Conclusion

In conclusion, we argue that eigenstates of the time-dependent Schrodinger equation are physical. One may take a linear superposition using the idea of OR situations from probability. If the series is infinite, this is equivalent to an infinite Fourier series and represents a function $W(x)$. A point we make is that according to (2), the derivative of such a function $W(x)$ is not necessarily the same as the derivative of the Fourier series if the endpoint values of dW/dx do not match d/dx Fourier series. This is the case for the wavefunction $W(x) = Cx(L-x)$ presented in (1). Thus one may use the Fourier series when calculating expectation values of derivatives, but must be cautious using derivatives of $W(x)$. In particular, $\langle W | H | W \rangle = 0$ which is unphysical and does not match $\langle W(\text{Fourier}) | H | W(\text{Fourier}) \rangle$. (1) provides an in-depth study of this problem. They suggest one use: $\langle HW | HW \rangle$. In such a case, this yields the same result as $\langle HW(\text{Fourier}) | HW(\text{Fourier}) \rangle$. We show that this is the case because $HW = \text{constant}$ and $\langle HW(\text{Fourier}) | HW(\text{Fourier}) \rangle$ is equivalent to $\int dx (\text{Fourier representation of a constant})^2$ (Fourier representation of a constant). One may note that the Fourier representation of a constant does not equal the constant at $x=0$.

References

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