Average Force on the Wavefunction Versus Force on Plane Wave Constituents

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The Schrodinger equation for a bound state includes the classical potential V(r) for which –d/dxj V represents Fj or force in the j direction. It has been argued in a previous note (1), that one may attribute physical meaning to the Fourier series of V(r). In such a case, V(r) and W(r) (the wavefunction) are quantities averaged over momentum (or vectors) as well as being averages over time. One may write the product of V(r)W(r) as one of two Fourier series and then reorganize into a series with basis exp(ikr). In such a case, one examines an interaction with V at each momentum wave level. Then the average is only over time as different k momentum states of in W combine with different p momentum states of the Fourier series of V(r). For a p momentum wave, one may write:

p^2/2m fp + Sum k Vk f(p-k) = E fp where W= Sum over p fp exp(ipx) in one dimension ((1))

The objective of this note is to observe differences in the interaction of a single plane wave with a potential ((1)) and the interaction of W with V in the Schrodinger equation. In particular, for a particle in a box with infinite walls, V(x)=0 inside the one dimensional box, yet the Fourier series of W includes all p values. From ((1)), even though V(x)=0 as an average, there seems to still be an interaction with various Vk values (Vk= the kth Fourier transform) in the interior of the box as ((1)) holds at all x points.

Particle in a Box with Infinite Walls

The problem of a particle in a box with infinite walls has been solved spatially a long time ago. V(x) is zero in the interior and so a simple sin(kave x) solution is obtainable, with W(x) vanishing at 0 and L. (One may also solve the problem for x extending from –L/2 to L/2). More recently, the Fourier transform for this problem was obtained in (2), noting that W(x)= sin(kave x) rect(x). Here rect(x) is the rectangle function which is 1 for -L/2 <x<L/2 and 0 elsewhere. Thus, one does not simply take the Fourier transform of sin(kave x). As a result, all p momentum waves contribute to W(x). In particular (2):

fp = sqrt(L/3.14) (3.14n)/(3.14n +pL) sinc(.5(3.14n -pL)) exp((i(n-1)3.14/2) ((2))

Here L is the length of a box centered at x=0 and hbar is 1. The momentum corresponding to the overall energy is +/-3.14n/L. Also, f-p =-fp for n even and f-p=fp for n odd.

On average, p momentum waves combine to yield sin(kave x) in the interior -L/2 <x<L/2 and zero elsewhere. In quantum mechanics, however, plane wave states of W are taken to have physical meaning. Thus, the picture seems to be one has all possible momentum waves inside the box.

Consider n odd. Then, fp goes as 1/ ((3.14n +pL) (3.14n -pL)). This blows up for p near +/- 3.14/L i.e. the average momentum associated with the average energy. Thus, these two p values and nearby ones should dominate, yet other p may be important as ((1)) applies to all p waves and a factor of Vo (approaching infinite) exists for the infinite potential. This factor can combine with a tiny fp value to yield a finite value, it seems.

If one examines ((1)), a conservation of energy type equation for a single momentum wavefunction which holds at all x points, it seems that for fp from ((2)), the interaction term with Vk cannot be zero even though V(x), the average over all momentum states is zero. In other words, even though on average there may appear to be no potential interaction or force, a momentum state (which exists for an instant in time) feels an interaction or force. The momentum state of the quantum particle changes from one instant to another, so the interaction in ((1)) is different for each p. In addition, it should be noted that ((1)) seems to represent an average over time. In particular, the term:

Sum over k Vk f(p-k)

,which represents the interaction, involves all possible f(p-k), but only one such state can exist at each instant. Thus, even though at t1 one may have a momentum state p-k, it may interact with a Fourier transform value, say Vk, to create the momentum state p. This may happen in many different ways. The resulting equation shows that a single momentum state (in an average over time) undergoes an interaction Sum over k Vk f(p-k). In this note, we argue that this may be nonzero even if V(x) is zero as in the case of the interior of a box with infinite potential walls. Thus, interactions may be occurring even though V(x) is zero.

One may attempt to examine the Fourier series for the potential in a box. The potential is 0 for -L/2 $<$x$<$L/2 and infinite elsewhere. Let Vo be a very large number (instead of infinite). Then, it seems the potential may be written as:

Vo (- rectangle(x) +1) where rectangle(x)=1 for -L/2 $<$x$<$L/2 and 0 elsewhere. ((3))

The Fourier transform for rectangle(x) is (3):

Sin(3.14 p) / (3.14 p) ((4))

Thus, the overall Fourier transform becomes:

-Vo Sin(3.14 p) / (3.14 p) + Vo ((5))

If this is the case, then ((1)) becomes:

p^2/2m fp + Vo fp - Vo Sum over k sin(3.14k) / (3.14 k) f(p-k) = E fp ((6))

Equation ((6)) should hold for all x, including the interior of the box.

Thus, for ((6)) to be consistent one needs:

Sum over k sin(3.14k) / (3.14 k) f(p-k) = fp –(E-p^2/2m)fp/Vo

At first, this seems difficult as Vo does not appear on the LHS.

Consider n odd for sake of argument.

Next as examples, let us examine in a hand-wavy manner two p values. The first is p=+3.14/L, i.e. one of the average momentum value (the other being the negative). In such a case, $p^2/2m$ =E and the sum involving the potential should vanish. Let us use discrete values of k. For k=0 f(p-k)=f(p) which blows up. Sinc(0)=0 so one obtains from the Sum term a +Vofp which cancels –Vofp. There is another peak, however, for k=2p. Then f(p-k)=f(-p)=f(p) for n odd. This still leaves the factor sinc(3.14p).

Examine the form of sinc(3.14k), the Fourier transform of a piece of the potential. This transform peaks at 1 for k=0 and then drops rapidly to zero (outside a range). Thus, if p=+3.14/L is fairly large, i.e. away from zero, sinc(3.14k) approaches 0 in such a momentum region. Thus, Vo times sinc(3.14k) has a chance of being 0 or small which it must be because $p^2/2m$ =E and there can be no contribution from the potential for this value of p.

As a second example, consider a p value such that $p^2/2m$ does not equal E, but sinc(3.14p) is roughly 0. In other words p is a region for which sinc(3.14p) has already reached 0.Then:

-Vofp + VoSum j+k=p sinc(3.14k) f(j) cannot be 0 because this term must balance $p^2/2m$ fp to create Efp.

For k=0, sinc(3.14k)=1 and one obtains Vofp which cancels –Vofp. Next, consider small values of k, both positive and negative on either side of k=0. Sinc(3.14k) is an even function and is roughly one. Thus, one may examine:

f(p-k) = 1/(3.14n +(p-k)L) sinc(.5(3.14n –(p-k)L))

For n odd, sin(.5(3.14n –(p-k)L))= cos((p-k)L) approx = cos(pL)-kL sin(pL) ((7))

The two other factors are of the form 1/(a-kL) and 1/(b+kL) and their product is approx = 1/(ab) +kL(1/a-1/b) Multiplying by ((7)) yields:

cos(pL)/(ab) + kL (cos(pL)(1/a-1/b) –sin(pL)/(ab))

Thus, positive tiny k terms cancel with negative tiny k ones.

Thus, one must consider k values in the region for which sinc(3.14k), the Fourier transform of part of V(x) is almost 0. In such a case, this small value has a chance of combining with Vo, which is extremely large, to create a finite term which is needed to balance $p^2/2m$ fp with Efp.

It seems that for all p values other than +/- 3.14/L, one requires a contribution from the potential to allow for a balanced energy equation for the p (momentum wave) in question. Thus, even though V(x)W(x) may be 0, it seems this combination may contribute nonzero values to all p wave energy equations except for p=+/-3.14/L. In other words, it may be decomposed into nonzero terms which combine to yield 0. In such a case, it may seem one has a zero potential in the interior of the box, but plane waves may still feel a force.

Conclusion

In conclusion, although V(x)W(x) may be zero in the Schrodinger equation, if one takes a Fourier series of both V(x) and W(x) and isolates terms for each exp(ipx), one may obtain an energy conservation for each p wave. If V(x) is 0 in certain regions as in the case of a particle in a box with an infinite potential at the walls, it seems there may still be potential interactions through Sum over k Vk f(p-k) and hence a force for some of the p waves (all but p=+/- 3.14/L for the box). It is only on average that there appears to be a V(x)=0. Thus, there seems to be a distinction between a classical average V(r) and its microscopic effect on a quantum particle.

References

1. Ruggeri, Francesco R. Does the Quantum Wavefunction Follow from a Fourier Series Treatment of a Classical Potential? (preprint, zenodo, 2019)

2. https://en.wikipedia.org/wiki/Particle_in_a_box

3. https://en.wikipedia.org/wiki/Rectangular_function

4. https://en.wikipedia.org/wiki/Rectangular_potential_barrier#E_%3C_V0