Fourier Transform for Bound States in a Step Potential

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In (1) the Fourier transform for a particle in a box with an infinite potential at the walls is calculated to show that all plane waves exp(ipx) are stirred up by collisions with the wall even though the spatial wavefunction is proportional to sin(kave x+b). In this note, we consider the case of a finite potential wall and investigate the Fourier transform. We argue that one must calculate the Fourier transform for x ranging from -infinite to + infinite. Thus, if the potential is very different in different regions, one may have W(x), the wavefunction, equaling different functions in each region. (Each is a solution to the time independent Schrodinger equation with the appropriate potential for the region in question.) If one wishes to keep the integration bounds of the Fourier transform at -/+ infinite, one may need to multiply the various W(x) functions by step like functions to ensure that a particular function is nonzero only in its appropriate region. The Fourier transform of a step function multiplied by a general function, however, is not the same as the Fourier transform of the function itself. Furthermore, one obtains an overall Fourier transform which is influenced by each spatial region. Thus, weights f(p) in W(x)= Sum over p f(p) exp(ipx) in a damped region within a potential barrier include contributions from a region where there is no potential and one has sinusoidal behaviour (and vice versa).

Finite Potential Wall

We consider the potential: V(x)= Vo for x>0, V(x)=infinite for x= -L V(x)= 0 for -L <= x<=0

W(x)=0 for x<-L

For the region with V=0, one may solve the time independent Schrodinger equation to obtain the well-known result:

W(x)=A sin(k1x) + B cos(k1x) but W(-L)=0 for -L <= x<=0 ((1a))

And W(x)= C exp(-k2 x) for x>0. ((1b))

The two W(x)'s directly above as well as d/dx W(x) are matched at x=0.

A question arises as to whether this system should also stir up all possible plane waves in the momentum representation. We rewrite the wavefunction ((1a)) and ((1b)) in terms of step type functions:

W(x)= [A sin(k1x) + B cos(k1x)] v(x) where v(x)=0 for x>0 and x<-L and u(x)=1 for -L <= x<=0

And W(x)= C exp(-k2 x) u(x) where u(x)=0 for x<=0 and 1 for x>0

These step type functions help make the Fourier transform nonzero for all p values, although exp(-k2 x) already by itself has a Fourier transform which includes all p. One, however, does not use the Fourier transform of exp(-k2 x) by itself

For the region -L<=x<=0, we use the same result as for the case V=infinite at the walls except that the wavefunction is not required to be zero at x=0, although it is zero at x=-L. Rather at x=0, it must match the value and the spatial derivative of C exp(-k2 x) outside the barrier. The Fourier transform for W(x)= [A sin(k1x) + B cos(k1x)] v(x) where v(x)=0 for x>0 and x<-L and u(x)=1 for -L <= x<=0 is given by (2):

f(p)= A1 [k1/ (k1 + k)] sin(.5L(k1-k))/ [L(k1-k)] exp(-ikxc) exp[i(.5Lk1 -3.14/2] ((2))

hbar=1 xc=center of the box i.e .-L/2

For the region x>0 we use (3) i.e.

Fourier transform of u(x) exp(-k2 x) = 1/ (k2 - i k) ((3))

Thus, the overall Fourier transform seems to be ((2)) + ((3))

A1 [k1/ (k1 + k)] sin(.5L(k1-k))/ [L(k1-k)] exp(-ik xc) exp[i(.5Lk1 -3.14/2] + 1/(k2 + ik) ((4))

If one examines the kinetic energy density in the region x>0, one sees it is negative:

W(x) (-1/2m) d/dx d/dx W(x) i.e. (-1/2m) k2*k2 exp(-2 k2 x) ((5))

If one considers kinetic energy in the momentum representation, one has:

Sum over p p*p/2m fp* fp or:

Sum over p p*p/2m { A*(p)A(p) + [A(p)/(k2-ik) + A*(p)/(k2+ik)] + 1/($k2^2$-p^2) } ((6))

For k2 very small, i.e. for E close to Vo, the last two terms in ((6)) are negative, lowering the KE for each exp(ipx) (as long as Im(A(p))>0. The last term is almost always negative (for k2 almost 0.)

Here A(p) = is given by ((2)).

For the particle in the region $-L<=x<=0$, it seems all exp(ipx) waves should be stirred up, if they are stirred up by in box with an infinite potential at the walls. This problem seems similar, even though the wavefunction can penetrate into the nonclassical region where V=Vo. On the other hand, the step like potential is often used in scattering problems, where a single exp(ikx) encounters a barrier. This problem is often solved in textbooks and the solutions are similar to those above, although exp(-k2 x) and exp(k2 x) are used within the V=Vo barrier. Both of these however, have Fourier transforms including all exp(ipx) waves. Does one have a single exp(ik1 x) incident wave which stirs up all possible exp(ipx) upon hitting the barrier? If the exp(i k1 x) wave reflects and becomes trapped (i.e. the wavefunction becomes real), it seems it should be interacting with the barrier and stirring up exp(ipx) waves within the region where V=0 .

Conditional Probability

Another point to consider is conditional probability:

P(p/x) = f(p) exp(ipx) / W(x) ((7))

W(x) is the wavefunction at a point x. Thus, one may solve the Schrodinger equation in a particular region to find W(x) in that region. f(p), however, does not seem to be x-region specific. Thus, it seems that for the problem here, one must use the full value ((4)) of the Fourier transform, even at a point within the potential barrier. Thus, part of the f(p) weight from within the box where V=0 is part of f(p) as is the part from the barrier. Thus,

P(p/x1)= f(p) exp(ipx)/ (exp(-k2x1) in the barrier and P(p/x2) = f(p) exp(ipx2) / (A sin(k1x2) + B cos(k1x2)) ((8))

Thus:

P(p/x1) / P(p/x2) = exp(-k2x1) / [A sin(k1x2) + B sin(k1 x2)] ((9))

In the barrier region, the conditional probability ratio for two different p values is:

P(pa/ x1) / P(pb / x1) = f(pa) exp(ipa x1) / [f(pb) exp(ipb x1)] ((10))

From ((10)), one sees that it is not the Fourier transform of exp(-k2 x) u(x) which influences the ratio, but the full Fourier transform. Thus, even in the barrier region, the weights of different plane waves are affected by the result in the region with no potential and vice versa.

Alternatively:

P(x1/p)= exp(-k2 x1) exp(-ip x1) / f(p)   and P(x2/p) = [A sin(k1x) + B cos(k2 x)] exp(-ip x2) / f(p) ((11))

Thus, it seems that one must be careful to avoid thinking that for W(x)=Sum over p f(p) exp(ipx), the f(p) values at a point x, only depend on the interaction of the p waves with the potential at that point. Thus, in the momentum view, spatial locality which is strongly present in the x representation is partially lost. In other words, one cannot consider too strongly the p representation as a statistical mechanical picture of different p-momentum particles colliding with a local potential as the weight f(p) depends on the entire Fourier transform. A special case, however, occurs for the ground state of the oscillator.

Ground State Oscillator

The Fourier transform of the wavefunction applies to each point in space at which the particle may exist. For a ground state oscillator, the Fourier transform of the wavefunction is of the form exp(-ap^2), thus this applies to each point on the x axis. In classical statistical mechanics, for an equilibrium situation one must have the same temperature at each point in space. This leads to the same Boltzmann factor exp(-p^2/2mT) existing at each point. This is not related to a Fourier transform it seems, but the result is the same as in the ground state oscillator. Thus, there seems to be a link between quantum mechanics and classical statistical mechanics for this case. (The spatial dependent portion for statistical mechanics is exp(-V(x)/T). For the ground state oscillator it is exp(- sqrt(km) xx) = W(x)W(x).)

Conclusion

In conclusion, it seems that in calculating a Fourier transform of a wavefunction which has different potential values in different regions, one calculates one Fourier transform for x from -infinite to + infinite, even though the spatial wavefunction may be calculated separately in each region, using the Schrodinger equation and the potential appropriate for that region. Thus, the wavefunction W(x)= Sum over p   f(p) exp(ipx) has an f(p) which is influenced by the behaviour of the wavefunction in all regions. This carries through even if one is calculating conditional probabilities such as P(p/x) = f(p) exp(ipx) / W(x). W(x) may be local, but f(p) incorporates all spatial regions.

References

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