

Time Independent Schrodinger Type Equations

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In this note, we wish to consider a derivation of sorts of time independent Schrodinger type equations from general principles related to a function which is the square root of a density. This derivation is not aimed at quantum mechanics, in fact it is classical, yet it appears to apply to quantum mechanics and the oscillator potential of statistical mechanics and not to the $1/v(x)$ density of classical mechanics. We try to consider the reason for this.

Formulation of the Problem

Let us consider a classical problem in which there is conservation of energy:

$$.5m v(x)^2 + V(x) = E \quad ((1))$$

One can also consider a situation in which there is a spatial density because in (1) even a single particle moving according to ((1)) is said to have a spatial density proportional to $1/v(x)$.

In such a case, the average kinetic energy is: $KE_{ave} = \int dx \, d(x) \cdot .5 m v(x)v(x) d(x)$ that of potential energy $PE_{ave} = \int dx \, V(x) d(x)$, where $d(x)$ is density. It possible to make the integrand appear symmetrical by writing $d(x) = W(x)W(x)$. In addition, this anticipates the form used in linear algebra and so there is also a math motivation.

Now:

$$V(x)W(x) = PE_{ave} W(x) + [V(x)-PE_{ave}] W(x) \quad ((2))$$

The second term is orthogonal to the first as one can see by multiplying by $W(x)$ and integrating. Here we assume $\int dx \, W(x)W(x) = 1$. If $W(x)$ is the first function in a set of orthonormal functions then the second term in ((2)) is a linear combination of $W_i(x)$ with $i > 0$ and $W(x) = W_0(x)$. Also:

$$Op W(x) = .5m v(x)^2 W(x) = KE_{av} W(x) + [.5mv(x)^2 - KE_{ave}] W(x) \quad ((3))$$

Here Op is an operator which yields the classical kinetic energy at a point times $W(x)$. It is important that Op be an operator (contain derivatives) and not just a function of x , otherwise there is no derivation. The second term in ((3)) is orthogonal to $KE_{av} W(x)$ and is also the negative of the second term of ((2)).

To consider matters in terms of “linear algebra”, consider a complete set of orthonormal functions $W(x), W_1(x) \dots$

Then: $[PE_{ave} + V(x) - PE_{ave}]W(x) = PE_{ave} W(x) + \sum_{i>0} a_i W_i(x)$ and

$[KE_{ave} + Op - KE_{ave}]W(x) = KE_{ave} W(x) + \sum_{i>0} b_i W_i(x)$.

Thus: $[Op + V(x)]W(x) = [KE_{ave} + PE_{ave}]W(x) + \sum_{i>0} a_i W_i(x) + \sum_{i>0} b_i W_i(x)$

If one considers:

$$M = \langle W(x) | [Op + V(x)] [Op + V(x)] | W(x) \rangle = \int dx W(x) E [EW(x) + Fluc1 + Fluc2] + H[Fluc1 + Fluc2]$$

Here $Fluc1 = \sum_{i>0} a_i W_i(x)$ and $Fluc2 = \sum_{i>0} b_i W_i(x)$

$$M = E^*E + \int W(x) H [Fluc1 + Fluc2]$$

If H is self-adjoint then

$$M = E^*E + [EW(x) + Fluc1 + Fluc2][Fluc1 + Fluc2] = E^*E + [Fluc1 + Fluc2]^2$$

Now $M = E^*E$ by definition so $Fluc1 = -Fluc2$ is a solution.

Thus, one can write:

$$Op W(x) + V(x) W(x) = [KE_{ave} + PE_{ave}] W(x) = E W(x)$$

This equation is of the form of a time independent Schrodinger equation, but no mention of quantum mechanics has been made, In fact, the arguments used are entirely classical together with the idea of a density and an operator acting upon it. It should be noted, however, that this approach implicitly contains the result:

$Ed(x) = E(x)$ i.e. total energy times the spatial density is $E(x)$, the energy density.

The next step is to attempt to obtain Op , the kinetic energy operator.

$$\exp(-b\partial) W(x) = W(x+b) \quad \text{Here } \partial = d/dx$$

$$Op W(x) = .5mv(x)^*v(x)W(x) \quad \text{and} \quad Op W(x+b) = Op \exp(-b\partial) W(x) = .5m v(x+b)^*v(x+b)W(x+b)$$

$$\exp(-b\partial)OpW(x) = .5m v(x+b)^*v(x+b)W(x+b)$$

Thus, $[Op, \exp(b\delta)] = 0$.

As a result, the kinetic energy operator Op commutes with all powers of $\delta = d/dx$ so one might consider Op to be a function of derivatives. Given that kinetic energy is positive, one might consider $m/2 (-d/dx)(d/dx)$ as a solution, although there could be various other solutions. The point is that a choice of Op proportional to δ^2 results in time independent quantum mechanics, but also the oscillator of classical statistical mechanics. The classical mechanical oscillator of statistical mechanics does not only hold for a one dimensional problem, but also applies to a gas rotating in a cylindrical container (2). A question arises as to whether this choice of Op applies to a classical mechanics oscillator. Consider:

$$Op W(x) = .5mv(x)v(x) W(x) \quad \text{with} \quad W(x) = \exp[g(x)]$$

$$\text{Then} \quad \exp[g(x)] \{ (d/dx)(d/dx)g(x) + [d/dx g(x)][d/dx g(x)] \} = (E - V(x)) W(x)$$

If $g(x) = ax^2$, one has a solution, but this restricts the relationship between E and $V(x)$ and so does not seem to apply to a classical oscillator.

One could suggest using $Op = -d/dx$ for $x > 0$. Then:

$\exp(Ex - (1/3).5k x^3)$ would yield a solution for all E and $.5kx^2$ situations, but this $W(x)$ is not at all similar to $1/v(x)$. (Note: $d(x) = W(x)W'(x)$). In fact, neither of these scenarios for Op is similar to $d(x)$ proportional to $1/v(x)$.

The Classical Mechanical Case

According to (1), a classical mechanical object moving according to ((1)), has a spatial density proportional to $1/v(x)$. This is obtained only considering motion determined by acceleration and calculating the time spent in each little region δx . To clarify this, note that:

$$d(x) v(x) = \text{constant for the classical case so}$$

$$[d/dx d(x)] v(x) + d(x) d/dx v(x) = 0 \quad \text{i.e. the density changes only due to acceleration.}$$

The statement:

$$Op W(x) = .5mv(x)v(x) W(x) \quad \text{with} \quad d(x) = W(x)W'(x)$$

seems to be of a very different nature. To attempt to see what is happening, take d/dx of the above.

$d/dx(.5mv(x)*v(x)) W(x) + .5mv(x)v(x) d/dxW(x) = d/dx [Op W(x)]$ which is not equal to 0.

Thus, the change in $W(x)$ and hence the change in density $d(x)$ is not strictly governed by acceleration if one considers a initial equation of $Op W(x)=.5mv(x)v(x) W(x)$. Thus, such an equation excludes the classical mechanical in the first place. To consider the oscillator in classical statistical mechanics, it was noted in (3), that the density $d(x)=\exp(-V(x)/T)$ can be arrived at by comparing the weights of the Maxwell-Boltzmann velocity distribution at a place where the potential is V_0 and there is no collective motion and a point x where there is collective kinetic energy. At V_0 , (the wall), one will have a certain weight for a velocity v_1 . At x , v_1 will have become a larger velocity v_2 (but relative probabilities are the same). Thus, at x one has v_2 , but with the higher weight of v_1 . This makes it look like density has increased. It should be noted that there are two factors here, the acceleration and the original Maxwell-Boltzmann distribution.

Conclusion

In conclusion, we try to develop a type of time-independent Schrodinger equation from very simple assumptions involving density and its square root. We try to see if this can be applied to any current theories and note that it matches quantum mechanical bound states and oscillator potentials in classical statistical mechanics. It does not apply to classical mechanics because the theory is not based on a density change due solely to acceleration. This, we think, may give some insight into differences between densities in quantum mechanics and classical statistical mechanics as opposed to classical mechanics,

References

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