

Math 5757: Look at section 2 to see how Schrödinger's eq'n is the asymptotic limit of the Klein-Gordon equation.

Dear Rodica,

In our last conversation, if I remember correctly, you directed attention to the problem of the quantum dynamics of a particle subjected to periodic potential like the one in Figure 1 below. Systems mathematized by such periodic structures are fundamental to physics (and engineering), not only in the context of quantum mechanics, but also in laser holography, transmission through periodic optical fibers, etc. The Epilogue below concretizes aspects of this in mathematical terms.

Below is a more readable account of my hand written e-mail from Thursday..

1 THE FRAMEWORK

Consider Klein-Gordon (K-K) wave equation

$$\frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} - \nabla^2 \psi + \left(\frac{mc}{\hbar} \right)^2 \psi + V(t, x, y, z) \psi = 0 \quad (1)$$

The asymptotic non-relativistic limit of its solutions can be obtained in two ways:"

1: First exhibit the asymptotic non-relativistic wave equation, and then solve it, or

2: First solve the K-G equation, and then go to the asymptotic non-relativistic limit of its solutions.

When the potential $V(t, x, y, z)$ depends on time and varies with sufficiently high frequency, e.g. like in Figure 1,

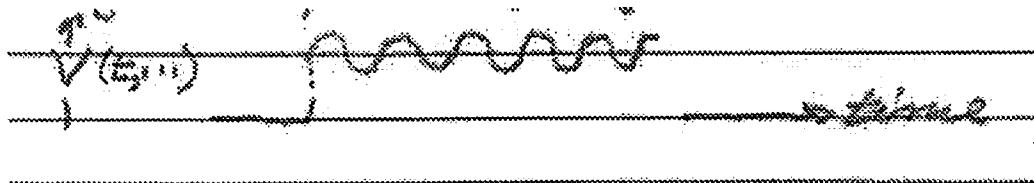


Figure 1: Ramped-up sinusoid

then approach # 1 does not really mathematize all the facts of the matter. This is because approach # 1 excludes the possibility of particle-antiparticle pair creation from the very start of one's formulation.

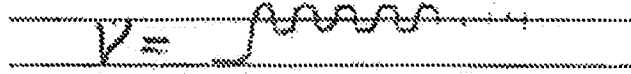
If the potential

$$V(t, x, y, z) \sim \sin \omega t$$

has Fourier components of frequency ω sufficiently high (i.e. $\omega \geq 2 \frac{mc^2}{\hbar}$) then there is the possibility of non-zero amplitude (i.e. inner product) between positive and negative energy solutions to the K-G wave equation. Such a non-zerosness mathematizes the creation process of particles and anti-particles. A

mathematical formulation in terms of the (non-relativistic) Schrödinger equation would exclude such a process from the beginning.

Nevertheless, a formulation in terms of the Schrödinger equation would be very desirable for a number of reasons. The least one is by no means the fact that most workers in this field feel more comfortable with the Schrödinger equation. This is in spite of the fact that the problem is easier in the context of a K-G



equation like

$$\frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} - \frac{\partial^2 \psi}{\partial x^2} + \left(\frac{mc}{\hbar} \right)^2 \psi + V(t, x) \psi = 0 \quad (2)$$

instead of a Schrödinger equation like

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \phi}{\partial x^2} + V(t, x) \phi = i \hbar \frac{\partial \phi}{\partial t}. \quad (3)$$

However, if one takes into account the fact that both the K-G approach and the Schrödinger approach are valid in their respective domains, then there should be a line of asymptotic mathematical reasoning in which one derives the Schrödinger equation from the K-G wave equation.

2 SCHRÖDINGER AS THE ASYMPTOTIC LIMIT OF KLEIN-GORDON

The derivation of the asymptotic non-relativistic limit in the form of the Schrödinger equation hinges on a specific type of solutions to the K-G Eq.(1), namely those whose space-time propagation vector

$$\left\{ \frac{1}{c} \frac{\partial \psi}{\partial t}, \frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial z} \right\}$$

point primarily into the time direction, i.e.

$$\left| \frac{\partial \psi}{\partial x} \right|, \left| \frac{\partial \psi}{\partial y} \right|, \left| \frac{\partial \psi}{\partial z} \right| \ll \left| \frac{1}{c} \frac{\partial \psi}{\partial t} \right|. \quad (4)$$

This means that the spatial momenta $|p_x|$, $|p_y|$, $|p_z|$ are small compared to mc . Thus the phase fronts in t, x, y, z -space have only a slight tilt with respect to the $t = 0$. By contrast to a highly relativistic particle has phase fronts whose vectorial gradient is close to the speed of light ($x = ct$) as in Figure 3.

Question:

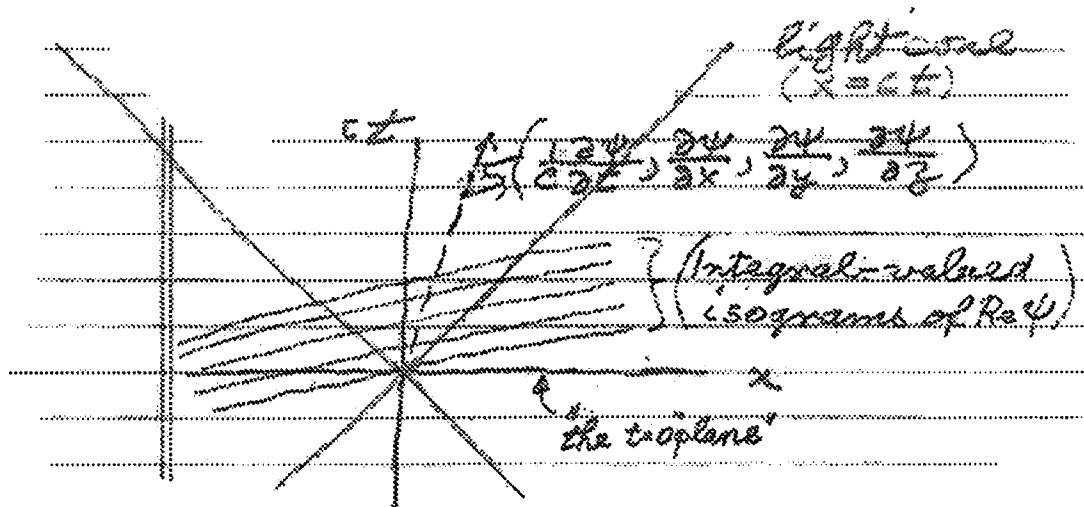


Figure 2: Phase fronts of ψ for a non-relativistic particle

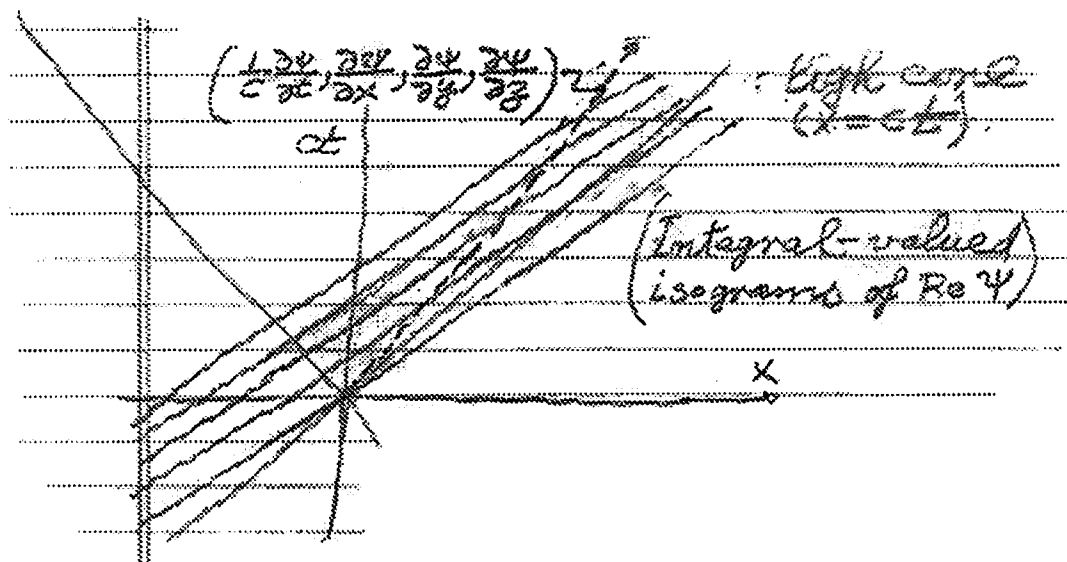


Figure 3: Phase fronts of ψ for a highly relativistic particle

By what mathematical relation does one conceptualize a K-G wave solution $\psi(t, x, y, z)$ as being non-relativistic?

Answer:

STEP I: Consider a K-G solution $\psi(t, x, y, z)$ which is non-relativistic

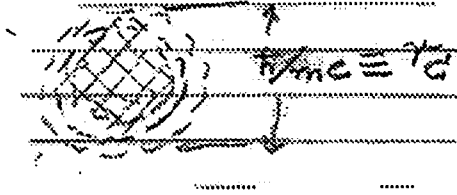


Figure 4: The Compton wave length of a particle of mass m

and thus obeys inequality (4).

STEP II: Introduce the new non-relativistic wave function $\phi(t, x, y, z)$ by setting

$$\psi = e^{i(\frac{mc}{\hbar})ct} \phi, \quad (5)$$

so that

$$\left| \frac{1}{c} \frac{\partial \psi}{\partial t} \right| = \frac{mc}{\hbar} |\phi| + \left| \frac{1}{c} \frac{\partial \phi}{\partial t} \right|.$$

Then mathematize the non-relativistic condition on ϕ by the condition that the second term on the r.h.s. is much smaller than the first:

$$\boxed{\frac{mc}{\hbar} |\phi| \gg \left| \frac{1}{c} \frac{\partial \phi}{\partial t} \right|}. \quad (6)$$

The (inverse of the) coefficient $\frac{\hbar}{mc} \equiv r_C$ is the quantum mechanical Compton wave length of the particle and c is the speed of light. Thus

$$\frac{r_C}{c} = \left(\begin{array}{l} \text{the amount of time it would} \\ \text{take for light to travel} \\ \text{one Compton wave length} \end{array} \right)$$

This time,

$$\frac{r_C}{c} = \frac{\hbar}{mc^2} \equiv \Delta t_C,$$

is called the Compton time. Inequality (6), the temporal non-relativistic condition, stipulates that

$$\boxed{|\phi| \gg \left| \frac{\partial \phi}{\partial t} \right| \Delta t_C}, \quad (7)$$

namely, namely that the non-relativistic wave function ϕ changes very little over the q.m. Compton time of the particle.

STEP III: Taking the time derivative of inequality (6) on page 4 results in the condition

$$\left| \frac{\partial \phi}{\partial t} \right| \gg \left| \frac{\partial^2 \phi}{\partial t^2} \right| \Delta t_C . \quad (8)$$

STEP IV: Introduce Eq.(5) into the K-G Eq.(1) on page 1. The resulting exact equation for ϕ is

$$-\left(\frac{mc}{\hbar}\right)^2 \phi + 2i \frac{m}{\hbar} \frac{\partial \phi}{\partial t} + \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} - \nabla^2 \phi + \left(\frac{mc}{\hbar}\right)^2 \phi + V\phi = 0$$

Multiply by $\frac{\hbar^2}{2m}$ and obtain the equivalent exact equation:

$$-\hbar \left(i \frac{\partial \phi}{\partial t} + \frac{\hbar}{2m} \frac{1}{c^2} \frac{\partial^2 \phi}{\partial t^2} \right) = -\frac{\hbar^2}{2m} \nabla^2 \phi + \frac{\hbar^2}{2m} V\phi.$$

Handwritten notes on the right side of the equation show the derivation of the non-relativistic potential:

$$\begin{aligned} &= \frac{2m}{\hbar^2} V_{nonrel} \\ &\left(mc^2 + \frac{V_{nonrel}}{c^2} \right) = \\ &= \left(m^2 c^2 + 2m V_{nonrel} + \frac{V_{nonrel}^2}{c^2} \right) \\ &= m^2 c^2 + \end{aligned}$$

STEP V: Taking note of inequality (8), we note that the 2nd term on the the l.h.s. of this exact equation is negligible compared to the first. Thus

$$\frac{\hbar}{i} \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \phi + V_{nonrel} \phi . \quad (9)$$

This is the Schrödinger equation whose non-relativistic potential V_{nonrel} is related to the relativistic V on page 1 by

$$V_{nonrel}(t, x, y, z) = \frac{\hbar^2}{2m} V(t, x, y, z)$$

3 CONCLUSION

The mathematical relation by which one conceptualizes a K-G wave solution ψ to be asymptotically non-relativistic is the condition (4). Its implementation consists of introducing via Eq.(5) the new function ϕ , which, because of (4), satisfies (7) and (8), and hence the Schrödinger Eq.(9).

4 EPILOGUE

The mathematical analysis of Schrödinger waves in the ramped up periodic potential, Figure 1, also applies to Euclidean optics. There one has a *paraxial*¹ laser beam passing through a medium with a periodic refractive index whose spatial variations have the same mathematical form as V has in Figure 1. In fact, in that Euclidean scenario one must use Kokelnik's equation for paraxial

¹the Euclidean analogue of being *non-relativistic* in space-time

wave patterns. This equation is the Euclidean analogue of the Schrödinger equation. The Kogelnik equation is

$$ik \frac{\partial \phi}{\partial z} = -\frac{1}{2k} \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) + \varepsilon(x, y, z) \phi \quad (10)$$

It is the result of an asymptotic analysis applied to the Helmholtz equation,

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + k^2 \psi + \varepsilon(x, y, z) \psi = 0, \quad (11)$$

in a medium whose refractive index n is $n(x, y, z) = 1 + \varepsilon(x, y, z)$. If ε is periodic in x and z but uniform in y , then such a periodic structure is a thick hologram, and ψ is the amplitude of laser radiation propagating through it. Equations (10) and (11) are the Euclidean analogue of what in space-time are the Schrödinger and the K-G equations.