On the properties of simple quantum graphs

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Contents

PART 1

1 Introduction

Recent development in nanotechnology put us on the threshold of new era when new nano scale devices with desired properties will be designed and fabricated. To be able to advance to that stage good mathematical models capturing significant properties of such devices are necessary. Because of the nanometer scale this models have to be necessarily quantum mechanical.

First part of this thesis study one such a model represented by quantum graph. A model useful for modelling propagation of quantum particle through a nanodevice consisting of a number of parts connected together by quantum wires. Features which quantum graph is able to capture is how the geometry and connection conditions affects the functioning of such a device. Particularly the question of connecting different parts together turns out to be nontrivial and leads to many possible alternatives. The region of connection can be considered as a short range limit of potential known as quantum point interaction. Quantum point interaction is a model of potentials possessing discontinuities or potentials varying wildly on a scale small when compared to the wavelength of the wavefuncton of the particle. The mathematical approach to such a problem is considering the potential to be point like and imposing proper boundary conditions on the wave function at given point. These conditions of course cannot be arbitrary. They depend on the nature of the connection and must be consistent with quantum mechanics, which in other words mean that the Hamiltonian describing the dynamics of such a system must be selfadjoint. This requirement of self adjointness of the Hamiltonian gives us all possible boundary conditions how two or more pieces of material can be connected together. For example in the case of one dimensional model, representing systems whose one dimension is much larger than other, the family of connection conditions is very rich and can be fully described by the unitary group $U(2)$. Properties of some of these boundary conditions are familiar to us and have been described in detail in literature. Let's name for example δ interaction or Dirichlet and Neumann boundary conditions. On the other hand there are other less known conditions often with unique and exotic properties waiting for detailed examination.

Among these less known point interactions we have chosen scale invariant point interaction first mentioned by Fulop and Tsutsui [1] whose properties are independent of energy of incident particle. As the system doesn't change its properties as the energy changes this point interaction is useful for studying the spectral and scattering properties of other point interaction in the "middle" energy region where the propagation is fully stochastic.

Studying quantum graphs as a system consisting of point interactions connected by bonds where the particle moves freely, helps us with understanding another phenomena known as a quantum chaos. As is described later in this thesis in more details, quantum chaos theory is trying to explain how classical chaotic behaviour arises from quantum dynamics. It has been shown that quantum systems with classical chaotic limit possess certain qualities regular quantum systems don't. These qualities which might be considered as seeds of

the classical chaos in quantum world are present in the wave function, energy spectra and also in scattering properties of quantum chaotic systems. More about that in the chapter 4 dedicated to quantum chaos. One of the central result of the first part of these thesis is that this features formerly considered to be a properties of quantum chaotic systems only are reproducible with simple, integrable, fully solvable system possessing no chaotic limit at all. This system consists of a number of point interactions arranging on the line and/or circle in incommensurable manner and a free electron moving on such a structure. This findings brings back the question If there exist any property of a quantum system which tells us that the classical limit of the system is chaotic.

References

[1] Tamas Fulop, Izumi Tsutsui, Taksu Cheon, J. of Phys. Soc. Jpn 72 (2003) 2737-2746

2 Review of basics of quantum mechanics in one dimension

Before we start talking about quantum graphs and point interactions let's review some basic properties of one dimensional quantum systems first.

We adopt the Schrödinger picture of quantum mechanics where the state of the system is represented by a vector Ψ in a Hilbert space $L^2(A)$ consisting of all square integrable complex functions defined on a subset $A \subseteq R$ where R represents the real line. Apart from square integrability which is mathematically described as

$$\int_{-\infty}^{\infty} |\Psi|^2 \, dx < \infty \tag{1}$$

the wave function must satisfy the one dimensional Schrödinger equation (SE) together with certain boundary conditions.

2.1 1D Schrödinger equation

The general time dependent SE is of the form

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H} \Psi(x,t) \tag{2}$$

$$\hat{H} = \nabla^2 + V \tag{3}$$

Here $\hat{H}$ is the Hamiltonian of the system.

In this thesis we deal with one dimensional systems and time independent potentials only and therefore when we talk about SE we mean the time independent SE of the form

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x) \tag{4a}$$

where $V(x)$ is time independent potential and E is energy of the system.

General time dependent solution for Hamiltonian with discrete or continuous spectrum is then of the usual form

$$\Psi(x,t) = \sum_{n=0}^{\infty} \psi_n(x) e^{-iE_n t/\hbar} \tag{5}$$

$$\Psi(x,t) = \int_{-\infty}^{\infty} \rho(k) \psi(x) e^{-iEt/\hbar} \tag{6}$$

The propagation of a quantum particle can be described either by its wave function or with the help of quantity derived from the wave function and called probability current. This concept of probability current have some advantages against the wave function and as we show later plays an important role in specifying boundary conditions for certain type of quantum systems.

The 1-dimensional probability current is defined as

$$j(x) = -\frac{i\hbar}{2m}(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}) \tag{7}$$

Since we suppose that the total number of particles in our system is constant we will require that the total probability current is conserved. This fact is mathematically expressed as the conservation equation

$$\frac{\partial |\Psi|^2}{\partial t} + \overrightarrow{\nabla}.\overrightarrow{j} = 0 \tag{8}$$

2.2 Solution of 1D Schrödinger equation for simple systems

2.2.1 Free solution

The free time independent Schrödinger equation is of the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \tag{9}$$

$$E = \frac{\hbar^2 k^2}{2m} \tag{10}$$

where k is a real continuous parameter.

This is well known equation for harmonic oscillator with the solution

$$\psi(x) = Ae^{ikx} \pm Be^{-ikx} \tag{11}$$

The time dependent solution is

$$\psi(x,t) = Ae^{i(kx-\omega t)} \pm Be^{-i(kx-\omega t)} \tag{12}$$

$$\omega = \frac{E}{\hbar} \tag{13}$$

The solution consists of a linear combination of two waves. The first term e^{ikx} represents wave propagating from left to right and the second term e^{-ikx} represents wave propagating in opposite direction.

It should be mentioned here that solution for one particular choice of k does not represent valid state because it is not normalizable.

We can nevertheless construct the general solution of the time dependent SE as a wave-packet consisting of linear combination of waves of different energy.

$$\psi(x,t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} dk \tag{14}$$

The probability current of a free particle is given by

$$\overrightarrow{j} = \overrightarrow{j_A} - \overrightarrow{j_B} = |A|^2 \frac{\hbar \overrightarrow{k}}{m} - |B|^2 \frac{\hbar \overrightarrow{k}}{m} = (|A|^2 - |B|^2) \frac{\hbar \overrightarrow{k}}{m} \tag{15}$$

2.2.2   Particle in constant potential

Now let's consider particle propagating in a region with constant potential.

The SE now takes the form

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V_0 \psi(x) = E\psi(x) \tag{16}$$

or equivalently

$$\frac{d^2\psi(x)}{dx^2} = -k_1^2 \psi(x) \tag{17}$$

$$k_1^2 = \frac{2m}{\hbar^2}(E - V_0) \tag{18}$$

These equations are similar to those we solved for free case and we can immediately write the solution as a linear combination of two waves propagating in opposite directions. The time independent part is

$$\psi(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x} \tag{19}$$

Spectrum is again continuous and consists of all points on the real line R.

Important fact that should be noticed here is how the general solution depends on the energy of particles. In case $E > V_0$ coefficient k is real and the solution is a periodic wave. In case when $E < V_0$ coefficient k become imaginary and the solution consist of linear combination of exponentials

$$\psi(x) = A_1 e^{-k_1 x} + B_1 e^{k_1 x} \tag{20}$$

since exponential function is not normalizable we drop the increasing part $e^{k_1 x}$ and consider only the exponentially decreasing part $e^{-k_1 x}$.

In the region where the energy of the particle is lower than the potential energy (classically prohibited region) the wave function is decreasing exponentially with the distance x.

$$\psi(x) = A_1 e^{-k_1 x} \tag{21}$$

This result represents the well known quantum mechanical effect called quantum tunneling when quantum particle enters classically prohibited region and vanishes exponentially.

2.2.3 Potential step

Now let's investigate the situation when quantum particle propagates from one region of constant potential V_1 to second region of constant potential V_2. Of special interest are the boundary conditions a wave function must satisfy at the point of potential change and consequences following these conditions.

Requirements we have on our wave functions are continuity at the point where potential change and in case that the change is finite we require also continuity of the derivative of the wave function.

Suppose that the change of the potential takes place at point $x = a$ than the continuity conditions are expressed as follows

$$\psi_1(a) = \psi_2(a) \tag{22}$$
$$A_1 e^{ik_1 a} + B_1 e^{-ik_1 a} = A_2 e^{ik_2 a} + B_2 e^{-ik_2 a} \tag{23}$$

and

$$\psi_1'(a) = \psi_2'(a) \tag{24}$$
$$ik_1 A_1 e^{ik_1 a} - ik_1 B_1 e^{-ik_1 a} = ik_2 A_2 e^{ik_2 a} - ik_2 B_2 e^{-ik_2 a} \tag{25}$$

Using matrix notation these conditions can be rewritten as

$$\begin{bmatrix} A_1 \\ B_1 \end{bmatrix} = M \begin{bmatrix} A_2 \\ B_2 \end{bmatrix} \tag{26}$$

where

$$M = \frac{1}{2} \begin{pmatrix} 1 + \frac{k_2}{k_1} & 1 - \frac{k_2}{k_1} \\ 1 - \frac{k_2}{k_1} & 1 + \frac{k_2}{k_1} \end{pmatrix} \tag{27}$$

Matrix M is called transfer matrix and its job is to transmit particles through the boundary between the two regions of different potential energy.

Propagation matrix is a very useful tool which can help us to find the transmission and reflection coefficients which represent the probabilities of transmission and reflection of the particle on the potential step.

To be able to derive these coefficients let's rewrite the general wave function in more convenient form

$$\psi(x) = e^{ik_1 x} + R.e^{-ik_1 x}, \text{for } x < a \tag{28}$$

$$\psi(x) = Te^{ik_2 x}, \text{for } x > a \tag{29}$$

using the transfer matrix we get

$$\begin{bmatrix} T \\ 0 \end{bmatrix} = \frac{1}{2} \begin{pmatrix} 1 + \frac{k_2}{k_1} & 1 - \frac{k_2}{k_1} \\ 1 - \frac{k_2}{k_1} & 1 + \frac{k_2}{k_1} \end{pmatrix} \begin{bmatrix} 1 \\ R \end{bmatrix} \tag{30}$$

Evaluating this system gives us

$$T = \frac{2k_2}{k_1 + k_2} \tag{31}$$

$$R = \frac{k_2 - k_1}{k_2 + k_1} \tag{32}$$

Notice that we supposed positive energy on both sides of the potential step and got nonzero reflection coefficient. A situation which is impossible in our classical Newtonian world.

2.2.4 Delta function potential well

In this last section from introductory chapter we will deal with special type of potential called delta potential which is defined as

$$\delta(x) = \begin{cases} \infty, x = 0 \\ 0, x \neq 0 \end{cases} \tag{33}$$

where $\delta(x)$ is so called delta function with additional property

$$\int_{-\infty}^{\infty} \delta(x) \psi(x) \, dx = \psi(0) \tag{34}$$

Schrödinger equation has the form

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} - \alpha\delta(x)\psi(x) = E\psi(x) \tag{35}$$

where α is some real constant defining the strength of the potential.

Solution for $x \neq 0$ yields

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x} \tag{36}$$

with different A, B for $x > 0$ and $x < 0$.

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Coefficient κ is defined as

$$\kappa = \frac{\sqrt{-2mE}}{\hbar} \tag{37}$$

For bound states $E < 0$ is κ real and the solution is of the form

$$\psi(x) = \begin{cases} B_1 e^{\kappa x}, x < 0 \\ A_2 e^{-\kappa x}, x > 0 \end{cases} \tag{38}$$

To find the wave function of the whole system we have to stitch the solutions together. The requirement of continuity gives us $B_1 = A_2 = B$ so we can write the solution

$$\psi(x) = \begin{cases} B e^{\kappa x}, x < 0 \\ B e^{-\kappa x}, x > 0 \end{cases} \tag{39}$$

Requirement of continuity of the derivative of the wave function cannot be applied here because of the infinite value of the potential at the point $x = 0$.

The relation between derivatives can be nevertheless obtained by integrating the Schrödinger equation.

$$-\frac{\hbar^2}{2m} \int_{-\varepsilon}^{+\varepsilon} \frac{d^2\psi(x)}{dx^2} dx - \int_{-\varepsilon}^{+\varepsilon} \alpha \delta(x) \psi(x) dx = E \int_{-\varepsilon}^{+\varepsilon} \psi(x) dx \tag{40}$$

Evaluation of integrals gives

$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{-2m\alpha}{\hbar^2}\psi(0) \tag{41}$$

Difference in derivative is proportional to the value of the wave function at the point of discontinuity.

After inserting our wave function we get

$$\kappa = \frac{m\alpha}{\hbar^2} \tag{42}$$

Which gives us the allowed energy

$$E = -\frac{m\alpha^2}{2\hbar^2} \tag{43}$$

Normalization gives us the wave function

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-\frac{m\alpha|x|}{\hbar^2}} \tag{44a}$$

For scattering states $E > 0$ is situation slightly more complicated. In that case coefficient κ is imaginary $\kappa = ik$ and the general solution is of the form

$$\psi(x) = \begin{cases} A e^{-ikx} + B e^{ikx}, x < 0 \\ F e^{-ikx} + G e^{ikx}, x > 0 \end{cases} \tag{45}$$

The application of continuity requirement and relation for derivatives (41) results in

$$F + G = A + B \tag{46}$$

$$ikF - G - A + B) = \frac{-2m\alpha}{\hbar^2}A + B) \tag{47}$$

If we consider incident particle coming from the left we can set the constant $G = 0$.

Coefficients B and F can be then expressed as following functions of A

$$B = \frac{i\beta}{1 - i\beta}A \tag{48}$$

$$F = \frac{1}{1 - i\beta}A \tag{49}$$

where $\beta = \frac{m\alpha}{\hbar^2 k}$

Reflection and transmission coefficients are defined as

$$|R|^2 = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1 + \beta^2} \tag{50}$$

$$|T|^2 = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \beta^2} \tag{51}$$

Where coefficient R tells us the probability of reflection and coefficient T the probability of transmission respectively. Obviously

$$|R|^2 + |T|^2 = 1 \tag{52}$$

In case of delta function barrier ($\alpha > 0$) bounded states are not possible. All expressions containing α^2 like transmission and reflection coefficients are still valid.

Fig.1 shows the probability of transmission through the delta potential as a function of energy. The higher the energy the higher probability of transmission.Low energies are suppressed. This property make delta potential a good candidate for a quantum mechanical low energy filter.
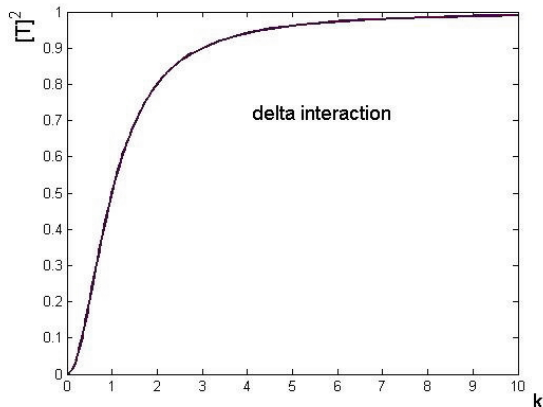
Figure 1: Transmission as a function of energy for delta potential

3   Point interaction

A point interaction is a model approximating systems consisting of a particle interacting with a potential of size negligible relative to the wavelength of the particle's wave function. Such situation often arises in applications of quantum mechanics where we frequently have to deal with discontinuities of various kinds. As an example might serve heterostructure semiconductor where materials of different nature are connected together. In this model the size of the potential or discontinuity is considered to be point-like and we are seeking appropriate boundary conditions which are consistent with quantum mechanics. To solve this problem we are not going to seek conditions for any specific potential but rather we are interested in general formula allowing us to describe all possible types of interactions. In order to derive this general formula we impose a simple condition of probability flux conservation at the point of discontinuity. This requirement is natural since the probability flux conservation guarantees that no particle is created or lost at the point of interaction. We don't impose any requirement on the continuity of the wave function or its derivative alone. This means that discontinuities in both are allowed. As we will see this generalization leads to a surprising number of new possible solutions.

In order to derive the general formula let's consider first a system consisting of a quantum spinless particle moving freely on a straight line with one point removed. Hilbert space $L^2(R - \{x_0\})$ of such a system consists of all square integrable complex functions defined on $R - \{x_0\}$ and the dynamics is described by Hamiltonian represented by one dimensional Laplace operator $-\frac{d^2}{dx^2}$. If we want our system to be consistent with reality we have to ensure that the Hamil-

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tonian generates unitary time evolution which in other words mean that the Hamiltonian must be self adjoint.

In our case the condition of self adjointness reads

$$\int_R \left[\psi^* \hat{H} \phi - \left(\hat{H}\psi\right)^* \phi\right] dx = W[\psi^*, \phi]_+ - W[\psi^*, \phi]_- = 0, \forall \psi, \phi \in L^2(R - \{0\}) \tag{53}$$

where $W[\psi^*, \phi]_\pm$ are the limiting values of Wronskian and the point defect. Recall that Wronskian is defined as determinant $W[\psi, \phi] = \begin{vmatrix} \psi & \psi' \\ \phi & \phi' \end{vmatrix}$ where ψ', ϕ' are derivatives.

Since the differential operator $-\frac{d^2}{dx^2}$ is symmetric the only place where a possible problem might arise is in the domain of the operator. This in practice means that we have to find suitable boundary conditions a wave function must satisfy at the point of discontinuity in order to guarantee self adjointness. This conditions are given by the requirement that the difference of wronskians in (53) is equal to zero. Different choices of these boundary conditions then represent different kind of point interaction. In other words a point interaction is unambiguously determined by certain boundary conditions at the point of interaction.

For one dimensional systems the requirement of self adjointness is equivalent to probability flux conservation.

As we already know the probability flux is defined as

$$j(x) = -\frac{i\hbar}{2m}(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}) = -\frac{i\hbar}{2m} W[\psi^*, \psi] \tag{54}$$

Let's place the discontinuity at the point $x_0 = 0$ and define vectors

$$\Psi = \left(\begin{array}{c} \psi_+ \\ \psi_- \end{array} \right), \Psi' = \left(\begin{array}{c} \psi'_+ \\ -\psi'_- \end{array} \right) \tag{55}$$

where $\psi_\pm$ and $\psi'_\pm$ are left and right limits of the wave function and its derivative at $x = 0$. Using these new vectors we can rewrite the equation (54) as

$$\Psi'^\dagger \Psi - \Psi^\dagger \Psi' = 0 \tag{56}$$

where $\Psi^\dagger = (\Psi^*)^T$.

Equation (56) can be rewritten as

$$|\Psi - iL_0\Psi'|^2 - |\Psi + iL_0\Psi'|^2 = 0 \tag{57}$$

where $L_0 \in R - \{0\}$ is arbitrary constant in the unit of length. Last equation means that the lengths of both vectors $\Psi - iL_0\Psi'$ and $\Psi + iL_0\Psi'$ are equal. Therefore there exist a unitary transformation U which maps one vector on the other. It is

$$\Psi - iL_0\Psi' = U\left(\Psi + iL_0\Psi'\right) \tag{58}$$

From this last expression immediately follow the general formula describing all possible one dimensional point interactions

$$(U - I)\Psi + iL_0(U + I)\Psi' = 0 \tag{59}$$

U is a 2×2 unitary matrix representing transformation (58) and I is 2×2 unit matrix. According to this equation, any unitary matrix represents possible self adjoint extension and therefore point interaction. There is a one to one correspondence between the set of all point interactions and the group $U(2)$ of unitary matrices.

For example

- Dirichlet boundary conditions $\psi_- = \psi_+ = 0$ which cause the straight line to decouple into two independent pieces are represented by matrix $U = I$

$$U = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{60}$$

- Neumann boundary conditions $\psi'_- = \psi'_+ = 0$ can be obtained if we choose $U = -I$

$$U = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \tag{61}$$

- Free case, where no interaction is present and wave function as well as its derivative is continuous $\psi_- = \psi_+, \psi'_- = \psi'_+$ is represented by matrix

$$U = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{62}$$

- δ interaction - $\sum_{j=1}^{2}\psi'_j(0) = \alpha\psi(0)$ $\psi_1(0) = \psi_2(0) = \psi(0)$ which we described in details in previous chapter is hidden behind the matrix

$$U = \frac{2}{2 + i\alpha}J - I, \ J = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \tag{63}$$

Besides those well known cases mentioned above let's introduce here a new type of point interaction known as δ' (delta prime) interaction and represented by matrix

$$U = I - \frac{2}{2 - i\beta}J, \ J = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \tag{64}$$

This matrix leads to boundary conditions of the form

$$\sum_{j=1}^{2} \psi_j(0) = \beta\psi'(0) \quad \psi'_1(0) = \psi'_2(0) = \psi'(0) \tag{65}$$

which can be also considered to be the defining property of this interaction.

The delta prime interaction is a singular potential which can be considered as a derivative of the delta function $\delta(x)$.

Properties of delta prime interaction are inverse to those of delta interaction. Delta function behaves as a low energy filter blocking low energy particles and transmitting only the high energy ones depending on the strength of the potential. Delta prime interaction on the other hand acts as a high energy filter, blocking high energy particles and transmitting the low energy ones. See fig.2.

These results can be easily verified inserting the solution of a free Hamiltonian

$$f = \begin{cases} e^{ikx} + R.e^{-ikx}, x < 0 \\ Te^{ikx}, x > 0 \end{cases} \tag{66}$$

into conditions (65)

The transmission coefficient $|T|^2$ than takes the form

$$|T|^2 = \frac{4}{4 + k^2} \tag{67}$$

and the transmission $|T|^2$ as a function of energy $k = \sqrt{E}$ can be seen on fig.2.

We derived a general formula which allows us to describe any possible point interaction as a boundary condition imposed on the wave function and its derivative at the point in question. But what can we do if the wave function or its derivative diverge at that point? Is there any possibility to handle such a situation? It turns out that we can solve this problem defining the vectors Ψ and Ψ' in different way.

To show this construction [first described in [2]] let's return again to the definition of self adjoint operator. Operator $\hat{H}$ is selfadjoint if

$\left\langle \psi, \hat{H}\phi \right\rangle = \left\langle \psi\hat{H}, \phi \right\rangle$ for all ψ, ϕ from the domain of $\hat{H}$.

For our Hilbert space $R - \{0\}$ and Hamiltonian $\hat{H} = -\frac{d^2}{dx^2}$ it means that integral

$$\int_R \left[\psi^* \hat{H}\phi - \left(\hat{H}\psi\right)^* \phi \right] dx = W[\psi^*, \phi]_+ - W[\psi^*, \phi]_- \tag{68}$$

is equal to 0.

The self adjoint domain of the operator thus consists of all functions $\psi \in L^2(R)$ for which the r.h.s. of (68) vanishes.

Let φ_1, φ_2 are two independent square integrable eigenfunctions $H\varphi_i = E\varphi_i$ defined on some $\varepsilon-$ neighborhood of the point defect. And let the wronskian
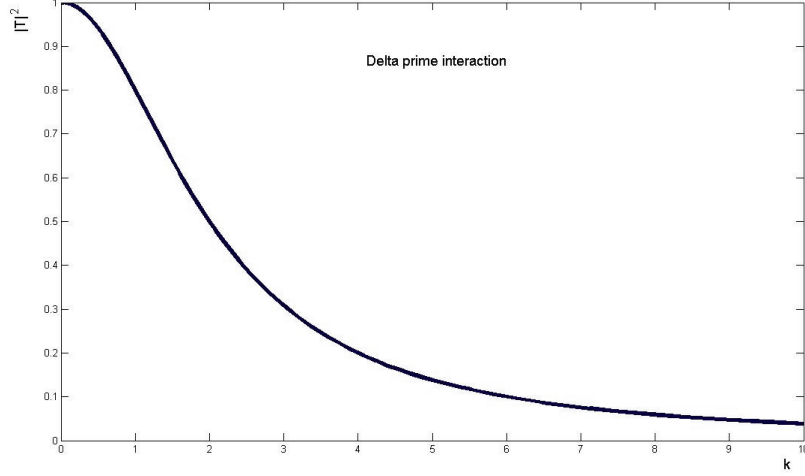
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Figure 2: Probability of transmission as a function of energy for delta prime interaction

$W[\varphi_1, \varphi_2] = 1$. Then for any square integrable wave function defined on the same neighborhood we can calculate the Wronskians $W[\psi, \varphi_1]$ and $W[\psi, \varphi_2]$ and define vectors Ψ and Ψ' as

$$\Psi = \begin{pmatrix} W[\psi, \varphi_1]_+ \\ W[\psi, \varphi_1]_- \end{pmatrix}, \Psi' = \begin{pmatrix} W[\psi, \varphi_2]_+ \\ -W[\psi, \varphi_2]_- \end{pmatrix} \tag{69}$$

where $W[\psi, \varphi_i]_\pm$ are again the limits taken from left and right respectively. It can be shown that these limits are finite even if one or both function diverge to $\pm\infty$.

With the help of these new vectors and eigenfunctions φ_1, φ_2 we can express any Wronskian of two arbitrary wave functions as

$$W[\phi^*, \psi] = \begin{vmatrix} \phi^* & \phi'^* \\ \psi & \psi' \end{vmatrix} = \begin{vmatrix} \phi^* & \phi'^* \\ \psi & \psi' \end{vmatrix} \begin{vmatrix} \varphi_1' & \varphi_2' \\ -\varphi_1 & -\varphi_2 \end{vmatrix} \tag{70}$$

$$= W[\phi^*, \varphi_1]W[\psi, \varphi_2] - W[\phi^*, \varphi_2]W[\psi, \varphi_1] \tag{71}$$

thus the r.h.s. of (68) can be conveniently written as

$$\Phi^\dagger \Psi' - \Phi'^\dagger \Psi \tag{72}$$

where Φ is constructed analogously to Ψ.
If ϕ, ψ belongs to the self adjoint domain then

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$$\Phi^\dagger \Psi' - \Phi'^\dagger \Psi = 0 \tag{73}$$

For $\psi = \phi$ and with the help of vectors $\Psi_\pm = \Psi \pm i L_0 \Psi'$ we get condition formally equal to (59) which holds even if the wave function or its derivative diverges.

In order to explore the properties of point interactions in more details (especially their spectra) let's change our system a little bit. Instead of dealing with a particle on a straight line, let's take a piece of line of length l and connect its ends together making a circle S^1 of the perimeter l. Let's place the point interaction at the point where these two ends are connected together.

It is also convenient to parametrize the unitary group $U(2)$ in the following standard way

$$U = e^{i\xi} \begin{pmatrix} \alpha & \beta \\ -\bar\beta & \bar\alpha \end{pmatrix} \tag{74}$$

$$\xi \in \langle 0, \pi) \ \alpha, \beta \in C \text{ and } |\alpha|^2 + |\beta|^2 = 1 \tag{75}$$

Now let's distinguish three cases

positive energy $E > 0$- in which case the general eigen functions are of the form

$$\psi_k = A_k e^{ikx} + B_k e^{-ikx} \tag{76}$$

negative energy $E < 0$

$$\psi_k = A_k e^{\kappa x} + B_k e^{-\kappa x} \tag{77}$$

and zero energy $E = 0$

$$\psi_0 = A_0 x + B_0 \tag{78}$$

Inserting these eigenfunctions together with parametrized matrix into (68) yields following system of equations
$E > 0$

$$\begin{pmatrix} \alpha S_- + \left(\beta e^{ikl} - e^{-i\xi}\right) S_+ & \alpha S_+ + \left(\beta e^{-ikl} - e^{-i\xi}\right) S_- \\ \alpha^* e^{ikl} S_+ - \left(\beta^* + e^{-i\xi} e^{ikl}\right) S_- & \alpha^* e^{-ikl} S_- - \left(\beta^* + e^{-i\xi} e^{-ikl}\right) S_+ \end{pmatrix} \begin{pmatrix} A_k \\ B_k \end{pmatrix} = 0 \tag{79}$$

where $S_\pm = (1 \pm k L_0)$

setting the determinant equal to zero and simplification gives

$$2k L_0 \left(\beta_I + \sin\xi \cos kl\right) + \left[(\cos\xi - \alpha_R) + (\cos\xi + \alpha_R)(k L_0)^2\right] \sin kl = 0 \tag{80}$$

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α_R is the real part of α and β_I is imaginary part of β

$E < 0$
substituting κ for ik gives

$$2\kappa L_0 \left(\beta_I + \sin\xi \cosh\kappa l\right) + \left[\left(\cos\xi - \alpha_R\right) + \left(\cos\xi + \alpha_R\right) \left(\kappa L_0\right)^2\right] \sinh\kappa l = 0 \tag{81}$$

$E = 0$

$$\left(\beta_I + \sin\xi\right) - \frac{l}{2L_0}\left(\alpha_R - \cos\xi\right) = 0 \tag{82}$$

Here we obtained a very interesting result. If we look at all the equations for spectrum carefully we see that they depend only on three parameters α_R, β_I, ξ . The physical properties of point interactions are therefore described only by these three numbers which means that not all different unitary matrices represent different physical situation. In other words different self adjoint extensions don't necessary lead to different physical realizations. We have freedom in choosing α_I and β_R to be anything without any physical consequence.

It is now possible to classify these distinct subfamilies which represent different realizations but we are not going to do that. Instead we focus on one of these subfamilies called the Fulop-Tsutsui scale invariant subfamily and describe its properties in more details. For more details on different subfamilies see [1]

Before we do so let's discuss some generalizations of the theory we derived so far.

Until now we dealt with a point interaction represented by connection conditions between two pieces of straight line. This model can be easily generalized considering case where more than two pieces are connected together at one point. Such a structure known as quantum graph has been intensively studied for last few decades. What follows in the next chapter is a summary of basic properties of this useful model.

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4 Quantum graph

In this paragraph we introduce the concept of quantum graph which is a useful model of various types of quantum systems consisting of a number of parts connected together. As an example let's mention the use of quantum graphs in calculating spectra of certain organic molecules or as a model of real systems consisting of combinations of quantum wires, where the width of the wire can be neglected in comparison to other length scales.

Quantum graphs also proved themselves useful in simulating quantum systems with strongly chaotic classical limit. One of the most significant features of such systems is that statistical properties of their spectra are coincident with spectral properties of certain class of random matrices studied by Random Matrix Theory. The importance of quantum graph is also supported by the fact that it is the only system for which we can write exact trace formula. By trace formula we mean relation which expresses spectral density function of given system in terms of periodic manifolds of its classical limit.

As a graph we generally mean a set of vertices and edges connected together in some specific way. For our purpose we don't impose any restrictions on how the vertices should be connected. Arbitrary vertex can be connected to any number of other vertices and the connection can be realized with one or more bonds.

If we define a metric on such a structure we get a new mathematical object known as metric graph.

Metric graph is thus an arbitrary graph consisting of V vertices and B bonds together with a metric defined on each bond. If we decide the order of the vertices assigning an index to every vertex the metric is defined in natural way as a distance from the vertex of lower index measured on a particular bond.

If we equip the metric graph with a self adjoint operator we get a mathematical structure called quantum graph.

So we may define quantum graph as a metric graph together with a self adjoint differential operator acting on it.

Typical operators considered in quantum graph theory are

- negative second derivative $-\frac{\partial^2}{\partial x^2}$

- general Schrödinger operator $-\frac{\partial^2}{\partial x^2} + V(x)$.

- Schrödinger operator with magnetic field $(\frac{d}{idx} - A(x))^2 + V(x)$.

In order to satisfy self adjoint property of the operator a certain kind of boundary conditions must be imposed at every vertex of the graph.

The most general condition is of the form

$$A_v F + B_v F' = 0 \qquad (83)$$

Where F and F' are vectors $(f_1(v), f_2(v), .., f_d(v))^T$ and $(f_1'(v), f_2'(v), .., f_d'(v))^T$ respectively. Prime represents derivative along the edges taken in the outgoing direction and d is the number of bonds connected to a specific vertex. Matrices A_v and B_v are $d \times d$ matrices with the property that their product $A_v B_v^*$ is self adjoint. Notice the similarity between [83] and [59]. Actually these two conditions are equivalent and we can rewrite equation [83] in the form of [59] with matrix $U \in U(n)$ where n is the number of edges connected to given vertex.

A concrete example of a self adjoint condition is for example the δ - type condition with matrices

$$A_v = \begin{pmatrix} 1 & -1 & 0 & ... & 0 \\ 0 & 1 & -1 & ... & 0 \\ ... & ... & 0 & 1 & -1 \\ -\alpha_v & 0 & ... & 0 & 0 \end{pmatrix}, B_v = \begin{pmatrix} 0 & 0 & ... & 0 \\ ... & ... & ... & 0 \\ 0 & 0 & ... & 0 \\ 1 & 1 & ... & 1 \end{pmatrix} \qquad (84)$$

and

$$A_v B_v^* = \begin{pmatrix} 0 & ... & 0 \\ ... & ... & ... \\ 0 & ... & -\alpha_v \end{pmatrix} \qquad (85)$$

Which can be written in the form

$$\sum_{e \in E_v} \frac{df}{dx}(v) = \alpha_v f(v), \forall v, \alpha_v\text{-real number} \qquad (86)$$

Where the sum goes through all bonds connected to vertex v and the value of the function f_e at the vertex v is same for all bonds $e \in E_v$.

The condition that α_v must be real for all v follows from the self adjoint requirement imposed on $A_v B_v^*$.

For $\alpha_v = 0$ we get the Kirchhoff conditions

$$\sum_{e \in E_v} \frac{df}{dx}(v) = 0 \qquad (87)$$

Another frequently used condition called δ'-condition can be obtained by interchanging the matrices A_v and B_v. The result can be again written as

$$\sum_{e \in E_v} f_e(v) = \alpha_v \frac{df}{dx}(v), \forall v, \alpha_v - \text{real number} \qquad (88)$$

Where similarly the value of the derivative $\frac{df_e}{dx_e}$ at the vertex v has the same value for all bonds $e \in E_v$.

4.1 Properties of spectrum

It can be shown that the spectrum of a finite graph with a negative second derivative operator has discrete spectrum.

The solution of the equation

$$-\frac{d^2 f}{dx^2} = \lambda f \tag{89}$$

can be rewritten using the values of the function f at vertices v and w belonging to the same edge as

$$f_e(x) = \frac{1}{\sin\sqrt{\lambda}l_e}(f_e(v)\sin\sqrt{\lambda}(l_e - x) + f_e(w)\sin\sqrt{\lambda}x) \tag{90}$$

Applying conditions at vertices then leads to secular equation and spectra. Particularly we get the equation

$$T(\lambda)F = 0 \tag{91}$$

Where F is a vector of dimension $D = \sum_v d_v$ combining all possible values of the function f at vertices. $T(\lambda)$ is a $D \times D$ matrix.

A following theorem holds

A point $\lambda \neq \frac{n^2\pi^2}{l_e^2}$ belongs to the spectrum of H if and only if zero belongs to the spectrum of the matrix $T(\lambda)$.

For graph which has all edges equal and δ - condition at all vertices we can show based on this last theorem that $\lambda \neq \frac{n^2\pi^2}{l_e^2}$ belongs to the spectrum of H iff $\alpha\frac{\sin l\sqrt{\lambda}}{l\sqrt{\lambda}} + d\cos\sqrt{\lambda}$ belongs to the spectrum of $\sum_{\{w,e=(v,w)\in E_v\}} f(w)$.

$$\sum_{\{w,e=(v,w)\in E_v\}} f(w) = (\alpha\frac{\sin l\sqrt{\lambda}}{l\sqrt{\lambda}} + d_v\cos\sqrt{\lambda})f(v) \tag{92}$$

For Dirichlet boundary conditions which represent the decoupled case the spectrum consists solely of eigenvalues $\lambda = \frac{n^2\pi^2}{l_e^2}$. In the case when the lengths of the edges are rationally independent numbers none of those Dirichlet eigenvalues are in spectrum.

Another method which gives us the spectrum of the graph is based on the concept of scattering matrix S connecting incoming and outgoing waves.

For more information about quantum graphs see for example

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5 Quantum Chaos

Quantum chaos or quantum chaology is a discipline whose goal is to explain the transition between quantum and classically chaotic systems. Quantum chaology studies the differences between quantum systems with regular classical limit and those which end up to be chaotic as the $\hbar \to 0$.

As is well known, classically chaotic system is a system whose evolution is sensitive to initial condition. As the system evolves, phase space trajectories diverge exponentially with the consequence of impossibility of long time predictions.

In contrast quantum evolution is smooth and unitary. Small difference in initial conditions leads to small difference in final result. The question therefore is how chaos emerges from regular quantum evolution and how can we distinguish whether given quantum system have regular or chaotic classical limit.

Let's first answer the second question. It has been found that the seed of chaos is present in certain characteristics of quantum systems. Namely in the distribution of energy levels in spectra, in the wave function of stationary states and also in the scattering matrix. In the spectra chaos manifests itself as repulsion between adjacent levels. Unlike regular quantum systems whose energy levels are "attracted" to each other (which means that the probability of finding two levels close to each other is higher than finding them far from each other) energy levels of quantum chaotic systems repel each other. This is immediately visible if we look at the level spacings distributions depicted on Fig. 3.

The black curve is graph of Poisson distribution which characterizes the properties of spectra of regular quantum systems. The red and blue curve are distributions known from random matrix theory as GOE (general orthogonal ensemble) and GUE (general unitary ensemble) characterizing spectral properties of random matrices with certain symmetries and describe the spectra of quantum chaotic systems. On the x axis are the distances between adjacent energy levels rescaled so that the mean is equal to 1. On the y axis is the probability density. The repulsion in the spectra of quantum chaotic systems is clearly visible.

In the wave function characteristics chaos appears as a wave pattern called scar. Stationary states of such a system do not display a random pattern but instead waves form pattern consisting of simple regular shapes.

Example of such patterns can be seen on Fig.4

The third way chaos represents itself in quantum systems is as a wild fluctuation in scattering function. Scattering properties such as transmission, time a particle spend in the scattering region and other similar characteristics display nonperiodic wild fluctuation. As an example is the conductance fluctuation in a
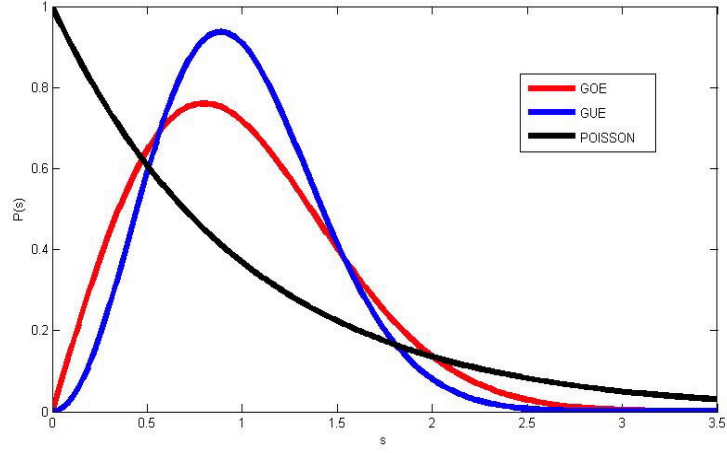
Figure 3: GOE GUE and Poisson distribution. GOE and GUE fits the energy level spacing distribution of systems with classical chaotic limit.
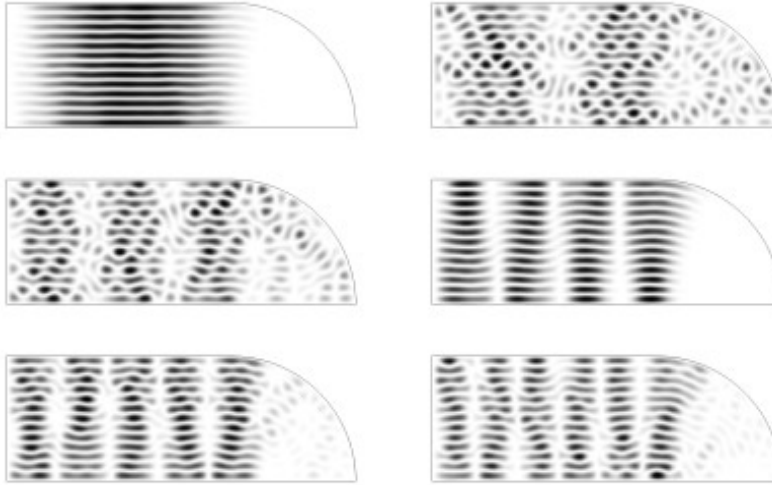

Figure 4: An example of wavefunction patterns (scars) a sign of quantum chaotic behaviour
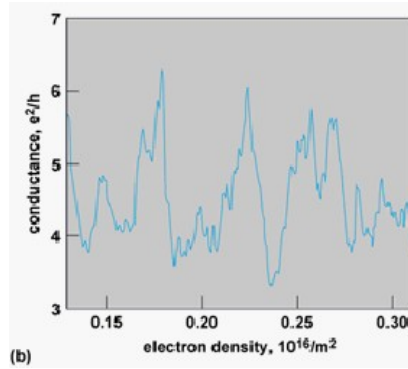
28

Figure 5: conductance fluctuations

semiconducting heterostructure as a function of electron density as can be seen on Fig.5 (picture taken from Douglas stone's homepage at Yale university)

All mention features, level repulsion, scars and wild fluctuations in scattering characteristics are believed to be a sign of classical chaotic limit.

Now we can ask a question if these chaotic properties of quantum systems can be derived from their classical counterparts. First who partly answered this question was Martin Gutzwiller [1] who derived so called trace formula which expresses the density of energy states of a quantum mechanical system as a sum over all classical periodic orbits. Periodic orbit is an orbit in phase space which repeats itself as the systems evolves. Gutzwiller's formula is not universal and applies only to systems with isolated orbits. Generalized version of Gutzwiller formula was presented by Strutinsky [2] and coworkers and later by Creagh and Littlejohn [3].

But still we have a problem how it is possible that from regular quantum mechanics arises chaos. The answer to this question lies in quantum break time. Quantum mechanics allows chaotic, seemingly random evolution only for a very short time known as a quantum break time. After this time the quantum laws suppress further chaotic evolution and the system retraces its path being caught in a kind of evolution loop. The difference between the classical and quantum systems is that for classical chaotic systems the break time is too long to be observable. The system is so complex that for retracing its evolution we need time bigger than the age of the universe. This quantum mechanical suppression was observed experimentally by Mark Raizen and co. from University in Texas who made a quantum version of kicked rotator using ultra-cold sodium atoms and laser.[4]

The existence of chaotic systems can also be understand in terms of decoherence. The inevitable interaction of a quantum system with environment leads to collapse of a wave function and losing unitarity of the evolution of the system.

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6 Scale invariant point interaction

The scale invariant point interaction is a less known subclass of one-dimensional point interactions compared to the standard δ potential and δ' potential.

As the name of the interaction suggests the properties of scale invariant potential are independent of the scale parameter. To derive the boundary conditions with such a property we seek a matrix U for which the general expression $(U - I) \Psi_i + iL_0 (U + I) \Psi'_i = 0$ derived in chapter 3 decouples.

This situation occurs when $(U - I) = 0$ or/and $(U + I) = 0$ for any vector Ψ. These equations are satisfied either when $U = \pm I$ or when the eigenvalues of the matrix are equal ± 1. First two conditions represent Dirichlet resp. Neumann boundary conditions the second condition defines the scale invariant potential.

A matrix U has eigenvalues ± 1Iff

$$\det(U - I) = \det(U + I) = 0. \tag{93}$$

This condition guarantees that the general expression is independent of the scale parameter L_0. The standard parametrization for this class of U is

$$U = \begin{pmatrix} \cos\theta & e^{i\phi}\sin\theta \\ e^{-i\phi}\sin\theta & -\cos\theta \end{pmatrix} \tag{94}$$

This gives the connection condition which reads

$$\frac{e^{i\phi}}{\alpha}\psi_- - \psi_+ = 0 \tag{95}$$

$$e^{i\phi}\alpha\psi'_- - \psi'_+ = 0 \tag{96}$$

where the "strength" α is defined by

$$\alpha = \cot\frac{\theta}{2}, \theta \in (0, \pi) \tag{97}$$

These boundary conditions can be conveniently expressed using transfer matrix notation. For general case (95)(96) when the interaction is at the point x the transfer matrix is of the form

$$M_T = \frac{1}{2}e^{i\phi}\begin{pmatrix} \frac{1}{\alpha} + \alpha & e^{-2ikx}(\frac{1}{\alpha} - \alpha) \\ e^{2ikx}(\frac{1}{\alpha} - \alpha) & \frac{1}{\alpha} + \alpha \end{pmatrix} \tag{98}$$

Let us, for a moment, suppose that there is only one single defect located at $x = s$. Let the particle approaches the defect from the region where $x < s$. The wave function then is of the usual form

$$\psi(x) = e^{ikx} - R_1(s)e^{-ikx} \quad (x < s) \tag{99}$$

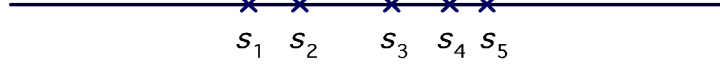$$\psi(x) = T_1(s)e^{ikx} \quad (x > s) \tag{100}$$

Figure 6:

and the transmission and reflection coefficients can be easily derived using the transmission matrix getting following system of linear equations

$$\begin{pmatrix} T \\ 0 \end{pmatrix} = \frac{1}{2}e^{i\phi} \begin{pmatrix} \frac{1}{\alpha} + \alpha & e^{-2iks}(\frac{1}{\alpha} - \alpha) \\ e^{2iks}(\frac{1}{\alpha} - \alpha) & \frac{1}{\alpha} + \alpha \end{pmatrix} \begin{pmatrix} 1 \\ R \end{pmatrix} \tag{101}$$

Solving this system yields

$$R(s) = \frac{1 - \alpha^2}{1 + \alpha^2} e^{2iks} \tag{102}$$

$$T(s) = \frac{2\alpha}{1 + \alpha^2} e^{i\phi} \tag{103}$$

As we can see the absence of the scale parameter L_0 results in the energy independence of scattering amplitude.

Similarly for the scattering from the opposite side $x > s$ we get

$$\psi(x) = T_1'(s)e^{-ikx} \qquad (x > s) \tag{104}$$

$$\psi(x) = e^{-ikx} - R_1'(s)e^{ikx} \quad (x < s) \tag{105}$$

Comparing amplitudes from both sides gives

$$T_1'(s) = T_1^*(s), \quad R_1'(s) = -R_1^*(s) \tag{106}$$

Now let's consider a quantum particle, moving on a one-dimensional line with N point-like defects whose locations are given by $x = s_i$ with $i = 1, 2, ..N$ (see fig.6) and explore scattering properties of such a system

The Hamiltonian is given, in appropriately rescaled unit, by

$$H = -\frac{1}{2}\frac{d^2}{dx^2}, \quad x \in (-\infty, s_1) \cup (s_1, s_2) \cup ...(s_{N-1}, s_N) \cup (s_N, \infty). \tag{107}$$

The dynamics of the system is described by the Schrödinger equation

$$H\psi(x) = E\psi(x) \tag{108}$$

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supplemented by the $U(2)$ connection conditions at the defects, which is conveniently specified by

$$(U - I)\,\Psi(s_i) + iL_0\,(U + I)\,\Psi'(s_i) = 0 \tag{109}$$

where i runs as $i = 1, 2, ..., N$, and U_i is a unitary matrix belonging to $U(2)$ group. The boundary vectors $\Psi(s_i)$ and $\Psi'(s_i)$ are defined by

$$\Psi(s_i) = \begin{pmatrix} \psi_-(s_i) \\ \psi_+(s_i) \end{pmatrix}, \Psi'(s_i) = \begin{pmatrix} \psi'_-(s_i) \\ \psi'_+(s_i) \end{pmatrix} \tag{110}$$

where $\psi_\pm(s_i)$ and $\psi'_\pm(s_i)$ denote the limit value of $\psi(x)$ and its derivative from the upper and lower regions of the defects s_i, $x \to s_i \pm 0$.

For technical simplicity, we assume all U_i to be identical, $U = U_i$.

With some elementary algebra, we can generalize results (102) and (103) and write the scattering amplitudes for N defects in the recursive forms; For the left-right amplitudes T_N and R_N, we have

$$T_N(s_1, ..., s_N) = \frac{T_1(s_1)T_{N-1}(s_2, ..., s_N)}{1 + R_1^*(s_1)R_{N-1}(s_2, ..., s_N)} \tag{111}$$

$$R_N(s_1, ..., s_N) = \frac{R_1(s_1) + R_{N-1}(s_2, ..., s_N)}{1 + R_1^*(s_1)R_{N-1}(s_2, ..., s_N)} \tag{112}$$

The right-left amplitude T' R' are obtained from

$$T'_N(s_1, ..., s_N) = T_N^*(s_N, ..., s_1) \tag{113}$$

$$R'_N(s_1, ..., s_N) = -R_N^*(s_N, ..., s_1) \tag{114}$$

Note the reversed ordering of s_i in right and left hand sides of the equations. With repeated iteration, we obtain explicit expressions for scattering matrices in the form

$$T_N(k) = \frac{\gamma^N}{D_N(k)}, \quad R_N(k) = \frac{B_N(k)}{D_N(k)}, \tag{115}$$

where $B_N(k)$ and $D_N(k)$ are defined as

$$B_N(k) = \beta \sum_i^N e^{2iks_i} + \beta^3 \sum_{i>j>m}^N e^{2ik(s_i - s_j + s_m)} + \beta^5 \sum_{i>j>m>n>p}^N e^{2ik(s_i - s_j + s_m - s_n + s_p)} +$$
...

$$D_N(k)=1+\beta^2\sum_{i>j}^N e^{2ik(s_i-s_j)}+\beta^4\sum_{i>j>m>n}^N e^{2ik(s_i-s_j+s_m-s_n)}$$
$$+\beta^6\sum_{i>j>m>n>p>q}^N e^{2ik(s_i-s_j+s_m-s_n+s_p-s_q)}+...$$

using abbreviations $\beta=\frac{1-\alpha^2}{1+\alpha^2},\gamma=\frac{2\alpha}{1+\alpha^2}e^{i\phi}$.

The sum runs over all indices in the range between 1 and N with the specified constraint, and the numerator contains terms up to the order of $\beta^{[N/2]}$ where the exponent signifies the integer part of $N/2$. For given N, there are $_NC_l$ terms with order β^l, and the scattering matrices are the multi-periodic oscillatory functions with 2^{N-1} frequencies.

The same result can be again obtained using the transfer matrix formalism and the fact that the transfer matrix through n defects is equal to the product of matrices for each single potential combined with the transfer matrix of free space between individual defects

$$M_{free}=\begin{pmatrix}e^{ik(x_2-x_1)} & 0 \\ 0 & e^{-ik(x_2-x_1)}\end{pmatrix} \tag{116}$$

.

$$M_T=M_n...M_{free}M_2M_{free}M_1 \tag{117}$$

$$\begin{pmatrix}A_n \\ B_n\end{pmatrix}=M_n...M_{free}M_2M_{free}M_1\begin{pmatrix}A_1 \\ B_1\end{pmatrix} \tag{118}$$

In order to reveal the physical content of the scattering matrices (111) (112), we plot $|T_N|^2$ as the function of incident momentum k for various number of defects. Fig.7 shows the result for $\alpha=3/2$ and the number of point defects equal to $N=3$, $N=5$ and $N=7$. The angle ϕ is set to be zero for all cases. We have chosen the locations of the defects to be the sum of square roots of primes; $s_1=1$, $s_2=1+\sqrt{2}$, $s_3=1+\sqrt{2}+\sqrt{3}$, $s_4=1+\sqrt{2}+\sqrt{3}+\sqrt{5}$, $s_5=1+\sqrt{2}+\sqrt{3}+\sqrt{5}+\sqrt{7}$, *etc.* to guarantee the incommensurability of s_i. This also models a generic case of random sequencing of successive s_i. We have checked that different choice of s_i, different ordering of relative size $s_{i+1}-s_i$ does not alter the essential characteristics of the results.

Despite the very simple analytic expression (115) of the scattering amplitude, as we increase N, the scattering quickly acquires "quantum chaotic" features, which are characterized by wild oscillations of scattering amplitudes (Ericson fluctuations). These fluctuations are the result of interference among multi-periodic oscillations with incommensurate frequencies, whose number of periods 2^{N-1} proliferates very fast with increasing N. Because of the scale invariance of each interaction, the fluctuation appears in arbitrary energy scale.
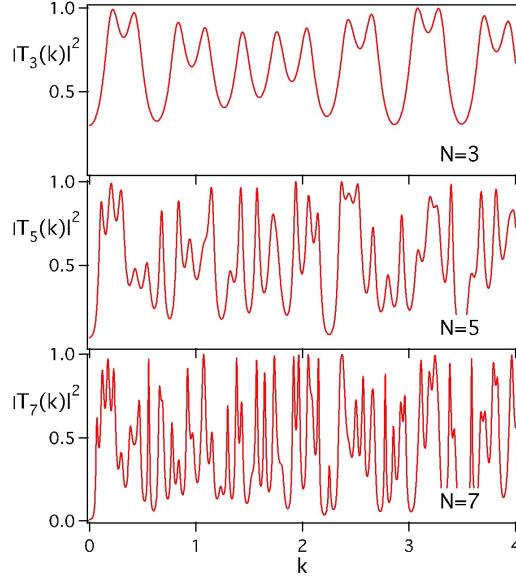
Figure 7: scattering function for N=3,5 and 7 point interactions on the line.

Along with the scattering properties, we can also study the spectral characteristics of the system by limiting it to a finite line of size $L \geq s_N$. One of the easiest way to do so is to impose periodic boundary conditions at $x = -L$ and $x = L$, $\psi(L) = \psi(-L) = 0$. This leads, for the case of $\phi = 0$, to the eigenvalue equation

$$\left(R_N(k) - e^{-2ikL}\right)\left(R'_N(k) - e^{-2ikL}\right) = T_N(k)T'_N(k) \qquad (119)$$

Explicit calculations yield the secular equation

$$0 = \sin 2kL + \beta \sum_i^N \sin 2ks_i + \beta^2 \sum_{i>j}^N \sin 2k(s_j - s_i + L) + \beta^3 \sum_{i>j>m}^N \sin 2k(s_m - s_j + s_i) +$$

$$+ \beta^4 \sum_{i>j>m>n}^N \sin 2k(s_n - s_m + s_j - s_i + L) + \beta^5 \sum_{i>j>m>n>p}^N \sin 2k(s_p - s_n + s_m - s_j + s_i) + \dots \qquad (120)$$

which is a bound state counterpart of (115).
Solving equation (120) gives the spectrum of the system.

On Fig. 8,9 and 10 level spacing distribution $P(s)$ for several α and N are shown. The distances s_i are chosen to be $s_1 : s_2 - s_1 : s_3 - s_2 : s_4 - s_3 : s_5 - s_4 : s_6 - s_5 : s_7 - s_6 = 1 : \sqrt{2} : \sqrt{3} : \sqrt{5} : \sqrt{7} : \sqrt{11} : \sqrt{13}$. The total length L is set to be $s_1 : 2L = 1 : 1 + \sqrt{2} + \sqrt{3} + \sqrt{5} + \sqrt{7} + \sqrt{11} + \sqrt{13} + \sqrt{17}$. We have chosen $\alpha = 27$ to approximate disconnected large coupling limit, and $\alpha = 2$ as the strong coupling limit, while, as an intermediate coupling, we chose the value $\alpha = 5$. These graphs clearly show the approach of $P(s)$ to the Wigner distribution (also known as GOE distribution), which is regarded as the quantum signature of classically chaotic dynamics, at the strong coupling value as we increase the number of points N. The convergence appears to be fast as the Wigner-like level statistics already takes shape even with $N = 3$.

Let's now discuss the implication of our findings in a broader context. The central result of this article is the generation of the "random" or irregular' properties in quantum dynamics out of fully analytic quantum spectral functions obtained from a one-dimensional system. This type of properties are usually associated to the nonintegrable system. Since the classical counterpart of conservative one-dimensional system necessarily is integrable, the well-established correspondence between the chaotic classical dynamics and the random quantum dynamics seems to fail for our model.

The clue to understand this seeming contradiction might be found in the singular nature of the high-energy limit of our system. Because of the special property of scale invariance present in Fülöp-Tsutsui point interaction, high energy limit, $k \to \infty$ does not bring the system to classical limit. Instead of either perfect bouncing wall or free pass, two legitimate deterministic classical limits of a point interaction, we are presented with semi-transparent wall with finite penetration probability. Therefore, if we were to identify the high energy limit as a classical limit, we are forced to consider stochastic dynamics whose randomness originates directly from the probabilistic nature of quantum mechanics itself.

Irrespective to the problem of classical limit and correspondence, our analytical expressions shed light on how irregular quantum dynamics emerge as the infinite-period limit of multi-periodic scattering matrices, just as chaotic classical dynamics emerge as the infinite-period limit of multi-periodic motion. In this connection, it should be useful to consider a complementary approach of trace-formula based analysis to our model. With appropriate modifications, existing semiclassical treatments of quantum graphs appear capable of handling the problem, and the comparison to the current approach should yield further insight into the singular and irregular dynamics in quantum mechanics.

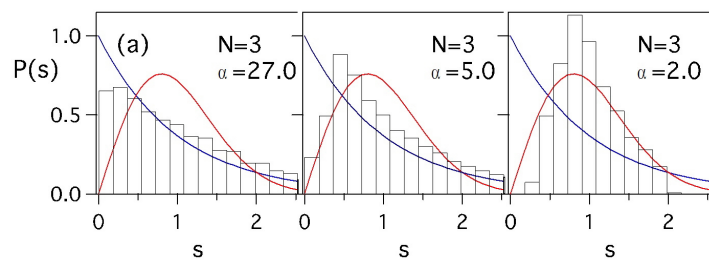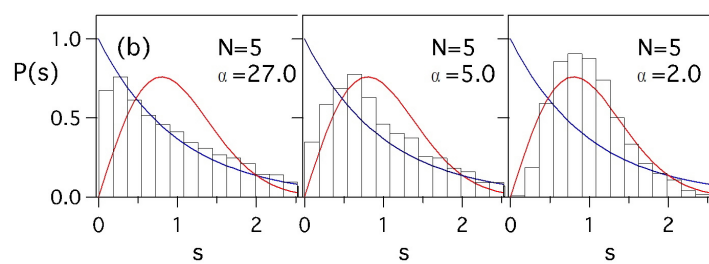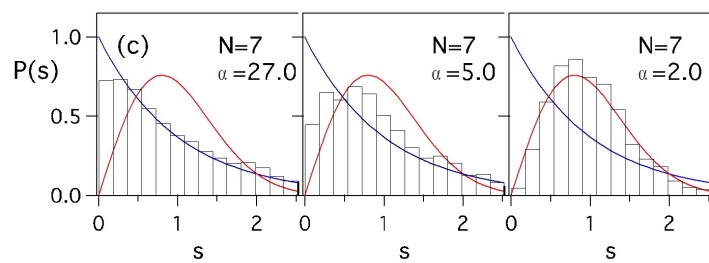These results were published in [1]

Figure 8:

Figure 9:

Figure 10:

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6.1 Detailed analysis of statistical properties of the spectrum

It has been shown by Seba and Vasata [2] that level spacing statistics of a system consisting of a number of scale invariant point interactions placed on a ring display statistical properties which are for some value of coefficient α closer to real GOE than the Wigner approximation.

Consider the secular equation of the form.

$$\cos 2k\pi - \left(1 - \beta^2\right)^{N/2} + \beta^2 \sum_{i>j}^{N} \cos(2k(s_j - s_i + \pi)) + \beta^4 \sum_{i>j>m>n}^{N} \cos 2k(s_n - s_m + s_j - s_i + \pi) + ... = 0 \tag{121}$$

For simplifying expressions we consider the length of the ring to be equal to 2π.

Solution of this equation gives us the spectrum of the system.

We won't deal with the energies itself but rather with the wave number $e = 2k$. The advantage of switching to this new variable is that their values don't have to be unfolded. It is their mean density is already equal to 1.

To show how the random matrix properties appear let's consider first the free case and then investigate what happens when we switch the potential on.

The secular equation for the free case $\alpha = 1, \beta = 0$ is of the form

$$\cos 2k\pi = 1 \tag{122}$$

and the solution is $k_j = j$ which gives us $e_j = 2j$.

The density function of the level spacings distribution $q_j = k_{j+1} - k_j$ of such a system is made of two peaks. Peak at zero is due to degeneracy.

Now let's investigate the case when we slowly turn the interaction on.

In that case $\alpha = 1 + \delta$ where $|\delta| \ll 1$, $\beta \approx -\delta$ and the solution of the secular equation (121) can be considered as a perturbation of the free case solution. Suppose the solution is of the form

$$k_j = j + \beta\lambda_j \tag{123}$$

substituting this expression in the secular equation (121) and simplifying using the properties of goniometric functions yield

$$-2\pi^2\lambda^2 + \frac{N}{2} + \sum_{k<l}^{N} \cos\left(2j(x_k - x_l)\right) = 0 \tag{124}$$

and the solution

$$\lambda_j^{\pm} = \pm\frac{1}{2\pi}\sqrt{\left(\sum_{k=1}^{N} \cos\left(2jx_k\right)\right)^2 + \left(\sum_{k=1}^{N} \sin\left(2jx_k\right)\right)^2} \tag{125}$$

39

we can see that the degenerate eigenvalues split and the new values are

$k_{2j-1} = j + |\beta| \lambda_j^-$ and $k_{2j} = j + |\beta| \lambda_j^+$

The unfolded level spacings then are

$q_{2j-1} = 4 |\beta| \lambda_j^+$ and $q_{2j} = 2 - 2 |\beta| (\lambda_{j+1}^+ + \lambda_j^+)$

As a result of switching on the potentials the degenerate levels split and the spacings distribution function changes. Peaks at 0 and 1 are broaden and as the interaction gets stronger the distribution of odd level spacings approaches the GOE distribution.

To show that we use some results of random matrix theory and theory of sequences modulo 1. It is known see [3] that the argument of $\cos(2jx_i) = \cos(2\pi((jx_i/\pi) \, mod \, 1))$ behaves like independent random variable uniformly distributed in interval $\langle 0, 2\pi \rangle$. The sequence $\{\cos(2jx_j)\}_{j=1}^{\infty}$ has probability distribution of the form

$$f(x) = \begin{cases} \frac{1}{\pi\sqrt{1-x^2}}, x \in (-1, 1) \\ 0, x \in R - (-1, 1) \end{cases} \tag{126}$$

for different x_i $i = 1, .., n$ the sequences behave like independent variables. What's more, it can be proven that the sums $\sum_{k=1}^{N} \cos(2jx_k)$ and $\sum_{k=1}^{N} \sin(2jx_k)$ if properly normalized converge to two statistically independent normally distributed random variables. From this fact follows that the distribution of the odd level spacings which is given by the square root of the sum of the squares of two independent normally distributed variables follow the χ^2 distribution which is nothing else but the Wigner distribution approximating the spacing levels of eigenvalues of the Gaussian orthogonal ensemble of random matrices.

$$P(q) = \frac{\pi}{2} q e^{-\frac{\pi q^2}{4}} \tag{127}$$

The even level spacings distribution is given by the distribution of the sum of two variables with Wigner distribution and doesn't follow the predictions made by random matrix theory.

It can be shown that the distribution of odd level spacings follow the random matrix predictions even outside the perturbative region and for some values of the parameter α approximates the real GOE distribution even better than the Wigner distribution.

For more details see (Seba Vasata arXiv:0808.2930)

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7   Conclusion

In the first part of this thesis we gave the summary of an important class of solvable quantum mechanical models known as quantum point interaction. We have shown that despite its relative simplicity this model is able to capture many significant features of more complex systems and we also discussed possible consequences of some of their properties for modern technology.

We discussed in more details the properties of one special subfamily of these systems known as the scale invariant subfamily which has the property that its scattering matrix is independent of energy. We showed that this innocent looking interaction is capable of displaying quantum chaotic features represented by wild fluctuations in the scattering matrix and the level repulsion in the spectrum described by random matrix spectral statistics.

This surprising findings not only shed new light on the origin of mentioned quantum chaotic phenomena (which have been so far considered as a property of more complicated systems with classical chaotic limit) but also have some important ramifications for future nanotechnology development.

PART 2

8 Introduction

In the second part of this thesis we study behaviour of a relativistic electron under the influence of vector and scalar potential.

Relativistic equivalent of Schrodinger equation for electron is the Dirac equation. Since its derivation by Dirac in 1928 Dirac equation faced problem with unbounded negative spectra coming from its solution. Dirac solved this problem by introducing the concept of Dirac sea where all states of negative energy are occupied and therefore because of the Pauli principle no electron can spontaneously move from the positive to negative part of the spectra.

Dirac equation was soon after its introduction surpassed by quantum field theory but in spite of this fact it is still a useful tool for describing behaviour of an electron in strong fields existing for example in heavy atoms or big molecules.

We present a solution of Dirac equation for an electron moving through a barrier of scalar and vector potentials and we show that certain combination of these potentials leads to an exotic phenomena of zero energy tunnelling. This phenomena was also recently observed in the Bose Einstein condensate where the tunnelling of phonon excitations through a barrier separating two bodies of the condensate display a perfect transmission at zero energy limit.[1] [2] This special barrier have also another mathematical peculiarity hidden in its short range classical limit. As the width of the barrier approach zero we obtain the δ' point interaction under the condition that the volume integral remains constant. An interaction which can be otherwise obtained after a rather complicated mathematical treatment.

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9 Dirac equation

Dirac equation is of the form

$$i\frac{\partial \psi}{\partial t} = (-i\alpha\nabla + m\beta)\,\psi \tag{128}$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ and β are mathematical objects satisfying following relations known as Clifford Algebra (these relations can be obtained by taking the "square" of both sides and comparing the result with Klein Gordon equation.)

$$\alpha_i^2 = 1 \tag{129}$$
$$\alpha_i\alpha_j + \alpha_j\alpha_i = 0 \tag{130}$$
$$\alpha_i\beta + \beta\alpha_i = 0 \tag{131}$$
$$\beta^2 = 1 \tag{132}$$

These anticommuting objects α_i and β cannot be ordinary real or complex numbers. The simplest objects satisfying these relations are 2×2 complex matrices and one possible representation is as follows

$$\alpha_1 = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix}, \alpha_2 = \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}, \alpha_2 = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}, \beta = \begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix} \tag{133}$$

Where $\sigma_i, i = 1, 2, 3$ are Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{134}$$

9.1 Dirac equation for free particle and its solution

The free Dirac equation has the form

$$i\hbar\frac{\partial \Psi(r,t)}{\partial t} = \left(-i\hbar c\,\overrightarrow{\alpha}\,\nabla + mc^2\beta\right)\Psi(r,t) \tag{135}$$

Where the vector $\Psi(r,t)$ is a four component vector (Dirac spinor)

$$\Psi(r,t) = \begin{pmatrix} \Psi_1(r,t) \\ \Psi_2(r,t) \\ \Psi_3(r,t) \\ \Psi_4(r,t) \end{pmatrix} \tag{136}$$

We will seek the solution in the form

$$\Psi(r,t) = \psi(r)e^{-\frac{iEt}{\hbar}} \tag{137}$$

which when substituted into the (135) gives

$$E\psi(r) = \left(-i\hbar c\, \overrightarrow{\alpha}\nabla + mc^2\beta\right)\psi(r) \tag{138}$$

Which is nothing but eigenvalue equation.

As the Hamiltonian on the r.h.s. obviously commute with momentum operator $[P,H] = 0$. we can look for the solution of the form

$$\psi_p(r) = u_p e^{-\frac{ip.x}{\hbar}} \tag{139}$$

where u_p is a four component vector which satisfies

$$Eu_p = \left(c\,\overrightarrow{\alpha}.\overrightarrow{p} + mc^2\beta\right)u_p \tag{140}$$

The matrix on the r.h.s. is a block matrix so the common strategy is to express the vector u_p as a vector composed of a two two components vectors

$$u_p = \begin{pmatrix} \phi_p \\ \chi_p \end{pmatrix} \tag{141}$$

and write the equation (140) in matrix form

$$\begin{pmatrix} mc^2 & c\,\overrightarrow{\sigma}.\overrightarrow{p} \\ c\,\overrightarrow{\sigma}.\overrightarrow{p} & -mc^2 \end{pmatrix}\begin{pmatrix} \phi_p \\ \chi_p \end{pmatrix} = \begin{pmatrix} E & 0 \\ 0 & E \end{pmatrix}\begin{pmatrix} \phi_p \\ \chi_p \end{pmatrix} \tag{142}$$

$$\begin{pmatrix} E - mc^2 & -c\,\overrightarrow{\sigma}.\overrightarrow{p} \\ -c\,\overrightarrow{\sigma}.\overrightarrow{p} & E + mc^2 \end{pmatrix}\begin{pmatrix} \phi_p \\ \chi_p \end{pmatrix} = 0 \tag{143}$$

which yields

$$\phi_p = \frac{c\,\overrightarrow{\sigma}.\overrightarrow{p}}{E - mc^2}\chi_p \tag{144}$$

$$\chi_p = \frac{c\,\overrightarrow{\sigma}.\overrightarrow{p}}{E + mc^2}\phi_p \tag{145}$$

Combining these equation and using the equality $\left(\overrightarrow{\sigma}.\overrightarrow{p}\right)^2 = p^2$ gives us

$$[E^2 - (m^2c^4 + c^2p^2)]\phi_p = 0 \tag{146}$$

and the energy eigenvalues are

$$E = \pm\sqrt{m^2c^4 + c^2p^2} \tag{147}$$

The spectrum of free particle consists of two continuous bands (one band for positive and one for negative energy) separated by a gap of width $2mc^2$.

Now we have to specify the vectors ϕ_p and χ_p to find u_p.

For $E > 0$ the simplest choices are $\phi_p = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\phi_p = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ which leads to

$$\chi_p = \frac{c\,\overrightarrow{\sigma}.\overrightarrow{p}}{E + mc^2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \chi_p = \frac{c\,\overrightarrow{\sigma}.\overrightarrow{p}}{E + mc^2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{148}$$

. Then as $\overrightarrow{\sigma}.\overrightarrow{p} = \begin{pmatrix} p_z & p_x - ip_y \\ p_x + ip_y & -p_z \end{pmatrix}$ we get

$$\chi_p = \begin{pmatrix} \frac{cp_z}{E+mc^2} \\ \frac{c(p_x+ip_y)}{E+mc^2} \end{pmatrix} \text{ and } \chi_p = \begin{pmatrix} \frac{c(p_x-ip_y)}{E+mc^2} \\ \frac{-cp_z}{E+mc^2} \end{pmatrix} \tag{149}$$

.And the solution for u_p is

$$u_p = \begin{pmatrix} 1 \\ 0 \\ \frac{cp_z}{E+mc^2} \\ \frac{c(p_x+ip_y)}{E+mc^2} \end{pmatrix} \text{ and } u_p = \begin{pmatrix} 0 \\ 1 \\ \frac{c(p_x-ip_y)}{E+mc^2} \\ \frac{-cp_z}{E+mc^2} \end{pmatrix} \tag{150}$$

representing the particle with spin up and down respectively.

9.2   Klein Paradox

On the problem of Klein paradox we will show the solution of Dirac equation for potential step.

Let's consider a potential of the form

$$V = \begin{cases} V_0, z > 0 \\ 0, z < 0 \end{cases} \tag{151}$$

and an electron of energy E approaching this potential from the left.

Outside the potential we have

$$\left(\frac{E}{c} \right)^2 = p^2 + m^2 c^2 \tag{152}$$

$$pc = \sqrt{E^2 - m^2 c^4} \tag{153}$$

Inside the potential the total energy changes and we get

$$\left(\frac{E - V_0}{c} \right)^2 = p'^2 + m^2 c^2 \tag{154}$$

$$p'c = \sqrt{(E - V_0)^2 - m^2 c^4} \tag{155}$$

where p' is the momentum inside potential.

Region I, $z < 0$
The incident wave is of the form
$$\psi_I = a \begin{pmatrix} 1 \\ 0 \\ \frac{cp}{E+mc^2} \\ 0 \end{pmatrix} e^{\frac{ip.z}{\hbar}}$$
Reflected wave
$$\psi_R = b \begin{pmatrix} 1 \\ 0 \\ \frac{-cp}{E+mc^2} \\ 0 \end{pmatrix} e^{\frac{-ip.z}{\hbar}} + b' \begin{pmatrix} 0 \\ 1 \\ 0 \\ \frac{cp}{E+mc^2} \end{pmatrix} e^{\frac{-ip.z}{\hbar}}$$
Region II, $z < 0$
Transmitted wave
$$\psi_R = d \begin{pmatrix} 1 \\ 0 \\ \frac{cp'}{E-V_0+mc^2} \\ 0 \end{pmatrix} e^{\frac{ip'.z}{\hbar}} + d' \begin{pmatrix} 0 \\ 1 \\ 0 \\ \frac{-cp'}{E-V_0+mc^2} \end{pmatrix} e^{\frac{ip'.z}{\hbar}}$$

Let's consider $V_0 > E + mc^2$ which yields real momentum p'.

The continuity condition $\psi_I + \psi_R = \psi_T$ gives us the relations between amplitudes a, b, b', d, d' as follows

$$b' = d' = 0 \tag{156}$$

$$a = \frac{d}{2} \left(1 - r\right) \tag{157}$$

$$b = \frac{d}{2} \left(1 + r\right) \tag{158}$$

$$r = \sqrt{\frac{\left(V_0 - E + mc^2\right)\left(E + mc^2\right)}{\left(V_0 - E - mc^2\right)\left(E - mc^2\right)}} \tag{159}$$

The probability current for relativistic particle is defined as

$$j\left(x\right) = c\psi'\left(x\right)\alpha_3\psi\left(x\right) \tag{160}$$

Which leads to

$$j_I = aa^* \frac{2pc^2}{E + mc^2} \tag{161}$$

$$j_R = -bb^* \frac{2pc^2}{E + mc^2} \tag{162}$$

$$j_T = -dd^* \frac{2p'c^2}{V_0 - E - mc^2} \tag{163}$$

r is real and we get for the ratio of currents

$$\frac{j_R}{j_I} = -\frac{bb^*}{aa^*} = -\frac{(1+r)^2}{(1-r)^2} \tag{164}$$

$$\frac{j_T}{j_I} = -\frac{p'}{p}\frac{E+mc^2}{V_0-E-mc^2}\frac{dd^*}{aa^*} = -\frac{4r}{(1-r)^2} \tag{165}$$

Now as $V_0 > E + mc^2$ the coefficient r is real and we get $j_R > j_I$ which paradoxically means that the number of reflected particles coming from the potential is bigger than the number of particles bouncing of the potential. This paradox can be explained using the idea of particle creation in the presence of strong field. Since the positive spectrum of free particle overlaps with the negative spectrum of a particle in the potential the incident particle is able to knock additional particles out of the vacuum, creating electron positron pair.

10 Anomalous Relativistic Tunneling and Exotic Point Interactions

In this chapter we present new results concerning a subtle effect of negative spectra on simple one dimensional potential scattering of a Dirac particle off relativistic potential barriers.

We show that proper consideration of Dirac sea has intriguing ramifications for low energy scattering matrices. In particular, we show that scattering off a relativistic potential having the same magnitudes and opposite signs for scalar and vector components ($S = -V$) leads to anomalous tunneling at zero incident energy.

We further show, that the short-range limit of this particular potential scattering, converges to an exotic low-pass Gaussian wave filter whose non-relativistic kinematics limit is "delta-prime" point interaction (see chapter 3 equation (65).

We start by considering Dirac equation in one dimension that takes the following two-component form

$$\begin{pmatrix} \varphi' \\ \chi' \end{pmatrix} = \begin{pmatrix} 0 & m + \varepsilon + S - V \\ m - \varepsilon + S + V & 0 \end{pmatrix} \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \tag{166}$$

where m, ε stand for the mass and relativistic energy of a Dirac particle, and S and V are scalar and (time component of) vector potentials. We only treat time-symmetric systems, so the spatial components of vector potential is absent. The *prime* signifies the spatial derivative $\frac{d}{dx}$.

Let's first consider one dimensional potential barrier of constant height located in positive x region, formally given by

$$V(x) = v\,\Theta(x), \quad S(x) = s\,\Theta(x) \tag{167}$$

where $\Theta(x)$ is a Heaviside step function which is equal to 1 for $x > 0$ and 0 for $x < 0$. We define "mass excluded" energy w by

$$w = \varepsilon - m \tag{168}$$

which we assume to be positive. The spectra of a Dirac particle inside the potential barrier is composed of two disjoint continuous spectra separated by a gap. (see fig. 11.)

The scattering wave functions at $x < 0$ and $x > 0$ are given, respectively as
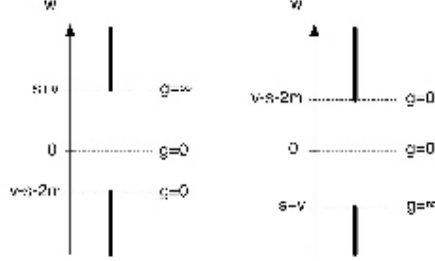
Figure 11:

$$
\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{ik}{m+\varepsilon} \end{pmatrix} e^{ikx} - R \begin{pmatrix} 1 \\ \frac{-ik}{m+\varepsilon} \end{pmatrix} e^{-ikx} \tag{169}
$$

$$
\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = T \begin{pmatrix} 1 \\ \frac{ip}{m+\varepsilon+s-v} \end{pmatrix} e^{ipx} \tag{170}
$$

with the free momentum $k = \sqrt{\varepsilon^2 - m^2}$ and the momentum $p = \sqrt{(\varepsilon - v)^2 - (m + s)^2}$ inside the potential barrier. Expressions (169) and (170) are valid for the case of continuous spectra for barrier region, $\varepsilon > |m + s| + v$. For the case of $|m + s| > \varepsilon > -|m + s| + v$, we need to make replacement, $p = i\kappa$ with $\kappa = \sqrt{-(\varepsilon - v)^2 + (m + s)^2}$. The case of $\varepsilon < -|m + s| + v$ corresponds to a particle under the Dirac sea, for which a $p \to -p$ is needed in (170), but this case is soon shown to be irrelevant. Reflection and transmission rate is given by the squared absolute values of coefficients R and T respectively, when p is real. When κ is real, on the other hand, T is the amplitude of wave function at classically forbidden region.

Expressing the momenta in terms of the energy w, we have

$$
k = \sqrt{w(w + 2m)} \tag{171}
$$

$$
p = \sqrt{(w - s - v)(w + 2m + s - v)} \tag{172}
$$

Matching of wave functions (169) (170) at $x = 0$ gives

$$
1 - R = T, \quad g(1 + R) = T \tag{173}
$$

with

$$
g = \sqrt{\frac{w(w+2m+s-v)}{(w+2m)(w-s-v)}} Q = \frac{1}{i} \sqrt{\frac{w(w+2m+s-v)}{(w+2m)(s+v-w)}} Q \tag{174}
$$

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Here, Q is the *Giachetti-Sorace factor* given by

$$Q = 1 - \Theta(v - s - 2m - w)\Theta(s + v - w) \tag{175}$$

that represents the exclusion of wave function to the barrier region $x > 0$ when the energy w hits the negative energy spectra of Dirac equation with potentials s and v. It is technically obtained from the proper connection condition $\varphi(0_-) = 0$, $\chi(0_-) = constant$, which is obtainable as the $n \to \infty$ limit of $(x - 1)^n$ potential, for which $\varphi(0_-) = 0$, $\chi(0_-) = constant$ is found to be the correct condition (see no.5 in reference) . Fuller picture of this peculiar boundary condition may require the treatment of the problem with proper field theoretical setup (see no.2 in reference), where the exclusion factor Q could be understood as a result of many-body Pauli blocking.

The solution of the problem (173) is elementary, and we have

$$T = \frac{2g}{1 + g}, \quad R = \frac{1 - g}{1 + g} \tag{176}$$

For large enough w, that satisfies the condition $w > |m + s| - m + v$, the spectra inside the potential region is continuous, and we have partial transmission and reflection specified by (176) with (174). We naturally have unitary relation $|R|^2 + |T|^2 = 1$. As we decrease w down to the threshold energy $w = v - m + |m + s|$, p approaches zero, and g becomes either zero (if $s < -m$ and therefore $w = v - s - 2m$) or infinity (if $s > -m$ and therefore $w = v + s$). They respectively correspond to perfect reflection $R = 1$ with Dirichlet boundary $\varphi(0_-) = 0$ or $R = -1$ with Neumann boundary $\chi(0_-) = 0$.

Below this threshold, $|m + s| - m + v > w > -|m + s| - m + v$ (or $|\varepsilon - v| < |m + s|$, if it occurs with positive w), the particle hits the spectral gap and we get exponential wave function with decay constant κ. The full reflection $|R| = 1$ with quantum penetration $0 < T < 2$ to the classically forbidden area is observed. Note that there is no problem in having $|T| > 1$ in this case, since the unitarity is guaranteed by decaying wave function $e^{-\kappa x}$. At the "Dirac sea" threshold, $w = v - m - |m + s|$, κ approaches zero, and g becomes either infinity (if $s < -m$ and therefore $w = v + s$) or zero (if $s > -m$ and therefore $w = v - s - 2m$) which correspond to perfect reflection $R = -1$ with Neumann boundary $\chi(0_-) = 0$ or $R = 1$ with Dirichlet boundary $\varphi(0_-) = 0$.

Below the Dirac sea threshold, $w < -|m + w| - m + v$ we have perfect reflection with Dirichlet condition $R = 1$ as a result of Giachetti-Sorace factor.

When the energy w approaches 0, we have $\kappa \to 0$, which signifies that the quantum penetration length to classically forbidden region $x > 0$ becoming infinite. However, (174) tells us that we have $g = 0$, and thus no penetration amplitude $T = 0$ and, as a result, the perfect "classical" reflection $R = 1$ occurs.

Above statements are true in generic case, depicted in the left hand graph on fig.12 for example, but there is an exception to the case when potentials v
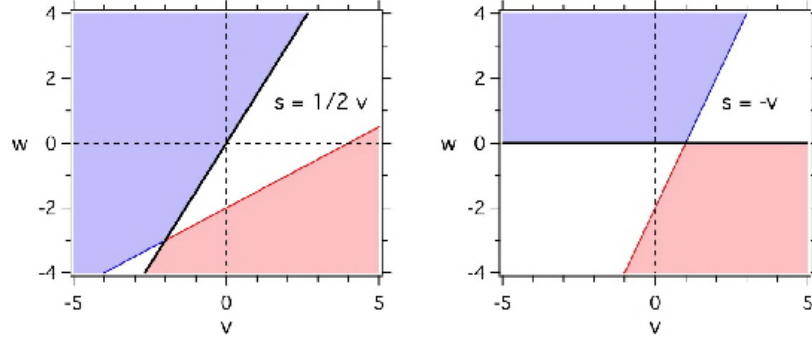
Figure 12: spectrum of Dirac particle in relativistic field. Blue region represents positive part of the spectra, red region represents the Dirac sea. White regions represent spectral gap

and s are related by $s + v = 0$, depicted in the right hand graph of fig.12. In this case, there is a cancellation in the expression for g, (174) and we have

$$g = \sqrt{\frac{w + 2m - 2v}{w + 2m}} = \frac{1}{i}\sqrt{\frac{2v - w - 2m}{w + 2m}} \qquad (177)$$

which is finite as a results of "merging" of $w = v + s$ line, on which $g = \infty$ holds, and $w = 0$ line, on which $g = 0$ holds.

This means that for this special case of opposite-sign but equal-magnitude scalar and vector potential, $s + v = 0$, we have singular infinite-range penetration limit $\kappa \to 0$ with finite amplitude $0 < |T| < 2$ for zero energy barrier reflection $w \to 0$. We rush to note that this poses no paradox of any sort, since we still have full reflection $|R| = 1$ albeit with some nontrivial phase for R. This is a subtle but an exotic exception, nonetheless, whose significance soon becomes obvious in the following.

We now consider one dimensional scattering off a square barrier of constant height (see fig. 13) potential with spatial extension L formally given by

$$V(x) = v\,\Theta(x)\Theta(L - x), \quad S(x) = s\,\Theta(x)\Theta(L - x) \qquad (178)$$

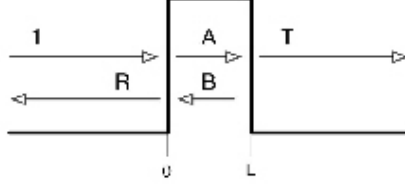The scattering wave functions at $x < 0$, $0 < x < L$ and $L < x$ are given, respectively as

Figure 13:

$$\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{ik}{m+\varepsilon} \end{pmatrix} e^{ikx} - R \begin{pmatrix} 1 \\ \frac{-ik}{m+\varepsilon} \end{pmatrix} e^{-ikx} \tag{179}$$

$$\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = A \begin{pmatrix} 1 \\ \frac{ip}{m+\varepsilon+s-v} \end{pmatrix} e^{ipx} - B \begin{pmatrix} 1 \\ \frac{-ip}{m+\varepsilon+s-v} \end{pmatrix} e^{-ipx} \tag{180}$$

$$\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = T \begin{pmatrix} 1 \\ \frac{ik}{m+\varepsilon} \end{pmatrix} e^{ikx} \tag{181}$$

In a similar manner to the previous case, smooth connection conditions for both large and small components at $x = 0$ and $x = L$ gives

$$1 - R = A - B \tag{182}$$

$$g(1 + R) = A + B \tag{183}$$

$$Ae^{ipL} - Be^{-ipL} = Te^{ikL} \tag{184}$$

$$Ae^{ipL} + Be^{-ipL} = gTe^{ikL} \tag{185}$$

Elementary calculation yields following expressions for transmission and reflection amplitudes;

$$T = \frac{e^{-ikL}}{\cos pL - \frac{i}{2}(1/g + g)\sin pL} \tag{186}$$

$$R = \frac{-\frac{i}{2}(1/g - g)\sin pL}{\cos pL - \frac{i}{2}(1/g + g)\sin pL} \tag{187}$$

This expression is literally valid for the energy $w > |m+s|+v$. For the energy $|m + s| + v > w > -|m + s| + v$, we have to make replacement $p = i\kappa$ as before, which will result in the replacements $\cos pL \to \cosh \kappa L$ and $\sin pL \to i \sinh \kappa L$ in (186) (187). This expression is reduced to $T = 0$, $R = 1$ for the energy $w < -|m + s| + v$ with which we hit the Dirac sea spectra inside the potential barrier, where we have $Q = 0$, thus $g = 0$.
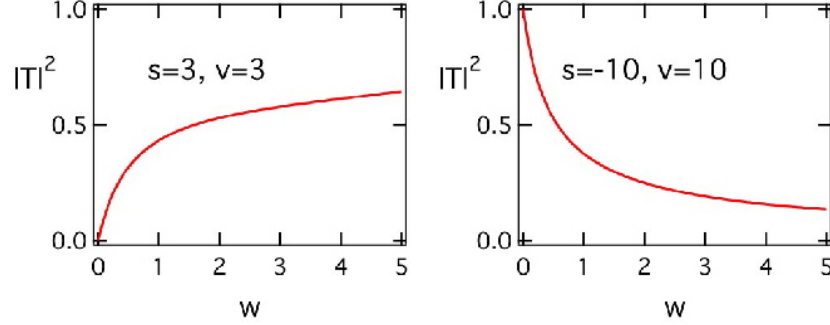
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Figure 14:

We look at the low energy limit of the scattering matrix T. Generically, for the case of $s \neq -v$, we have the quantity g that approaches to zero as we take $w \to 0$ limit, causing the divergence of $1/g$, which guarantees the perfect reflection

$$T \to 0, \quad R \to 1 \quad \text{as} \quad w \to 0 \qquad (s + v \neq 0) \tag{188}$$

This simply is an exact expression of the intuitive statement that a generic obstacle works as a reflecting block for low energy projectile, or in other word, if we hit any barrier too slowly, we are bound to get reflected all the time.

However, for the special case of $s + v = 0$, g takes the form (177) after cancellation of w in both denominator and enumerator of (174), and we have $g = \text{finite}$ and $\kappa \to 0$ (or $p \to 0$) as we take $w \to 0$ limit. We therefore obtain, from (186)(187), a peculiar limit

$$T \to 1, \quad R \to 0 \quad \text{as} \quad w \to 0 \qquad (s + v = 0) \tag{189}$$

which signifies an anomalous *full transmission at zero energy*. This is particularly intriguing for the case of decaying wave in the gap region, in which κ is real, where decaying length $1/\kappa$ becomes infinity at $w \to 0$ limit.

The situation is immediately understood by inspecting the illustrations on fig.14. Here, the graph in the left depicts a generic case that has normal perfect reflection at $w \to 0$ limit, while the graph in the right shows the anomalous zero energy transparency. The reason behind this transparency lies in the enhanced long range tunneling inside the barrier, which occurs because, at $w \to 0$, the energy approaches to the threshold of negative continuous spectra that exists right below $w = 0$ for $s + v = 0$ potentials. The presence of Dirac sea not only induces the perfect reflection for $w > 0$ with $v > |s|$, for example, it also affects the decaying length and induces the anomalous tunneling, and transmission at $w \to 0$ limit for the case of $s + v = 0$ potentials.
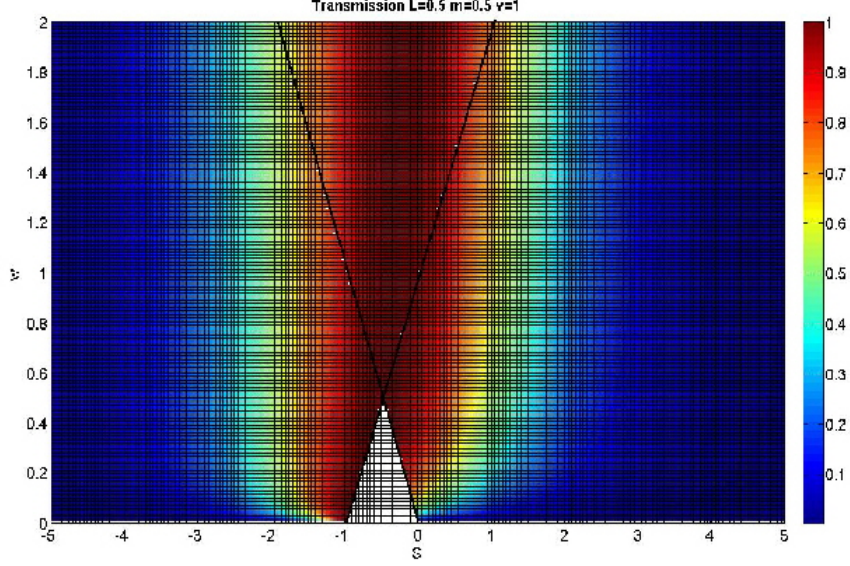
Figure 15: Transmission as a function of the kinetic energy w of incident particle and scalar component s of relativistic potential. Vector component v is set to be equal 1

The zero energy transmission is clearly visible on fig. 15, which shows the transmission coefficient as a function of energy w and scalar potential s for fixed value of vector potential $v = 1$. We can see that for $s = -v = -1$ the transmission coefficient approach 1 as $w \to 0$.

The meaning of the black lines is that they divide the graph into regions depending on which part of spectra particle hits in the barrier region. (see fig. 16)

Let us now consider the $L \to 0$ limit of relativistic scattering. Straightforward limit will, of course, lead to disappearance of the barrier, $T \to 1$. Limit $L \to 0$ with constant volume integrals,

$$v = \frac{\bar{v}}{L}, \quad s = \frac{\bar{s}}{L}, \qquad (L \to 0) \tag{190}$$
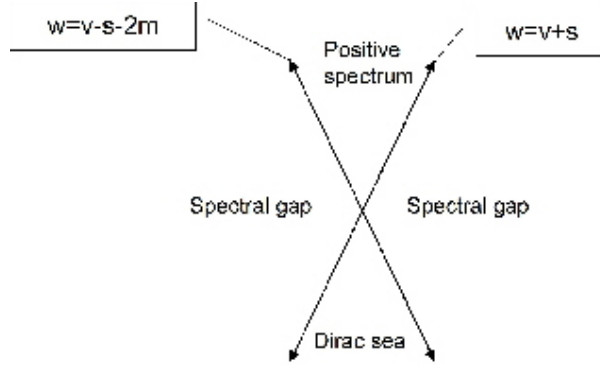
on the other hand, leads to

Figure 16:

$$T = \frac{1}{\cos\beta + \frac{i}{2\beta}\sin\beta\left[(\bar{v}+\bar{s})/K + (\bar{v}-\bar{s})K\right]}\Theta(\bar{v}+|\bar{s}|) \tag{191}$$

$$R = \frac{\frac{i}{2\beta}\sin\beta\left[(\bar{v}+\bar{s})/K - (\bar{v}-\bar{s})K\right]}{\cos\beta + \frac{i}{2\beta}\sin\beta\left[(\bar{v}+\bar{s})/K + (\bar{v}-\bar{s})K\right]}\Theta(-\bar{v}-|\bar{s}|) + \Theta(\bar{v}+|\bar{s}|) \tag{192}$$

with $\beta = \sqrt{\bar{v}^2 - \bar{s}^2} = i\sqrt{\bar{s}^2 - \bar{v}^2}$ and $K = \sqrt{\frac{w}{w+2m}}$.

We can interpret this result in terms of relativistic *point interactions* specified by the boundary condition which is a most general time-reversal symmetric one

$$\begin{pmatrix} \varphi(0_+) \\ \chi(0_+) \end{pmatrix} = \begin{pmatrix} \alpha & u_- \\ u_+ & \alpha \end{pmatrix} \begin{pmatrix} \varphi(0_-) \\ \chi(0-) \end{pmatrix} \tag{193}$$

with $\alpha^2 - u_+ u_- = 1$. The scattering off the point interaction (193) is given

$$T = \frac{1}{\alpha + \frac{i}{2}[u_+/K - u_- K]}, \quad R = \frac{\frac{i}{2}[u_+/K + u_- K]}{\alpha + \frac{i}{2}[u_+/K - u_- K]} \tag{194}$$

which comparing to (191) and (192) allows the identifications

$$u_+ = (\bar{s}+\bar{v})\frac{\sin\beta}{\beta}, \quad u_- = (\bar{s}-\bar{v})\frac{\sin\beta}{\beta} \tag{195}$$

The special cases $\bar{s} = \bar{v}$ and $\bar{s} = -\bar{v}$ can be considered as the limiting cases of (191) and (192), and we have, for $\bar{s} = \bar{v}$

$$T = \frac{1}{1 + i\bar{v}/K}, \quad R = \frac{i\bar{v}/K}{1 + i\bar{v}/K} \tag{196}$$

while, for $\bar{s} = -\bar{v}$, we have

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$$T = \frac{1}{1 + i\bar{v}K}, \quad R = \frac{-i\bar{v}K}{1 + i\bar{v}K} \tag{197}$$

If we take the *non-relativistic limit in kinematics*, $K \to k/(2m)$, these two cases are exactly identical to the scattering form *delta* and *delta-prime* point interactions , which represent high-pass and low-pass wave filters, respectively. Note that constructing non-standard point interactions, that results in (197), within non-relativistic framework involves highly singular procedures.

Finally, we ask a question whether we can construct an analogue of the phenomena we have found in the framework of non-relativistic Schrödinger equation. We rewrite the Dirac equation (166) by eliminating small component χ in the form

$$-\frac{d}{dx}\frac{1}{2m^*}\frac{d}{dx}\varphi + U\varphi = w\varphi \tag{198}$$

with effective mass m^* and potential U defined by

$$m^* = m + \frac{w}{2} + \frac{S - V}{2}, \quad U = S + V \tag{199}$$

Assuming the conditions $w << m$ and $|S - V| << m$, we obtain Schrödinger equation with effective potential which is given by the sum of vector and scalar potentials. This is nothing but the true non-relativistic limit. However, we obtain non-standard low-energy limit by assuming the non-relativistic kinematics $w << m$ in conjunction with strong relativistic potentials $|S - V| \sim m$. Specifically, we can reproduce anomalous transmission from Schrödinger equation (198) by setting $S = -V$ which results in $m^* \approx m - V$ and $U = 0$. This means that we can construct a purely non-relativistic model of anomalous scattering and delta-prime point interaction with *just effective mass and no potential*. Readers are warned, however, that this non-relativistic analogue scheme works only to an extent: When $S - V$ is negative in sign and so large, we obtain negative value for the effective mass m^*. For this *bona fide* relativistic dynamics, non-relativistic analogue (198) does not make sense, and therefore does not exist.

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11 Conclusion

In the second part we dealt with relativistic Dirac equation and showed that proper consideration of the Dirac sea leads to an interesting consequences for a low energy scattering systems. Specifically we showed that a set of relativistic potentials having the property of same strength but opposite signs for scalar and vector components displays anomalous tunneling and full transparency at zero energy, while barrier starts functioning at higher energy. The short range limit of this phenomenon leads to a smooth relativistic realization of an exotic point interaction, delta-prime, that conventionally requires singular and esoteric constructions within non-relativistic dynamics. It has been pointed out that in three dimensions, the "$S = -V$" relativistic potentials have an esoteric property called *pseudospin symmetry* that has been found to play important role in the degeneracy structure of nuclear levels. Current work shows that there is yet another aspect to this pseudospin symmetric limit of relativistic potentials, which is revealed only in one dimensional systems.