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Application of Green's-Function techniques to quantum barrier penetration problems

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Abstract
We obtain a mathematical and algebraic expression of the Green-function method in treating quantum tunnelling in one-dimensional barrier systems. The retarded Green's function of the free-particle resolvent is then obtained consistently to obtain scattering amplitudes using the Lippmann-Schwinger equation. The technique is used to apply to the d-function barrier, the finite square barrier, and the double-barrier quantum-well structure in order to describe the transmission, penetration of the barrier, and resonance. With the Green, the pole structure in the case of the double-barrier directly traces the quasi-bound and the Breit-Wigner-type resonances.

Keywords: Schrödinger equation, green's function, delta potential, barrier, tunneling

Introduction
One of the most dramatic examples of the behavior of waves in quantum mechanics is quantum tunneling, which allows particles to tunnel through potential barriers where classical physics would prohibit such a result [1]. It is the main characteristic of a broad set of physical systems and electronic devices, most prominently tunnel diodes, resonant tunneling structures and current nanoscale heterostructures based on semiconductors [2]. With the reduction in device size, and the increased importance of quantum effects, it is both more important to develop a transparent and general mathematical model of tunneling, both to understand and to model. The functions of green give a strong and integrated method of the investigation of the penetration through barriers. In contrast to the older techniques of finding the scale factor between two different boundaries, the Green's-function formalism uses boundary conditions in the form of the analytic structure of the resolvent and offers a natural way to find scattering solutions using the Lippmann-Schwinger equation. The view point reveals the relevance of outgoing-wave conditions and complex-energy poles and resonance formation, without which it is difficult to engage in the study of tunneling between single and multiple barriers.
This paper gives a self-sufficient derivation of the retarded Green's function of one-dimensional systems and uses it to calculate barrier (canonical) systems central to quantum transport theory. We start by a δ-function barrier that gives a perfectly solvable model that gives a clear picture of the algebraic simplicity of the Green's-function method. The formalism is then generalized to the finite square barrier, in which it is shown that tunneling probabilities and penetration depths naturally occur in the framework of the formalism. We lastly investigate the quantum-well system of a double-barrier system where the pole structure of the resolvent will display quasi-bound states and Breit-Wigner-type resonances which determine resonant tunneling.
The Green's-function method got the transmission coefficients, which are related to popular quantum transport relations, such as the Landauer formula and the Tsu-Esaki expression of tunneling currents. This conceptual synthesis goes beyond the understanding into a set of tools to be applied in the analysis of semiconductor systems in which quantum coherence and energy-selective tunneling are predominant.

Schrödinger Equation and Green's Function
Consider a particle of mass m moving in one dimension under potential V (x). The time-independent Schr¨odinger equation at energy E reads

$$(E - H)\psi(x) = 0, \quad H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \tag{1}$$

Define the resolvent (retarded Green's function) G(x,x′;E) by

$$(E - H)G(x,x';E) = \delta(x - x') \tag{2}$$

with outgoing boundary conditions (retarded prescription) appropriate for scattering states [3].
Once G is known, a formal solution to the inhomogeneous equation (E-H)ψ =s is

$$\psi(x) = \int G(x,x';E)s(x')dx' \tag{3}$$

For scattering we use the Lippmann-Schwinger formulation to convert the homogeneous Schro¨dinger equation to an integral equation.
For free particle, We first compute the free Green's function G0(x,x′;E) solving

$$(E - H_0)G_0(x,x';E) = \delta(x - x'), \quad H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \tag{4}$$

Assume E > 0 and define the wave number

$$E = \frac{\hbar^2 k^2}{2m}, \quad k > 0 \tag{5}$$

Then for x ≠ x′ the homogeneous equation is

$$\left(\frac{d^2}{dx^2} + k^2\right)G_0(x,x';E) = 0 \tag{6}$$

General solution for regions x < x′ and x > x′ are linear combination of e±ikx. Impose continuity at x = x′ and the jump condition obtained by integrating (4) across x′

$$\frac{d}{dx}G_0(x,x';E)|_{x=x'+0} - \frac{d}{dx}G_0(x,x';E)|_{x=x'-0} = \frac{2m}{\hbar^2} \tag{7}$$

Impose outgoing (radiation) boundary condition: as |x − x′| → ∞ the solution is proportional to eik|x−x′| with outgoing waves [4].
The unique solution is

$$G_0(x,x';E) = \frac{im}{\hbar^2 k}e^{ik|x-x'|} \tag{8}$$

We can verify by direct differentiation and distributional identities that (8) satisfies (4). Note the retarded +i0 prescription in energy corresponds to k ⟶ k + i0.

Lippmann-Schwinger equation and Dyson series
Writing H = H0 + V and using the definition of G_0 and G we obtain the Dyson equation

$$G = G_0 + G_0VG, \tag{9}$$

in kernel form:

$$G(x,x';E) = G_0(x,x';E) + \int G_0(x,y;E)V(y)G(y,x';E)dy \tag{10}$$

For scattering states with incident wave ϕ(x) (solution of free Schro¨dinger equation) the Lippmann- Schwinger equation is

$$\psi(x) = \phi(x) + \int G_0(x,x';E)V(x')\psi(x')dx' \tag{11}$$

This integral equation is equivalent to the differential Schro¨dinger equation with outgoing boundary conditions [5].
If we consider a right-incident plane wave ϕ(x) = eikx. The physical scattering state behaves asymptotically as,

$$\psi(x) \overset{x\to-\infty}{\to} e^{ikx} + r(E)e^{-ikx}, \quad \psi(x) \overset{x\to+\infty}{\to} t(E)e^{ikx} \tag{12}$$

To extract t(E) and r(E) from (11), use the large-|x| asymptotics of for x → +∞,
G_0 (x,x';E)~im/(h^2 k) e^ikx e^(-ikx'). Hence from (11)

$$\psi(x \to +\infty) = e^{ikx} + \int G_0(x,x';E)V(x')\psi(x')dx'$$

$$\sim e^{ikx} + \frac{im}{\hbar^2 k} e^{ikx} \int e^{-ikx'} V(x')\psi(x')dx' \tag{13}$$

Therefore, the transmission amplitude is,

$$t(E) = 1 - \frac{im}{\hbar^2 k} \int e^{-ikx} V(x)\psi(x)dx \tag{14}$$

Similarly, using x → −∞ asymptotics one can extract r(E).

Case1: δ-function barrier
Let V (x) = λδ(x) with real λ. This is exactly solvable and illustrates the Green's-function method. From (11) with ϕ(x) = eikx and using the support of V

$$\psi(x) = e^{ikx} + \lambda G_0(x,0;E)\psi(0) \tag{15}$$

Evaluating at x = 0 gives

$$\psi(0) = 1 + \lambda G_0(0,0;E)\psi(0) \Rightarrow \psi(0) = \frac{1}{1-\lambda G_0(0,0;E)} \tag{16}$$

Using (8): G_0 (0,0;E)=-im/(ℏ^2 k) Thus

$$\psi(x) = e^{ikx} + \frac{e^{ik|x|}}{1+im\lambda/(\hbar^2 k)} \frac{im\lambda}{\hbar^2 k} \tag{17}$$

For x → +∞, the coefficient of eikx is

$$t(E) = \frac{1}{1+i\frac{m\lambda}{\hbar^2 k}} \tag{18}$$

Hence the transmission probability is

$$T(E) = |t(E)|^2 = \frac{1}{1+\left(\frac{m\lambda}{\hbar^2 k}\right)^2} \tag{20}$$

Reflection amplitude r(E) = t(E) − 1 and R(E) = 1 - T

Case 2: Finite square barrier (step-by-step)
Consider the potential barrier of the form

$$V(x) = \begin{cases} V_0, & 0 \le x \le a, \\ 0, & \text{otherwise.} \end{cases}$$

Defining $k = \frac{\sqrt{2mE}}{\hbar}$ and $q = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

If E < V0, q = iκ with κ= $\frac{\sqrt{2m(V_0-E)}}{\hbar}$
Since V (x) is supported on [0,a], restrict (11) to x ∈ [0,a]:

$$\psi(x) = e^{ikx} + V_0 \int_0^a G_0(x,x';E)\psi(x')dx', \quad 0 \le x \le a. \tag{21}$$

This is a linear integral equation (second-kind) for ψ on [0,a]. Using the explicit form of G0(x,x′) one may convert it to algebraic equations by projecting onto suitable basis functions (e.g. e±iqx) — equivalently, the differential-equation matching method is algebraically simpler.
Solving Schro¨dinger equation in three regions yields;

$$\psi_L(x) = e^{ikx} + re^{-ikx}, \quad x < 0, \tag{22}$$

$$\psi_M(x) = Ae^{iqx} + Be^{-iqx}, \quad 0 < x < a, \tag{23}$$

$$\psi_R(x) = te^{ikx}, \quad x > a. \tag{24}$$

Impose continuity of ψ and ψ′ at x = 0 and x = a (four equations for A,B,r,t). After algebraic elimination one obtains (standard result)

$$t(E) = \frac{4kq\,e^{-ika}}{(k+q)^2 e^{-iqa} - (k-q)^2 e^{iqa}} \tag{25}$$

This expression can be algebraically manipulated to common alternative forms. For E < V0 put q = iκ and simplify to see the exponential tunneling dependence ~ e−κa in the transmission.

Double-barrier and resonant tunneling (application to RTD and Esaki-like devices)

A double-barrier structure (two finite barriers separated by a quantum well) supports quasi-bound states in the well. When an incoming electron energy coincides with a quasi-bound level, transmission is resonantly enhanced. Green's functions make pole structure and resonance widths explicit.

Barriers: region I (x < 0) free, region II (0 < x < b) barrier V0, region III (b < x < b + w) well (V = 0), region IV (b + w < x < 2b + w) barrier V0, region V (x > 2b + w) free. Solve by transfer-matrix or Green's function matching; the transmission amplitude takes the form

$$t(E) = \frac{e^{-ik(2b+w)}}{D(E)} \tag{26}$$

where the denominator D(E) contains terms like cos(qw) and sin(qw) with coeficients depend-ing on barrier parameters [6]. Zeros of D(E) in complex energy plane correspond to poles of G(E) (resonances).

If a resonance occurs at complex energy Er − iΓ/2 then near the resonance

$$G(E) \sim \frac{R}{E - E_r + i\Gamma/2} \tag{27}$$

and the transmission near the resonance has Breit-Wigner form with full width at half maximum Γ. Lifetime τ of quasi-bound state relates by τ = ħ/Γ.

Poles of G(x,x′;E) under analytic continuation to complex E mark bound states (real nega-tive energy poles for localized potentials) and resonances (complex poles in lower half-plane). Methods to find poles include solving determinant conditions from matching/transfer-matrix denominators or evaluating det(1 − V G_0) when using operator formalism.

Conclusion

In this work, we formulate algebraically an algebraic and self-contained formulation of the retarded Green's function in one-dimensional quantum tunnelling and show that it can be effective in a variety of barrier problems typically encountered. Standing up with the free resolvent and the Lippmann-Schwinger equation, we obtain the explicit Green functions and scattering amplitudes, and we do not have to deal with the complexities of traditional boundary-matching. The delta-function model and square-barrier model demonstrate the simplicity in determining transmission and penetration, and the double-barrier model indicates the pole structure of the resolvent and the appearance of Breit-Wigner resonances. The framework has connected in a straightforward manner microscopic scattering physics to quantifiable currents in tunneling devices by relating the resulting transmission coefficients to the Landauer and Tsu Esaki transport formulas.

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