

A Model System for Dimensional Competition in Nanostructures: A Quantum Wire on a Surface

Rainer Dick

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Abstract The retarded Green's function $(E - H + i\epsilon)^{-1}$ is given for a dimensionally hybrid Hamiltonian which interpolates between one and two dimensions. This is used as a model for dimensional competition in propagation effects in the presence of one-dimensional subsystems on a surface. The presence of a quantum wire generates additional exponential terms in the Green's function. The result shows how the location of the one-dimensional subsystem affects propagation of particles.

Keywords Fermions in reduced dimensions · Nanowires · Quantum wires

Introduction

One-dimensional field theory is frequently used for quantum wires or nanowires [1–3] or nanotubes [4–7]. Two-dimensional field theory has become a universally accepted tool for the theoretical modeling of particles and quasiparticles on surfaces, interfaces, and thin films. The success of low-dimensional field theory in applications to the quantum hall effects [8–10], impurity scattering in low-dimensional system (see e.g. [11–16]), and the confirmation of low-dimensional critical exponents in experimental samples [17–22] confirm that low-dimensional field theories are useful tools for the description of low-dimensional condensed matter systems.

The properties of a physical system have a strong dependence on the number of dimensions d . A straightforward

example is provided by the zero energy Green's function $G(r)|_{E=0}$, which is proportional to r in $d = 1$ and proportional to $\ln r$ in $d = 2$, and decays like r^{2-d} in higher dimensions. Green's functions determine correlation functions, two-particle interaction potentials, propagation of initial conditions, scattering off perturbations, susceptibilities, and densities of states in quantum physics. It is therefore of interest to study systems of mixed dimensionality, where competition of dimensions can manifest itself in the properties of particle propagators.

To address questions of dimensional competition analytically in the framework of interfaces in a bulk material, dimensionally hybrid Hamiltonians of the form

$$H = \frac{\hbar^2}{2m} \int d^2\mathbf{x} \int dz (\nabla\psi^+ \cdot \nabla\psi + \partial_z\psi^+ \cdot \partial_z\psi) + \frac{\hbar^2}{2\mu} \int d^2\mathbf{x} \nabla\psi^+ \cdot \nabla\psi \Big|_{z=z_0} \quad (1)$$

were introduced in [23]. The corresponding first quantized Hamiltonian is

$$H = \frac{\mathbf{p}^2 + p_z^2}{2m} + |z_0\rangle\langle z_0| \frac{\mathbf{p}^2}{2\mu}. \quad (2)$$

Here the convention is to use vector notation $\mathbf{x} = (x, y)$, $\nabla = (\partial_x, \partial_y)$ for directions parallel to an interface, while z is orthogonal to the interface. From a practical side, Hamiltonians of the form (2) may be used to investigate propagation effects of weakly coupled particles in the presence of an interface. From a theoretical side, the Hamiltonians (1,2) are of interest for the analytic study of competition between two-dimensional and three-dimensional motion.

The two-dimensional mass parameter μ is a mass per length. In simple models it is given by

R. Dick (✉)
 Physics and Engineering Physics, University of Saskatchewan,
 116 Science Place, Saskatoon, SK, Canada S7N 5E2
 e-mail: rainer.dick@usask.ca

$$\mu = \frac{m}{L_{\perp}},$$

where depending on the model, $L_{\perp}$ is either a bulk penetration depth of states bound to the interface at $z = z_0$ or a thickness of the interface, see [24].

The zero energy Green's function for the Hamiltonians (1,2) for perturbations in the interface ($z' = z_0 = 0$), $G(\mathbf{x} - \mathbf{x}', z) = \langle \mathbf{x}, z | G | \mathbf{x}', 0 \rangle$ satisfies

$$(\Delta + \partial_z^2)G(\mathbf{x} - \mathbf{x}', z) + \frac{m}{\mu}\delta(z)\Delta G(\mathbf{x} - \mathbf{x}', 0) = -\delta(\mathbf{x} - \mathbf{x}')\delta(z)$$

and was found in [23] ($r = |\mathbf{x} - \mathbf{x}'|$),

$$G(\mathbf{x} - \mathbf{x}', z) = \frac{1}{4\pi} \int_0^{\infty} dk \frac{\exp(-k|z|)}{1 + k\ell} J_0(kr), \quad \ell = \frac{m}{2\mu}. \quad (3)$$

The Green's function in the interface is given in terms of a Struve function and a Bessel function,

$$G(\mathbf{x} - \mathbf{x}', 0) = \frac{1}{8\ell} \left[H_0\left(\frac{r}{\ell}\right) - Y_0\left(\frac{r}{\ell}\right) \right] \quad (4)$$

and interpolates between two-dimensional and three-dimensional distance laws (see Fig. 1),

$$r \ll \ell: \quad G(\mathbf{x} - \mathbf{x}', 0) = \frac{1}{4\pi\ell} \left[-\gamma - \ln\left(\frac{r}{2\ell}\right) + \frac{r}{\ell} + \mathcal{O}\left(\frac{r^2}{\ell^2}\right) \right], \quad (5)$$

$$r \gg \ell: \quad G(\mathbf{x} - \mathbf{x}', 0) = \frac{1}{4\pi r} \left[1 - \frac{\ell^2}{r^2} + \mathcal{O}\left(\frac{\ell^4}{r^4}\right) \right]. \quad (6)$$

The corresponding energy-dependent Green's function was also recently reported [24]. However, another system of great practical and theoretical interest concerns quantum wires or nanowires on surfaces. Preparation techniques for one-dimensional nanostructures were recently reviewed in reference [25]. We will examine the corresponding dimensionally hybrid Hamiltonian and its Green's function in this paper.

The Hamiltonian

We wish to discuss effects of dimensionality of nanostructures on the propagation of weakly coupled particles in the framework of a simple model system. We assume large de Broglie wavelengths $\hbar/p$ compared to lateral dimensions of nanostructures, and for our model system we also neglect electromagnetic effects or interactions, bearing in mind that these effects are highly relevant in realistic nanostructures [26, 27].

The model system which we have in mind consists of non-relativistic particles or quasi-particles tied to a surface. The surface carries a one-dimensional wire. The x direction

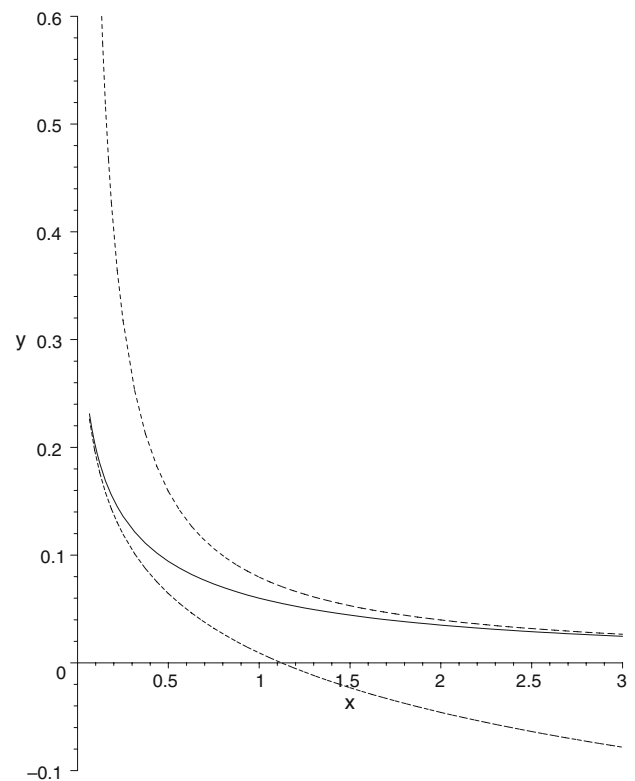


Fig. 1 The upper dotted line is the three-dimensional Green's function $(4\pi r)^{-1}$ in units of ℓ^{-1} , the continuous line is the Green's function (4), and the lower dotted line is the two-dimensional logarithmic Green's function. $x = r/\ell$

is along the wire and the y direction is orthogonal to the wire. The wire is located at $y = y_0$. The particles can move with a mass m on the surface, but motion along the wire may be described by a different effective mass m_* . In case of a weak attraction to substructures, kinetic operators can be split between bulk motion and motion along substructures [24]. Alternatively, for large lateral de Broglie wavelength relative to lateral extension $L_{\perp}$ of a substructure, one can also argue that the lateral integral of the kinetic energy density along a substructure only yields a factor $L_{\perp}$ in the kinetic energy for motion along the substructure. In either case we end up with an approximation for the kinetic energy operator of the particles of the form

$$H = \int dx \int dy \frac{\hbar^2}{2m} \times \left(\frac{\partial \psi^+(x, y)}{\partial x} \frac{\partial \psi(x, y)}{\partial x} + \frac{\partial \psi^+(x, y)}{\partial y} \frac{\partial \psi(x, y)}{\partial y} \right) + \int dx \frac{\hbar^2}{2\mu} \frac{\partial \psi^+(x, y_0)}{\partial x} \frac{\partial \psi(x, y_0)}{\partial x}, \quad (7)$$

where the mass parameter $\mu = m_*/L_{\perp}$ is a mass per lateral attenuation length of bound states, or a mass per lateral extension of the substructure. The operator (7) is the

second quantized kinetic Hamiltonian for the particles. The corresponding first quantized Hamiltonian is

$$H = \frac{p_x^2 + p_y^2}{2m} + |y_0\rangle\langle y_0| \frac{p_x^2}{2\mu}. \quad (8)$$

The wire corresponds to a channel in which propagation of a particle comes with a different cost in terms of kinetic energy. It is intuitively clear that existence of this channel will affect propagation of the particles on the surface, and we will discuss this in terms of a resulting Green's function for the Hamiltonians (7,8).

The Green's Function in k Space

The Hamiltonians (7,8) yield the Schrödinger equation

$$E\psi(x, y) = -\frac{\hbar^2}{2m}(\partial_x^2 + \partial_y^2)\psi(x, y) - \frac{\hbar^2}{2\mu}\delta(y - y_0)\partial_x^2\psi(x, y_0), \quad (9)$$

and the corresponding equation for the Green's function in the energy representation,

$$\left(E - \frac{p_x^2 + p_y^2}{2m} - |y_0\rangle\langle y_0| \frac{p_x^2}{2\mu}\right)G(E) = 1.$$

The last equation reads in (x, y) representation and with the convention $G(E) \equiv -2mG(E)/\hbar^2$

$$\left(\frac{2m}{\hbar^2}E + \partial_x^2 + \partial_y^2 + \delta(y - y_0)\frac{m}{\mu}\partial_x^2\right)\langle x, y|G(E)|x', y'\rangle = -\delta(x - x')\delta(y - y'). \quad (10)$$

Substitution of the Fourier transform

$$\begin{aligned} \langle x, y|G(E)|x', y'\rangle &= \frac{1}{4\pi^2} \int dk_x \int dk'_x \int dk_y \\ &\times \int dk'_y \langle k_x, k_y|G(E)|k'_x, k'_y\rangle \\ &\times \exp[i(k_x x + k_y y - k'_x x' - k'_y y')] \end{aligned}$$

yields

$$\begin{aligned} &\left(\frac{2m}{\hbar^2}E - k_x^2 - k_y^2\right)\langle k_x, k_y|G(E)|k'_x, k'_y\rangle \\ &- \frac{m}{\mu} \frac{k_x^2}{2\pi} \int d\kappa \exp[i(\kappa - k_y)y_0] \langle k_x, \kappa|G(E)|k'_x, k'_y\rangle \\ &= -\delta(k_x - k'_x)\delta(k_y - k'_y). \end{aligned} \quad (11)$$

This yields with

$$\langle k_x, k_y|G(E)|k'_x, k'_y\rangle = \langle k_y|G(E, k_x)|k'_y\rangle \delta(k_x - k'_x)$$

the condition

$$\begin{aligned} &\left(k_x^2 + k_y^2 - \frac{2m}{\hbar^2}E\right)\langle k_y|G(E, k_x)|k'_y\rangle \\ &+ \frac{m}{\mu} \frac{k_x^2}{2\pi} \int d\kappa \exp[i(\kappa - k_y)y_0] \langle \kappa|G(E, k_x)|k'_y\rangle \\ &= \delta(k_y - k'_y). \end{aligned} \quad (12)$$

This result implies that $\langle k_y|G(E, k_x)|k'_y\rangle$ must have the form

$$\begin{aligned} &\exp(ik_y y_0) \langle k_y|G(E, k_x)|k'_y\rangle \\ &= \frac{\exp(ik_y y_0) \delta(k_y - k'_y) + f(E, k_x, k'_y)}{k_x^2 + k_y^2 - (2mE/\hbar^2) - i\epsilon}, \end{aligned}$$

with the yet to be determined function $f(E, k_x, k'_y)$ satisfying

$$\begin{aligned} &\left(1 + \frac{m}{\mu} \frac{k_x^2}{2\pi} \int \frac{d\kappa}{\kappa^2 + k_x^2 - (2mE/\hbar^2) - i\epsilon}\right) f(E, k_x, k'_y) \\ &= -\frac{m}{\mu} \frac{k_x^2}{2\pi} \frac{\exp(ik'_y y_0)}{k_y'^2 + k_x^2 - (2mE/\hbar^2) - i\epsilon}. \end{aligned} \quad (13)$$

Substitution of

$$\begin{aligned} \int \frac{d\kappa}{\kappa^2 + k_x^2 - (2mE/\hbar^2) - i\epsilon} &= \pi\hbar \frac{\Theta(\hbar^2 k_x^2 - 2mE)}{\sqrt{\hbar^2 k_x^2 - 2mE}} \\ &+ i\pi\hbar \frac{\Theta(2mE - \hbar^2 k_x^2)}{\sqrt{2mE - \hbar^2 k_x^2}} \end{aligned}$$

yields

$$\begin{aligned} &\left[1 + \frac{m\hbar}{2\mu} k_x^2 \left(\frac{\Theta(\hbar^2 k_x^2 - 2mE)}{\sqrt{\hbar^2 k_x^2 - 2mE}} + i \frac{\Theta(2mE - \hbar^2 k_x^2)}{\sqrt{2mE - \hbar^2 k_x^2}}\right)\right] \\ &\times f(E, k_x, k'_y) \\ &= -\frac{m}{\mu} \frac{k_x^2}{2\pi} \frac{\exp(ik'_y y_0)}{k_y'^2 + k_x^2 - (2mE/\hbar^2) - i\epsilon}. \end{aligned}$$

We finally find

$$\begin{aligned} &\langle k_y|G(E, k_x)|k'_y\rangle \\ &= \frac{1}{k_y^2 + k_x^2 - (2mE/\hbar^2) - i\epsilon} \\ &\times \left[\delta(k_y - k'_y) - \frac{k_x^2 \ell}{\pi} \frac{\exp[i(k'_y - k_y)y_0]}{k_y^2 + k_x^2 - (2mE/\hbar^2) - i\epsilon}\right. \\ &\times \left(\frac{\sqrt{\hbar^2 k_x^2 - 2mE} \Theta(\hbar^2 k_x^2 - 2mE)}{\sqrt{\hbar^2 k_x^2 - 2mE} + \hbar k_x^2 \ell}\right. \\ &\left. \left. + \frac{\sqrt{2mE - \hbar^2 k_x^2} \Theta(2mE - \hbar^2 k_x^2)}{\sqrt{2mE - \hbar^2 k_x^2} + i\hbar k_x^2 \ell}\right)\right], \end{aligned} \quad (14)$$

where the definition

$$\ell = \frac{m}{2\mu} = \frac{m}{2m_*} L_{\perp}$$

was used. $\langle k_x, k_y | G(E) | k'_x, k'_y \rangle = \langle k_y | G(E, k_x) | k'_y \rangle \delta(k_x - k'_x)$ is the Green's function which we would use in k space Feynman rules. It is also instructive to switch to y representation for the transverse direction to see the impact of the wire on particle propagation.

The Green's Function in Mixed Representations and Impurity Scattering

It is well known in surface science that Green's functions can also be given in closed form in mixed representations, where momentum coordinates are used along the surface and configuration space coordinates are used for the transverse directions. The same observation applies here. In particular, the Green's function with one transverse momentum replaced by a transverse coordinate is given by

$$\begin{aligned} \langle k_y | G(E, k_x) | y' \rangle &= \frac{1}{\sqrt{2\pi}} \int dk'_y \exp(-ik'_y y') \langle k_y | G(E, k_x) | k'_y \rangle \\ &= \frac{1}{\sqrt{2\pi}} \frac{1}{k_y^2 + k_x^2 - (2mE/\hbar^2) - i\epsilon} \\ &\quad \times \left[\exp(-ik_y y') - \frac{\hbar k_x^2 \ell \Theta(\hbar^2 k_x^2 - 2mE)}{\sqrt{\hbar^2 k_x^2 - 2mE} + \hbar k_x^2 \ell} \exp\left(-ik_y y_0 - \sqrt{\hbar^2 k_x^2 - 2mE} \frac{|y' - y_0|}{\hbar}\right) \right. \\ &\quad \left. - i \frac{\hbar k_x^2 \ell \Theta(2mE - \hbar^2 k_x^2)}{\sqrt{2mE - \hbar^2 k_x^2} + i\hbar k_x^2 \ell} \exp\left(-ik_y y_0 + i\sqrt{2mE - \hbar^2 k_x^2} \frac{|y' - y_0|}{\hbar}\right) \right]. \end{aligned} \quad (15)$$

The Green's function with both arguments for the transverse direction given in terms of configuration space coordinates is

$$\begin{aligned} \langle y | G(E, k_x) | y' \rangle &= \frac{\hbar \Theta(\hbar^2 k_x^2 - 2mE)}{2\sqrt{\hbar^2 k_x^2 - 2mE}} \left[\exp\left(-\sqrt{\hbar^2 k_x^2 - 2mE} \frac{|y - y'|}{\hbar}\right) \right. \\ &\quad \left. - \frac{\hbar k_x^2 \ell}{\sqrt{\hbar^2 k_x^2 - 2mE} + \hbar k_x^2 \ell} \exp\left(-\sqrt{\hbar^2 k_x^2 - 2mE} \frac{|y - y_0| + |y' - y_0|}{\hbar}\right) \right] \\ &\quad + \frac{\hbar \Theta(2mE - \hbar^2 k_x^2)}{2\sqrt{2mE - \hbar^2 k_x^2}} \left[i \exp\left(i\sqrt{2mE - \hbar^2 k_x^2} \frac{|y - y'|}{\hbar}\right) \right. \\ &\quad \left. + \frac{\hbar k_x^2 \ell}{\sqrt{2mE - \hbar^2 k_x^2} + i\hbar k_x^2 \ell} \exp\left(i\sqrt{2mE - \hbar^2 k_x^2} \frac{|y - y_0| + |y' - y_0|}{\hbar}\right) \right]. \end{aligned} \quad (16)$$

The first order perturbation of a state $\psi_0(x, y)$ due to scattering off an impurity potential $V(x, y)$ corresponds to

$$\begin{aligned} \psi(x, y) &= \psi_0(x, y) - \frac{2m}{\hbar^2} \int dx' \int dy' \langle y | G(E, x - x') | y' \rangle \\ &\quad \times V(x', y') \psi_0(x', y') \\ &= \psi_0(x, y) \\ &\quad - \frac{m}{\pi \hbar^2} \int dx' \int dy' \int dk_x \langle y | G(E, k_x) | y' \rangle \\ &\quad \times \exp[ik_x(x - x')] V(x', y') \psi_0(x', y'). \end{aligned} \quad (17)$$

The result (16) shows peculiar distance effects between the location of the wire and the perturbation or impurity on the one hand, and between the location of the wire and the y coordinate of the wave function on the other hand. In both cases, the wavelength (for $2mE > \hbar^2 k_x^2$) or attenuation length (for $2mE < \hbar^2 k_x^2$) are the same as in the terms from the unperturbed surface propagator. In the evanescent case,

the impact of the wire on impurity scattering is exponentially suppressed if either the impurity is located far from the wire or if the wave function is considered far from the

wire. In the non-evanescent case the perturbation of the propagator due to the wire becomes a strongly oscillating function of $\sqrt{2mE - \hbar^2 k_x^2}/\hbar$ far from the wire. Therefore the impact of the wire will also be small if we consider wave packets far from the wire.

For a simple application of (17) consider a wire at $y_0 = 0$ and an impurity potential

$$V(x, y) = W\delta(x)\delta(y).$$

The plane wave $\psi_0(x, y) = \exp(iy\sqrt{2mE}/\hbar)$ with $\hbar \gg \sqrt{2mEL_\perp}$ is a solution of the Schrödinger Eq. 9 which satisfies the conditions for the approximation (7). In this case we get a scattering amplitude

$$\begin{aligned} \delta\psi(x, y) = & -\frac{mW}{\pi\hbar} \left[\int_0^{\sqrt{2mE}/\hbar} dk_x \frac{i \exp(ik_x x)}{\sqrt{2mE - \hbar^2 k_x^2 + i\hbar k_x^2 \ell}} \right. \\ & \times \exp\left(i\sqrt{2mE - \hbar^2 k_x^2} \frac{|y|}{\hbar}\right) \\ & + \int_{\sqrt{2mE}/\hbar}^\infty dk_x \frac{\exp(ik_x x)}{\sqrt{\hbar^2 k_x^2 - 2mE + i\hbar k_x^2 \ell}} \\ & \left. \times \exp\left(-\sqrt{\hbar^2 k_x^2 - 2mE} \frac{|y|}{\hbar}\right) \right]. \quad (18) \end{aligned}$$

The equation for $\ell = 0$ is just the standard result for scattering from a pointlike impurity in mixed representation. The presence of the wire reduces the scattering cross section of the impurity for orthogonal in fall.

Equations 15 and 16 also show that the effects of the additional terms should be most noticeable if $k_x \ell \gg 1$. Since $\ell = m/2\mu = mL_\perp/2m_*$, promising samples should have an effective mass m_* for motion along a quantum or nanowire which is much smaller than the effective mass m for motion along the surface. What comes to mind is an InSb nanowire on a Si surface. Scattering of surface particles off impurities in the presence of the wire should exhibit the additional propagator terms.

Conclusion

A simple model system for dimensional competition in nanostructures has been proposed. The system assumes that motion along a wire on a surface comes with a different cost in terms of kinetic energy, e.g. due to effective mass effects. The dimensionally hybrid retarded Green's function for the propagation of free particles in the system was found in closed analytic form both in k space and in mixed (k_x, y) representations. The wire generates extra exponential terms in the propagator of the particles. The attenuation

lengths or wavelengths in the evanescent or oscillating case, respectively, are the same as for the unperturbed propagator, but the extra terms exhibit distance effects between the particles and the wire.

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