Dimensionally hybrid Green’s functions and density of states for interfaces

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Abstract: The energy dependent Green’s function \((E - H)^{-1}\) for an interface Hamiltonian which interpolates between two and three dimensions can be calculated explicitly. This yields an expression for the density of states \(\rho(E, z_0)\) on the interface which interpolates continuously between the two-dimensional \(\rho(E) = \text{constant}\) behavior for high energies and the three-dimensional \(\rho(E) \propto \sqrt{E}\) behavior for low energies.

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1 Introduction

Many quantities of physical interest depend on the number \(d\) of spatial dimensions. This includes potentials and two-point correlation functions, which are proportional to the zero energy Green’s function

\[
G_{(d)}(r) = \begin{cases} 
-r/2, & d = 1, \\
-(2\pi)^{-1} \ln(r/a), & d = 2, \\
\Gamma\left(\frac{d-2}{2}\right) \left(4\pi^{d/2} r^{d-2}\right)^{-1}, & d \geq 3,
\end{cases}
\]

as well as densities of states, which e.g. for non-relativistic free particles are

\[
\rho_{(d)}(E) = g \Theta(E) \sqrt{\frac{m}{2\pi}} \frac{\sqrt{E}^{d-2}}{\Gamma(d/2)\hbar^d}.
\]

These are densities of states per \(d\)-dimensional volume and per unit of energy. The factor \(g\) is the number of helicity or spin states of the particles.

The corresponding dependence of the relation between the Fermi energy and the density \(n\) of electrons on \(d\) is

\[
n_{(d)} = \frac{2}{\hbar d \Gamma((d + 2)/2)} \sqrt{\frac{m E_F^{d-1}}{2\pi}}.
\]

The generic case of physical interest is \(d = 3\), of course. Yet we frequently use mathematical techniques in \(d = 2\) for the theoretical modeling of electrons or quasi-particles.
on surfaces or interfaces. But how two-dimensional is e.g. an ensemble of electrons in an interface? Is the two-dimensional logarithmic two-point correlation function appropriate for the description of a gas of particles in an interface? Or should we rather expect the three-dimensional \( r^{-1} \) correlation? The correct answer will certainly lie somewhere in between, and how much in between will depend both on the specific system and its parameters.

To address these kinds of questions analytically, dimensionally hybrid Hamiltonians of the form

\[
H = \frac{\hbar^2}{2m} \int d^2x \int dz \left( \nabla \psi^+ \cdot \nabla \psi + \partial_z \psi^+ \cdot \partial_z \psi \right) + \int d^2x \int dz \psi^+ V \psi
\]

\[
+ \frac{\hbar^2}{2\mu} \int d^2x \nabla \psi^+ \cdot \nabla \psi \bigg|_{z=0}
\]

were introduced in \[1\]. Here the convention is to use vector notation \( x = (x, y) \), \( \nabla = (\partial_x, \partial_y) \) for directions parallel to the interface, while \( z \) is orthogonal to the interface.

The potential term will generically also include three-dimensional and two-dimensional terms,

\[
V(x, z) = V_b(x, z) + V_i(x) \delta(z),
\]

but the competition between two-dimensional and three-dimensional behavior of physical quantities turns out to be mostly a consequence of competition between the two-dimensional and three-dimensional kinetic terms.

The two-dimensional mass parameter \( \mu \) is a mass per length. In simple models it is given by

\[
\mu = \frac{m}{L_\perp},
\]

where \( L_\perp \) is a bulk penetration depth of states bound to the interface at \( z = 0 \), see Section \[2\].

The zero energy Green’s function for the Hamiltonian

\[
H_0 = \frac{\hbar^2}{2m} \int d^2x \int dz \left( \nabla \psi^+ \cdot \nabla \psi + \partial_z \psi^+ \cdot \partial_z \psi \right) + \frac{\hbar^2}{2\mu} \int d^2x \nabla \psi^+ \cdot \nabla \psi \bigg|_{z=0}
\]

for perturbations in the interface \( (z' = 0) \), \( G(x - x', z) = \langle x, z | G | x', 0 \rangle \) satisfies

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

and was found in \[1\] \( (r = |x - x'|) \),

\[
G(x - x', z) = \frac{1}{4\pi} \int_0^\infty dk \frac{\exp(-k|z|)}{1 + k\ell} J_0(kr), \quad \ell = \frac{m}{2\mu}.
\]
The Green’s function in the interface is given in terms of a Struve function and a Bessel function,
\[ G(x - x', 0) = \frac{1}{8\ell} \left[ H_0 \left( \frac{r}{\ell} \right) - Y_0 \left( \frac{r}{\ell} \right) \right] \] (7)
and interpolates between two-dimensional and three-dimensional distance laws,
\[ r \ll \ell : \quad G(x - x', 0) = \frac{1}{4\pi \ell} \left[ -\gamma - \ln \left( \frac{r}{2\ell} \right) + \frac{r}{\ell} + O \left( \frac{r^2}{\ell^2} \right) \right], \] (8)
\[ r \gg \ell : \quad G(x - x', 0) = \frac{1}{4\pi r} \left[ 1 - \frac{\ell^2}{r^2} + O \left( \frac{\ell^4}{r^4} \right) \right]. \] (9)

For the model (5) the Green’s function \( G(x, 0) \) appears in the first place as a two-point correlation function in the interface, but it can also be realized as an electromagnetic potential for an electromagnetic Hamiltonian
\[ H[F] = \frac{1}{2} \int d^2x \int dz \left( E^2 + E_{\perp}^2 + B^2 + B_{\perp}^2 \right) + \ell \int d^2x \left( E^2 + B_{\perp}^2 \right) \bigg|_{z=0}, \] (10)
if the fields which are continuous across the interface yield a special interface contribution due to a finite limit
\[ 2\ell = \lim_{L \to 0} \epsilon_r L. \]

Here \( \epsilon_r \) is the relative permittivity of the interface and \( L \) is its thickness.

The correspondence between electronic two-point correlation functions and electrostatic potentials is often used to map the quantum partition function of a free
fermion gas into the partition function of a classical Coulomb gas or plasma. The two-dimensionial Coulomb gas also plays an important role in the variational treatment of the fractional quantum Hall effect [2, 3, 4]. The appearance of $G(x, 0)$ as the Green’s function for both of the dimensionally hybrid Hamiltonians (5) and (10) indicates that the free fermion gas – Coulomb gas duality persists in the transition regime between two and three dimensions. However, the objective of the present paper is the extension of $G$ to non-zero energy and for perturbations off the interface, and the discussion of implications on the density of states.

I will further elaborate on the motivation and justification for dimensionally hybrid Hamiltonians of the form (4) in Section 2. The calculation of the energy dependent Green’s functions and the resulting density of states on the interface will be discussed in Sections 3 and 4. Section 5 contains the conclusions.

2 Dimensionally hybrid Hamiltonians

The interesting part about the Hamiltonian (4) is the competition between two-dimensional and three-dimensional kinetic terms. Hamiltonians with low-dimensional $\delta$ contributions to the potential $V$ are standard in quantum mechanics, and we easily understand the model assumptions behind the use of low-dimensional potentials. On the other hand, Hamiltonians with competing low-dimensional and three-dimensional kinetic terms are certainly not as common as superpositions of low-dimensional and three-dimensional potentials. I will denote Hamiltonians with superpositions of low-dimensional and three-dimensional kinetic terms as dimensionally hybrid Hamiltonians. The introduction of these Hamiltonians in [1] was based on physical intuition and mathematical curiosity. The primary physical justification for the mixed kinetic terms is electrons or quasi-particles which can propagate with an effective mass $m^*$ in a thin layer of thickness $L$ and with mass $m$ outside of the layer. In that case we would expect that particle propagation in the bulk-layer-bulk system should be described by a Hamiltonian of the form (4) with $\mu \simeq m^*/L$. The purpose of this section is to point out that models of the kind (4) can also be motivated in a different way from simple standard Hamiltonians with a standard three-dimensional kinetic term.

As the simplest possible model consider an interface with an attractive potential

$$V(x, z) = -W\delta(z),$$

$$H = \int d^2 x \int dz \left( \frac{\hbar^2}{2m} \left( \nabla \psi^+ \cdot \nabla \psi + \partial_z \psi^+ \cdot \partial_z \psi \right) + \psi^+ V \psi \right).$$

The eigenvalues and eigenfunctions factorize with one set of states bound to the interface,

$$\psi_{k, \kappa, +}(x, z) = \langle x, z|k, \kappa, +\rangle = \frac{\exp(ik \cdot x) \sqrt{mW}}{2\pi \hbar} \exp\left(-\frac{m}{\hbar^2}W|z|\right), \quad (11)$$
$$E = \frac{\hbar^2}{2m} (k^2 - \kappa^2) = \frac{\hbar^2}{2m} k^2 - \frac{m}{2\hbar^2} W^2, \quad \kappa = \frac{mW}{\hbar^2},$$

and two orthogonal sets of transversally free states with transversal wavenumber $k_{\perp} \geq 0$ and energy $E = \hbar^2 (k^2 + k_{\perp}^2) / 2m$,

$$\psi_{k,k_{\perp},+}(x, z) = \langle x, z | k, k_{\perp}, + \rangle = \frac{\exp(ik \cdot x) \hbar k_{\perp} \cos(k_{\perp} z) - mW \sin(k_{\perp} |z|)}{2\pi \sqrt{\hbar^4 k_{\perp}^2 + m^2 W^2}}, \quad (12)$$

$$\psi_{k,k_{\perp},-}(x, z) = \langle x, z | k, k_{\perp}, - \rangle = \frac{\exp(ik \cdot x) \hbar k_{\perp} \sin(k_{\perp} z)}{2\pi \sqrt{\hbar^4 k_{\perp}^2 + m^2 W^2}}. \quad (13)$$

The completeness relation for the factor $\chi(z)$ in $\psi(x, z) = \phi(x)\chi(z)$ is [5]

$$|\kappa, +\rangle \langle \kappa, +| + \int_0^\infty dk_{\perp} (|k_{\perp}, +\rangle \langle k_{\perp}, +| + |k_{\perp}, -\rangle \langle k_{\perp}, -|) = 1.$$

This implies a decomposition of the kinetic operator

$$\frac{\hbar^2}{2m} \int d^2x \int_{-\infty}^\infty dz \left( \chi^+(z) \nabla \phi^+(x) \cdot \nabla \phi(x) \chi(z) + \partial_z \chi^+(z) \phi^+(x) \cdot \phi(x) \partial_z \chi(z) \right)$$

$$= \frac{\hbar^2}{2m} \int d^2x \int_{-\infty}^\infty dz \left( \nabla \psi^+(x, z) \cdot \nabla \psi(x, z) + \partial_z \psi^+(x, z) \cdot \partial_z \psi(x, z) \right)_{\text{free}}$$

$$+ \frac{\hbar^2}{2m} \int d^2x \nabla \phi^+(x) \cdot \nabla \phi(x) + \frac{mW^2}{2\hbar^2} \int d^2x \phi^+(x) \cdot \phi(x),$$

where the first kinetic term on the right hand side only acts on components which are unbound in $z$ direction, while the last two terms arise from the bound states. If we now express both the operators acting on free states and the operators acting on bound states of $\psi(x, z)$, we find

$$\frac{\hbar^2}{2m} \int d^2x \int_{-\infty}^\infty dz \left( \nabla \psi^+(x, z) \cdot \nabla \psi(x, z) + \partial_z \psi^+(x, z) \cdot \partial_z \psi(x, z) \right)$$

$$= \frac{\hbar^2}{2m} \int d^2x \int_{-\infty}^\infty dz \left( \nabla \psi^+(x, z) \cdot \nabla \psi(x, z) + \partial_z \psi^+(x, z) \cdot \partial_z \psi(x, z) \right)_{\text{free}}$$

$$+ \frac{\hbar^4}{2m^2 W} \int d^2x \nabla \psi^+(x, 0) \cdot \nabla \psi(x, 0)_{\text{bound}} + \frac{W}{2} \int d^2x \psi^+(x, 0) \cdot \psi(x, 0).$$

This includes a superposition of kinetic terms similar to $H_0$ [5] with

$$\mu = \frac{m^2 W}{\hbar^2} = \frac{m}{L_{\perp}}.$$
where \( L_\perp = \kappa^{-1} \) is the bulk penetration depth of the bound states \(|k, \kappa, +\rangle\). Superposition of two-dimensional and three-dimensional kinetic terms might appear like an exotic concept for the description of particle propagation in the presence of surfaces or interfaces, but on a qualitative level the concept can be justified. And we have already seen in equations (6) and (7) that it allows us to provide simple analytic estimates on the impact of dimensional competition on propagation effects. In the following we will focus on a study of the competition between the different kinetic terms, i.e. we will neglect any potential terms and study the Hamiltonian \( H_0 \).

3 The energy dependent Green’s function

The energy dependent Green’s function \( G(E) \) satisfies

\[
(E - H)G(E) = 1.
\]

The Green’s function \( G(E) \) which has \( E = 0, z' = 0 \) limit is related to \( G(E) \) through

\[
G(E) = -\frac{2m}{\hbar^2}G(E).
\]

Our objective is to find the energy dependent Green’s function \( G(E) \) for the dimensionally hybrid Hamiltonian \( H_0 \) in equation (5). For later comparison, we will first revisit the free Green’s function \( G_0(E) \) of the Hamiltonian \( H_0 \) without the interface term, \( 1/\mu \to 0 \), and then calculate \( G(E) \).

3.1 The free Green’s function

The free retarded Green’s function is translation invariant,

\[
\langle x, z|G_0(E)|x', z'\rangle = G_0(E; x - x', z - z')
\]

and is well known to be

\[
G_0(E; x, z) = \frac{\Theta(-E)}{4\pi \sqrt{r^2 + z^2}} \exp \left( \frac{-1}{\hbar} \sqrt{-2mE(r^2 + z^2)} \right) + \frac{\Theta(E)}{4\pi \sqrt{r^2 + z^2}} \exp \left( \frac{i}{\hbar} \sqrt{2mE(r^2 + z^2)} \right),
\]

where we continue to use cylinder coordinates. For positive energy this corresponds to the standard choice of poles in \( G_0(E; k, k_\perp) \) to generate outgoing spherical waves without any incoming spherical component, in symbolic notation

\[
G(E) = \frac{1}{E - H + i\epsilon} = \sum_{n, \nu} \frac{|n, \nu\rangle\langle n, \nu|}{E - E_n + i\epsilon}
\]

\[
= \mathcal{P} \sum_{n, \nu} \frac{|n, \nu\rangle\langle n, \nu|}{E - E_n} - i\pi \sum_{n, \nu} \delta(E - E_n)|n, \nu\rangle\langle n, \nu|,
\]
where \( \nu \) is a degeneracy index.

Green’s functions for surfaces or interfaces are commonly parametrized in an axially symmetric mixed representation like \( G(E; \mathbf{k}, z, z') \), see e.g. \([6]\). In bra-ket notation this corresponds for the free Green’s function \( G_0(E) \), which is also translation invariant in \( z \) direction, to

\[
(k, z | G_0(E) | k', z') = G_0(E; k, z - z') \delta(k - k').
\]

For later comparison we will also briefly recall the explicit form of the free Green’s function \( G_0(E) \) in the axially symmetric mixed parametrization. The equation

\[
\left( \frac{\partial^2}{\partial z^2} - k^2 + \frac{2mE}{\hbar^2} \right) G_0(E; k, z) = -\delta(z)
\]

yields

\[
G_0(E; k, z) = \frac{1}{2\pi} \int dk_\perp \frac{\exp(ik_\perp z)}{k_\perp^2 + k^2 - (2mE/\hbar^2) - i\epsilon}
\]

\[
= \frac{\hbar \Theta(\hbar^2k^2 - 2mE)}{2\sqrt{\hbar^2k^2 - 2mE}} \exp\left(-\sqrt{\hbar^2k^2 - 2mE} \frac{|z|}{\hbar}\right)
\]

\[
+ \frac{i\hbar \Theta(2mE - \hbar^2k^2)}{2\sqrt{2mE - \hbar^2k^2}} \exp\left(i\sqrt{2mE - \hbar^2k^2} \frac{|z|}{\hbar}\right).
\]

Note that this axially symmetric representation of the free Green’s function depends on the number \( d - 1 \) of dimensions perpendicular to \( z \) only through the number of components of the wavevector \( \mathbf{k} \).

### 3.2 The interface Green’s function \( G(E) \)

Our objective is to generalize the Green’s function \( G(x - x', z) = \langle x, z | G(0) | x', 0 \rangle \) both to general values of \( E \) and \( z' \), \( \langle x, z | G(E) | x', z' \rangle \). We will also keep the general value \( z_0 \) for the location of the interface and investigate the dependence of \( G(E) \) on this parameter.

The Hamiltonian

\[
H_0 = \int d^2x \int dz \left( \frac{\hbar^2}{2m} \left( \nabla \psi^+ \cdot \nabla \psi + \partial_z \psi^+ \cdot \partial_z \psi \right) + \frac{\hbar^2}{2\mu} \delta(z - z_0) \nabla \psi^+ \cdot \nabla \psi \right)
\]

yields the Schrödinger equation

\[
E \psi(x, z) = -\frac{\hbar^2}{2m} (\Delta + \partial_z^2) \psi(x, z) - \frac{\hbar^2}{2\mu} \delta(z - z_0) \Delta \psi(x, z),
\]

or

\[
\left( E - \frac{p_x^2 + p_z^2}{2m} - |z_0\rangle \langle z_0 | \frac{p_z^2}{2\mu} \right) \psi = 0, \quad \left( E - \frac{p_x^2 + p_z^2}{2m} - |z_0\rangle \langle z_0 | \frac{p_z^2}{2\mu} \right) G(E) = 1.
\]
The last equation in \((x, z)\) representation is
\[
\left( \frac{2m}{\hbar^2} E + \Delta + \partial_z^2 + \delta(z - z_0) \frac{m}{\mu} \Delta \right) \langle x, z | G(E) | x', z' \rangle = -\delta(x - x') \delta(z - z'). \tag{17}
\]
Substitution of the Fourier transform
\[
\langle x, z | G(E) | x', z' \rangle = \frac{1}{4\pi^2} \int d^2k \int d^2k' \langle k, z | G(E) | k', z' \rangle \exp[i(k \cdot x - k' \cdot x')]
\]
yields
\[
\left( \frac{2m}{\hbar^2} E - k^2 + \partial_z^2 \right) \langle k, z | G(E) | k', z' \rangle - \frac{m}{\mu} k^2 \delta(z - z_0) \langle k, z | G(E) | k', z' \rangle = -\delta(k - k') \delta(z - z'). \tag{18}
\]
This yields with
\[
\langle k, z | G(E) | k', z' \rangle = \langle z | G(E, k) | z' \rangle \delta(k - k')
\]
the condition
\[
\left( \frac{2m}{\hbar^2} E - k^2 - k_\perp^2 \right) \langle k_\perp | G(E, k) | z' \rangle - \frac{m}{2\pi\mu} k^2 \delta(z - z_0) \langle z | G(E, k) | z' \rangle = -\delta(z - z'). \tag{19}
\]
Fourier transformation with respect to \(z\) yields
\[
\left( \frac{2m}{\hbar^2} E - k^2 - k_\perp^2 \right) \langle k_\perp | G(E, k) | z' \rangle
- \frac{m}{2\pi\mu} k^2 \int d\kappa_\perp \exp[i(\kappa_\perp - k_\perp)z_0] \langle \kappa_\perp | G(E, k) | z' \rangle = -\frac{1}{\sqrt{2\pi}} \exp(-ik_\perp z').
\]
This result implies that \(\langle k_\perp | G(E, k) | z' \rangle\) has the form
\[
\exp(ik_\perp z_0) \langle k_\perp | G(E, k) | z' \rangle = \frac{\exp[ik_\perp(z_0 - z')] / \sqrt{2\pi} + f(E, k, z')}{k^2_\perp + k^2 - (2mE/\hbar^2)}
\]
with the yet to be determined function \(f(E, k, z')\) satisfying
\[
f(E, k, z') + \frac{m}{2\pi\mu} k^2 \int d\kappa_\perp \frac{\exp[ik_\perp(z_0 - z')] / \sqrt{2\pi} + f(E, k, z')}{\kappa_\perp^2 + k^2 - (2mE/\hbar^2)} = 0.
\]
For the treatment of the integrals we should be consistent with the calculation of the free retarded Green’s function \(\langle 16 \rangle\),
\[
\int \frac{d\kappa_\perp}{2\pi} \frac{\exp(ik_\perp z)}{k^2_\perp + k^2 - (2mE/\hbar^2)} = \frac{\hbar}{2} \Theta(h^2k^2 - 2mE) \exp\left(-\frac{\sqrt{h^2k^2 - 2mE}}{\hbar} |z| / \hbar \right)
+ \frac{\hbar}{2} \Theta(2mE - h^2k^2) \exp\left(\frac{i\sqrt{2mE - h^2k^2}}{\sqrt{2mE - h^2k^2}} |z| / \hbar \right).
\]
This yields
\[
\left[ 1 + \frac{m\hbar}{2\mu} k^2 \left( \frac{\Theta(h^2k^2 - 2mE)}{\sqrt{h^2k^2 - 2mE}} + i\Theta(2mE - h^2k^2) \right) \right] f(E, k, z') \\
= -\frac{m\hbar}{2\mu\sqrt{2\pi}} k^2 \left[ \frac{\Theta(h^2k^2 - 2mE)}{\sqrt{h^2k^2 - 2mE}} \exp\left( -\sqrt{h^2k^2 - 2mE}\frac{|z' - z_0|}{\hbar} \right) \right] \\
+ \frac{i\Theta(2mE - h^2k^2)}{\sqrt{2mE - h^2k^2}} \exp\left( i\sqrt{2mE - h^2k^2}\frac{|z' - z_0|}{\hbar} \right) \right],
\]
and therefore
\[
\langle k_\perp | G(E, k) | z' \rangle = \frac{1}{\sqrt{2\pi k_\perp^2 + k^2 - (2mE/\hbar^2)}} \left[ \exp(-ik_\perp z') \\
- \frac{\hbar k^2\ell\Theta(h^2k^2 - 2mE)}{\sqrt{h^2k^2 - 2mE} + \hbar k^2\ell} \exp\left( -ik_\perp z_0 - \sqrt{h^2k^2 - 2mE}\frac{|z' - z_0|}{\hbar} \right) \right] \\
- \frac{i\hbar k^2\ell\Theta(2mE - h^2k^2)}{\sqrt{2mE - h^2k^2} + i\hbar k^2\ell} \exp\left( -ik_\perp z_0 + i\sqrt{2mE - h^2k^2}\frac{|z' - z_0|}{\hbar} \right) \right].
\]
Here we use the definition\(^3\)
\[
\ell \equiv \frac{m}{2\mu}.
\]
Fourier transformation with respect to \(k_\perp\) yields finally
\[
\langle z | G(E, k) | z' \rangle = \frac{\hbar\Theta(h^2k^2 - 2mE)}{2\sqrt{h^2k^2 - 2mE}} \left[ \exp\left( -\sqrt{h^2k^2 - 2mE}\frac{|z - z'|}{\hbar} \right) \right] \\
- \frac{\hbar k^2\ell}{\sqrt{h^2k^2 - 2mE} + \hbar k^2\ell} \exp\left( -\sqrt{h^2k^2 - 2mE}\frac{|z - z_0| + |z' - z_0|}{\hbar} \right) \right] \\
+ \frac{\hbar\Theta(2mE - h^2k^2)}{2\sqrt{2mE - h^2k^2}} \left[ \exp\left( i\sqrt{2mE - h^2k^2}\frac{|z - z'|}{\hbar} \right) \right] \\
- \frac{i\hbar k^2\ell}{\sqrt{2mE - h^2k^2} + i\hbar k^2\ell} \exp\left( i\sqrt{2mE - h^2k^2}\frac{|z - z_0| + |z' - z_0|}{\hbar} \right) \right].
\]
This result is translation invariant in the transverse \(z\) direction for scattering off perturbations on the interface, \(z' = z_0\),
\[
\langle z | G(E, k) | z' \rangle \bigg|_{z'=z_0} = G(E, k, z - z_0).
\]
\(^3\) In the simple model from Section\(^2\) \(\ell = L_\perp/2 = (2\kappa)^{-1}\) would be the bulk penetration depth of the probability densities \(|\langle x, z | k, \kappa, \pm \rangle|^2\) of the bound states. But note that we have neglected any potential contribution in \(H_0\), such that the results derived here are not directly applicable to the model from Section\(^2\).
4 Density of states and Fermi energy on the interface in the dimensionally hybrid model

The equation (15) yields a standard expression for the density of states in terms of the imaginary part of Green’s functions, see e.g. [7],

\[
\varrho(E_n, x, z) = \sum_\nu \langle x, z|n, \nu\rangle\langle n, \nu|x, z\rangle = -\frac{g}{\pi} \Im \langle x, z|\mathcal{G}(E_n)|x, z\rangle
\]

(22)

Here we explicitly included a factor \(g\) for the number of spin or helicity states, because the summation over degeneracy indices in (15) usually only involves orbital indices. For translation invariant Green’s functions

\[
\langle x, z|\mathcal{G}(E)|x', z'\rangle = \mathcal{G}(E; x-x', z-z')
\]

we have

\[
\varrho(E) = -\frac{g}{\pi} \Im \mathcal{G}(E; x=0, z=0) = -\frac{g}{\pi(2\pi)^{d-1}} \Im \int d^{d-1}k \mathcal{G}(E; k, z=0).
\]

(23)

Insertion of the free retarded propagator (16) reproduces the standard density of states (2), of course,

\[
\varrho(d)(E) = \frac{2mg}{\pi \hbar^2} \frac{\hbar \Theta(E)}{2^{d-1} \sqrt{\pi^{d-1} \Gamma((d-1)/2)}} \int_0^{\sqrt{2mE/\hbar}} dk \frac{k^{d-2}}{\sqrt{2mE - \hbar^2 k^2}}
\]

\[
= g \Theta(E) \sqrt{\frac{m}{2\pi}} \frac{\sqrt{E}}{\Gamma(d/2)\hbar^d}.
\]

The interface at \(z_0\) breaks translational invariance in \(z\) direction, and we have with

\[
\langle k, z|\mathcal{G}(E)|k', z\rangle = \langle z|\mathcal{G}(E, k)|z\rangle \delta(k - k')
\]

\[
\varrho(E, z) = \frac{2mg}{\pi \hbar^2} \Im \langle x, z|\mathcal{G}(E)|x, z\rangle = \frac{2mg}{\pi \hbar^2} \Im \int \frac{d^3k}{4\pi^2} \langle z|\mathcal{G}(E, k)|z\rangle.
\]

We will use the result (21) to calculate the density of states \(\varrho(E, z_0)\) for the Hamiltonian (5) on the interface. Substitution yields

\[
\varrho(E, z_0) = \frac{gm}{2\pi^3 \hbar^2} \Im \int d^2k \langle z_0|\mathcal{G}(E, k)|z_0\rangle
\]

\[
= \frac{gm}{2\pi^2 \hbar} \Theta(E) \int_0^{\sqrt{2mE/\hbar}} dk k \frac{\sqrt{2mE - \hbar^2 k^2}}{2mE - \hbar^2 k^2 + \hbar^2 k^4 \ell^2}.
\]
The evaluation of the integral yields

$$\rho(E, z_0) = \frac{gm\Theta(E)}{4\pi^2\hbar^2\ell\sqrt{\hbar^2 - 8mE\ell^2}} \Theta(h^2 - 8mE\ell^2)$$

$$\times \left[ \left( h + \sqrt{\hbar^2 - 8mE\ell^2} \right) \arctan \left( \frac{\ell\sqrt{8mE}}{h + \sqrt{\hbar^2 - 8mE\ell^2}} \right) \ight.$$

$$- \left( h - \sqrt{\hbar^2 - 8mE\ell^2} \right) \arctan \left( \frac{\ell\sqrt{8mE}}{h - \sqrt{\hbar^2 - 8mE\ell^2}} \right) \right]$$

$$+ \frac{gm\Theta(8mE\ell^2 - h^2)}{4\pi^2\hbar^2\ell} \left[ \frac{h}{\sqrt{8mE\ell^2 - h^2}} \ln \left( \frac{\ell\sqrt{8mE} - \sqrt{8mE\ell^2 - h^2}}{h} \right) \right.$$

$$+ \arctan \left( \frac{\sqrt{8mE\ell^2 - h^2} + \ell\sqrt{8mE}}{h} \right) + \arctan \left( \frac{\ell\sqrt{8mE} - \sqrt{8mE\ell^2 - h^2}}{h} \right) \right].$$

This is a more complicated result than the density (24) for \( d = 2 \) or \( d = 3 \). However, it reduces to either the two-dimensional or three-dimensional density of states in the appropriate limits. For large energies, i.e. if the states only probe length scales smaller than the transverse penetration depth \( \ell \), we find the two-dimensional density of states properly rescaled by a dimensional factor to reflect that it is a density of states per three-dimensional volume,

$$8mE\ell^2 \gg \hbar^2 : \quad \rho(E, z_0) \rightarrow \Theta(E) \frac{gm}{8\pi\hbar^2\ell} = \frac{1}{4\ell} \rho_{(d=2)}(E).$$

$$\text{(25)}$$
For small energies, i.e. if the states probe length scales larger than the transverse penetration depth $\ell$, we find the three-dimensional density of states

$$8mE\ell^2 \ll \hbar^2 : \quad \varrho(E, z_0) \to \Theta(E) \frac{g\sqrt{m^3}}{\sqrt{2\pi^2\hbar^3}} \sqrt{E} = \varrho_{(d=3)}(E). \quad (26)$$

This limiting behavior for interpolation between two and three dimensions is consistent with what was observed already for the zero energy Green’s function in the interface (7-9).

Equation (24) also implies interpolating behavior for the relation between electron density and Fermi energy on the interface for the Hamiltonian (5). The full relation is with $g = 2$

$$n(z_0) = \int_0^{E_F} dE \varrho(E, z_0) = \frac{\sqrt{m E_F}}{\sqrt{8\pi^2\hbar^2\ell^2}} - \frac{1}{16\pi\ell^2} \left[ \Theta(\hbar^2 - 8mE_F\ell^2) \left( 4mE_F\ell^2 - \hbar \sqrt{\hbar^2 - 8mE_F\ell^2} \right) \arctan \left( \frac{\sqrt{8mE_F\ell}}{\hbar + \sqrt{\hbar^2 - 8mE_F\ell^2}} \right) 
+ (4mE_F\ell^2 + \hbar \sqrt{\hbar^2 - 8mE_F\ell^2}) \arctan \left( \frac{\sqrt{8mE_F\ell}}{\hbar - \sqrt{\hbar^2 - 8mE_F\ell^2}} \right) 
+ \frac{\Theta(8mE_F\ell^2 - \hbar^2)}{8\pi^2\hbar^2\ell^3} \left( \sqrt{8mE_F\ell^2 - \hbar^2 \ln \left( \frac{\sqrt{8mE_F\ell} - \sqrt{8mE_F\ell^2 - \hbar^2}}{\hbar} \right) } 
+ \frac{4mE_F\ell^2}{\hbar} \arctan \left( \frac{\sqrt{8mE_F\ell} + \sqrt{8mE_F\ell^2 - \hbar^2}}{\hbar} \right) 
+ \frac{4mE_F\ell^2}{\hbar} \arctan \left( \frac{\sqrt{8mE_F\ell} - \sqrt{8mE_F\ell^2 - \hbar^2}}{\hbar} \right) \right] \right].$$

This approximates two-dimensional behavior for $mE_F\ell^2 \gg \hbar^2$,

$$n(z_0) \simeq \frac{m E_F}{4\pi \hbar^2 \ell} = \frac{1}{4\ell} n_{(d=2)},$$

and three-dimensional behavior for $mE_F\ell^2 \ll \hbar^2$,

$$n(z_0) \simeq \frac{\sqrt{2mE_F}^3}{3\pi^2\hbar^3} = n_{(d=3)}.$$

It is intuitively understandable that the presence of a layer increases the Fermi energy for a given density of electrons. The presence of a layer implies boundary or matching conditions which reduce the number of available states at a given energy.
5 Conclusion and Outlook

Inclusion of competing kinetic terms for effective propagation of particles in low-dimensional subsystems and bulk materials implies dimensional interpolation effects for Green’s functions and for quantities derived from the Green’s functions in such systems. Simple model systems with competing kinetic terms can be solved exactly and yield analytic insights into the transition between two-dimensional and three-dimensional properties in materials with low-dimensional subsystems.

The present paper focused on the study of the competition between two-dimensional and three-dimensional kinetic terms, thereby neglecting any bulk and layer potentials. In that case the transition scale between two-dimensional and three-dimensional behavior is given by \( \ell \sim m/\mu \sim (m/m_*)L \). Please note that inclusion of the confining layer potentials will change this scale for most systems. The approximation \( H_0 \) per se as an approximation for specific systems is only useful for the study of propagation effects and impurity scattering of particles which are not strongly bound to a thin layer, but which are affected by its presence to the extent that propagation in the thin layer is described by an effective mass.

The purpose of the present investigation was to further advance a novel tool for the study of low-dimensional systems, not to derive generic quantitative properties of these systems. The Green’s function \( G(E) \) calculated here should nevertheless prove useful for the study of impurity scattering of weakly coupled particles in thin layer systems, with the impurity potentials treated as perturbations.

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