Chapter 20
Dimensional Effects in Low-dimensional Systems

Surfaces, interfaces, thin films, and quantum wires provide abundant examples of quasi two-dimensional or one-dimensional systems in science and technology. Quantum mechanics in low dimensions has become an important tool for modeling properties of these systems. Here we wish to go beyond the simple low-dimensional potential models of Chapter 3 and discuss in particular implications of the dependence of energy-dependent Green's functions on the number d of spatial dimensions. However, if it is true that the behavior of electrons in certain systems and parameter ranges can be described by low-dimensional quantum mechanics, then there must also exist ranges of parameters for quasi low-dimensional systems where the behavior of electrons exhibits *inter-dimensional* behavior in the sense that there must exist continuous interpolations e.g. between two-dimensional and three-dimensional behavior. We will see that inter-dimensional (or "dimensionally hybrid") Green's functions provide a possible avenue to the identification and discussion of inter-dimensional behavior in physical systems.

20.1 Quantum mechanics in d dimensions

Suppose an electron is strictly confined to a two-dimensional quantum well. Unless the material in the quantum well has special dielectric properties, that electron would still "know" that it exists in three spatial dimensions, because it feels the $1/r$ Coulomb interaction with other charged particles, and this $1/r$ distance law is characteristic for three dimensions. If the electron would not just be confined to two dimensions, but exist in a genuine two-dimensional world, it would experience a logarithmic distance law for the Coulomb potential. The reason for the $1/r$ Coulomb law in three dimensions is that the solution of the equation

$$\Delta G(r) = -\delta(\boldsymbol{x}) \tag{20.1}$$

R. Dick, *Advanced Quantum Mechanics*, Graduate Texts in Physics,
DOI 10.1007/978-3-319-25675-7_20

in three dimensions is given by

$$G(r) = \frac{1}{4\pi r},$$

but in general the solution of equation (20.1) depends on the number d of spatial dimensions. Appendix J explains in detail the derivation of the d-dimensional version of $G(r)$ with the result

$$G_d(r) = \begin{cases} (a-r)/2, & d = 1, \\ -(2\pi)^{-1} \ln(r/a), & d = 2, \\ \Gamma\left(\frac{d-2}{2}\right) \left(4\sqrt{\pi}^d r^{d-2}\right)^{-1}, & d \geq 3. \end{cases} \tag{20.2}$$

The most direct application of these results are electrostatic potentials. Equation (20.1) implies that the electrostatic potential of a point charge q in d dimensions is given by

$$\Phi_d(r) = \frac{q}{\epsilon_0} G_d(r). \tag{20.3}$$

However, from the point of view of non-relativistic quantum mechanics, the Green's functions (20.2) are the special zero energy values of the energy-dependent free Schrödinger Green's functions, $G_d(r) = G_d(\boldsymbol{x}, E = 0)$. These energy dependent Green's functions satisfy

$$\Delta G_d(\boldsymbol{x}, E) + \frac{2m}{\hbar^2} E G_d(\boldsymbol{x}, E) = -\delta(\boldsymbol{x}). \tag{20.4}$$

We have solved this condition in three dimensions in Section 11.1, see equation (11.17). The solution in d dimensions by two different methods is described in Appendix J, with the result (J.27)

$$\begin{aligned} G_d(\boldsymbol{x}, E) = {} & \frac{\Theta(-E)}{\sqrt{2\pi}^d} \left(\frac{\sqrt{-2mE}}{\hbar r}\right)^{\frac{d-2}{2}} K_{\frac{d-2}{2}}\left(\sqrt{-2mE}\frac{r}{\hbar}\right) \\ & + \mathrm{i}\frac{\pi}{2} \frac{\Theta(E)}{\sqrt{2\pi}^d} \left(\frac{\sqrt{2mE}}{\hbar r}\right)^{\frac{d-2}{2}} H^{(1)}_{\frac{d-2}{2}}\left(\sqrt{2mE}\frac{r}{\hbar}\right). \end{aligned} \tag{20.5}$$

The functions K_ν and $H^{(1)}_\nu$ are modified Bessel functions and Hankel functions of the first kind, respectively. These are exponential functions for $d = 1$ or $d = 3$,

$$K_{-\frac{1}{2}}(x) = K_{\frac{1}{2}}(x) = \sqrt{\frac{\pi}{2x}} \exp(-x), \quad H^{(1)}_{-\frac{1}{2}}(x) = \mathrm{i} H^{(1)}_{\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}} \exp(\mathrm{i}x),$$

and therefore

$$G_1(x,E) = \frac{\hbar\Theta(-E)}{2\sqrt{-2mE}}\exp\left(-\sqrt{-2mE}\frac{|x|}{\hbar}\right) + \mathrm{i}\frac{\hbar\Theta(E)}{2\sqrt{2mE}}\exp\left(\mathrm{i}\sqrt{2mE}\frac{|x|}{\hbar}\right), \tag{20.6}$$

and we recover the already known three-dimensional result from Section 11.1,

$$G_3(\boldsymbol{x},E) = \frac{\Theta(-E)}{4\pi r}\exp\left(-\sqrt{-2mE}\frac{r}{\hbar}\right) + \frac{\Theta(E)}{4\pi r}\exp\left(\mathrm{i}\sqrt{2mE}\frac{r}{\hbar}\right). \tag{20.7}$$

These results also give us the screened or Yukawa potentials in d dimensions if we substitute $\hbar/\sqrt{-2mE} \to \lambda$, see Figure 20.2.

The Figures 20.1 and 20.2 illustrate that long distance effects of interactions become more prominent in lower dimensions, while short distance effects become stronger with increasing number of dimensions.

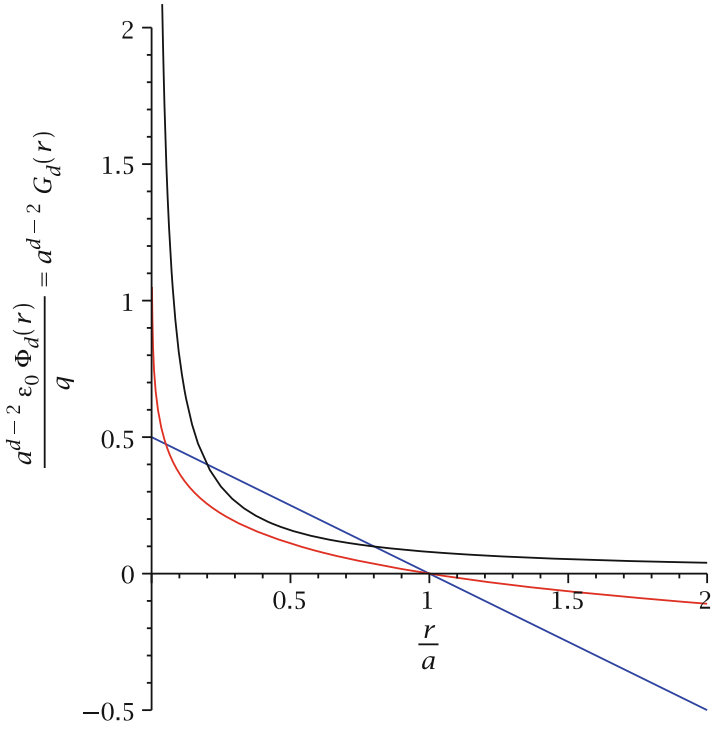

Fig. 20.1 The Green's functions (20.2) and the related specific electrostatic potentials $\Phi_d(r)/q$ in 1, 2 and 3 dimensions. The blue curve is for $d = 1$, red is for $d = 2$ and the black curve is the 3-dimensional Coulomb potential

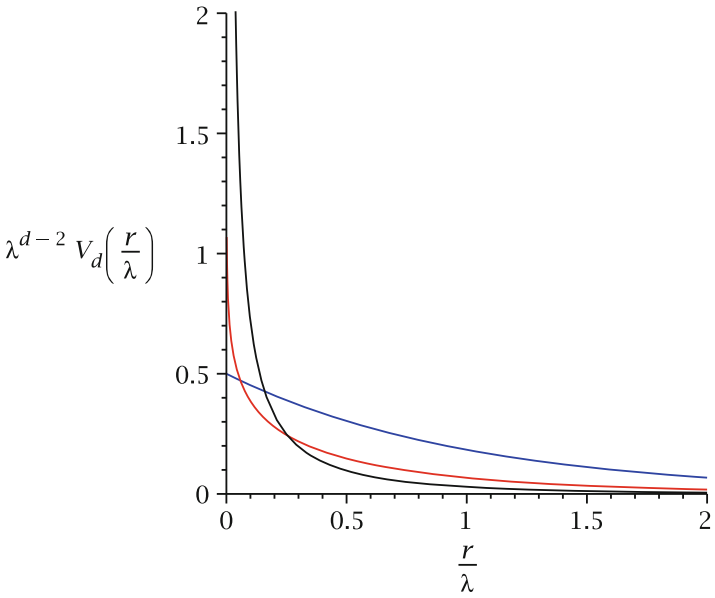

Fig. 20.2 Yukawa potentials $V_d(r)$ with screening length λ. The blue curve corresponds to $d = 1$, red to $d = 2$ and black to $d = 3$

The Green's function does not only determine interaction potentials, but also has other profound implications for the behavior of particles in d dimensions. We have already seen in Chapter 11 that potential scattering of particles of energy $E = \hbar^2 k^2/2m$ is described by energy-dependent Green's functions. The d-dimensional version of equation (11.20) is

$$\begin{aligned}\psi(\boldsymbol{x}) &= \frac{\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})}{(2\pi)^{d/2}} - \frac{2m}{\hbar^2}\int d^d\boldsymbol{x}'\, G_d(\boldsymbol{x}-\boldsymbol{x}', \hbar^2k^2/2m)V(\boldsymbol{x}')\psi(\boldsymbol{x}') \\ &= \frac{\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})}{(2\pi)^{d/2}} - \frac{\mathrm{i}\pi m}{(2\pi)^{d/2}\hbar^2}\int d^d\boldsymbol{x}'\left(\frac{k}{|\boldsymbol{x}-\boldsymbol{x}'|}\right)^{\frac{d-2}{2}} \\ &\quad \times H^{(1)}_{\frac{d-2}{2}}\left(k|\boldsymbol{x}-\boldsymbol{x}'|\right) V(\boldsymbol{x}')\psi(\boldsymbol{x}'), \end{aligned} \tag{20.8}$$

and we get the d-dimensional version of the leading order Born approximation through the substitution of $\psi(\boldsymbol{x}')$ with the incoming plane wave.

Suppose the scattering potential $V(\boldsymbol{x}')$ is concentrated around $\boldsymbol{x}' = 0$ with finite range R. The asymptotic form of the Hankel function for large argument $x \gg 1$,

$$H^{(1)}_{\frac{d-2}{2}}(x) \to \sqrt{\frac{2}{\pi x}}\exp\left(\mathrm{i}x - \mathrm{i}\pi\frac{d-1}{4}\right),$$

yields the asymptotic form for the scattered wave function in the limit $|\boldsymbol{x}| \gg R$ (here we neglect again the normalization factors $(2\pi)^{-d/2}$ because they cancel in the cross section),

$$\begin{aligned}\psi(\boldsymbol{x}) &= \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}) - \frac{m}{(2\pi)^{(d-1)/2}\hbar^2}\frac{k^{(d-3)/2}}{r^{(d-1)/2}}\exp\left(\mathrm{i}kr - \mathrm{i}\pi\frac{d-3}{4}\right)\\ &\quad\times\int d^d\boldsymbol{x}'\,\exp[\mathrm{i}(\boldsymbol{k}-k\hat{\boldsymbol{x}})\cdot\boldsymbol{x}']V(\boldsymbol{x}')\\ &= \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}) + f(k\hat{\boldsymbol{x}}-\boldsymbol{k})\frac{1}{r^{(d-1)/2}}\exp(\mathrm{i}kr)\\ &= \psi^{(\mathrm{in})}(\boldsymbol{x}) + \psi^{(\mathrm{out})}(\boldsymbol{x}),\end{aligned} \tag{20.9}$$

with the scattering amplitude

$$\begin{aligned}f(\Delta\boldsymbol{k}) &= -\frac{mk^{(d-3)/2}}{(2\pi)^{(d-1)/2}\hbar^2}\exp\left(-\mathrm{i}\pi\frac{d-3}{4}\right)\int d^d\boldsymbol{x}\,\exp(-\mathrm{i}\Delta\boldsymbol{k}\cdot\boldsymbol{x})V(\boldsymbol{x})\\ &= -\sqrt{2\pi}\frac{mk^{(d-3)/2}}{\hbar^2}\exp\left(-\mathrm{i}\pi\frac{d-3}{4}\right)V(\Delta\boldsymbol{k}).\end{aligned} \tag{20.10}$$

The d-dimensional version of (11.2),

$$\frac{d\sigma}{d\Omega} = \frac{1}{j_{in}(\hat{\boldsymbol{k}})}\frac{dn(\Omega)}{d\Omega dt} = \lim_{r\to\infty} r^{d-1}\frac{j_{out}(\hat{\boldsymbol{k}}')}{j_{in}(\hat{\boldsymbol{k}})}, \tag{20.11}$$

then yields the same relation between the scattering cross section and the scattering amplitude as in three dimensions,

$$\frac{d\sigma_k}{d\Omega} = |f(k\hat{\boldsymbol{x}}-\boldsymbol{k})|^2\,.$$

Note that the relative prominence of long distance effects in low dimensions should be amplified in scattering effects, because the Green's function generically determines *both* the scattering potentials $V(\boldsymbol{x}')$ *and* the kernels $G_d(\boldsymbol{x}-\boldsymbol{x}', E)$ which are convoluted into the potentials to calculate the scattered wave functions.

Yet another instance where the number of dimensions plays a prominent role is the density of states. We have seen this already in equations (12.12, 12.13). However, this result is also closely linked to the energy-dependent Green's functions.

First we note that we can write the generalization of equation (20.4) for the Hamilton operator $H = H_0 + V$,

$$\Delta G_{d,V}(\boldsymbol{x},\boldsymbol{x}';E) + \frac{2m}{\hbar^2}[E - V(\boldsymbol{x})]G_{d,V}(\boldsymbol{x},\boldsymbol{x}';E) = -\delta(\boldsymbol{x}-\boldsymbol{x}'). \tag{20.12}$$

also in representation free operator notation,

$$(E-H)\mathcal{G}_{d,V}(E) = 1, \tag{20.13}$$

where the connection to (20.12) is recovered through the matrix elements[1]

$$\langle \boldsymbol{x}|\mathcal{G}_{d,V}(E)|\boldsymbol{x}'\rangle = -\frac{2m}{\hbar^2} G_{d,V}(\boldsymbol{x},\boldsymbol{x}';E)$$

The solution of (20.13) requires a small complex shift in E to avoid the singularities on the real axis which arise from the real spectrum of H,

$$\mathcal{G}_{d,V}(E) = \frac{1}{E - H + \mathrm{i}\epsilon}.$$

The positive imaginary shift yields the retarded Green's function with only outgoing spherical waves from scattering centers in scattering theory, and only forward evolution in time, see Section 11.1.

The Hamilton operator in the denominator of $\mathcal{G}(E)$ can be replaced by energy eigenvalues if we use energy eigenstates

$$H|E', \nu(E')\rangle = E'|E', \nu(E')\rangle, \quad \sum\!\!\!\!\!\!\int dE'\, d\nu(E')\, |E', \nu(E')\rangle\langle E', \nu(E')| = 1,$$

where $\nu(E')$ is a set of degeneracy indices for energy level E'. This yields

$$\mathcal{G}_{d,V}(E) = \sum\!\!\!\!\!\!\int dE'\, d\nu(E')\, \frac{|E', \nu(E')\rangle\langle E', \nu(E')|}{E - E' + \mathrm{i}\epsilon}. \tag{20.14}$$

The connection to the density of states follows if we rewrite this with the Sokhotsky-Plemelj relation (2.11),

$$\begin{aligned}\mathcal{G}_{d,V}(E) = \mathcal{P} \sum\!\!\!\!\!\!\int dE'\, d\nu(E')\, \frac{|E', \nu(E')\rangle\langle E', \nu(E')|}{E - E'} \\ - \mathrm{i}\pi \sum\!\!\!\!\!\!\int dE'\, d\nu(E')\, \delta(E - E')|E', \nu(E')\rangle\langle E', \nu(E')|.\end{aligned} \tag{20.15}$$

Comparison with equation (12.17) shows that

$$\varrho_d(E, \boldsymbol{x}) = -\frac{1}{\pi}\Im\langle \boldsymbol{x}|\mathcal{G}_{d,V}(E)|\boldsymbol{x}\rangle = \frac{2m}{\pi\hbar^2}\Im\langle \boldsymbol{x}|G_{d,V}(E)|\boldsymbol{x}\rangle. \tag{20.16}$$

In particular, substitution of the free Green's functions (20.5) yields again the result (12.13) which we had initially derived from equation (12.12)

$$\varrho_d(E) = g\Theta(E)\sqrt{\frac{m}{2\pi}}^d \frac{\sqrt{E}^{d-2}}{\Gamma(d/2)\hbar^d}. \tag{20.17}$$

[1]These concepts are further discussed in Appendix J. However, it is not necessary to read Appendix J before reading this section.

For the derivation of (20.17) from (20.16) and (20.5), we recall that

$$\langle \boldsymbol{x}|G_{d,V}(E)|\boldsymbol{x}'\rangle\big|_{V=0} \equiv G_{d,V}(\boldsymbol{x},\boldsymbol{x}';E)\big|_{V=0} = G_d(\boldsymbol{x}-\boldsymbol{x}',E)$$

is translation invariant for free particles, and use the property

$$\Re H^{(1)}_{\frac{d-2}{2}}\left(\sqrt{2mE}\frac{r}{\hbar}\right)\Big|_{r\to 0} = J_{\frac{d-2}{2}}\left(\sqrt{2mE}\frac{r}{\hbar}\right)\Big|_{r\to 0} \sim \frac{1}{\Gamma(d/2)}\left(\sqrt{\frac{mE}{2}}\frac{r}{\hbar}\right)^{\frac{d-2}{2}}$$

of the Hankel functions. The spin or helicity factor g arises from the summation over spin states included in the summation over degeneracy indices ν in equation (20.15) if we take into account that the Green's functions (20.5) in the presence of spin multiply $g \times g$ unit matrices in spin space[2].

20.2 Inter-dimensional effects in interfaces and thin layers

The dependence of energy-dependent Green's functions on the number of dimensions begs the question whether this can have observable consequences in (quasi)two-dimensional or one-dimensional systems like interfaces, layers, thin films, or nanowires. Indeed, the density of states $\varrho_d(E)$ (20.16) is often used to estimate densities of electron states in low-dimensional systems in nanotechnology. However, is this really justified? After all, we are still dealing with electrons with non-vanishing extensions of their wave functions in every direction, including directions perpendicular to any confining potential barriers. Wave functions can be squeezed, but they will will never be genuine two-dimensional or one-dimensional. Furthermore, if the behavior of low-energy particles in confining structures can be approximated by the laws of one-dimensional or two-dimensional quantum mechanics, there must exist a transition regime at higher energy levels, where inter-dimensional effects between low-dimensional and three-dimensional behavior should be observable.

To examine these questions, we consider a model system of electrons moving in a bulk material which also contains a layer of thickness $2a$ located at $z = z_0$. The potential energy of the electrons inside the layer is shifted by an amount V_0,

$$V(\boldsymbol{x}) \equiv V(z) = V_0\Theta(z_0 + a - z)\Theta(z - z_0 + a), \tag{20.18}$$

and we also assume that electrons in the bulk move with (effective) mass m, while the effective mass inside the layer is m_*. This yields a Hamiltonian which in the first

[2]For spin or helicity, there is actually a transition from a tensor product to a trace operation in making the connection between (20.15) and (20.16): $1 = \sum_s |s\rangle\langle s| \to \sum_s \langle s|s\rangle = g$. Otherwise equation (20.16) would yield the density of states per spin state.

quantized formalism has the form

$$H = \frac{\mathbf{p}^2}{2m}\left[1 - \Theta(z_0 + a - z)\Theta(z - z_0 + a)\right] + \Theta(z_0 + a - z)\Theta(z - z_0 + a)\left(\frac{\mathbf{p}^2}{2m_*} + V_0\right). \tag{20.19}$$

We might expect two-dimensional behavior in the limit $a \to 0$ both from the difference of effective mass in the interface and from the interface potential. Indeed, the different effective mass m_* in the interface implies different propagation properties inside the interface and yields quasi two-dimensional behavior both in terms of propagators and in the density of states[3], even for vanishing interface potential. The corresponding second quantized Hamiltonian is

$$H = \int d^2\boldsymbol{x}_\parallel \int dz\, \frac{\hbar^2}{2m} \nabla\psi^+(\boldsymbol{x}_\parallel, z) \cdot \nabla\psi(\boldsymbol{x}_\parallel, z) + \int d^2\boldsymbol{x}_\parallel \frac{\hbar^2}{2\mu} \nabla_\parallel \psi^+(\boldsymbol{x}, z_0) \cdot \nabla_\parallel \psi(\boldsymbol{x}_\parallel, z_0), \tag{20.20}$$

where the index $\parallel$ is used for two-dimensional vectors parallel to the interface at z_0. The parameter μ has dimensions of mass per length.

In the following we will investigate the emergence of quasi two-dimensional behavior from an attractive interface potential.

Two-dimensional behavior from a thin quantum well

We wish to examine the appearance of quasi two-dimensional behavior from a quantum well potential, i.e. we assume $m_* = m$. An infinitely thin attractive quantum well arises from the potential (20.18) if we set $V_0 = -\mathcal{W}/2a$ and take the limit $a \to 0$,

$$H = \frac{\mathbf{p}^2}{2m} - \mathcal{W}\delta(z - z_0).$$

The corresponding Schrödinger equation separates, and the z component is the Schrödinger equation with the attractive δ potential that we had solved in Section 3.3. This implies three kinds of energy eigenstates. First we have eigenstates which are moving along the interface,

$$\langle \boldsymbol{x}|\boldsymbol{k}_\parallel, \kappa\rangle = \frac{\sqrt{\kappa}}{2\pi} \exp\left(\mathrm{i}\boldsymbol{k}_\parallel \cdot \boldsymbol{x}_\parallel - \kappa|z - z_0|\right), \quad \kappa = \frac{m}{\hbar^2}\mathcal{W}, \tag{20.21}$$

$$E(\boldsymbol{k}_\parallel, \kappa) = \frac{\hbar^2}{2m}\boldsymbol{k}_\parallel^2 - \frac{m}{2\hbar^2}\mathcal{W}^2.$$

[3] R. Dick, Physica E 40, 2973 (2008); Nanoscale Res. Lett. 5, 1546 (2010).

We also have free states with odd or even parity under $z \to 2z_0 - z$, cf. (3.21, 3.22),

$$\langle \boldsymbol{x}|\boldsymbol{k}_\parallel, k_\perp, -\rangle = \frac{1}{2\sqrt{\pi}^3} \exp\bigl(\mathrm{i}\boldsymbol{k}_\parallel \cdot \boldsymbol{x}_\parallel\bigr) \sin[k_\perp(z - z_0)], \tag{20.22}$$

$$\langle \boldsymbol{x}|\boldsymbol{k}_\parallel, k_\perp, +\rangle = \exp\bigl(\mathrm{i}\boldsymbol{k}_\parallel \cdot \boldsymbol{x}_\parallel\bigr) \frac{k_\perp \cos[k_\perp(z - z_0)] - \kappa \sin[k_\perp|z - z_0|]}{2\sqrt{\pi^3(\kappa^2 + k_\perp^2)}}. \tag{20.23}$$

The wave number $k_\perp$ in (20.22) and (20.23) is constrained to the positive half-line $k_\perp > 0$, and the energy levels of the free states are

$$E(\boldsymbol{k}_\parallel, k_\perp) = \frac{\hbar^2}{2m}\left(\boldsymbol{k}_\parallel^2 + k_\perp^2\right).$$

The energy-dependent Green's function

$$\langle \boldsymbol{x}_\parallel, z|G(E)|\boldsymbol{x}'_\parallel, z'\rangle \equiv \langle z|G(\boldsymbol{x}_\parallel - \boldsymbol{x}'_\parallel, E)|z'\rangle \equiv -\frac{\hbar^2}{2m}\langle z|\mathcal{G}(\boldsymbol{x}_\parallel - \boldsymbol{x}'_\parallel, E)|z'\rangle$$

of this system must satisfy

$$\left(\Delta + \frac{2m}{\hbar^2}\left[E + \mathcal{W}\delta(z - z_0)\right]\right)\langle z|G(\boldsymbol{x}_\parallel, E)|z'\rangle = -\,\delta(\boldsymbol{x}_\parallel)\delta(z - z'). \tag{20.24}$$

We would not have to solve this equation explicitly, since we know the complete set of energy eigenstates of the system. However, there is a neat way to solve these kinds of problems which also works for interfaces in which particles move with different effective mass[4].

We can solve equation (20.24) in a mixed representation using

$$\begin{aligned}\langle \boldsymbol{k}_\parallel, k_\perp|G(E)|\boldsymbol{k}'_\parallel, z'\rangle &= \frac{1}{\sqrt{2\pi}^5}\int d^2\boldsymbol{x}_\parallel \int d^2\boldsymbol{x}'_\parallel \int dz\, \langle \boldsymbol{x}_\parallel, z|G(E)|\boldsymbol{x}'_\parallel, z'\rangle \\ &\quad \times \exp\Bigl[\mathrm{i}\Bigl(\boldsymbol{k}'_\parallel \cdot \boldsymbol{x}'_\parallel - \boldsymbol{k}_\parallel \cdot \boldsymbol{x}_\parallel - k_\perp z\Bigr)\Bigr] \qquad (20.25)\\ &= \langle k_\perp|G(\boldsymbol{k}_\parallel, E)|z'\rangle \delta\Bigl(\boldsymbol{k}_\parallel - \boldsymbol{k}'_\parallel\Bigr), \qquad (20.26)\end{aligned}$$

$$\begin{aligned}\langle k_\perp|G(\boldsymbol{k}_\parallel, E)|z'\rangle &= \frac{1}{\sqrt{2\pi}}\int d^2\boldsymbol{x}_\parallel \int dz\, \langle z|G(\boldsymbol{x}_\parallel, E)|z'\rangle \\ &\quad \times \exp\bigl[-\mathrm{i}\bigl(\boldsymbol{k}_\parallel \cdot \boldsymbol{x}_\parallel + k_\perp z\bigr)\bigr]. \qquad (20.27)\end{aligned}$$

[4] R. Dick, Int. J. Theor. Phys. 42, 569 (2003). See also the previous references.

Substitution into equation (20.24) yields with $\kappa = m\mathcal{W}/\hbar^2$

$$\frac{\exp[\mathrm{i}k_\perp(z_0 - z')]}{\sqrt{2\pi}} = \left(\boldsymbol{k}_\parallel^2 + k_\perp^2 - \frac{2mE}{\hbar^2}\right)\exp(\mathrm{i}k_\perp z_0)\,\langle k_\perp|G(\boldsymbol{k}_\parallel, E)|z'\rangle - \frac{\kappa}{\pi}\int dq_\perp\,\exp(\mathrm{i}q_\perp z_0)\,\langle q_\perp|G(\boldsymbol{k}_\parallel, E)|z'\rangle. \tag{20.28}$$

This result implies that the retarded Green's function $\langle k_\perp|G(\boldsymbol{k}_\parallel, E)|z'\rangle$ must have the form

$$\exp(\mathrm{i}k_\perp z_0)\,\langle k_\perp|G(\boldsymbol{k}_\parallel, E)|z'\rangle = \left(\frac{\exp[\mathrm{i}k_\perp(z_0 - z')]}{\sqrt{2\pi}} + f(\boldsymbol{k}_\parallel, E, z')\right) \times \frac{1}{k_\perp^2 + \boldsymbol{k}_\parallel^2 - (2mE/\hbar^2) - \mathrm{i}\epsilon}, \tag{20.29}$$

with the yet to be determined function $f(\boldsymbol{k}_\parallel, E, z')$ satisfying

$$f(\boldsymbol{k}_\parallel, E, z') - \frac{\kappa}{\pi}\int dk_\perp \frac{\left(\exp[\mathrm{i}k_\perp(z_0 - z')]/\sqrt{2\pi}\right) + f(\boldsymbol{k}_\parallel, E, z')}{k_\perp^2 + \boldsymbol{k}_\parallel^2 - (2mE/\hbar^2) - \mathrm{i}\epsilon} = 0,$$

which follows from substituting (20.29) back into (20.28).

The integral is readily evaluated with the residue theorem,

$$\int \frac{dk_\perp}{\pi}\frac{\exp(\mathrm{i}k_\perp z)}{k_\perp^2 + \boldsymbol{k}_\parallel^2 - (2mE/\hbar^2) - \mathrm{i}\epsilon} = \frac{\Theta(\hbar^2\boldsymbol{k}_\parallel^2 - 2mE)}{\sqrt{\boldsymbol{k}_\parallel^2 - (2mE/\hbar^2)}} \times \exp\left(-\sqrt{\boldsymbol{k}_\parallel^2 - \frac{2mE}{\hbar^2}}|z|\right) + \mathrm{i}\frac{\Theta(2mE - \hbar^2\boldsymbol{k}_\parallel^2)}{\sqrt{(2mE/\hbar^2) - \boldsymbol{k}_\parallel^2}}\exp\left(\mathrm{i}\sqrt{\frac{2mE}{\hbar^2} - \boldsymbol{k}_\parallel^2}|z|\right).$$

This yields the condition for $f(\boldsymbol{k}_\parallel, E, z')$ in the form

$$\left[1 - \hbar\kappa\left(\frac{\Theta(\hbar^2\boldsymbol{k}_\parallel^2 - 2mE)}{\sqrt{\hbar^2\boldsymbol{k}_\parallel^2 - 2mE}} + \mathrm{i}\frac{\Theta(2mE - \hbar^2\boldsymbol{k}_\parallel^2)}{\sqrt{2mE - \hbar^2\boldsymbol{k}_\parallel^2}}\right)\right] f(\boldsymbol{k}_\parallel, E, z') = \frac{\hbar\kappa}{\sqrt{2\pi}}\left[\frac{\Theta(\hbar^2\boldsymbol{k}_\parallel^2 - 2mE)}{\sqrt{\hbar^2\boldsymbol{k}_\parallel^2 - 2mE}}\exp\left(-\sqrt{\hbar^2\boldsymbol{k}_\parallel^2 - 2mE}\frac{|z' - z_0|}{\hbar}\right) + \mathrm{i}\,\frac{\Theta(2mE - \hbar^2\boldsymbol{k}_\parallel^2)}{\sqrt{2mE - \hbar^2\boldsymbol{k}_\parallel^2}}\exp\left(\mathrm{i}\sqrt{2mE - \hbar^2\boldsymbol{k}_\parallel^2}\frac{|z' - z_0|}{\hbar}\right)\right],$$

and therefore we find with the proper treatment of poles for retarded Green's functions the result

$$\begin{aligned}\langle k_\perp|G(\boldsymbol{k}_\parallel,E)|z'\rangle &= \frac{1}{\sqrt{2\pi}}\frac{1}{k_\perp^2+\boldsymbol{k}_\parallel^2-(2mE/\hbar^2)-\mathrm{i}\epsilon}\Bigg[\exp(-\mathrm{i}k_\perp z')\\ &+\frac{\hbar\kappa\Theta(\hbar^2\boldsymbol{k}_\parallel^2-2mE)}{\sqrt{\hbar^2\boldsymbol{k}_\parallel^2-2mE}-\hbar\kappa-\mathrm{i}\epsilon}\exp\left(-\mathrm{i}k_\perp z_0-\sqrt{\hbar^2\boldsymbol{k}_\parallel^2-2mE}\frac{|z'-z_0|}{\hbar}\right)\\ &+\frac{\mathrm{i}\hbar\kappa\Theta(2mE-\hbar^2\boldsymbol{k}_\parallel^2)}{\sqrt{2mE-\hbar^2\boldsymbol{k}_\parallel^2}-\mathrm{i}\hbar\kappa}\exp\left(-\mathrm{i}k_\perp z_0+\mathrm{i}\sqrt{2mE-\hbar^2\boldsymbol{k}_\parallel^2}\frac{|z'-z_0|}{\hbar}\right)\Bigg].\end{aligned} \tag{20.30}$$

Fourier transformation of equation (20.30) with respect to $k_\perp$ yields finally

$$\begin{aligned}\langle z|G(\boldsymbol{k}_\parallel,E)|z'\rangle &= \frac{\hbar\Theta(\hbar^2\boldsymbol{k}_\parallel^2-2mE)}{2\sqrt{\hbar^2\boldsymbol{k}_\parallel^2-2mE}}\Bigg[\exp\left(-\sqrt{\hbar^2\boldsymbol{k}_\parallel^2-2mE}\frac{|z-z'|}{\hbar}\right)\\ &+\frac{\hbar\kappa}{\sqrt{\hbar^2\boldsymbol{k}_\parallel^2-2mE}-\hbar\kappa-\mathrm{i}\epsilon}\exp\left(-\sqrt{\hbar^2\boldsymbol{k}_\parallel^2-2mE}\frac{|z-z_0|+|z'-z_0|}{\hbar}\right)\Bigg]\\ &+\mathrm{i}\frac{\hbar\Theta(2mE-\hbar^2\boldsymbol{k}_\parallel^2)}{2\sqrt{2mE-\hbar^2\boldsymbol{k}_\parallel^2}}\Bigg[\exp\left(\mathrm{i}\sqrt{2mE-\hbar^2\boldsymbol{k}_\parallel^2}\frac{|z-z'|}{\hbar}\right)\\ &+\frac{\mathrm{i}\hbar\kappa}{\sqrt{2mE-\hbar^2\boldsymbol{k}_\parallel^2}-\mathrm{i}\hbar\kappa}\exp\left(\mathrm{i}\sqrt{2mE-\hbar^2\boldsymbol{k}_\parallel^2}\frac{|z-z_0|+|z'-z_0|}{\hbar}\right)\Bigg].\end{aligned} \tag{20.31}$$

The limit $\kappa \to 0$ in equations (20.30, 20.31), as well as in equation (20.34) below reproduces the corresponding representations of the free retarded Green's function in three dimensions.

Our results describe the Green's function for a particle in the presence of the thin quantum well, but for arbitrary energy and both near and far from the quantum well. Therefore we cannot easily identify any two-dimensional limit from the Green's function. To explore this question further, we will look at the density of electron states in the presence of the quantum well.

The quantum well at z_0 breaks translational invariance in z direction, and we have with equation (20.16)

$$\varrho(E,z) = \frac{4m}{\pi\hbar^2}\Im\langle\boldsymbol{x}_\parallel,z|G(E)|\boldsymbol{x}_\parallel,z\rangle = \frac{m}{\pi^3\hbar^2}\Im\int d^2\boldsymbol{k}_\parallel\,\langle z|G(\boldsymbol{k}_\parallel,E)|z\rangle,$$

where a factor $g = 2$ was taken into account for spin 1/2 states.

If there is any quasi two-dimensional behavior in this system, we would expect it in the quantum well region. Therefore we use the result (20.31) to calculate the density of states $\varrho(E, z_0)$ in the quantum well. Substitution yields

$$\begin{aligned}\varrho(E, z_0) &= \frac{m}{\pi^3\hbar^2}\Im\int d^2\boldsymbol{k}_\parallel\,\langle z_0|G(\boldsymbol{k}_\parallel, E)|z_0\rangle \\ &= \frac{m}{\pi\hbar}\int_0^\infty dk\,k\,\delta\Big(\sqrt{\hbar^2k^2 - 2mE} - \hbar\kappa\Big) \\ &\quad + \frac{m}{\pi^2\hbar}\Theta(E)\int_0^{\sqrt{2mE}/\hbar} dk\,\frac{k\sqrt{2mE - \hbar^2k^2}}{2mE - \hbar^2k^2 + \hbar^2\kappa^2},\end{aligned}$$

and after evaluation of the integrals,

$$\begin{aligned}\varrho(E, z_0) &= \Theta(2mE + \hbar^2\kappa^2)\kappa\frac{m}{\pi\hbar^2} \\ &\quad + \Theta(E)\frac{m}{\pi^2\hbar^3}\left[\sqrt{2mE} - \hbar\kappa\arctan\left(\frac{\sqrt{2mE}}{\hbar\kappa}\right)\right].\end{aligned} \tag{20.32}$$

We can also express this in terms of the free two-dimensional and three-dimensional densities of electron states (cf. (20.17)),

$$\begin{aligned}\varrho(E, z_0) &= \kappa\varrho_{d=2}\big(E + (\hbar^2\kappa^2/2m)\big) \\ &\quad + \varrho_{d=3}(E)\left[1 - \frac{\hbar\kappa}{\sqrt{2mE}}\arctan\left(\frac{\sqrt{2mE}}{\hbar\kappa}\right)\right].\end{aligned} \tag{20.33}$$

We note that the states which are exponentially suppressed perpendicular to the quantum well indeed contribute a term proportional to the two-dimensional density of states $\varrho_{d=2}(E')$ with the kinetic energy E' of motion of particles along the quantum well, but with a dimensional proportionality constant κ which is the inverse penetration depth of those states. Such a dimensional factor has to be there, because densities of states in three dimensions enumerate states per energy and per volume, while $\varrho_{d=2}(E')$ counts states per energy and per area. Furthermore, the unbound states yield a contribution which approaches the free three-dimensional density of states $\varrho_{d=3}(E)$ in the limit $\kappa \to 0$. The result can also be derived directly from the energy eigenstates (20.21–20.23) and the definition (12.15) of the local density of states, see Problem 20.7. However, the derivation from the Green's function, while more lengthy for the pure quantum well, has the advantage to also work in the case of an interface in which the electrons move with different effective mass.

The density of states in the quantum well region is displayed for binding energy $B = \hbar^2\kappa^2/2m = 1\,\text{eV}$, mass $m = m_e = 511\,\text{keV}/c^2$, and different energy ranges in Figures 20.3 and 20.4.

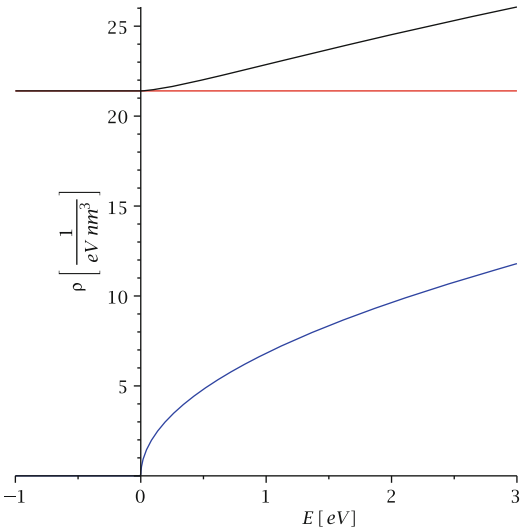

Fig. 20.3 The density of states in the quantum well location $z = z_0$ for binding energy $B = 1\,\text{eV}$, mass $m = m_e = 511\,\text{keV}/c^2$, and energies $-B \leq E \leq 3\,\text{eV}$. The red curve is the contribution from states bound inside the quantum well, the blue curve is the pure three-dimensional density of states in absence of a quantum well, and the black curve is the density of states according to equation (20.32)

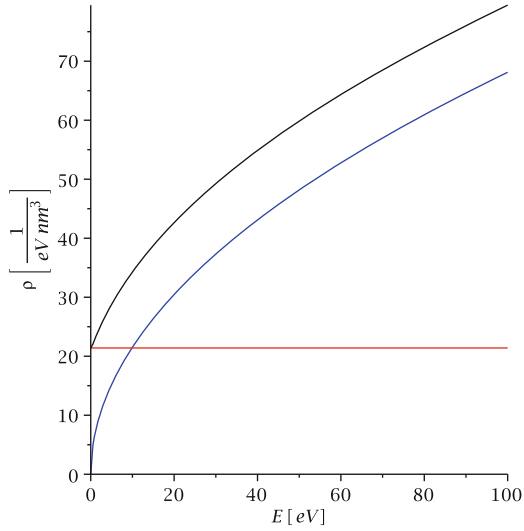

Fig. 20.4 The density of states (20.32) in the quantum well location $z = z_0$ for higher energies $0 \leq E \leq 100\,\text{eV}$. The binding energy, mass and color coding are the same as in Figure 20.3. The full density of states (20.32) approximates the three-dimensional $\sqrt{E}$ behavior for energies $E \gg B$, but there remains a finite offset compared to $\varrho_{d=3}$ due to the presence of the quantum well

20.3 Problems

20.1. Derive the d-dimensional version of equation (11.28) for scattering off spherically symmetric potentials.

20.2. Calculate the differential scattering cross sections for the potentials

20.2a. $V(r) = V_0\Theta(R - r)$,

20.2b. $V(r) = V_0 \exp(-r/R)$,

20.2c. $V(r) = V_0 \exp(-r^2/R^2)$,
in d dimensions in Born approximation. Which results do you find in particular for $d = 2$?

20.3. Derive the optical theorem in d dimensions.

20.4. The solution (3.16) can also be considered as the bound state in a one-dimensional pointlike quantum dot $V(x) = -\mathcal{W}\delta(x)$,

$$\psi_{d=1}(x) = \kappa \exp(-\kappa|x|), \quad \kappa = \frac{m}{\hbar^2}\mathcal{W},$$

with binding energy

$$B = -E = \frac{\hbar^2\kappa^2}{2m} = \frac{m}{2\hbar^2}\mathcal{W}^2.$$

No such states exist for higher-dimensional pointlike quantum dots $V(\boldsymbol{x}) = -\mathcal{W}\delta(\boldsymbol{x})$, unless we also let the depth $\mathcal{W}$ go to zero in a judicious way.

Show that the following wave functions describe bound states in two-dimensional and three-dimensional pointlike quantum dots if we let $\mathcal{W}$ go to zero,

$$\psi_{d=2}(r) = \frac{\kappa}{\sqrt{\pi}} K_0(\kappa r), \quad \psi_{d=3}(r) = \sqrt{\frac{\kappa}{2\pi}} \frac{\exp(-\kappa r)}{r}.$$

The binding energy of the states is

$$B = -E = \frac{\hbar^2\kappa^2}{2m}.$$

Hint: Show that the bound states must be proportional to the energy-dependent retarded Green's functions.

Note that we cannot extend this construction to four or more dimensions because the corresponding Green's functions are not square integrable any more.

20.5. Suppose we consider a proton and an electron in $d \geq 3$ spatial dimensions. The electromagnetic interaction potential of these particles is

$$V_d(r) = -\frac{e^2}{\epsilon_0} G_d(r).$$

Suppose that there are normalizable bound energy eigenstates in this system. Which relation between the expectation values $\langle K \rangle$ and $\langle V \rangle$ of kinetic and potential energy would then be implied by the virial theorem (4.41)? Can atoms exist in $d \geq 4$ dimensions?

20.6. Show that substitution of the Fourier transform

$$\begin{aligned}\langle \boldsymbol{k}_\parallel, k_\perp | G(E) | \boldsymbol{k}'_\parallel, k'_\perp \rangle &= \int d^2\boldsymbol{x}_\parallel \int d^2\boldsymbol{x}'_\parallel \int dz \int dz' \, \frac{\langle \boldsymbol{x}_\parallel, z | G(E) | \boldsymbol{x}'_\parallel, z' \rangle}{(2\pi)^3} \\ &\quad \times \exp\Big[\mathrm{i}\Big(\boldsymbol{k}'_\parallel \cdot \boldsymbol{x}'_\parallel + k'_\perp z' - \boldsymbol{k}_\parallel \cdot \boldsymbol{x}_\parallel - k_\perp z\Big)\Big] \\ &= \langle k_\perp | G(\boldsymbol{k}_\parallel, E) | k'_\perp \rangle \delta\Big(\boldsymbol{k}_\parallel - \boldsymbol{k}'_\parallel\Big) ,\end{aligned}$$

with

$$\begin{aligned}\langle k_\perp | G(\boldsymbol{k}_\parallel, E) | k'_\perp \rangle = \frac{1}{2\pi} \int d^2\boldsymbol{x}_\parallel \int dz \, \langle z | G(\boldsymbol{x}_\parallel, E) | z' \rangle \\ \times \exp\big[-\mathrm{i}\big(\boldsymbol{k}_\parallel \cdot \boldsymbol{x}_\parallel + k_\perp z - k'_\perp z'\big)\big]\end{aligned}$$

in equation (20.24) yields with the same technique that we used to solve (20.28) the result

$$\begin{aligned}\langle k_\perp | G(E, \boldsymbol{k}_\parallel) | k'_\perp \rangle = \frac{1}{k_\perp^2 + \boldsymbol{k}_\parallel^2 - (2mE/\hbar^2) - \mathrm{i}\epsilon} \Bigg[\delta(k_\perp - k'_\perp) \\ + \frac{\kappa}{\pi} \frac{\exp[\mathrm{i}(k'_\perp - k_\perp) z_0]}{k'^2_\perp + \boldsymbol{k}_\parallel^2 - (2mE/\hbar^2) - \mathrm{i}\epsilon} \Bigg(\frac{\sqrt{\hbar^2 \boldsymbol{k}_\parallel^2 - 2mE}\, \Theta(\hbar^2 \boldsymbol{k}_\parallel^2 - 2mE)}{\sqrt{\hbar^2 \boldsymbol{k}_\parallel^2 - 2mE} - \hbar\kappa - \mathrm{i}\epsilon} \\ + \frac{\sqrt{2mE - \hbar^2 \boldsymbol{k}_\parallel^2}\, \Theta(2mE - \hbar^2 \boldsymbol{k}_\parallel^2)}{\sqrt{2mE - \hbar^2 \boldsymbol{k}_\parallel^2} - \mathrm{i}\hbar\kappa} \Bigg) \Bigg] . \qquad (20.34)\end{aligned}$$

Show also that Fourier transformation yields again the result (20.30).

20.7. Derive the result (20.32) directly from the energy eigenstates (20.21), (20.22) and (20.23) for particles in the presence of the quantum well.

Solution.
The decomposition of unity in terms of the eigenstates is

$$\int d^2\boldsymbol{k}_\parallel \, |\boldsymbol{k}_\parallel, \kappa\rangle\langle \boldsymbol{k}_\parallel, \kappa| + \sum_{\pm} \int d^2\boldsymbol{k}_\parallel \int_0^\infty dk_\perp \, |\boldsymbol{k}_\parallel, k_\perp, \pm\rangle\langle \boldsymbol{k}_\parallel, k_\perp, \pm| = 1.$$

For the application of the definition (12.15) we have to take into account that

$$d^2\boldsymbol{k}_\parallel = k_\parallel dk_\parallel d\varphi \to \frac{m}{\hbar^2} dE d\varphi$$

holds both for the two dimensional integration measure $d^2\boldsymbol{k}_\parallel$ from $E = \hbar^2(\boldsymbol{k}_\parallel^2 - \kappa^2)/2m$, and also in the three-dimensional integration measure $d^2\boldsymbol{k}_\parallel \wedge dk_\perp$, where $E = \hbar^2(\boldsymbol{k}_\parallel^2 + k_\perp^2)/2m$. This yields with a factor of 4π from $g = 2$ for electrons and from integration over φ the result

$$\varrho(E, z_0) = \frac{4\pi m}{\hbar^2}\left(\Theta(2mE+\hbar^2\kappa^2)\frac{\kappa}{4\pi^2} + \Theta(E)\int_0^{\sqrt{2mE}/\hbar}\frac{k_\perp^2\, dk_\perp}{4\pi^3(\kappa^2+k_\perp^2)}\right).$$

Evaluation of the integral yields again the result (20.32).

20.8. Generalize the derivation of the relation (20.16) to the relativistic case.

Solution.
The relativistic scalar Green's function is

$$G = \frac{\hbar^2}{p^2 + m^2c^2 - \mathrm{i}\epsilon}, \quad \langle k|G|k'\rangle = \frac{\delta(k-k')}{k^2 + (mc/\hbar)^2 - \mathrm{i}\epsilon},$$

see also (J.66–J.70). We can write this with $H = c\sqrt{\boldsymbol{p}^2 + (mc)^2}$ in the form

$$G = -\frac{\hbar^2c^2}{E^2 - H^2 + \mathrm{i}\epsilon} = -\frac{\hbar^2c^2}{2E}\left(\frac{1}{E - H + \mathrm{i}\epsilon} + \frac{1}{E + H - \mathrm{i}\epsilon}\right).$$

Here $E = cp^0$ is still an operator, but we can make the transition to the energy-dependent Green's operator $G(E)$ with classical variable $E = \hbar ck^0$ through $|k\rangle = |\boldsymbol{k}\rangle \otimes |k^0\rangle$ and

$$\langle k^0|G|k'^0\rangle = G(E)\delta(k^0 - k'^0). \tag{20.35}$$

Use of the Sokhotsky-Plemelj relation (2.11) yields

$$\begin{aligned}\Im G(E) &= \frac{\pi\hbar^2c^2}{2E}\left[\delta(E-H) - \delta(E+H)\right] \\ &= \frac{\pi\hbar^2c^2}{2E}\sum_{n,\nu}\left[\delta(E-E_n) - \delta(E+E_n)\right]|n,\nu\rangle\langle n,\nu|,\end{aligned} \tag{20.36}$$

and therefore[5]

$$\Im\langle\boldsymbol{x}|G(E)|\boldsymbol{x}\rangle = \frac{\pi\hbar^2c^2}{2E}\left[\varrho(E) - \overline{\varrho}(\overline{E})\right]. \tag{20.37}$$

[5] A.C. Zulkoskey, R. Dick, K. Tanaka, Phys. Rev. A 89, 052103 (2014).

Here $\varrho(E)$ and $\overline{\varrho}(\overline{E})$ denote the densities of states of particles of energy E, and of anti-particles (or holes) of energy $\overline{E} = -E$, respectively.

We can test our result in the free (anti-)particle case where the density of states per helicity state is

$$\hat{\varrho}(E) = \varrho(E) + \overline{\varrho}(\overline{E}) = \frac{2\Theta(E^2 - m^2c^4)}{(2\sqrt{\pi}\hbar c)^d \Gamma(d/2)} |E| \sqrt{E^2 - m^2c^4}^{d-2}, \tag{20.38}$$

see equation (12.23).

The $\boldsymbol{x}$-representation $\langle \boldsymbol{x}|G(E)|\boldsymbol{x}'\rangle = G(\boldsymbol{x} - \boldsymbol{x}', \omega)$ of the energy-dependent free Green's function has been calculated in Appendix J, equation (J.42). The modified Bessel function $K_\nu(z)$ with real argument is real, and the imaginary part of the Hankel function $\mathrm{i}H_\nu^{(1)}(z)$ for real z satisfies [1]

$$\lim_{z \to 0} \Re H_\nu^{(1)}(z) = \frac{(z/2)^\nu}{\Gamma(\nu + 1)}.$$

Substitution into (J.42) for $r = |\boldsymbol{x} - \boldsymbol{x}'| \to 0$ yields

$$\Im \langle \boldsymbol{x}|G(E)|\boldsymbol{x}\rangle = \frac{\pi\hbar^2 c^2}{\Gamma(d/2)} \frac{\Theta(E^2 - m^2c^4)}{(2\sqrt{\pi}\hbar c)^d} \sqrt{E^2 - m^2c^4}^{d-2},$$

in agreement with equations (20.37) and (20.38).