Interdimensional effects in systems with quasirelativistic dispersion relations

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We examine Green's functions and densities of states for bosons which move in materials with interfaces. Motivated by the interest in materials with quasirelativistic dispersion relations, we demonstrate that modification of Klein-Gordon-type contributions to the Hamiltonian in an interface yields Green's functions and densities of states which exhibit two-dimensional behavior at high energies. Three-dimensional behavior in a low-energy range is recovered if the shift of the mass parameter in the interface is small.

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I. INTRODUCTION

Low-dimensional models of quantum mechanics or electrodynamics are commonly employed to describe the behavior of electrons, photons, or quasiparticles like phonons and magnons in layers or wires with confining properties. Low-dimensional densities of states are also frequently used to estimate, e.g., the availability of carriers for charge or heat transport in these structures. This begs the question for analytic models which describe the transition from low-dimensional to three-dimensional behavior for (quasi-)particles in the presence of low-dimensional substructures.

Substructures can induce low-dimensional propagation or transport properties through the generation of potential wells, and it is easy to derive, e.g., the density of states in the energy scale for particles in a thin quantum well with binding energy $B = \hbar^2\kappa^2/2m$ and penetration depth κ^{-1} of the bound states into the substrate,

$$H = \frac{\boldsymbol{p}^2}{2m} - \frac{\hbar^2\kappa}{m}\delta(z - z_0). \tag{1}$$

The density of states in this system is a superposition of the two-dimensional and three-dimensional density of states [1],

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

Here

$$\varrho_d(E) = \Theta(E)\sqrt{\frac{m}{2\pi}}^{d}\frac{\sqrt{E}^{d-2}}{\Gamma(d/2)\hbar^d} \tag{3}$$

is the density of states (per spin or helicity state) for nonrelativistic particles of mass m in d space dimensions, and the correction factor $1 - (\hbar\kappa/\sqrt{2mE})\arctan(\sqrt{2mE}/\hbar\kappa)$ smoothly turns on the three-dimensional contribution to the density of states. The analytic result (2) confirms the intuitive assumption that bound states which can move along a quantum well contribute to a two-dimensional density of states, which is made dimensionally correct in three dimensions through scaling with the inverse penetration depth κ. Note that $E + (\hbar^2\kappa^2/2m) = \hbar^2\boldsymbol{k}_\parallel^2/2m$ is the kinetic energy of the particles moving along the well with momentum $\hbar\boldsymbol{k}_\parallel$.

On the other hand, low-dimensional structures in materials can also modify the propagation properties of particles through differences in effective mass for motion in a layer and in the surrounding substrate, and it is not as intuitively clear as for quantum wells how this should affect the density of states. This problem has been analyzed in [2] under the assumption of parabolic band approximations for motion in a layer and in the surrounding substrate or bulk material. The assumption of parabolic band approximations leads to interdimensional Schrödinger-type Hamiltonians of the form

$$\begin{aligned}H &= \int d^3\boldsymbol{x}\,\frac{\hbar^2}{2m}\nabla\psi^\dagger(\boldsymbol{x})\cdot\nabla\psi(\boldsymbol{x})\\ &\quad+ \int d^2\boldsymbol{x}_\parallel\,\frac{\hbar^2}{2\mu}\nabla_\parallel\psi^\dagger(\boldsymbol{x}_\parallel,z_0)\cdot\nabla_\parallel\psi(\boldsymbol{x}_\parallel,z_0).\end{aligned} \tag{4}$$

Here $\boldsymbol{x} = (\boldsymbol{x}_\parallel,z)$ splits vectors into components parallel and perpendicular to an interface at $z = z_0$. The parameter μ has the dimension of mass per length, and the coefficient $\hbar^2/2\mu$ parametrizes the change in effective mass due to motion in the interface or layer at $z = z_0$. Equation (4) would describe the Hamiltonian of the particles in second quantization. The corresponding first quantized Hamiltonian is

$$H = \frac{\boldsymbol{p}^2}{2m} + |z_0\rangle\langle z_0|\frac{\boldsymbol{p}_\parallel^2}{2\mu}. \tag{5}$$

These operators yield analytic results for Green's functions and densities of states which interpolate between two-dimensional behavior at small distances or high energies and three-dimensional behavior for large distances or small energies even without attractive potential wells [2].

Motivated by the recent interest in systems with quasirelativistic dispersion relations, we would like to generalize the study of Hamiltonians with linear combinations of two-dimensional and three-dimensional kinetic terms to the case of interdimensional Klein-Gordon or Dirac-type terms. Materials with quasirelativistic properties which are under intense scrutiny include graphene [3,4], topological insulators from time-reversal invariance [5] or crystal symmetry [6], and topological Dirac semimetals [7,8]. However, photons and low-energy acoustic phonons also provide systems with relativistic or approximately quasirelativistic dispersion

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relations in materials. In the present study we will focus on the combination of two-dimensional and three-dimensional Klein-Gordon terms. Our findings generalize the results from the earlier studies of interdimensional Schrödinger-type Hamiltonians (4) and reproduce those results in the "nonrelativistic" limit.

The layout of the paper is as follows. We derive the relativistic generalization of the well-known relation

$$\varrho(E,\boldsymbol{x}) = -\frac{1}{\pi}\mathrm{Im}\langle \boldsymbol{x}|\mathcal{G}(E)|\boldsymbol{x}\rangle = \frac{2m}{\pi\hbar^2}\mathrm{Im}\langle \boldsymbol{x}|G(E)|\boldsymbol{x}\rangle \quad (6)$$

between the local density of states $\varrho(E,\boldsymbol{x})$ and the energy-dependent Green's operator

$$\mathcal{G}(E) = \frac{1}{E - H + i\epsilon} = -\frac{2m}{\hbar^2}G(E)$$

in Sec. II. The interdimensional Klein-Gordon system is introduced in Sec. III. We calculate in particular the Green's functions and the density of states in the interface and analyze under which circumstances we find two-dimensional or three-dimensional behavior in the system. Our conclusions are summarized in Sec. IV. The technical details of the calculation of the Green's function in the presence of a layer with Klein-Gordon-type contributions to the Hamiltonian are described in the Appendix.

II. GREEN'S FUNCTIONS AND DENSITIES OF STATES IN RELATIVISTIC SYSTEMS

We wish to generalize the derivation of relation (6) to the relativistic case. The relativistic scalar Green's operator is, with the convention $\eta_{00} = -1$ for the Minkowski metric, given by

$$G = \frac{\hbar^2}{p^2 + m^2c^2 - i\epsilon}. \quad (7)$$

This yields in plane wave states with wave vectors $k = (k^0,\boldsymbol{k})$ the momentum space Green's function

$$\langle k|G|k'\rangle = \frac{\delta(k-k')}{k^2 + (mc/\hbar)^2 - i\epsilon}.$$

We can write the relativistic Green's operator G (7) with the relativistic Hamiltonian $H = c\sqrt{\boldsymbol{p}^2 + (mc)^2}$ in the form

$$G = -\frac{\hbar^2c^2}{E^2 - H^2 + i\epsilon} = -\frac{\hbar^2c^2}{2E}\left(\frac{1}{E - H + i\epsilon} + \frac{1}{E + H - i\epsilon}\right). \quad (8)$$

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

$$\langle k^0|G|k'^0\rangle = G(E)\delta(k^0 - k'^0). \quad (9)$$

Use of the Sokhotsky-Plemelj relation then yields

$$\mathrm{Im}G(E) = \frac{\pi\hbar^2c^2}{2E}[\delta(E-H) - \delta(E+H)] = \frac{\pi\hbar^2c^2}{2E}\sum\!\!\!\!\!\!\int_{n,\nu}[\delta(E-E_n) - \delta(E+E_n)]|n,\nu\rangle\langle n,\nu|, \quad (10)$$

where $\sum\!\!\!\!\!\!\int$ refers to integration or summation over continuous or discrete quantum numbers, respectively.

Equation (10) yields the sought-after relation between relativistic scalar Green's functions and densities of states,

$$\mathrm{Im}\langle \boldsymbol{x}|G(E)|\boldsymbol{x}\rangle = \frac{\pi\hbar^2c^2}{2E}[\varrho(E) - \overline{\varrho}(\overline{E})]. \quad (11)$$

Here $\varrho(E)$ and $\overline{\varrho}(\overline{E})$ denote the densities of states of particles of energy E and of antiparticles (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 in d space dimensions is

$$\hat{\varrho}(E) = \varrho(E) + \overline{\varrho}(\overline{E}) = \frac{2\Theta(E^2 - m^2c^4)}{(2\sqrt{\pi}\hbar c)^d\Gamma(d/2)}|E|\sqrt{E^2 - m^2c^4}^{\,d-2}. \quad (12)$$

The $\boldsymbol{x}$ representation $\langle \boldsymbol{x}|G(E)|\boldsymbol{x}'\rangle = G(\boldsymbol{x}-\boldsymbol{x}',\omega)$ of the energy-dependent relativistic scalar Green's function in d space dimensions can be found, e.g., in Appendix I of Ref. [1],

$$G(\boldsymbol{x},\omega) = \frac{\Theta(mc^2 - \hbar|\omega|)}{\sqrt{2\pi}^d}\left(\frac{\sqrt{m^2c^4 - \hbar^2\omega^2}}{\hbar cr}\right)^{\frac{d-2}{2}} \times K_{\frac{d-2}{2}}\left(\sqrt{m^2c^4 - \hbar^2\omega^2}\frac{r}{\hbar c}\right) + i\frac{\pi}{2}\frac{\Theta(\hbar|\omega| - mc^2)}{\sqrt{2\pi}^d}\left(\frac{\sqrt{\hbar^2\omega^2 - m^2c^4}}{\hbar cr}\right)^{\frac{d-2}{2}} \times H^{(1)}_{\frac{d-2}{2}}\left(\sqrt{\hbar^2\omega^2 - m^2c^4}\frac{r}{\hbar c}\right). \quad (13)$$

The functions $K_\nu(z)$ and $H^{(1)}_\nu(z)$ are modified Bessel functions and Hankel functions of the first kind, respectively, and we follow the definitions and conventions from [9].

The modified Bessel function $K_\nu(z)$ with the real argument is real, and the Hankel function satisfies [9]

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

Substitution into (13) for $r = |\boldsymbol{x} - \boldsymbol{x}'| \to 0$ yields

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

in agreement with Eqs. (11) and (12).

III. INTERDIMENSIONAL EFFECTS WITH QUASIRELATIVISTIC BOSONS

Relativistic wave equations imply a dispersion relation

$$E^2 = c^2p^2 + m^2c^4. \quad (14)$$

In the band structure for electrons, photons or phonons in materials this can be realized through the emergence of Dirac cones $E^2 = c^2p^2$ with group velocity or sound velocity c. Indeed, $E = \pm cp$ is the case of interest for Dirac semimetals. However, we will see that models with Klein-Gordon-type mass terms (14) in interfaces or in the substrate are also solvable, and inclusion of mass terms allows us to connect to the results with parabolic band approximations (i.e., Schrödinger-type models) through the "nonrelativistic limit" $p \ll mc$. Furthermore it is known that the topological insulator $Bi_{1-x}Sb_x$ has massive Dirac fermions in the bulk [10,11], and the existence of massive Dirac hyperboloids in the bulk of the topological crystalline insulator $Pb_{1-x}Sn_xSe$ [12] has also recently been confirmed [13]. Similar results are expected for $Pb_{1-x}Sn_xTe$.

The mass term could also arise through lifting the degeneracy at $p = 0$ such that $E^2 = c^2p^2$ near $p = 0$ becomes

$$E^2 = c^2p^2 + \Delta_g^2, \tag{15}$$

where $2\Delta_g$ parametrizes the energy gap between the resulting Dirac hyperboloids after distortion of the discrete symmetry and c is the group velocity for $cp \gg \Delta_g$. Dirac points in materials are usually protected by discrete symmetries [5–7], and breaking the discrete symmetries while preserving the continuous symmetries of the Dirac cones should yield Dirac hyperboloids. We recover the mass from expansion of E near $p = 0$,

$$E \simeq \pm\left(\Delta_g + \frac{c^2p^2}{2\Delta_g}\right), \tag{16}$$

which confirms that $m = \Delta_g/c^2$ is the effective mass parameter for the Dirac hyperboloids (15). The direct proportionality between effective mass and energy gap for perturbed Dirac cones might not appear intuitive from a physical point of view, but it is a simple consequence of basic geometry: Perturbing a Dirac cone for given asymptotic velocity parameter $c \simeq E/p$ requires higher band curvature and therefore smaller effective mass for smaller energy gap.

We emphasize that this model can only be used in an energy and momentum range around Dirac points in semimetals or on the surface of topological insulators or around approximate Dirac points in narrow-gap semiconductors. For example, in $Pb_{1-x}Sn_xTe$ with $x \lesssim 0.3$ the results in [12,14] indicate that (perturbed) Dirac cones can be used in the momentum range up to $\Delta k = 0.1\,\text{Å}^{-1}$ and in the energy range $\Delta E = \pm 400$ meV above and below the Fermi level. The gap parameter in the bulk is $\Delta_g \lesssim 95$ meV at 4.2 K, and the velocity parameter is $c \simeq 2 \times 10^{-3}c_0 = 600\,\text{km/s}$, where c_0 is the vacuum speed of light. These parameters correspond to a mass parameter $m = 24\,\text{keV}/c_0^2$ in the quasirelativistic dispersion relation (14). We are concerned in the following with the simplest possible quantum-mechanical representation of coexistence of Dirac cones or hyperboloids of different dimensionality which neglects spin. As such, the results directly apply to systems with scalar quasirelativistic excitations (e.g., acoustic phonons in symmetric compounds) or systems where spin-orbit effects are negligible. However, Dirac operators are roots of Klein-Gordon operators, and therefore quasirelativistic spin states also satisfy Klein-Gordon equations. This implies that our observations about transitions from three-dimensional behavior in an interface at low energies to two-dimensional behavior at high energies will also persist for systems with quasirelativistic fermions. We will use the parameters from $Pb_{1-x}Sn_xTe$ for illustrations of the transition from three-dimensional to two-dimensional behavior.

The simplest quantum-mechanical model for particles with dispersion relation (14) is a Klein-Gordon field with Hamiltonian density

$$\mathcal{H} = \hbar\dot{\phi}^\dagger\dot{\phi} + \hbar c^2\nabla\phi^\dagger \cdot \nabla\phi + \frac{m^2c^4}{\hbar}\phi^\dagger\phi. \tag{17}$$

The normalization is chosen for convenience with second quantization. The Lagrange density corresponding to (17) yields canonical commutation relations in $\boldsymbol{x}$ space,

$$\begin{aligned}[\phi(\boldsymbol{x},t),\dot{\phi}^\dagger(\boldsymbol{x}',t)] &= i\delta(\boldsymbol{x}-\boldsymbol{x}'),\\ [\phi^\dagger(\boldsymbol{x},t),\dot{\phi}(\boldsymbol{x}',t)] &= i\delta(\boldsymbol{x}-\boldsymbol{x}'),\end{aligned} \tag{18}$$

and the decomposition in terms of $\boldsymbol{k}$-space annihilation and creation operators is

$$\begin{aligned}\phi(\boldsymbol{x},t) = \frac{1}{\sqrt{2\pi}^3}\int \frac{d^3\boldsymbol{k}}{\sqrt{2\omega_{\boldsymbol{k}}}}\{&a(\boldsymbol{k})\exp[i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_{\boldsymbol{k}}t)]\\ &+ b^\dagger(\boldsymbol{k})\exp[-i(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_{\boldsymbol{k}}t)]\},\end{aligned} \tag{19}$$

$$[a(\boldsymbol{k}),a^\dagger(\boldsymbol{k}')] = \delta(\boldsymbol{k}-\boldsymbol{k}'), \quad [b(\boldsymbol{k}),b^\dagger(\boldsymbol{k}')] = \delta(\boldsymbol{k}-\boldsymbol{k}').$$

The frequency in Eq. (19) is

$$\omega_{\boldsymbol{k}} = c\sqrt{\boldsymbol{k}^2 + (m^2c^2/\hbar^2)}.$$

From Eq. (17) we can infer that an interdimensional Hamiltonian for quasirelativistic bosons has the form

$$\begin{aligned}H = \frac{1}{\hbar}\int d^2\boldsymbol{x}_\parallel \int dz[&\hbar^2\dot{\phi}^\dagger(\boldsymbol{x}_\parallel,z,t)\dot{\phi}(\boldsymbol{x}_\parallel,z,t)\\ &+ \hbar^2c^2\nabla\phi^\dagger(\boldsymbol{x}_\parallel,z,t)\cdot\nabla\phi(\boldsymbol{x}_\parallel,z,t)\\ &+ m^2c^4\phi^\dagger(\boldsymbol{x}_\parallel,z,t)\phi(\boldsymbol{x}_\parallel,z,t)]\\ &+ \frac{\ell}{\hbar}\int d^2\boldsymbol{x}_\parallel[\hbar^2c^2\nabla_\parallel\phi^\dagger(\boldsymbol{x}_\parallel,z_0,t)\cdot\nabla_\parallel\phi(\boldsymbol{x}_\parallel,z_0,t)\\ &+ \Delta m^2c^4\phi^\dagger(\boldsymbol{x}_\parallel,z_0,t)\phi(\boldsymbol{x}_\parallel,z_0,t)],\end{aligned} \tag{20}$$

where $\ell\Delta m^2 \equiv \ell\Delta(m^2)$ parametrizes the product of interface thickness and change of the bulk gap parameter m^2 due to motion in the interface at z_0. In models with quasirelativistic dispersion relations, the length scale ℓ also parametrizes the change in kinetic energy from different wave-function curvatures in the interface. This is different from models like (1) where an infinitely thin attractive quantum well generates bound states with a penetration depth κ^{-1} into the surrounding substrate. In nonrelativistic models the contributions from change in mass and wave-function curvature are always combined in a single term.

The interface contribution in (20) only affects mass and spatial gradient terms, and therefore the x-space commutation relations (18) are unchanged. Substitution of the Hamiltonian (20) into the iterated Heisenberg equation

$$\frac{\partial^2}{\partial t^2}\phi(\boldsymbol{x},t) = -\frac{1}{\hbar^2}[H,[H,\phi(\boldsymbol{x},t)]] \tag{21}$$

therefore yields an equation of motion $[\partial^2 = \nabla^2 - (\partial_t/c)^2]$

$$\partial^2\phi - \frac{m^2c^2}{\hbar^2}\phi + \ell\delta(z-z_0)\left(\nabla_\parallel^2\phi - \frac{\Delta m^2c^2}{\hbar^2}\phi\right) = 0.$$

The corresponding interdimensional Green's function has to satisfy

$$\ell\delta(z-z_0)\left(\nabla_\parallel^2-\frac{\Delta m^2c^2}{\hbar^2}\right)\langle x|G|x'\rangle + \left(\partial^2-\frac{m^2c^2}{\hbar^2}\right)\langle x|G|x'\rangle = -\delta(x-x'). \quad (22)$$

The Green's function $\langle x|G|x'\rangle$ is related to the energy-dependent Green's function $\langle \boldsymbol{x}|G(E)|\boldsymbol{x}'\rangle$ through [see (9)]

$$\langle k^0,\boldsymbol{x}|G|k'^0,\boldsymbol{x}'\rangle = \langle \boldsymbol{x}|G(E)|\boldsymbol{x}'\rangle\delta(k^0-k'^0)|_{E=\hbar ck^0} \quad (23)$$

and

$$\langle x|G|x'\rangle = \frac{1}{2\pi}\int dk^0\int dk'^0\,\langle k^0,\boldsymbol{x}|G|k'^0,\boldsymbol{x}'\rangle \times \exp[i(k'^0x'^0-k^0x^0)]. \quad (24)$$

The equivalent equation to (22) for $\langle \boldsymbol{x}|G(E)|\boldsymbol{x}'\rangle$ is therefore

$$\ell\delta(z-z_0)\left(\nabla_\parallel^2-\frac{\Delta m^2c^2}{\hbar^2}\right)\langle \boldsymbol{x}|G(E)|\boldsymbol{x}'\rangle + \left(\nabla^2+\frac{E^2}{\hbar^2c^2}-\frac{m^2c^2}{\hbar^2}\right)\langle \boldsymbol{x}|G(E)|\boldsymbol{x}'\rangle = -\delta(\boldsymbol{x}-\boldsymbol{x}'). \quad (25)$$

Equations (22) and (25) can be solved analytically for $z=z_0$ and $E\geqslant mc^2$. The energy-dependent Green's function in $\boldsymbol{x}$ representation is found in the Appendix in the form of a Hankel transform,

$$\langle \boldsymbol{x}|G(E)|\boldsymbol{x}'\rangle = \frac{1}{2\pi}\int_0^\infty dk_\parallel\,k_\parallel J_0(k_\parallel|\boldsymbol{x}_\parallel-\boldsymbol{x}'_\parallel|) \times \langle z|G(k^0,k_\parallel)|z'\rangle|_{E=\hbar ck^0}, \quad (26)$$

where

$$\langle z|G(k^0,k_\parallel)|z'\rangle = i\frac{\Theta[(k^0)^2-k_\parallel^2-(mc/\hbar)^2]}{2\sqrt{(k^0)^2-k_\parallel^2-(mc/\hbar)^2}}\left\{\exp[i\sqrt{(k^0)^2-k_\parallel^2-(mc/\hbar)^2}|z-z'|] - \frac{i\ell[k_\parallel^2+\Delta m^2(c/\hbar)^2]}{2\sqrt{(k^0)^2-k_\parallel^2-(mc/\hbar)^2}+i\ell[k_\parallel^2+\Delta m^2(c/\hbar)^2]}\exp[i\sqrt{(k^0)^2-k_\parallel^2-(mc/\hbar)^2}(|z-z_0|+|z'-z_0|)]\right\}$$
$$+\frac{\Theta[k_\parallel^2+(mc/\hbar)^2-(k^0)^2]}{2\sqrt{k_\parallel^2+(mc/\hbar)^2-(k^0)^2}}\left\{\exp[-\sqrt{k_\parallel^2+(mc/\hbar)^2-(k^0)^2}|z-z'|] - \frac{\ell[k_\parallel^2+\Delta m^2(c/\hbar)^2]}{2\sqrt{k_\parallel^2+(mc/\hbar)^2-(k^0)^2}+\ell[k_\parallel^2+\Delta m^2(c/\hbar)^2]}\exp[-\sqrt{k_\parallel^2+(mc/\hbar)^2-(k^0)^2}(|z-z_0|+|z'-z_0|)]\right\}.$$

The Green's function in the interface is

$$\langle z_0|G(k^0,k_\parallel)|z_0\rangle = \Theta[(k^0)^2-k_\parallel^2-(mc/\hbar)^2]\frac{1}{\ell[k_\parallel^2+\Delta m^2(c/\hbar)^2]-2i\sqrt{(k^0)^2-k_\parallel^2-(mc/\hbar)^2}} + \frac{\Theta[k_\parallel^2+(mc/\hbar)^2-(k^0)^2]}{\ell[k_\parallel^2+\Delta m^2(c/\hbar)^2]+2\sqrt{k_\parallel^2+(mc/\hbar)^2-(k^0)^2}}.$$

This yields with (11) the following expression for the density of states in the interface (with $E=-\overline{E}=\hbar ck^0$):

$$\varrho(E,z_0)-\overline{\varrho}(\overline{E},z_0) = \frac{E\Theta(E^2-m^2c^4)}{2(\pi\hbar c)^2\ell}\left[\arctan\left(\frac{\ell\sqrt{E^2-m^2c^4}+\sqrt{g(E,\ell,m,\Delta m^2)}}{\hbar c}\right) + \arctan\left(\frac{\ell\sqrt{E^2-m^2c^4}-\sqrt{g(E,\ell,m,\Delta m^2)}}{\hbar c}\right)\right] + \frac{E\Theta(E^2-m^2c^4)}{4\pi^2\hbar c\ell\sqrt{g(E,\ell,m,\Delta m^2)}}\ln\frac{f_-(E,\ell,m,\Delta m^2)}{f_+(E,\ell,m,\Delta m^2)} \quad (27)$$

with

$$g(E,\ell,m,\Delta m^2) = \ell^2(E^2-m^2c^4+\Delta m^2c^4)-\hbar^2c^2$$

and

$$f_\pm(E,\ell,m,\Delta m^2) = 2\ell(E^2-m^2c^4)+\ell\Delta m^2c^4 \pm 2\sqrt{E^2-m^2c^4}\sqrt{g(E,\ell,m,\Delta m^2)}.$$

From this result and Eq. (27) we can infer the particle density of states for $E>mc^2$ and the antiparticle or hole density of states in the interface for $E=-\overline{E}<-mc^2$. The result does not imply that the bulk energy gap of $2mc^2$ between the particle and hole states is preserved in the interface because the Green's function $\langle \boldsymbol{x}|G(E)|\boldsymbol{x}\rangle$ only tells us the difference between the particle and hole densities of states.

The right-hand side of Eq. (27) remains real also for $g(E,\ell,m,\Delta m^2) < 0$. If we wish to express $\varrho(E) - \overline{\varrho}(\overline{E})$ explicitly in terms of real functions in this case we can use that for $x \geqslant 0, y \geqslant 0$,

$$\frac{1}{i}\ln\left(\frac{x+iy}{x-iy}\right) = 2\arctan(y/x), \tag{28}$$

and

$$\arctan(x+iy) + \arctan(x-iy) = \arctan\left(\frac{x}{1+y}\right) + \arctan\left(\frac{x}{1-y}\right). \tag{29}$$

This yields the representation

$$\varrho(E,z_0) - \overline{\varrho}(\overline{E},z_0) = \frac{E\Theta(E^2-m^2c^4)}{2(\pi\hbar c)^2\ell}\left[\arctan\left(\frac{\ell\sqrt{E^2-m^2c^4}}{\hbar c+\sqrt{-g(E,\ell,m,\Delta m^2)}}\right) + \arctan\left(\frac{\ell\sqrt{E^2-m^2c^4}}{\hbar c-\sqrt{-g(E,\ell,m,\Delta m^2)}}\right)\right] + \frac{E\Theta(E^2-m^2c^4)}{2\pi^2\hbar c\ell\sqrt{-g(E,\ell,m,\Delta m^2)}}\left[\arctan\left(\frac{\ell\sqrt{E^2-m^2c^4}}{\hbar c+\sqrt{-g(E,\ell,m,\Delta m^2)}}\right) - \arctan\left(\frac{\ell\sqrt{E^2-m^2c^4}}{\hbar c-\sqrt{-g(E,\ell,m,\Delta m^2)}}\right)\right]. \tag{30}$$

Equations (27)–(30) use $0 \leqslant \arctan(x) < \pi$. Otherwise, we would have to add π to every inverse tangent function with negative argument, $\arctan(x) \to \arctan(x) + \pi\Theta(-x)$, to properly reflect the continuity and smoothness properties of the Green's function from which $\varrho(E,z_0) - \overline{\varrho}(\overline{E},z_0)$ was derived.

Equation (30) also applies in the limit $\ell \to 0$ and yields

$$[\varrho(E,z_0) - \overline{\varrho}(\overline{E},z_0)]_{\ell\to 0} = \Theta(E^2-m^2c^4)\frac{E\sqrt{E^2-m^2c^4}}{2\pi^2(\hbar c)^3} = [\varrho(E) - \overline{\varrho}(\overline{E})]_{d=3}, \tag{31}$$

as expected. The three-dimensional limit (31) can also be derived for low energies

$$|\Delta m^2c^4| \ll E^2 - m^2c^4 \ll \hbar^2c^2/\ell^2 \tag{32}$$

if the magnitude of the shift parameter for the gap in the interface is small.

On the other hand, the density of states in the interface shows two-dimensional behavior up to logarithmic corrections if

$$E^2 - m^2c^4 \gg (\hbar c/\ell)^2 - \Delta m^2c^4. \tag{33}$$

This yields for the particle density of states ($E > mc^2$)

$$\varrho(E,z_0)|_{(33)} \simeq \frac{E}{4\pi(\hbar c)^2|\ell|} - \frac{E}{\sqrt{E^2-m^2c^4}}\frac{\ln(2|\ell|\sqrt{E^2-m^2c^4}/\hbar c)}{2\pi^2\hbar c\ell^2} = \frac{\varrho_{d=2}(E)}{2|\ell|} - \frac{E}{\sqrt{E^2-m^2c^4}}\frac{\ln(2|\ell|\sqrt{E^2-m^2c^4}/\hbar c)}{2\pi^2\hbar c\ell^2}. \tag{34}$$

The resulting density of states for length parameter $\ell = 3$ nm, bulk gap parameter $\Delta_g = 95$ meV, and $\Delta m^2c^4 = 0$ along with the limiting three-dimensional and two-dimensional asymptotic cases is illustrated in Figs. 1 and 2, respectively. Note that the interface can also affect the density of states without a change in effective mass due to a change in wave function curvature contributions to the energy density of particles in the interface.

Figure 3 illustrates the result for gap shift $\Delta m^2c^4 < -\Delta_g^2$. Negative gap shift Δm^2c^4 in the interface generates a finite offset

$$\varrho(\Delta_g,z_0)|_{\Delta m^2<0} = \frac{\Delta_g}{2\pi\hbar^2c^2\ell}\left(1 - \frac{\hbar c}{\sqrt{\hbar^2c^2 - \ell^2\Delta m^2c^4}}\right)$$

due to the generation of gap states.

The Green's function $\langle \boldsymbol{x}|G(E)|\boldsymbol{x}'\rangle$ and the results ensuing from it reproduce the results for interdimensional Schrödinger systems in the nonrelativistic limit $0 < K = E - mc^2 \ll mc^2$ and for $\Delta m^2 = 0$ (our ℓ here corresponds to 2ℓ in [2], and the densities of states there include an extra spin factor of 2 because the discussion explicitly referred to electrons). However, the nonrelativistic limit of the Hamiltonian (20) is richer because parabolic band approximation in the bulk does not

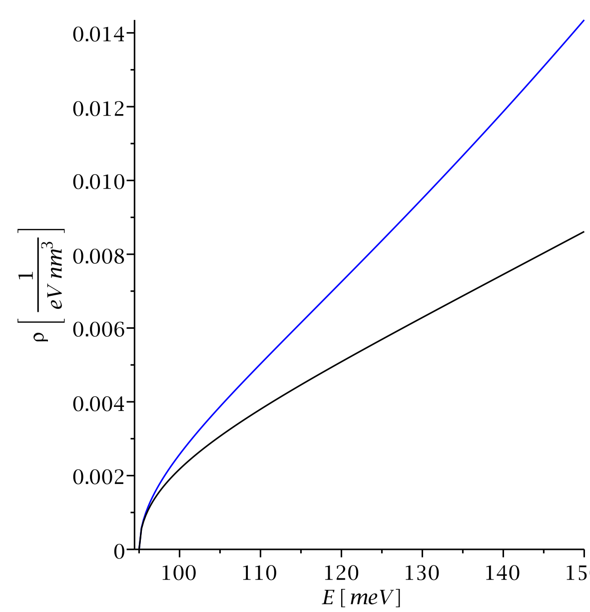

FIG. 1. (Color online) The density of states in the interface for $\ell = 3$ nm, $\Delta_g = 95$ meV, and $\Delta m^2c^4 = 0$. The three-dimensional density of states is included in blue (upper line) for comparison.

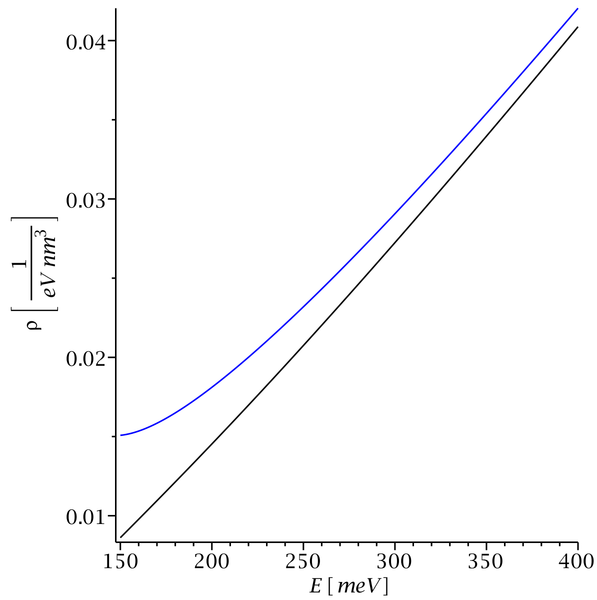

FIG. 2. (Color online) The density of states in the interface for $\ell = 3$ nm, $\Delta_g = 95$ meV, and $\Delta m^2c^4 = 0$. The corresponding two-dimensional limit plus logarithmic correction (34) is included in blue (upper line) for comparison.

constrain the low-dimensional Δm^2 term from quasirelativistic dispersion in the interface.

The nonrelativistic approximation for the complex scalar field is [1]

$$\phi(\boldsymbol{x},t) \simeq \sqrt{\frac{\hbar}{2mc^2}}\psi(\boldsymbol{x},t)\exp\left(-i\frac{mc^2}{\hbar}t\right). \tag{35}$$

This approximation is also relevant for the present investigation since the particles are nonrelativistic from the point of view of bulk motion if $0 < E - \Delta_g \ll \Delta_g$.

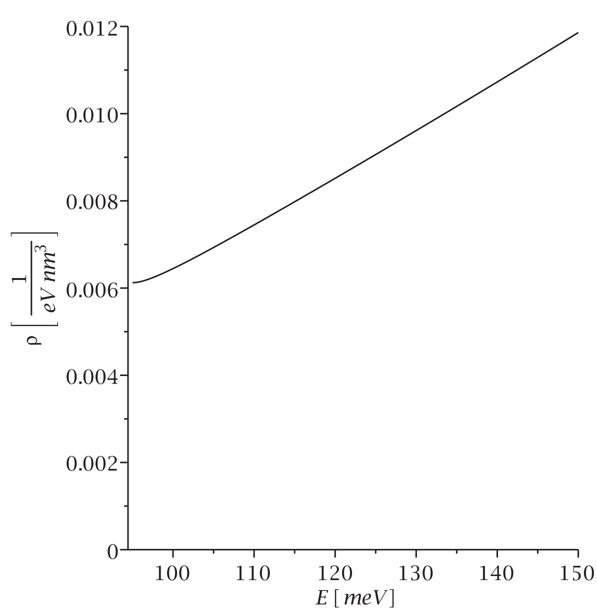

FIG. 3. The density of states in the interface for $\ell = 3$ nm, $E > \Delta_g = 95$ meV, and gap shift $\Delta m^2c^4 = -\Delta_g^2$.

Substitution of (35) into (20) and neglect of the usual subleading terms for nonrelativistic bulk motion yields a Hamiltonian,

$$\begin{aligned} H = &\int d^2\boldsymbol{x}_\parallel \int dz \left[\frac{\hbar^2}{2m}\nabla\psi^+(\boldsymbol{x}_\parallel,z)\cdot\nabla\psi(\boldsymbol{x}_\parallel,z)\right. \\ &\left.+ mc^2\psi^+(\boldsymbol{x}_\parallel,z)\psi(\boldsymbol{x}_\parallel,z)\right] \\ &+ \ell\int d^2\boldsymbol{x}_\parallel \left[\frac{\hbar^2}{2m}\nabla_\parallel\psi^+(\boldsymbol{x}_\parallel,z_0)\cdot\nabla_\parallel\psi(\boldsymbol{x}_\parallel,z_0)\right. \\ &\left.+ \frac{\Delta m^2c^2}{2m}\psi^+(\boldsymbol{x}_\parallel,z_0)\psi(\boldsymbol{x}_\parallel,z_0)\right], \end{aligned} \tag{36}$$

where we reduced to Schrödinger picture operators.

Note that the Δm^2 term in the nonrelativistic approximation for bulk motion does not reduce to a parabolic band approximation with effective mass $m_* = m_*(m,\Delta m^2)$ for motion in the interface. Removal of the bulk rest energy term can be accomplished in the standard way at the expense of removal of the phase factor $\exp(-imc^2t/\hbar)$ from the wave function or Heisenberg picture operator $\psi(\boldsymbol{x},t)$. However, using a two-dimensional Schrödinger Hamiltonian for the interface term requires that the magnitude of the contribution from the quasirelativistic Δm^2 term is small compared to the Schrödinger term involving the gradients of the operators. In terms of the kinetic energy $K = E - mc^2 \ll mc^2$, interference of the Δm^2 term with a parabolic approximation for both the interface and the bulk manifests itself in the fact that the speed c remains in all expressions for the densities of states in the form $2mK + \Delta m^2c^2$, while all the other powers of c cancel. In terms of the kinetic energy, the requirement of simultaneous parabolic approximation in the bulk and in the interface is

$$\frac{|\Delta m^2|c^2}{m} \ll K \ll mc^2, \tag{37}$$

i.e., a nonrelativistic kinetic-energy domain (37) exists if the modification of the energy gap in the interface is much smaller than the bulk gap parameter, $|\Delta m^2| \ll m^2$.

IV. CONCLUSIONS

We have calculated the Green's function and the density of states for quasirelativistic bosons which are moving in the presence of a thin interface under the assumption that motion in the interface affects mass and kinetic contributions to the energy of the bosons. The general analytic results for the density of states $\varrho(E,z_0)$ in the interface are displayed in Eqs. (27) and (30). We have found that $\varrho(E,z_0)$ always approaches two-dimensional behavior $\sim E$ for high energies (34). On the other hand, it approaches the three-dimensional behavior $\sim E\sqrt{E^2 - m^2c^4}$ displayed in Eq. (31) in a low-energy limit but only if the shift $\Delta(m^2)$ of the gap parameter in the interface satisfies the constraint $\ell^2|\Delta m^2| \ll \hbar^2/c^2$. Since $|\ell|$ should scale with the thickness of the interface, decreasing interface thickness in systems with quasirelativistic dispersion relations and sufficiently small $|\Delta m^2|$ should open up an energy range with three-dimensional behavior. Equation (37) explains when this also complies with a parabolic approximation in the bulk.

The results in the interface are analytic and in full compliance with the corresponding parabolic results. They confirm that the presence of an interface which only affects propagation properties of particles but does not necessarily exert an attractive potential on the particles still induces two-dimensional behavior in the high-energy limit.

ACKNOWLEDGMENT

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APPENDIX: SOLUTION OF EQ. (22)

Substitution of the Fourier representation

$$\langle x|G|x'\rangle = \frac{1}{\sqrt{2\pi}^7}\int d^2\boldsymbol{k}_\parallel \int d^2\boldsymbol{k}'_\parallel \int dk^0 \int dk'^0 \int dk_\perp \langle k^0,\boldsymbol{k}_\parallel,k_\perp|G|k'^0,\boldsymbol{k}'_\parallel,z'\rangle \times \exp[i(\boldsymbol{k}_\parallel\cdot\boldsymbol{x}_\parallel - \boldsymbol{k}'_\parallel\cdot\boldsymbol{x}'_\parallel - k^0x^0 + k'^0x'^0 + k_\perp z)]$$

into Eq. (22) yields

$$\frac{\ell}{2\pi}\int d\kappa_\perp \exp[i(\kappa_\perp - k_\perp)z_0]\left(\boldsymbol{k}_\parallel^2 + \frac{\Delta m^2c^2}{\hbar^2}\right)\langle k^0,\boldsymbol{k}_\parallel,\kappa_\perp|G|k'^0,\boldsymbol{k}'_\parallel,z'\rangle + \left(\boldsymbol{k}_\parallel^2 + k_\perp^2 - (k^0)^2 + \frac{m^2c^2}{\hbar^2}\right)\langle k^0,\boldsymbol{k}_\parallel,k_\perp|G|k'^0,\boldsymbol{k}'_\parallel,z'\rangle = \frac{\exp(-ik_\perp z')}{\sqrt{2\pi}}\delta(\boldsymbol{k}_\parallel - \boldsymbol{k}'_\parallel)\delta(k^0 - k'^0).$$

Substitution of

$$\langle k^0,\boldsymbol{k}_\parallel,k_\perp|G|k'^0,\boldsymbol{k}'_\parallel,z'\rangle = \langle k_\perp|G(k^0,\boldsymbol{k}_\parallel)|z'\rangle\delta(\boldsymbol{k}_\parallel - \boldsymbol{k}'_\parallel)\delta(k^0 - k'^0)$$

then yields

$$\left(\boldsymbol{k}_\parallel^2 + k_\perp^2 - (k^0)^2 + \frac{m^2c^2}{\hbar^2}\right)\langle k_\perp|G(k^0,\boldsymbol{k}_\parallel)|z'\rangle + \frac{\ell}{2\pi}\int d\kappa_\perp \exp[i(\kappa_\perp - k_\perp)z_0]\left(\boldsymbol{k}_\parallel^2 + \frac{\Delta m^2c^2}{\hbar^2}\right)\langle \kappa_\perp|G(k^0,\boldsymbol{k}_\parallel)|z'\rangle = \frac{\exp(-ik_\perp z')}{\sqrt{2\pi}}.$$

This implies that $\langle k_\perp|G(k^0,\boldsymbol{k}_\parallel)|z'\rangle$ must have the form

$$\exp(ik_\perp z_0)\langle k_\perp|G(k^0,k_\parallel)|z'\rangle = \frac{1}{(mc/\hbar)^2 + k^2 - i\epsilon}\left(\frac{\exp[ik_\perp(z_0 - z')]}{\sqrt{2\pi}} + f(k^0,k_\parallel,z')\right), \tag{A1}$$

where the factor $f(k^0,k_\parallel,z')$ has to satisfy

$$\frac{\ell}{2\pi}\int dk_\perp \left(\frac{\exp[ik_\perp(z_0 - z')]}{\sqrt{2\pi}} + f(k^0,k_\parallel,z')\right)\frac{\Delta m^2(c/\hbar)^2 + k_\parallel^2}{(mc/\hbar)^2 + k^2 - i\epsilon} + f(k^0,k_\parallel,z') = 0. \tag{A2}$$

The pole shift $-i\epsilon$ in the denominator is such that Eq. (A1) reproduces the retarded free Green's function for $\ell = 0$.

For the evaluation of the integral we observe

$$\begin{aligned}
&\int \frac{dk_\perp}{2\pi}\frac{\exp(ik_\perp z)F(k_\perp)}{k_\perp^2 + k_\parallel^2 - (k^0)^2 + (mc/\hbar)^2 - i\epsilon}\\
&= i\Theta(z)\Theta[(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2]F\left(\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2}\right)\frac{\exp\left(i\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2}z\right)}{2\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2}}\\
&\quad + i\Theta(-z)\Theta[(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2]F\left(-\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2}\right)\frac{\exp\left(-i\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2}z\right)}{2\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2}}\\
&\quad + \Theta(z)\Theta[k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2]F\left(i\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2}\right)\frac{\exp\left(-\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2}z\right)}{2\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2}}\\
&\quad + \Theta(-z)\Theta[k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2]F\left(-i\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2}\right)\frac{\exp\left(\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2}z\right)}{2\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2}}.
\end{aligned} \tag{A3}$$

Evaluating the integral in Eq. (A2) and solving for $f(k^0,k_\parallel,z')$ yield

$$f(k^0,k_\parallel,z') = -i\Theta[(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2]\frac{\ell(k_\parallel^2 + \Delta m^2(c/\hbar)^2)}{2\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2} + i\ell(k_\parallel^2 + \Delta m^2(c/\hbar)^2)}\frac{\exp(i\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2}|z'-z_0|)}{\sqrt{2\pi}}$$
$$- \frac{\Theta[k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2]\ell(k_\parallel^2 + \Delta m^2(c/\hbar)^2)}{2\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2} + \ell(k_\parallel^2 + \Delta m^2(c/\hbar)^2)}\frac{\exp(-\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2}|z'-z_0|)}{\sqrt{2\pi}},$$

and therefore

$$\langle k_\perp|G(k^0,k_\parallel)|z'\rangle = \frac{1}{\sqrt{2\pi}}\frac{1}{k_\perp^2 + k_\parallel^2 - (k^0)^2 + (mc/\hbar)^2 - i\epsilon}\Bigg\{\exp(-ik_\perp z')$$
$$- i\frac{\Theta[(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2]\ell(k_\parallel^2 + \Delta m^2(c/\hbar)^2)}{2\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2} + i\ell(k_\parallel^2 + \Delta m^2(c/\hbar)^2)}\exp[-ik_\perp z_0 + i\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2}|z'-z_0|]$$
$$- \frac{\Theta[k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2]\ell[k_\parallel^2 + \Delta m^2(c/\hbar)^2]}{2\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2} + \ell[k_\parallel^2 + \Delta m^2(c/\hbar)^2]}\exp[-ik_\perp z_0 - \sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2}|z'-z_0|]\Bigg\}.$$

Fourier transformation yields

$$\langle z|G(k^0,k_\parallel)|z'\rangle = \int dk_\perp\,\frac{\exp(ik_\perp z)}{\sqrt{2\pi}}\langle k_\perp|G(k^0,k_\parallel)|z'\rangle$$
$$= i\frac{\Theta[(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2]}{2\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2}}\Bigg\{\exp[i\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2}|z-z'|]$$
$$- \frac{i\ell[k_\parallel^2 + \Delta m^2(c/\hbar)^2]}{2\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2} + i\ell[k_\parallel^2 + \Delta m^2(c/\hbar)^2]}\exp[i\sqrt{(k^0)^2 - k_\parallel^2 - (mc/\hbar)^2}(|z-z_0| + |z'-z_0|)]\Bigg\}$$
$$+ \frac{\Theta[k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2]}{2\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2}}\Bigg\{\exp[-\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2}|z-z'|]$$
$$- \frac{\ell[k_\parallel^2 + \Delta m^2(c/\hbar)^2]}{2\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2} + \ell[k_\parallel^2 + \Delta m^2(c/\hbar)^2]}\exp[-\sqrt{k_\parallel^2 + (mc/\hbar)^2 - (k^0)^2}(|z-z_0| + |z'-z_0|)]\Bigg\}.$$

The energy-dependent Green's function in $\boldsymbol{x}$ space (9) is then

$$\langle \boldsymbol{x}|G(E)|\boldsymbol{x}'\rangle = \frac{1}{(2\pi)^2}\int d^2\boldsymbol{k}_\parallel\,\exp[i\boldsymbol{k}_\parallel\cdot(\boldsymbol{x}_\parallel - \boldsymbol{x}'_\parallel)]\langle z|G(k^0,k_\parallel)|z'\rangle|_{E=\hbar ck^0}$$
$$= \frac{1}{2\pi}\int_0^\infty dk_\parallel\,k_\parallel J_0(k_\parallel|\boldsymbol{x}_\parallel - \boldsymbol{x}'_\parallel|)\langle z|G(k^0,k_\parallel)|z'\rangle|_{E=\hbar ck^0}. \tag{A4}$$

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