Quasirelativistic electronic $T$-matrix for the short-range perturbation

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Exact $T$-matrix for the delta-function short-range perturbation of the (3+1)-Dirac equation has been derived. Separability of the potential in the angular momentum representation is used. A characteristic equation for the $T$-matric poles determining the bound and resonance states has been obtained. The calculated $T$-matrix determines transport properties of the narrow-gap and zero-gap semiconductors.

I. INTRODUCTION

Transport theory and theory of the electronic spectrum need in calculation of the $T$-matrix including its "nonphysical" part outside the mass shell. This makes it necessary to consider exactly solvable models of perturbation. One of them is the delta function potential. In the case of the two-band nonrelativistic problem described by the Dirac equation the problem of bound and resonance states was considered with a use of such potential in the paper [1]. The short radius potential $\delta (r - r_0)$ was considered. This potential has no a singularity at $r = 0$ and is separable in the angular momentum representation. Here were consider the problem of the bound and resonance states with slightly different approach and calculate an exact $T$-matrix. We take into account possible difference of the perturbation matrix elements calculated on wave functions of the upper and lower bands that is equivalent to consideration of both potential and mass perturbations.

II. CHARACTERISTIC EQUATION

As it is well known, the electronic states near the band edge are determined by the quasirelativistic Dirac equation [1]. It can be written in the momentum representation in the form:

$$s \sigma \mathbf{p} \chi (\mathbf{p}) + (m s^2 - E) \varphi (\mathbf{p}) + \int d^3p' V_i (\mathbf{p} - \mathbf{p}') \varphi (\mathbf{p}') = 0,$$

(1)

$$s \sigma \mathbf{p} \varphi (\mathbf{p}) - (m s^2 + E) \chi (\mathbf{p}) + \int d^3p' V_2 (\mathbf{p} - \mathbf{p}') \chi (\mathbf{p}') = 0,$$

(2)

where $\sigma$ is the Pauli matrix, $s$ is the quasirelativistic limiting velocity of band electrons, $2ms^2 = E_g$. The potential Fourier transform $V_i (\mathbf{p})$ can be expanded into a series of the Legendre polynomials $P_l (\cos \theta)$ in the case of the spherical symmetry [2]:

$$V_i (|\mathbf{p} - \mathbf{p}'|) = \sum_l V^l_i (p, p') P_l (\cos \theta) (2l + 1) / 4\pi,$$

(3)

$$V^l_i (p, p') = 2 \int_0^\infty dr r V_i (r) \frac{J_{l+1/2} (pr) J_{l+1/2} (p'r)}{\sqrt{pp'}},$$

(4)

where $J_{l+1/2} (pr)$ is the Bessel function. The wave functions can be expanded into a series of spherical spinors $\Omega_{jlm} (\mathbf{n})$ [3]:

$$\begin{pmatrix} \varphi^E_{l'm} (\mathbf{p}) \\ \chi^E_{l'm} (\mathbf{p}) \end{pmatrix} = \begin{pmatrix} f_E (p) i^{-l} \Omega_{jlm} (\mathbf{n}) \\ -g_E (p) i^{-l'} \Omega_{j'l'm} (\mathbf{n}) \end{pmatrix},$$

(5)

where $l = j \pm 1/2$, $l' = j \pm 1/2$, $j$ is the total angular momentum quantum number, $\mathbf{n} = \mathbf{p} / p$, $\theta$ is the angle between the vectors $\mathbf{p}$ and $\mathbf{p'}$, while

$$\sigma \mathbf{n} \Omega_{jlm} (\mathbf{n}) = i^{l'-l} \Omega_{j'l'm} (\mathbf{n}).$$

(6)

Signs ± correspond to $\varkappa = \pm (j + 1/2)$. Thus, eqs. (1), (2) take the form
where the equation is extremely sensitive to a singularity of the potential \( V_{j,l,m} \). Making use of the addition theorem for the spherical functions

\[
\sum_m Y_{lm}^* (\mathbf{n}) Y_{l'm'} (\mathbf{n'}) = \frac{2l+1}{4\pi} P_l (\cos \theta),
\]

we obtain from (??), (??)

\[
\Omega_{j=\pm 1/2, l, m} (\mathbf{n}) = \left( \frac{1}{\sqrt{2j+1}} \right) \frac{V_{j-1/2, l, m} (\mathbf{n})}{\sqrt{\Omega_{j=\pm 1/2, l, m} (\mathbf{n})}}
\]

we obtain from (??), (??)

\[
(V_{l'} (r) = \frac{V_{l'} (r)}{4\pi r_0^2} \delta (r - r_0).
\]

Substituting (??) into (??) we obtain the separable in the angular momentum-momentum modulus representation potential:

\[
V_{l'} (p, p') = v_{l'} (p) v_{l'} (p'),
\]

where

\[
v_{l'} (p) = \sqrt{\frac{V_{l'} (r)}{2\pi pr_0}} J_{l+1/2}(pr_0).
\]

Equations (??) become degenerate and can be written as follows:

\[
(ms^2 - E) f_E (p) + spg_E (p) + v_1 (p) \int_0^\infty dp' (p')^2 f_E (p') v_1 (p') = 0,
\]

\[
(ms^2 + E) f_E (p) + spg_E (p) - v_2 (p) \int_0^\infty dp' (p')^2 g_E (p') v_2 (p') = 0.
\]

Introducing the functions

\[
F (E) = \int_0^\infty dp p^2 f_E (p) v_1 (p), \quad G (E) = \int_0^\infty dp p^2 g_E (p) v_2 (p), \quad R (p) = (s^2 p^2 + m^2 s^4 - E^2)^{-1}.
\]
We obtain the algebraic equation set
\[ F = G \int_0^\infty dpp^2 sR(p) v'_1(p) v''_1(p) - (E + ms^2) F \int_0^\infty dpp^2 R(p) \left(v'_1(p)\right)^2, \]
\[ G = F \int_0^\infty dpp^2 sR(p) v'_1(p) v''_2(p) + (E - ms^2) G \int_0^\infty dpp^2 R(p) \left(v''_2(p)\right)^2. \] (17)

The solvability condition for this equation set gives the characteristic equation:
\[ \left[ 1 + \frac{E + ms^2}{\hbar^2 s^2} V_1^0 I_{+1/2} (\kappa r_0) K_{+1/2} (\kappa r_0) \right] \left[ 1 + \frac{E - ms^2}{\hbar^2 s^2} V_2^0 I'_{+1/2} (\kappa r_0) K'_{+1/2} (\kappa r_0) \right] = \frac{V_0 V_0'}{16 \pi^2 r_0^4 \hbar^2 s^2}, \] (18)

where \( \kappa^2 = (m^2 s^4 - E^2) h^{-2} s^{-2}, I_n(x), K_n(x) \) are the modified Bessel functions.

### III. Calculation of the T-Matrix

Let us determine the standard representation bispinor basis as follows
\[ (r, g | p, \chi, +) = \frac{i^l}{\sqrt{2 E_p}} \left( \begin{array}{c} \Omega_\kappa (r/r) \\ -\Omega_\kappa' (r/r) \end{array} \right), \] (19)
\[ (r, g | p, \chi, -) = \frac{i^{l'}}{\sqrt{2 E_p}} \left( \begin{array}{c} \Omega_\kappa (r/r) \\ \Omega_\kappa' (r/r) \end{array} \right), \] (20)

where \( \lambda = \pm, \kappa = (j, l, m); E_p = \sqrt{m^2 s^4 + p^2 s^2}; l - l' = \text{sgn} \kappa; \kappa = \pm 1, \pm 2, \ldots; R_{pl} (r) = \sqrt{p/r} H^{(1)}_{l+1/2} (pr); g \) is the bispinor index. We work in units with \( \hbar = s = 1 \). The exact wave function of the out-basis satisfies the Lippmann-Schwinger equation:
\[ \langle r, g | p, \chi, \lambda \rangle = (r, g | p, \chi, \lambda) - \sum_{g' g''} \int d^3 r G_{g' g''} (r - r') V_{g' g''} (r') \langle r', g'' | p, \chi, \lambda \rangle \] (21)

The perturbation matrix can be written in the form
\[ V_{gg'} (r) = V_g \delta_{gg'}. \] (22)

Distinct values for the upper and lower bands stem from different symmetries of the Kohn-Luttinger basic functions. We define \( V_1 = V_2 = V_+; V_3 = V_4 = V_- \). The \( T \)-matrix can be defined as follows:
\[ \langle p', \chi', \lambda' | T | p, \chi, \lambda \rangle = \sum_g \int d^3 r \langle p', \chi', \lambda g | r, g \rangle V_g (r) \langle r, g | p, \chi, \lambda \rangle. \] (23)

Using (21) and expanding the Green function into a series of the Dirac Hamiltonian eigenfunctions we obtain the equation for the \( T \)-matrix:
\[ \langle p', \chi', \lambda' | T (E) | p, \chi, \lambda \rangle = \langle p', \chi', \lambda' | V (r) | p, \chi, \lambda \rangle - \frac{\sum_{\chi_1, \lambda_1} \langle p', \chi', \lambda' | V (r) | p_1, \chi_1, \lambda_1 \rangle}{E_{p_1} \text{sgn} \lambda_1 - E - i0} \langle p_1, \chi_1, \lambda_1 | T (E) | p, \chi, \lambda \rangle. \] (24)

The perturbation matrix elements are determined as follows
\[ \langle p', \chi', \lambda' | V (r) | p, \chi, \lambda \rangle = \sum_g \int d^3 r \langle p', \chi', \lambda g | r, g \rangle V_g (r) \langle r, g | p, \chi, \lambda \rangle \] (25)
This matrix takes a form of a sum of the two factorized expressions in our case:

\[
(p', \chi', \lambda') V(r) | p, \chi, \lambda) = \int \tilde{d}r \, \langle p', \chi', \lambda' | r_0, n, + \rangle \langle r_0, n, + | p, \chi, \lambda) V_+ + \\
(p', \chi', \lambda') r_0, n, - \rangle \langle r_0, n, - | p, \chi, \lambda) V_-.
\]

(26)

We seek a solution of the Lippmann-Schwinger equation in the form:

\[
(\mathbf{r}, \mathbf{g} | p, \chi, +) = \frac{i}{\sqrt{2E_p}} \left( \sqrt{E_p + mR_{pl} (r)} F_{pl}^{(+)} (r) \Omega_\chi (\mathbf{r}/r) \right),
\]

(27)

\[
(\mathbf{r}, \mathbf{g} | p, \chi, -) = \frac{i}{\sqrt{2E_p}} \left( \sqrt{E_p - mR_{pl} (r)} F_{pl}^{(-)} (r) \Omega_\chi (\mathbf{r}/r) \right).
\]

(28)

The \(T\)-matrix can be expressed in terms of the \(F_{pl}^{\pm}\) and \(G_{pl}^\pm\) functions as follows:

\[
\langle p_1, \chi_1, + | T(E) | p, \chi, + \rangle = \frac{\delta_{\chi\chi'}}{2 \sqrt{E_p E_p'}} \left[ \sqrt{(E_{p_1} + m)(E_p + m)} V_+^0 F_{pl}^{(+)} (r) R_{pl_1} (r) + \sqrt{(E_{p_1} - m)(E_p - m)} V_+^0 G_{pl_1}^{(+)} (r) R_{pl_1} (r) \right],
\]

(29)

\[
\langle p_1, \chi_1, - | T(E) | p, \chi, - \rangle = \frac{\delta_{\chi\chi'}}{2 \sqrt{E_p E_p'}} \left[ \sqrt{(E_{p_1} - m)(E_p - m)} V_+^0 F_{pl}^{(-)} (r) R_{pl_1} (r) + \sqrt{(E_{p_1} + m)(E_p + m)} V_+^0 G_{pl_1}^{(-)} (r) R_{pl_1} (r) \right],
\]

(30)

\[
\langle p_1, \chi_1, + | T(E) | p, \chi, - \rangle = \frac{\delta_{\chi\chi'}}{2 \sqrt{E_p E_p'}} \left[ \sqrt{(E_{p_1} - m)(E_p + m)} V_+^0 F_{pl}^{(+)} (r) R_{pl_1} (r) - \sqrt{(E_{p_1} + m)(E_p - m)} V_+^0 G_{pl_1}^{(+)} (r) R_{pl_1} (r) \right],
\]

(31)

\[
\langle p_1, \chi_1, - | T(E) | p, \chi, + \rangle = \frac{\delta_{\chi\chi'}}{2 \sqrt{E_p E_p'}} \left[ \sqrt{(E_{p_1} + m)(E_p - m)} V_+^0 F_{pl}^{(-)} (r) R_{pl_1} (r) - \sqrt{(E_{p_1} - m)(E_p + m)} V_+^0 G_{pl_1}^{(-)} (r) R_{pl_1} (r) \right],
\]

(32)

Substituting (29), (30), (31) and (32) into (26) we obtain two independent sets of equations for the pairs of functions \(F^{(+)}\), \(G^{(+)}\) and \(F^{(-)}\), \(G^{(-)}\):

\[
\hat{A}^{(\pm)} \begin{pmatrix} F_{pl_1}^{(\pm)} \\ G_{pl_1}^{(\pm)} \end{pmatrix} = \begin{pmatrix} c^{\pm \pm}_{pl_1} V_0^0 R_{pl_1}^{(+)} + c^{\pm \mp}_{pl_1} V_0^0 R_{pl_1}^{(-)} \\ c^{\mp \pm}_{pl_1} V_0^0 R_{pl_1}^{(+)} - c^{\mp \mp}_{pl_1} V_0^0 R_{pl_1}^{(-)} \end{pmatrix},
\]

(33)

where

\[
c^{\pm \pm}_{pl_1} = \sqrt{(E_{p_1} \pm m)(E_p \pm m)}, \quad c^{\pm \mp}_{pl_1} = \sqrt{(E_{p_1} \pm m)(E_p \mp m)}
\]

(34)

\[
b^{(+)}_{pl_1} = R_{pl_1}^+ R_{pl_1}^+ R_{pl_1}^+ R_{pl_1}^-, \quad b^{(-)}_{pl_1} = R_{pl_1}^+ R_{pl_1}^+ R_{pl_1}^+ R_{pl_1}^-, \quad b^{(+)}_{pl_1} = pR_{pl_1}^+ R_{pl_1}^+ R_{pl_1}^+ R_{pl_1}^-, \quad b^{(-)}_{pl_1} = pR_{pl_1}^+ R_{pl_1}^+ R_{pl_1}^+ R_{pl_1}^-.
\]

(35)
Matrix elements of $\hat{A}$ read

$$\begin{align*}
A_{11}^± &= V_+^{0,±±} b_{pp}^{(++)} [1 + V_+^0 (E + m) B^{++} (E)] \pm \frac{V_+^{0,±±}}{p} c_{pp}^{±±} b_{pp}^{(++)} B^{±±} (E), \\
A_{22}^± &= -V_0^{0,±±} b_{pp}^{(--)} [1 + V_0^0 (E - m) B^{--} (E)] \pm \frac{V_0^{0,±±}}{p} c_{pp}^{±±} b_{pp}^{(--)} B^{±±} (E), \\
A_{12}^± &= V_0^{0,±±} b_{pp}^{(--)} [1 + V_0^0 (E - m) B^{--} (E)] \pm \frac{V_0^{0,±±}}{p} c_{pp}^{±±} b_{pp}^{(--)} B^{±±} (E), \\
A_{21}^± &= V_+^{0,±±} b_{pp}^{(++)} [1 + V_+^0 (E + m) B^{++} (E)] \pm \frac{V_+^{0,±±}}{p} c_{pp}^{±±} b_{pp}^{(++)} B^{±±} (E),
\end{align*}$$

where the matrix $\hat{B} (E)$ is determined as follows

$$\hat{B} (E) = \int_0^\infty dp \frac{b_{pp}}{E_p^2 - E^2 - i0}. \tag{37}$$

Equating the matrix $\hat{A}$ determinant $d$ to zero, we obtain the characteristic equation, which was derived in [?] and in the Section II using a different approach:

$$d (E) \equiv \det \hat{A} \equiv \left[1 + V_+^0 (E + m) \int_0^\infty dp \frac{|R_{p1l}|^2}{E_p^2 - E^2 - i0}\right] \left[1 + V_0^0 (E - m) \int_0^\infty dp \frac{|R_{p1l}|^2}{E_p^2 - E^2 - i0}\right] - \int_0^\infty dp \frac{p R_{p1l}^* R_{p1l}}{E_p^2 - E^2 - i0} \int_0^\infty dp' \frac{p' R_{p'1l}^* R_{p'1l}}{E_p^2 - E^2 - i0} = 0. \tag{38}$$

Solving the inhomogeneous equation set [33] we obtain an expression for the $T$-matrix:

$$\langle p_1, \chi_1, \lambda_1 | T (E) | p, \chi, \lambda \rangle = \frac{\delta_{\chi_1 \lambda_1}}{2d_E} t_{\lambda_1 \lambda} (E), \tag{40}$$

where the matrix elements of $\hat{t}$ are determined as follows

$$\begin{align*}
\langle \pm | t | \pm \rangle &= c_{pp}^{±±} V_+^{0,±±} b_{pp}^{(++)} [1 + V_+^0 (E - m) B^{--}] \mp c_{pp}^{±±} V_+^{0,±±} V_0^{0,±±} b_{pp}^{(++)} B^{±±}, \tag{41} \\
\langle \mp | t | \pm \rangle &= V_0^{0,±±} [1 + V_0^0 (E + m) B^{++}] \mp c_{pp}^{±±} V_0^{0,±±} V_0^{0,±±} b_{pp}^{(++)} B^{±±}, \tag{42} \\
\langle \pm | t | \mp \rangle &= (-1)^{l' \ell} \delta_{\ell' \ell} \frac{c_{pp}^{±±} V_+^{0,±±} V_0^{0,±±} b_{pp}^{(++)} [1 + V_+^0 (E - m) B^{--}] \pm c_{pp}^{±±} V_0^{0,±±} V_0^{0,±±} b_{pp}^{(++)} B^{±±}}{E_0^2 + m^2}, \tag{43}
\end{align*}$$

The formulae [10], [41], and [43] give an exact solution for the $T$-matrix for arbitrary $p, p_1$, and $E$. Taking these values on the mass shell $p = p_1, E = \sqrt{m^2 + p^2}$, we obtain the scattering matrix.

**Conclusion**

Non-relativistic problem of the electronic spectrum and scattering described by the Dirac equation is considered in the case of the two-component short-range perturbation. An exact $T$-matrix both on- and off-shell has been calculated.

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