Coherent quantum transport in ferromagnet/superconductor/ferromagnet structures

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The Blonder-Tinkham-Klapwijk (BTK) approach is extended to study coherent quantum transport in ferromagnet/superconductor/ferromagnet (FM/SC/SM) double tunnel junctions. In order to guarantee current conservation it is necessary to simultaneously consider spin-polarized electron currents along one direction and spin-polarized hole currents along the opposite direction, and to determine self-consistently the chemical potential in SC. It is found that all the reflection and transmission coefficients in BTK theory as well as conductance spectra oscillate with energy, exhibiting different behavior in the metallic and tunnel limits.

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I. INTRODUCTION

Since the discovery of giant magnetoresistance effects in magnetic multilayer,1 spin-polarized electron transport in various magnetic nanostructured systems has attracted much attention.2 A most noticeable effect is the large tunneling magnetoresistance (TMR) observed in a ferromagnet/ferromagnet (FM/FM) tunnel junction composed of two ferromagnetic metallic films separated by a thin insulating film.3–4 The tunneling conductance is minimal when the magnetizations of two ferromagnetic layers are antiparallel to each other, while it is maximal when the magnetizations are parallel aligned by a magnetic field, exhibiting a large TMR. On the other hand, the spin-polarized tunneling current in FM/superconductor (FM/SC) tunnel junctions is an interesting subject from the viewpoint of either basic physics or device applications. The conductance due to the Andreev reflection (AR) (Ref. 5) is strongly affected by the spin polarization of FM. This idea has been verified by experiments in the FM/SC thin film nanocontact,5 FM/SC metallic point contact,7 and FM/d-wave SC junction.8 Especially, Soulen et al.7 have successfully determined the spin polarization at the Fermi energy for several FM’s by measuring the differential conductance of the FM/SC metallic point contact. Theoretical works have clarified that the AR is suppressed by the exchange interaction in FM in the FM/SC (with d- or s-wave pairing) junctions. The effects of the exchange interaction in FM, the interfacial barrier strength, and the Fermi wavevector mismatch between FM and SC regions on differential conductances of FM/SC junctions have been investigated.9–13

Recently, the study of TMR has been extended to FM/s-wave SC/FM (Refs. 14,15) and FM/d-wave SC/FM (Ref. 16) double tunnel junctions. For the incoherent tunneling,14–16 the spin-polarized tunneling currents may induce a difference in the chemical potential between spin-up and spin-down electrons in SC for the antiparallel magnetizations of the two FM’s, and the resulting TMR exhibits anomalous voltage dependence on exchange potential and barrier strength. On the other hand, the coherent quantum tunneling may appear in FM/SC/FM double tunnel junctions if the thickness of SC interlayer is small enough. The coherent tunneling has been studied in SC/NM/SC tunnel junctions (with NM the normal metallic film) by considering the current-carrying Andreev bound states17,18 and multiple AR.19–21 Since earlier experiments by Tomasch,22 the geometric resonance nature of the differential conductance oscillations in SC/NM/SC and NM/SC/NM tunnel junctions has been ascribed to the quasipartical interference in the central film.23–26 Recently, The McMillan-Rowell oscillations were observed in SC/NM/SC edge junctions of d-wave SC, and used for measurements of the superconducting gap and the Fermi velocity.27

The Blonder-Tinkham-Klapwijk (BTK) approach28 has been widely used to calculate the conductance of NM/SC,29–35 FM/SC,10–13 and FM/FM/SC (Ref. 36) tunnel junctions. It is also suitable to the study of the TMR effect in FM/FM tunnel junctions,37 the coherent tunneling conductance in FM/NM/FM double tunnel junctions,38 and incoherent tunneling conductance in FM/SC/FM double tunnel junctions.15 Very recently, this approach was extended to the coherent tunneling case of the FM/SC/FM double tunnel junction with the SC interlayer thin enough.39 For a spin-s electron incident on the left FM/SC interface from the left FM, there are two sets of reflected quasiparticle waves in the left FM: normal reflection as an electron of spin-s with probability B_s(E) and Andreev reflection as a hole of the opposite spin s with probability A_s(E), as shown in Fig. 1(a). In the right FM, there are two sets of transmitted waves; electronlike quasiparticle with probability C_s(E) and holelike quasiparticle with probability D_s(E). The conservation of probability requires that A_s(E) + B_s(E) + C_s(E) + D_s(E) = 1. From this conservation condition, one finds that 1 + A_s(E) − B_s(E) cannot be equal to C_s(E) − D_s(E) pro-
condition 28 cannot be satisfied, i.e., the current calculated at
tions, if only the injection of electrons from the left FM to
the tunneling conductance and TMR in the FM/SC/SM struc-

ture. The motion of conduction electrons in FM can be de-

tribution with the hole contribution. The present approach is

Consider an FM/SC/FM double tunnel junction, in which

FIG. 1. Schematic illustration of reflections and transmissions of
quasiparticles in an FM/SC/SM structure.

provided that either $A_s(E)$ or $D_s(E)$ is not vanishing. It then
follows that in the present FM/SC/FM double tunnel junctions,
if only the injection of electrons from the left FM to SC is taken into account, the current conservation condition \cite{28} cannot be satisfied, i.e., the current calculated at the left FM/SC interface by use of $1 + A_s(E) - B_s(E)$ is unequal to that calculated at the right interface by use of $C_s(E) - D_s(E)$. It is found that the differential conductances calculated from $1 + A_s(E) - B_s(E)$ and from $C_s(E) - D_s(E)$ not only differ in magnitude from each other, but also have a phase difference in the metallic limit. The latter arises from the creation and annihilation of Cooper pairs in SC. In order to solve this difficulty, we propose that in the presence of a voltage drop between the two FM electrodes, not only there are spin-polarized electrons incident on the left FM/SC interface from the left FM, but also there are spin-polarized holes incident on the right SC/FM interface from the right FM, as shown in Fig. 1(b). In this case, the chemical potential in SC is determined by the current conservation condition, i.e., the currents through the left FM/SC interface and the right one must be equal to each other. Unlike in Ref. 39, the differential conductance obtained in the present approach is a result of combining the electron contribution with the hole contribution. The present approach is similar to that made by Lambert \cite{40} for an NM/SC/NM double tunnel junction. In the latter the chemical potential of SC was also chosen self-consistently in order to ensure quasiparticle charge conservation.

In this paper what we study is the coherent tunneling con-
ductance in the FM/SC/FM double tunnel junctions. It is quite different from incoherent tunneling conductance in the similar double tunnel junctions. In the latter case, the thickness of SC is large enough (but smaller than spin diffusion length) so that a double tunnel junction structure can be regarded as a simple series connection of two independent FM/SC tunnel junctions. In the present coherent transport, the quasiparticle interference in SC and resonant tunneling play an important role, giving rise to new quantum effects on the tunneling conductance and TMR in the FM/SC/SM struc-
tures.

II. QUASIPARTICLE TRANSPORT COEFFICIENTS

Consider an FM/SC/FM double tunnel junction, in which the left and right electrodes are made of the same FM, and they are separated from the central SC by two thin insulating interfaces, respectively. The layers are assumed to be the $y$-$z$ plane and to be stacked along the $x$ direction. The scattering Hamiltonian of two thin insulting interlayer is modeled by the two $\delta$-type barrier potentials $U(x) = U_0[\delta(x) + \delta(x - L)]$, where $L$ is the thickness of the SC interlayer and $U_0$ depends on the product of barrier height and width. The two FM’s have the same exchange splitting, which is described by $h(\mathbf{r}) = h_0[\Theta(-x) \pm \Theta(x - L)]$ where the plus [minus] sign corresponds to the parallel (P) [antiparallel (AP)] configuration of magnetizations, and $\Theta(x)$ is the Heaviside step function. We neglect for simplicity the self-consistency of spatial distribution of the pair potential in SC (Refs. 41,42) and take it as a step function $\Delta(x) = \Delta \Theta(x)(L-x)$, where $\Delta$ is the bulk superconducting gap.

The Bogoliubov–de Gennes (BdG) approach \cite{43} is applied to study the quasiparticle transport in the FM/SC/FM structure. The motion of conduction electrons in FM can be described by an effective single-particle Hamiltonian with an exchange splitting $2h_0$. In the absence of spin-flip scattering, the spin-dependent (four-component) BdG equations may be decoupled into two sets of two-component equations: one for the spin-up electronlike and spin-down hololelike quasiparticle wave functions $(u_\uparrow, v_\uparrow)$, the other for $(u_\downarrow, v_\downarrow)$. The BdG equation for $(u_\uparrow, v_\uparrow)$ is given by

$$
\begin{pmatrix}
H_0(\mathbf{r}) - h(\mathbf{r}) & \Delta(x) \\
\Delta^*(x) & -H_0^{\text{T}}(\mathbf{r}) - h(\mathbf{r})
\end{pmatrix}
\begin{pmatrix}
u_\uparrow(x) \\
v_\downarrow(x)
\end{pmatrix}
= E
\begin{pmatrix}
u_\uparrow(x) \\
v_\downarrow(x)
\end{pmatrix},
$$

(1)

where $H_0(\mathbf{r}) = -\hbar^2 \nabla^2/2m + V(\mathbf{r}) - E_F$ with $V(\mathbf{r})$ the usual static potential, and the excitation energy $E$ is measured relative to Fermi energy $E_F$.

For the injection of a spin-up electron from the left FM, as shown in Fig. 1(a), there are four possible trajectories: normal reflection ($b_\uparrow$), Andreev reflection ($a_\uparrow$), transmission to the right electrode as an electronlike quasiparticle ($c_\uparrow$), and as a hololelike quasiparticle ($d_\downarrow$). We wish to point out that AR coefficient $a_\uparrow$ is labeled with subscript $\uparrow$, for the AR results in an electron deficiency in the spin-down subband in the left FM. With general solutions of the BdG equation (1), the wave functions in three regions have the following form:

$$
\Psi_1 = \begin{pmatrix}
1 \\
e^{iq_1 x} + a_\uparrow
\end{pmatrix}
\begin{pmatrix}
0 \\
e^{iq_1 x} + b_\uparrow
\end{pmatrix}
\begin{pmatrix}
1 \\
e^{-iq_1 x}
\end{pmatrix}
$$

(2)

for $x < 0$,

$$
\Psi_2 = \begin{pmatrix}
u_\uparrow \\
e^{ik_1 x} + f \nu_\uparrow
\end{pmatrix}
\begin{pmatrix}
u_\downarrow \\
e^{-ik_1 x} + g \nu_\downarrow
\end{pmatrix}
\begin{pmatrix}
u_\uparrow \\
e^{ik_1 x}
\end{pmatrix}
$$

(3)

for $0 < x < L$, and

$$
\Psi_3 = \begin{pmatrix}
1 \\
e^{iq_1 x} + d_\downarrow
\end{pmatrix}
\begin{pmatrix}
0 \\
e^{-iq_1 x}
\end{pmatrix}
$$

(4)

for $x > L$. Here $q_\uparrow = \sqrt{2m(E_F + E + h_0)/\hbar}$ and $q_\downarrow = \sqrt{2m(E_F - E - h_0)/\hbar}$ indicate different Fermi wave vectors for the spin-up electron and spin-down hole in FM, and
COHERENT QUANTUM TRANSPORT IN . . .


FIG. 2. Reflection and transmission probabilities \( A_s \), \( B_s \), \( C_s \), and \( D_s \) (with \( s = \uparrow \) and \( s = \downarrow \)) as a function of \( E/\Delta \) for different \( h_0/E_F \) in the P (left column) and AP (right column) configurations. Here \( \Delta/E_F = 10^{-3} \), \( k_F L = 5000 \), and \( z = 0 \).

For the injection of an electron (a hole) with such a energy, we have \( A_\uparrow(E) = D_\downarrow(E) = \tilde{A}_\downarrow(E) = \tilde{D}_\downarrow(E) = 0 \). In this case, there is neither AR nor hole (electron) transmission, the quasiparticles pass from one FM electrode to the other via SC without creation or annihilation of Cooper pairs. The oscillation period is increased with \( E \), approaching to \( 2\pi E_F/(\Delta k_F L) \) for \( E \gg \Delta \).

Figures 2 and 3 show these coefficients as a function of \( E \) for different exchange splitting \( h_0 \) in FM’s and different barrier strength \( z \), exhibiting oscillatory behavior due to the coherent tunneling through the FM/SC/FM structure. The parameters used in the calculation are \( E_F/\Delta = 10^3 \) and \( k_F L = 5000 \). For \( z = 0 \), as shown in Fig. 2, the AR plays an important role in the coherent tunneling. In this case, for \( E < \Delta \), \( C_s \), \( \tilde{C}_s \), \( \tilde{C}_s \), and \( \tilde{D}_s \) are almost vanishing, so that in this energy range only \( A_s(E) = \tilde{A}_s(E) \), but also \( B_s(E) \approx \tilde{B}_s(E) \). The spin-\( s \) electron incident to the left FM/SC interface and its AR give rise to creating the Cooper pair in SC, while the spin-\( \bar{s} \) hole incident to the right FM/SC interface and its AR corresponds to the process that a couple of electrons due to the Cooper pair broken transmit into the right FM. It is found that with increasing \( h_0 \), the AR coefficients \( A_s \) are suppressed and the normal reflection coefficients \( B_s \) are increased. For \( E > \Delta \), as \( h_0 \) is increased, the oscillatory amplitudes for \( \tilde{C}_s \), \( B_s \), and \( \tilde{D}_s \) are increased. The oscillatory behavior stems from interference effects in SC between electronlike and holelike quasiparticles. The oscillation period for these coefficients is determined by Eq. (5),

\[
\left( \frac{E}{\Delta} \right)^2 = \frac{\left( \frac{2 \pi n(E_F/\Delta)}{k_F L} \right)^2}{1 + 1 - \frac{\Delta}{E \Delta}^2}/2.
\]
depending on the thickness of the SC interlayer at fixing $\Delta/E_F$ value. For a very thin superconducting film, the period is very large so that the oscillation is less pronounced.

An increase of the barrier strength gives rise to reducing $A_s$, $C_s$, $\tilde{A}_s$, and $\tilde{C}_s$ and to enhancing $B_s$, $D_s$, $\tilde{B}_s$, and $\tilde{D}_s$, as shown in Fig. 3. As $z$ is increased to be 1, each peak in $A_s$ has split across. In the tunnel limit ($z = 5$ in Fig. 4), each split peak becomes two sharp peaks, corresponding to a series of bound states of quasiparticles in SC. It is found that the positions of these peaks are determined by $k_+L = n\pi$ and $k_-L = n\pi$ and the minimum between the two adjacent peaks is determined by $(k_+ - k_-)L = (2n - 1)\pi$ with $n$ the positive

FIG. 3. The same as in Fig. 2 except that different values of $z$ are taken for $h_0/E_F = 0.5$ fixed.

FIG. 4. The same as in Fig. 3 except that $h_0/E_F = 0.2$. 
integer. This result may be understood by the following argument. In the large $z$ limit, Eq. (A1) is reduced to

$$a_{n} = \left( \frac{1}{2z^2} \right) \left( \frac{iuvr \cos[(k_{+} - k_{-})L/2] + O(1/z)}{(u^2 - v^2)\sin(k_{+}L)\sin(k_{-}L) + O(1/z)} \right) \times \sin[(k_{+} - k_{-})L/2],$$

(6)

where $O(1/z)$ stands for those terms proportional to $1/z$. In this case, in addition to the AR coefficients vanish at $(k_{+} - k_{-})L = 2\pi n$, same as in Eq. (5); they have additional minima at $(k_{+} - k_{-})L = (2n - 1)\pi$. In reality, these minima are close to zero in the large $z$ limit, so that each peak in $A_{z}$ or $\tilde{A}_{z}$ for $z = 0$ splits into two sharp peaks, as shown in Fig. 4. On the other hand, the dominant term in the denominator is proportional to $\sin(k_{+}L)\sin(k_{-}L)$, so that the AR coefficients exhibit maxima or peaks at $k_{+}L = n\pi$ and $k_{-}L = n\pi$. These bound states are the result of quantum interference between electronlike quasiparticles in the SC well and between holelike ones, respectively.

III. DIFFERENTIAL CONDUCTANCE

Once all the transmission and reflection probabilities are obtained, we can calculate the current in response to a difference in chemical potential between the two FM’s, $\mu_{L} - \mu_{R}$. Since the current must be conserved, it can be calculated in any plane. In the P configuration, the current coming into the SC interlayer via the left FM/SC interface is given by

$$I_{L} = e(\mu_{L} - \mu) \sum_{x = \pm} P_{x} \left[ 1 + A_{z} - B_{z} \right]$$

$$+ e(\mu - \mu_{R}) \sum_{x = \pm} P_{x} \left[ \tilde{C}_{z} - \tilde{D}_{z} \right],$$

(7)

where $\mu$ is the chemical potential of SC, and $P_{1} = 1 - P_{-} = \frac{1}{2}(1 + h_{0}/E_{F})$. The current coming out of the SC interlayer via the right FM/SC interface is given by

$$I_{R} = e(\mu_{L} - \mu) \sum_{x = \pm} P_{x} \left[ C_{z} - D_{z} \right]$$

$$+ e(\mu - \mu_{R}) \sum_{x = \pm} P_{x} \left[ 1 + \tilde{A}_{z} - \tilde{B}_{z} \right].$$

(8)

The current conservation requires $I_{L}$ equal to $I_{R}$, from which $\mu$ can be determined. For the present FM/SC/FM structure, the two FM’s are identical to each other. In this case we find that $\mu = (\mu_{L} + \mu_{R})/2$ in either P or AP configuration. The differential conductance is given by

$$G_{p}(E) = G_{0} \sum_{x = \pm} P_{x} \left[ 1 + A_{z}(E) - B_{z}(E) + \tilde{C}_{z}(E) - \tilde{D}_{z}(E) \right],$$

(9)

in the P configuration and

in the AP configuration with $G_{0} = 2e^{2}/h$. Although the same symbols of $A_{z}(E)$, $B_{z}(E)$, $\tilde{C}_{z}(E)$, and $\tilde{D}_{z}(E)$ are used in Eqs. (9) and (10) without difference, they have different expressions and values in the P and AP configurations, e.g., shown in Figs. 2–4. We wish to point out that the expressions for the differential conductance given by Eqs. (9) and (10) are quite different from Eq. (3.3) of Ref. 39. In the latter only the terms of $1 + A_{z}(E) - B_{z}(E)$ were taken into account, they correspond to the contribution of electron current via the left interface at $s = 0$. It is found that the differential conductance calculated by $1 + A_{z}(E) - B_{z}(E)$ is different from that calculated by $C_{z}(E) - D_{z}(E)$, as shown in Fig. 5. Here the solid and dashed lines correspond, respectively, to the contributions of electron currents via the left and right interfaces. They differ from each other not only in magnitude, but also in phase, especially in the metallic limit or for $E < \Delta$. Such a phase difference arises from the creation and annihilation of Cooper pairs with the electrons passing through the SC interlayer. We have numerically calculated the differential conductance spectrum $G$ by use of Eqs. (9) and (10) in the P and AP configurations of the two FM’s. Figure 6 shows the normalized conductance $G$ versus energy $E/\Delta$ for different $z$. Comparing Fig. 6 with Fig. 5, one finds that the present calculated result (the solid lines in Fig. 6) is a combined contribution of electron and hole tunneling processes in two opposite directions. Although the result in Fig. 6 is calculated at the left interface by use of Eqs. (9) and

\begin{figure}
\centering
\includegraphics[width=\textwidth]{Fig5}
\caption{Differential conductance as a function of $E/\Delta$ at different $z = 0$ (a), $z = 1$ (b), and $z = 2$ (c) in the P configuration, respectively, calculated by $1 + A_{z}(E) - B_{z}(E)$ (solid lines) and by $C_{z}(E) - D_{z}(E)$ (dashed lines). Here $\Delta/E_{F} = 10^{-3}$, $k_{F}L = 5000$, and $h_{0}/E_{F} = 0.6$.}
\end{figure}
along one direction and the hole currents along the other direction are simultaneously taken into account. Such an approach can guarantee the conservation of charge and spin currents in the present structure. The quantum interference effects of quasiparticle in the SC interlayer give rise to oscillations of reflection and transmission probabilities as well as conductances with energy above the superconducting gap, the Andreev reflection $A(E)$ and the corresponding transmission $D(s)$ vanishing for $k_+ - k_- = 2n\pi/L$. In the tunnel limit of large $z$, all the reflection and transmission coefficients exhibit sharp peaks at the energy satisfying $k_+L = n\pi$ or $k_-L = n\pi$. Another interesting result is that the conductance spectra in the P and AP magnetization configurations have a $\pi$ phase difference in the metallic limit, but they have the same phase in the tunnel case of finite $z$. The difference between $G_P(E)$ and $G_{AP}(E)$ exhibits oscillatory behavior from positive and negative.

It is expected that the theoretical results obtained will be confirmed in the future experiments. In principle, oscillation of differential conductance with the period of geometrical resonance could be used for spectroscopy of quasiparticle excitations in SC. In the present model, we have neglected the spatial variation of the pair potential in the SC due to proximity effects and the spin flip of the spin polarized currents. Inclusion of these effects would be necessary for a complete theory, which merits further study.

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APPENDIX: EXPRESSIONS FOR REFLECTION AND TRANSMISSION COEFFICIENTS

In the P configuration

Using the boundary conditions on the wave functions given by Eqs. (2)–(4) and carrying out a little tedious algebra, we find

$$\begin{align*}
A_1 &= -16r_1u\nu \sin[(k_+ - k_-)L/2](r_1 + r_1) \\
&\times \sin[(k_+ - k_-)L/2] + i(u^2 - v^2) \\
&\times [1 - (2zi + r_1)(2zi - r_1)] \\
&\times \cos[(k_+ - k_-)L/2]/M, \\
\end{align*}
$$

$$\begin{align*}
b_1 &= [(u^2 - v^2)^2(2zi + r_1 - 1)(2zi - r_1 - 1)(2zi - r_1 - 1)^2e^{i(k_+ + k_-)L} + (2zi + r_1 + 1)(2zi - r_1 + 1) \\
&\times (2zi - r_1 + 1)^2e^{-i(k_+ + k_-)L} - 2uw^2v^2[\cos(k_+ - k_-)L - 1][(2zi - r_1)^2 - 1][8z^2 + (r_1 + 1)^2 + (r_1 - 1)^2] \\
&\times [(2zi - 1)^2 - r_1^2](2zi - r_1 + 1)^2Q + [(2zi + 1)^2 - r_1^2](2zi - r_1 - 1)^2W]/M, \\
\end{align*}
$$
\[
\begin{align*}
    c_i &= -4r_1(u^2 - v^2)e^{-iq_1L}[(2zi - r_1 - 1)^2e^{ik\cdot L} - (2zi - r_1 + 1)^2e^{-ik\cdot L}]u^2 + [(2zi - r_1 + 1)^2e^{-ik\cdot L} - (2zi - r_1 - 1)^2e^{ik\cdot L}]u^2] / M, \\
    d_i &= 16ir_1uv(u^2 - v^2)e^{iq_1L}[(1 + (2zi + r_1)(2zi - r_1)] \\
    &\times \cos[(k + k_\perp)L/2] - i(4zi + r_1 - r_1) \\
    &\times \sin[(k + k_\perp)L/2]]\sin[(k + k_\perp)L/2]) / M, \\
    Q &= 2u^2v^2 - u^4e^{(k - k_\perp)L} - v^4e^{-ik\cdot L}, \\
    W &= 2u^2v^2 - u^4e^{-ik\cdot (k + k_\perp)L} - v^4e^{ik\cdot (k + k_\perp)L},
\end{align*}
\]

with

\[
\begin{align*}
    b_i &= -e^{2iq_1L}[(u^2 - v^2)^2[2zi + r_1 - 1)^2(2zi - r_1 - 1)e^{ik\cdot L} + (2zi + r_1 + 1)^2(2zi - r_1 + 1)^2(2zi - r_1 + 1)^2 + 2u^2v^2[cos(k + k_\perp)L - 1][2zi + r_1 + 1)^2 + (2zi + r_1 - 1)^2] \times [(2zi + r_1)^2 + (2zi + r_1 - 1)^2(2zi - r_1)^2]W / M, \\
    c_i &= -4r_1(u^2 - v^2)e^{iq_1L}[(2zi + r_1 + 1)^2e^{ik\cdot L} - (2zi + r_1 - 1)^2e^{-ik\cdot L}]u^2 + [(2zi + r_1 - 1)^2e^{ik\cdot L}]u^2] / M, \\
    \bar{d}_i &= r_1 \frac{d_i}{r_1}. 
\end{align*}
\]

Here \( r_1 = q_1/k_F = \sqrt{1 + h_0/E_F}, \) \( r_1 = q_1/k_F = \sqrt{1 - h_0/E_F}, \) and \( z = mU_0/(h^2k_F). \)