Junctions with ferromagnetic contacts to probe the pairing symmetry of iron pnictide superconductors

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Abstract. The quantum transport of junctions with an iron-based superconductor (SC) of antiphase s-wave pairing, sandwiched in between two ferromagnets, is studied by the use of an extended Blonder–Tinkham–Klapwijk approach. It is shown that due to novel interband interference in the SC, oscillations of not only reflection and transmission probabilities but also differential conductances with energy in both ferromagnetic and antiferromagnetic magnetization alignments exhibit conspicuously characteristic peak and dip behavior at two gap energies. More importantly, the behavior is found to be thoroughly different from those without antiphase s-wave pairing for the SC, which can be used to experimentally probe the antiphase s-wave pairing in iron-based SCs.

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1. Introduction

The recent discovery of superconductivity in iron pnictides has kindled much interest among members of the scientific community [1–12]. As faced by all newly discovered superconductors (SCs) with unconventional behavior, one of the important issues for iron-based SCs is the determination of pair potential symmetry. Although a number of works have contributed to this issue, final agreement has not yet been reached [7]; many order parameter (OP) symmetries such as s-wave and d-wave have been put forward. A leading contender is the so-called antiphase s-wave or \( s^\pm \)-pairing state of the multiband SC, where the pair potentials for the hole and electron bands are of isotropic s-wave state but have opposite signs.

It is important to confirm \( s^\pm \)-pairing in iron-based SCs by experiments [9]. The probe of low-energy quantum transport properties of SC materials in experiments has proven to be a highly useful tool to extract information about the symmetry of the superconducting OP [13–17]. In particular, Andreev spectroscopy is generally regarded as a powerful experimental probe to derive the superconducting OP. For instance, in a simple normal metal/SC junction [18], both the nodal and nodeless superconductivities can be deduced from the absence or presence of zero-bias conductance peaks due to the Andreev surface bound state, which contains important and clear signatures of the orbital structure of the OP [14, 17].

In this work, tunneling with ferromagnetic contacts is proposed, in which an iron-based SC is sandwiched in between two magnets (FMs), to be used for experimentally probing the \( s^\pm \)-pairing state. There are two typical cases [19]. One case is that the thickness of the SC is much larger than the SC coherence length and the majority of carriers form Cooper pairs. An electron-like excitation in an FM with energy lower than the \( s^\pm \)-SC energy gap cannot enter the \( s^\pm \)-SC region and performs only via Andreev reflection; it is either reflected from the first or second band of the \( s^\pm \)-SC at the left FM/\( s^\pm \)-SC interface as a hole or reflected back into the first or second band as an electron at the right \( s^\pm \)-SC/FM interface. Therefore, the constructively novel band interference of electron- and hole-like excitations coming from the two different bands results in the formation of the novel Andreev bound state in the \( s^\pm \)-SC, which plays an important role in the transfer of polarized electron-like particles through the junction. Moreover, the spin of quasiparticles may be reversed during the Andreev reflection process because of the spin splitting of the energy band, i.e. the Andreev reflected quasiparticle can gain or lose spin-splitting energy, so that the conductance spectrum of the FM/\( s^\pm \)-SC/FM junction can exhibit very different behavior, as the two magnetizations are parallel or antiparallel to each other. The other case is that the situation of the so-called subgap transport in the junction is quite

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opposite and the SC thickness is smaller than or comparable to the SC coherence length in which the majority of carriers is transferred directly from one FM to another at low energy below the superconducting gap. Similarly, due to the interband interference in the SC, the different magnetic alignments of the two magnetizations can lead to very different behavior of the conductance spectrum of the FM/s±-SC/FM junction. These, in turn, can all be used to more favorably discern the OP symmetry of the iron-based SC.

We extend the Blonder–Tinkham–Klapwijk (BTK) approach [20] to studying the FM/s±-SC/FM junction by taking into account the interference between the two relevant bands in the iron-based SC as also in other multiband SCs, in which the thickness of the SC is much larger than the SC coherence length. It is found that the parallel (F) and antiparallel (AF) magnetizations of two FMs can give rise to very different characteristics for conductances. For comparison, the results for FM/s±-SC/FM junctions without antiphase s-wave pairing or with s++-pairing for the SC including the conventional s-wave state are also presented. It is shown that, compared with s++-pairing, s±-pairing can lead to remarkable transport properties because of the novel interband interference in s±-SC, i.e. the reflection and transmission probabilities as well as differential conductances with energy exhibit conspicuous characteristic peak and dip structures, which can survive in both F and AF alignments; however, this is not the case for the s++-pairing model. Therefore, such features of the FM/s±-SC/FM junction may be used to experimentally probe and identify the antiphase s-wave pairing in iron-based SCs. This work is organized as follows. In section 2, the model and theory are presented. In section 3, we present the numerical calculations and the discussions. Finally, the summary is given in section 4.

2. Model and theory

A ferromagnetic contact can be modeled by the x-direction, in which the left and right FMs are assumed to be identical and separated from the central s±-pairing SC of thickness \( a \). The layers are in the y–z-plane and stacked along the x-direction. A subband model with spin-splitting energy \( \Delta \) is applied for the FMs. The two FMs have the same exchange energy described by \( h(\mathbf{r}) = h_0 [\Theta ( -x ) \pm \Theta ( x - a ) ] \), where the plus and minus signs, respectively, stand for the F and AF alignments, \( \Theta ( x ) \) is the Heaviside step function and \( h_0 \) equals \( \Delta / 2 \). The two interfaces are, respectively, described by \( \delta \)-type barrier potentials \( U(x) = U_0 [\delta(x) + \delta(x-a)] \) with \( U_0 \) being the barrier strength.

The iron-based SC possesses two superconducting gap energies \( \Delta_{1,2} \) in both bands with the corresponding Fermi wave vectors \( p \) and \( q \); moreover, the relevant superconducting phases of the gaps \( \Delta_{1,2} \) are \( \varphi_1 \) and \( \varphi_2 \). For the s±-pairing model with unequal s-wave gaps of opposite sign, we have \( \varphi_1 - \varphi_2 = \pi \), while for the s++-pairing model with gaps of the same sign, we have \( \varphi_1 = \varphi_2 \). The standard Bogoliubov coefficients \( u \) and \( v \) are, respectively, given by \( u_{1(2)} = \sqrt{1 + \Omega_{1(2)} / E} / 2 \) and \( v_{1(2)} = \sqrt{1 - \Omega_{1(2)} / E} / 2 \) with \( \Omega_{1(2)} = \sqrt{E^2 - \Delta_{1(2)}^2} \). The mixing coefficient \( \alpha_{0} \) is defined to describe the ratio of probability amplitudes for an electron crossing the interface from the left FM to tunnel into the first and second bands in the SC or for an electron crossing the interface from the two bands of the SC into the right FM [17].

We start with the Bogoliubov–de Gennes (BdG) equation for the quasiparticle spectrum [21]. In the absence of spin-flip scattering, the spin-dependent (four-component) BdG equation may be decoupled into two sets of two-component equations: one is for the spin-\( \sigma \) electron-like and spin-\( \bar{\sigma} \) hole-like quasiparticle wave functions \( (u_\sigma, v_\bar{\sigma}) \), and the other

\begin{equation}
\end{equation}
is \((u_\sigma, v_\sigma)\), where \(\sigma\) is the spin index with \(\uparrow\) or \(\downarrow\) and \(\bar{\sigma}\) is the spin opposite to \(\sigma\). The BdG equation for \((u_\sigma, v_\sigma)\) is given by

\[
\begin{pmatrix}
H_0(\mathbf{r}) - h(\mathbf{r}) & \Delta(x) \\
\Delta^*(x) & -H_0(\mathbf{r}) - h(\mathbf{r})
\end{pmatrix}
\begin{pmatrix}
\begin{pmatrix}
u_1 e^{-i\psi_1} \\
v_1 e^{i\psi_1}
\end{pmatrix} e^{ip_{\uparrow} x} + a_0 \begin{pmatrix}
u_2 e^{-i\psi_2} \\
v_2 e^{i\psi_2}
\end{pmatrix} e^{iq_{\uparrow} x}
\end{pmatrix} + f \begin{pmatrix}
u_1 e^{i\psi_1} \\
v_1 e^{-i\psi_1}
\end{pmatrix} e^{ip_{\uparrow} x} + a_0 \begin{pmatrix}
u_2 e^{i\psi_2} \\
v_2 e^{-i\psi_2}
\end{pmatrix} e^{iq_{\uparrow} x}
\end{array}
\begin{array}
\begin{pmatrix}
u_1 e^{-i\psi_1} \\
v_1 e^{i\psi_1}
\end{pmatrix} e^{ip_{\downarrow} x} + a_0 \begin{pmatrix}
u_2 e^{-i\psi_2} \\
v_2 e^{i\psi_2}
\end{pmatrix} e^{iq_{\downarrow} x}
\end{pmatrix} + h \begin{pmatrix}
u_1 e^{i\psi_1} \\
v_1 e^{-i\psi_1}
\end{pmatrix} e^{ip_{\downarrow} x} + a_0 \begin{pmatrix}
u_2 e^{i\psi_2} \\
v_2 e^{-i\psi_2}
\end{pmatrix} e^{iq_{\downarrow} x}
\end{array}
\begin{array}
\begin{pmatrix}
u_1 e^{-i\psi_1} \\
v_1 e^{i\psi_1}
\end{pmatrix} e^{ip_{\uparrow} x} + a_0 \begin{pmatrix}
u_2 e^{-i\psi_2} \\
v_2 e^{i\psi_2}
\end{pmatrix} e^{iq_{\uparrow} x}
\end{array}
\begin{array}
\begin{pmatrix}
u_1 e^{i\psi_1} \\
v_1 e^{-i\psi_1}
\end{pmatrix} e^{ip_{\downarrow} x} + a_0 \begin{pmatrix}
u_2 e^{i\psi_2} \\
v_2 e^{-i\psi_2}
\end{pmatrix} e^{iq_{\downarrow} x}
\end{array}
\end{pmatrix}
\end{equation}

for \(x < 0\), and

\[
\Psi_{\text{III}} = c_1 \begin{pmatrix}
1 \\
0
\end{pmatrix} e^{ik_{\text{left}, x}^1} + d_1 \begin{pmatrix}
0 \\
1
\end{pmatrix} e^{-ik_{\text{right}, x}^1}
\end{equation}

for \(x > a\), where \(k_{\text{left}, L, \sigma} = \sqrt{2m(E_F + (-E + \eta_\sigma h_0))/\hbar}\), \(k_{\text{right}, R, \sigma}\) is given by \(k_{\text{left}, L, \sigma}\) with \(L \rightarrow R\), \(p_{\pm} = \sqrt{2m(E_F \pm \Omega_1)/\hbar}\), \(q_{\pm} = \sqrt{2m(E_F \pm \Omega_2)/\hbar}\), \(\eta_\sigma = 1\) for \(\sigma = \uparrow\) and \(\eta_\sigma = -1\) for \(\sigma = \downarrow\).
In equations (2)–(4), all the transmission and reflection coefficients are determined by the following boundary conditions at $x = 0$ and $x = a$, which are given by

\[ \Psi_{\Pi}(0) = \Psi_{I}(0), \]  
\[ (d\Psi_{\Pi}/dx)_{x=0} = (d\Psi_{I}/dx)_{x=0} = 2mU_0\Psi_{I}(0)/\hbar^2, \]  
\[ \Psi_{\Pi}(a) = \Psi_{II}(a), \]  
\[ (d\Psi_{\Pi}/dx)_{x=a} = (d\Psi_{II}/dx)_{x=a} = 2mU_0\Psi_{II}(a)/\hbar^2. \]

Since the analytical results for these coefficients are tedious, we only present expressions for $a_\perp$, $b_\perp$, $c_\perp$ and $d_\perp$ for the F alignment in the appendix. From them, we get $A_{\sigma} = |a_{\sigma}|^2k_{hL,\sigma}/k_{cL,\sigma}$, $B_{\sigma} = |b_{\sigma}|^2$, $C_{\sigma} = |c_{\sigma}|^2$ and $D_{\sigma} = |d_{\sigma}|^2k_{hL,\sigma}/k_{cL,\sigma}$, respectively, corresponding to the AR and normal reflection probabilities, the transmission probabilities of hole-like and electron-like quasiparticles.

As in [22–24], to guarantee current conservation, it is necessary to simultaneously consider that not only are spin-polarized electrons incident on the left FM/$s_{\pm}$-SC interface from the left FM, but also the spin-polarized holes can tunnel through the right $s_{\pm}$-SC/FM interface from the right FM, as shown in figure 1(b). The corresponding $\vec{a}_\perp$, $\vec{b}_\perp$, $\vec{c}_\perp$ and $\vec{d}_\perp$ can be obtained by a similar calculation, and then all the related probabilities in the AR alignment can be similarly acquired. Here, a dimensionless parameter $Z = 2mU_0/(\hbar^2k_F)$, with $k_F$ being the Fermi wave vector in the SC, is introduced to describe the barrier strength at the two interfaces.

3. Results and discussions

In this section, we, respectively, perform the numerical calculations for $s_{\pm}$- and $s_{++}$-pairings, and mainly focus on the effects of the mixing coefficient $\alpha_0$, the superconducting gap ratio $\beta$ ($\Delta_2/\Delta_1$) and magnetization alignments. In figures 2 and 3, $A_{\sigma}$, $B_{\sigma}$, $C_{\sigma}$ and $D_{\sigma}$ are plotted as a function of $E$ for different $\alpha_0$ and $\beta$ with $s_{\pm}$- and $s_{++}$-pairings, respectively. The main characteristic of the variation of all probabilities with $E$ is the oscillating behavior, which stems from interference effects in the SC between electron- and hole-like quasiparticles as in FM/$s$-wave SC/FM junctions [23, 24]. The behavior in the vicinity of superconducting gap energy is quite important, which directly contains information on the superconducting OP; hence, much attention is paid to it. The parameters used in the calculations are $E_F/\Delta_2 = 10^3$, $k_F a = 5000$ [25] and $Z = 1.0$, which indicates very low interface transparency of the electron and hole. In figure 2(a), except for the normal reflection probability $B_{\sigma}$, other probabilities are found to have no significant differences between the F and AF alignments as in the FM/$s$-wave SC/FM junction [23, 24]. When $\alpha_0 = 0$, the $s_{\perp}$-SC reduces to the conventional $s$-wave one, so that the results shown in figure 2(a) are the same as those obtained in [23, 24]. When $\alpha_0 \neq 0$, the AR probability $A_{\sigma}$ has two peaks: one at $E/\Delta_2 = 1.0$ and the other at $E/\Delta_2 = 0.5$, which just indicates two OPs. For $C_{\sigma}$, the point at $E/\Delta_2 = 1.0$ is an inflection one, which arises from the $s_{\pm}$-pairing. It is noted that $D_{\sigma}$ at $E/\Delta_2 = 1.0$ has a dip accompanied by the splitting of a peak with $\alpha_0 \neq 0$, which is also just attributed to the $s_{\pm}$-pairing. Interestingly, one finds that the normal reflection probability $B_{\sigma}$ at $E/\Delta_2 = 0.5$ has a dip accompanied by a peak for both F and AF alignments. However, with $\alpha_0$ unequal to 0, $B_{\sigma}$ at $E/\Delta_2 = 1.0$ has a dip accompanied by the splitting of a peak for both F and AF alignments although the splitting is not pronounced in the F alignment. This also manifests the strong dependence of splitting for
Figure 2. Reflection and transmission probabilities $A_\sigma$, $B_\sigma$, $C_\sigma$ and $D_\sigma$ (with $\sigma = \uparrow$ and $\sigma = \downarrow$) as a function of $E/\Delta_2$ for $\alpha_0 = 0.0$, 0.3 and 0.5 in the F (the left column) and AF (the right column) alignments. Here, $\Delta \varphi = \pi$ (a) and 0 (b), $k_F a = 5000$, $h_0/E_F = 0.5$, $\beta = 2$, $\Delta_2/E_F = 10^{-3}$ and $Z = 1.0$. 

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Figure 3. Reflection and transmission probabilities $A_\sigma$, $B_\sigma$, $C_\sigma$ and $D_\sigma$ (with $\sigma = \uparrow$ and $\sigma = \downarrow$) as a function of $E/\Delta_2$ for $\beta = 1.0$, 2.0 and 4.0 in the $F$ (the left column) and $AF$ (the right column) alignments. Here $\Delta \phi = \pi$ (a) and 0 (b), $\alpha_0 = 0.3$, and the other parameters are the same as in figure 2.
$B_\sigma$ at $E/\Delta_2 = 1.0$ on magnetization alignments. The physical origin is that the reflected wave vector with the same energy at the $s_\pm$-SC/FM interface is different for different magnetization alignments, so that the interband interference in the $s_\pm$-SC is different. For comparison, we also present the relevant probabilities for the $s_{++}$-pairing model in figure 2(b). It is seen from figures 2(a) and (b), at $\alpha_0 = 0.0$, that the amplitudes of all relevant probabilities for both the $s_{++}$- and $s_\pm$-pairing models are the same because the two SCs are really the same $s$-wave conventional one with a single band. However, it is found that when $\alpha_0 \neq 0$, $\overline{C}_\sigma$ at $E/\Delta_2 = 1.0$ for the $s_{++}$-pairing model no longer has any inflection point. In particular, when $\alpha_0 \neq 0$, for the $s_{++}$-pairing model, the behavior of $B_\sigma$ at $E/\Delta_2 = 0.5$ with a dip accompanied by a peak and of $\overline{D}_\sigma$ at $E/\Delta_2 = 1.0$ with a dip accompanied by the splitting of a peak no longer appears, regardless of F and AF alignments. These differences can be explained as follows: for a single band, all incident electrons at the SC/FM interface are reflected into the same band; however, this situation is altered at $\alpha_0 \neq 0$ in a different manner for $s_\pm$- and $s_{++}$-pairings. For the former, all incident electrons at the SC/FM interface are reflected into the two different bands with OPs of opposite signs; however, for the latter, although two bands exist, they have OPs with the same signs; consequently, the interband interferences in the SC are very different from the former, giving rise to the above-mentioned different features of the correlative probabilities. The differences can also be explained by the fact that in the expressions for four probabilities in the appendix, $e^{-i\psi_1}$ and $e^{-i\psi_2}$ exert an important influence on the tunneling, which are unequal for the $s_\pm$-pairing model and equal for the $s_{++}$-pairing model.

In figures 3(a) and (b), it is clear that the features of the reflection and transmission probabilities in both F and AF alignments almost remain unchanged with increasing $\beta$ as in figure 2, except that $\beta = 1$. We find that at $\beta = 1$, the behavior of the four probabilities for the two models is virtually the same, respectively, although the values are different, which can be easily explained as expected. Here, it is worth noting that when $\beta = 1$ and $\Delta\psi = 0$, this exactly represents the case of conventional SC. Although the first peak of $A_\sigma$ in both figures 3(a) and (b), together with the dip of $B_\sigma$ in figure 3(a), is shown to shift to lower energy for both F and AF alignments when $\beta$ is enhanced, these only imply the increase in the ratios of OP magnitudes. As a result, compared with the situation for the $s_{++}$-pairing model, one key property for the $s_\pm$-pairing model is concluded: that novel features of $B_\sigma$ at $E/\Delta_2 = 0.5$ with a dip accompanied by a peak and of $\overline{D}_\sigma$ at $E/\Delta_2 = 1.0$ with a dip accompanied by splitting of a peak in both F and AF alignments appear, which are ascribed to a different interband interference from that for the $s_{++}$-pairing model.

After obtaining all the relevant transmission and reflection probabilities, we can calculate the conductances in the F and AF alignments, respectively, given by [23, 24]

$$G_F(E) = G_0 \sum_{\sigma = \uparrow, \downarrow} P_\sigma [1 + A_\sigma(E) - B_\sigma(E) + \overline{C}_\sigma(E) - \overline{D}_\sigma(E)]$$

(9)

in the F alignment and

$$G_{AF}(E) = G_0 \sum_{\sigma = \uparrow, \downarrow} P_\sigma [1 + A_\sigma(E) - B_\sigma(E) + \overline{C}_\sigma(E) - \overline{D}_\sigma(E)]$$

(10)

in the AF alignment with $G_0 = 2e^2/h$.

In figure 4, the differential conductances in the F and AF alignments are shown as a function of $E$ with different $\alpha_0$, in which the $s_\pm$- and $s_{++}$-pairing models are all included. When
\(\alpha_0 = 0\), the results for the \(s_{\pm}\)-pairing model are the same as those for the \(s_{++}\)-pairing model because the two models are all reduced to the same conventional \(s\)-wave pairing one. For the \(s_{++}\)-pairing model in the left column of figure 4, when \(\alpha_0 \neq 0\), \(G_{F(AF)}\) at \(E/\Delta_2 = 1\) and \(E/\Delta_2 = 0.5\) has a peak, respectively, regardless of \(\alpha_0\), which is natural and indicates the two OPs as in conventional multiband SC models. However, for the \(s_{\pm}\)-pairing model, as shown in the right column of figure 4, when \(\alpha_0 \neq 0\), there is at least one sharp peak no matter the magnetization alignment and the value of \(\alpha_0\). In particular, for \(\alpha_0 \neq 0\), there exists no peak at \(E/\Delta_2 = 1\) in spite of magnetization alignments. These are quite different from those in the \(s_{++}\)-pairing model.

Differential conductances as a function of \(E\) are plotted in figure 5 with different \(\beta\) for both the \(s_{\pm}\) (the right column) and \(s_{++}\)-pairing (the left column) models in the F and AF alignments. It is found that when \(\beta = 1.0\), the features of the curves for the two models remain almost the same as those at \(\alpha_0 = 0.0\) shown in figure 4 although there exists only a slight difference in the values owing to the different interband interferences, which just resemble the cases of previous probabilities. It is to be noted that with increasing \(\beta\), the main features of differential conductances in the F and AF alignments for the two models are not significantly changed except for trivial variations. For example, the first peak of differential conductances are all also found to shift towards the lower energy with an enhancement of the band ratio. These can be naturally explained by the probabilities shown in figure 3. Therefore, another key property is deduced that for the \(s_{\pm}\)-pairing model, there is no longer an oscillation peak of tunneling differential conductances at the bigger gap energy and at least one peak is very sharp in both the F and AF alignments.

Finally, we wish to briefly discuss the three-dimensional (3D) effects on the calculated results. The previous parts of this paper only dealt with a 1D system, corresponding to a
perpendicular incidence to replace various angles of incidence. It is very easy to extend the 1D approach to a 3D structure. After performing numerical calculations, we found that there is no significant difference in the calculated results between 1D and 3D approaches.

4. Conclusion

By developing the BTK approach, we have studied the tunneling junction composed of two FMs and one sandwiched iron-based SC with \( s_{\pm} \)-pairing. In comparison with the \( s_{++} \)-pairing, the \( s_{\pm} \)-pairing is shown to lead to different transport properties owing to the novel interband interference in the iron-based SC. Two key properties of the \( s_{\pm} \)-pairing are achieved: one is the novel features for \( B_{\sigma} \) at the smaller gap energy with a dip accompanied by a peak and for \( \overline{D}_{\sigma} \) with a dip accompanied by splitting of a peak in both F and AF alignments; the other is that there is no longer an oscillation peak of tunneling differential conductances at the bigger gap energy and at least one peak is very sharp in both the F and AF alignments. These conspicuous low-energy transport properties can be used to discern the \( s_{\pm} \)-pairing symmetry of iron-based SC in experiments. It is pointed out that after performing numerical calculations of the dependence of differential conductance on energy at different voltages, we found that there is no significant change of the features. In addition, the features of the peaks and dip of differential conductance at two gap energies are found to remain unchanged at temperatures much lower than the critical temperature \( T_{C} \).

Figure 5. Differential conductance as a function of \( E/\Delta_{2} \) for the F (solid line) and AF (dashed line) alignments with \( \Delta \phi = 0 \) (the left column) and \( \Delta \phi = \pi \) (the right column) at different values of \( \beta \). Here the parameters are the same as in figure 3.
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Appendix. Expressions for the reflection and transmission coefficients in the F alignment

\[ a_t = t (v_1 e^{-i\varphi_1} + \alpha_0 v_2 e^{-i\varphi_2}) + f (u_1 e^{-i\varphi_1} + \alpha_0 u_2 e^{-i\varphi_2}) + g (v_1 e^{-i\varphi_1} + \alpha_0 v_2 e^{-i\varphi_2}) + h (u_1 e^{-i\varphi_1} + \alpha_0 u_2 e^{-i\varphi_2}), \]  
(A.1)

\[ b_t = t (u_1 + \alpha_0 u_2) + f (v_1 + \alpha_0 v_2) + g (u_1 + \alpha_0 u_2) + h (v_1 + \alpha_0 v_2) - 1, \]  
(A.2)

\[ c_t = t [u_1 e^{i(p_s - k_{\text{er}})a} + \alpha_0 u_2 e^{i(q_s - k_{\text{er}})a}] + f [v_1 e^{i(p_s - k_{\text{er}})a} + \alpha_0 v_2 e^{i(q_s - k_{\text{er}})a}] + g [u_1 e^{-i(p_s - k_{\text{er}})a} + \alpha_0 u_2 e^{-i(q_s + k_{\text{er}})a}] \]  
\[ + h [v_1 e^{-i(p_s + k_{\text{er}})a} + \alpha_0 v_2 e^{-i(q_s - k_{\text{er}})a}], \]  
(A.3)

\[ d_t = t [v_1 e^{-i(p_i + k_{\text{el}}a)} + \alpha_0 v_2 e^{-i(q_i - k_{\text{el}}a)}] + f [u_1 e^{-i(p_i - k_{\text{el}}a)} + \alpha_0 u_2 e^{-i(q_i - k_{\text{el}}a)}] + g [v_1 e^{-i(p_i + k_{\text{el}}a)} + \alpha_0 v_2 e^{-i(q_i - k_{\text{el}}a)}] \]  
\[ + h [u_1 e^{-i(p_i - k_{\text{el}}a)} + \alpha_0 u_2 e^{-i(q_i - k_{\text{el}}a)}]. \]  
(A.4)

In these expressions,

\[ t = \frac{\alpha'_0}{\gamma_4 \gamma_1 - \gamma_3 \gamma_2} [(\alpha_{10} \alpha_5 - \alpha_9 \alpha_6)(\gamma_2 \alpha_7 - \gamma_1 \alpha_8) - \alpha_6 \gamma_1 (\alpha_{12} \alpha_5 - \alpha_9 \alpha_8)], \]  
(A.5)

\[ f = \frac{\alpha'_0 \alpha_5}{\gamma_4 \gamma_1 - \gamma_3 \gamma_2} [(\alpha_{5} \alpha_{11} - \alpha_9 \alpha_7) \gamma_2 - (\alpha_{5} \alpha_{12} - \alpha_9 \alpha_8) \gamma_1], \]  
(A.6)

\[ g = -\frac{\alpha'_0 \alpha_5 \gamma_2 (\alpha_{10} \alpha_5 - \alpha_9 \alpha_6)}{\gamma_4 \gamma_1 - \gamma_3 \gamma_2}, \]  
(A.7)

and

\[ h = \frac{\alpha'_0 \alpha_5 \gamma_1 (\alpha_{10} \alpha_5 - \alpha_9 \alpha_6)}{\gamma_4 \gamma_1 - \gamma_3 \gamma_2}, \]  
(A.8)

where

\[ \gamma_1 = (\alpha_{15} \alpha_5 - \alpha_{13} \alpha_7)(\alpha_{10} \alpha_5 - \alpha_9 \alpha_6) - (\alpha_{14} \alpha_5 - \alpha_{13} \alpha_6)(\alpha_{11} \alpha_5 - \alpha_9 \alpha_7), \]  
(A.9)

\[ \gamma_2 = (\alpha_{16} \alpha_5 - \alpha_{13} \alpha_7)(\alpha_{10} \alpha_5 - \alpha_9 \alpha_6) - (\alpha_{14} \alpha_5 - \alpha_{13} \alpha_6)(\alpha_{12} \alpha_5 - \alpha_9 \alpha_8), \]  
(A.10)

\[ \gamma_3 = (\alpha_{3} \alpha_5 - \alpha_{1} \alpha_7)(\alpha_{10} \alpha_5 - \alpha_9 \alpha_6) - (\alpha_{2} \alpha_5 - \alpha_1 \alpha_6)(\alpha_{11} \alpha_5 - \alpha_9 \alpha_7), \]  
(A.11)
\( \gamma_4 = (\alpha_3 \alpha_5 - \alpha_1 \alpha_8)(\alpha_{10} \alpha_5 - \alpha_9 \alpha_6) - (\alpha_2 \alpha_5 - \alpha_1 \alpha_6)(\alpha_{12} \alpha_5 - \alpha_9 \alpha_8), \)  
(\text{A.12})

\[ \alpha'_0 = 2k_{el} \frac{1}{i}, \]  
(\text{A.13})

\[ \alpha_1 = -Z_k F(u_1 + \alpha_0 u_2) + (p_+ u_1 + \alpha_0 q_+ u_2 + k_{el} \frac{1}{i} u_1 + k_{el} \frac{1}{i} \alpha_0 u_2)i, \]  
(\text{A.14})

\[ \alpha_2 = -Z_k F(v_1 + \alpha_0 v_2) + (p_- v_1 + \alpha_0 q_- v_2 + k_{el} \frac{1}{i} v_1 + k_{el} \frac{1}{i} \alpha_0 v_2)i, \]  
(\text{A.15})

\[ \alpha_3 = -Z_k F(u_1 + \alpha_0 u_2) - (p_+ u_1 + \alpha_0 q_+ u_2 - k_{el} \frac{1}{i} u_1 - k_{el} \frac{1}{i} \alpha_0 u_2)i, \]  
(\text{A.16})

\[ \alpha_4 = -Z_k F(v_1 + \alpha_0 v_2) - (p_- v_1 + \alpha_0 q_- v_2 - k_{el} \frac{1}{i} v_1 - k_{el} \frac{1}{i} \alpha_0 v_2)i, \]  
(\text{A.17})

\[ \alpha_5 = -Z_k F(v_1 e^{-i\phi_1} + \alpha_0 v_2 e^{-i\phi_2}) + (p_+ v_1 e^{-i\phi_1} + q_+ \alpha_0 v_2 e^{-i\phi_2} - k_{hl} \frac{1}{i} v_1 e^{-i\phi_1} - \alpha_0 k_{hl} \frac{1}{i} v_2 e^{-i\phi_2})i, \]  
(\text{A.18})

\[ \alpha_6 = -Z_k F(u_1 e^{-i\phi_1} + \alpha_0 u_2 e^{-i\phi_2}) + (p_- u_1 e^{-i\phi_1} + q_- \alpha_0 u_2 e^{-i\phi_2} - k_{hl} \frac{1}{i} u_1 e^{-i\phi_1} - \alpha_0 k_{hl} \frac{1}{i} u_2 e^{-i\phi_2})i, \]  
(\text{A.19})

\[ \alpha_7 = -Z_k F(v_1 e^{-i\phi_1} + \alpha_0 v_2 e^{-i\phi_2}) - (p_+ v_1 e^{-i\phi_1} + q_+ \alpha_0 v_2 e^{-i\phi_2} + k_{hl} \frac{1}{i} v_1 e^{-i\phi_1} + \alpha_0 k_{hl} \frac{1}{i} v_2 e^{-i\phi_2})i, \]  
(\text{A.20})

\[ \alpha_8 = -Z_k F(u_1 e^{-i\phi_1} + \alpha_0 u_2 e^{-i\phi_2}) - (p_- u_1 e^{-i\phi_1} + q_- \alpha_0 u_2 e^{-i\phi_2} + k_{hl} \frac{1}{i} u_1 e^{-i\phi_1} + \alpha_0 k_{hl} \frac{1}{i} u_2 e^{-i\phi_2})i, \]  
(\text{A.21})

\[ \alpha_9 = Z_k F(u_1 e^{i\phi_1} + \alpha_0 u_2 e^{i\phi_2}) + (p_+ u_1 e^{i\phi_1} + q_+ \alpha_0 u_2 e^{i\phi_2} - k_{er} \frac{1}{i} u_1 e^{i\phi_1} - \alpha_0 k_{er} \frac{1}{i} u_2 e^{i\phi_2}), \]  
(\text{A.22})

\[ \alpha_{10} = Z_k F(v_1 e^{i\phi_1} + \alpha_0 v_2 e^{i\phi_2}) + (p_- v_1 e^{i\phi_1} + q_- \alpha_0 v_2 e^{i\phi_2} - k_{er} \frac{1}{i} v_1 e^{i\phi_1} - \alpha_0 k_{er} \frac{1}{i} v_2 e^{i\phi_2})i, \]  
(\text{A.23})

\[ \alpha_{11} = Z_k F(u_1 e^{-i\phi_1} + \alpha_0 u_2 e^{-i\phi_2}) - (p_+ u_1 e^{-i\phi_1} + q_+ \alpha_0 u_2 e^{-i\phi_2} + k_{er} \frac{1}{i} u_1 e^{-i\phi_1} + \alpha_0 k_{er} \frac{1}{i} u_2 e^{-i\phi_2})i, \]  
(\text{A.24})

\[ \alpha_{12} = Z_k F(v_1 e^{-i\phi_1} + \alpha_0 v_2 e^{-i\phi_2}) - (p_- v_1 e^{-i\phi_1} + q_- \alpha_0 v_2 e^{-i\phi_2} + k_{er} \frac{1}{i} v_1 e^{-i\phi_1} + \alpha_0 k_{er} \frac{1}{i} v_2 e^{-i\phi_2})i, \]  
(\text{A.25})

\[ \alpha_{13} = Z_k F(v_1 e^{-i(\phi_1 - \frac{1}{2} \alpha_3 + \alpha_0 v_2 e^{-i(\phi_2 - q_0)})} + [p_+ v_1 e^{-i(\phi_1 - \frac{1}{2} \alpha_3 + \alpha_0 v_2 e^{-i(\phi_2 - q_0)})} + q_+ \alpha_0 v_2 e^{-i(\phi_2 - q_0)} + k_{hl} \frac{1}{i} v_1 e^{-i(\phi_2 - q_0)} + \alpha_0 k_{hl} \frac{1}{i} v_2 e^{-i(\phi_2 - q_0)}])i, \]  
(\text{A.26})
\[ \alpha_{14} = k_F[u_1 e^{-i(\phi_1 - p\alpha)} + \alpha_0 u_2 e^{-i(\phi_2 - q\alpha)}] + [p_- u_1 e^{-i(\phi_1 - p\alpha)} + q_- \alpha_0 u_2 e^{-i(\phi_2 - q\alpha)}] \\
+ k_{hR} u_1 e^{-i(\phi_1 - p\alpha)} + \alpha_0 k_{hR} u_2 e^{-i(\phi_2 - q\alpha)}]i, \quad (A.27) \]

\[ \alpha_{15} = Z k_F[u_1 e^{-i(\phi_1 + p\alpha)} + \alpha_0 u_2 e^{-i(\phi_2 + q\alpha)}] - [p_+ u_1 e^{-i(\phi_1 + p\alpha)} + q_+ \alpha_0 u_2 e^{-i(\phi_2 + q\alpha)}] \\
- k_{hR} u_1 e^{-i(\phi_1 + p\alpha)} - \alpha_0 k_{hR} u_2 e^{-i(\phi_2 + q\alpha)}]i, \quad (A.28) \]

and

\[ \alpha_{16} = Z k_F[u_1 e^{-i(\phi_1 + p\alpha)} + \alpha_0 u_2 e^{-i(\phi_2 + q\alpha)}] - [p_- u_1 e^{-i(\phi_1 + p\alpha)} + q_- \alpha_0 u_2 e^{-i(\phi_2 + q\alpha)}] \\
- k_{hR} u_1 e^{-i(\phi_1 + p\alpha)} - \alpha_0 k_{hR} u_2 e^{-i(\phi_2 + q\alpha)}]i. \quad (A.29) \]

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