Accurate Asymptotic Forms of RKKY Interaction in a Simple Anisotropic Band Model. II

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1. Introduction

At the beginning, the results in paper I [1] are summarized briefly (see also ref. [4]). The simple anisotropic band model has the symmetrical Fermi surface around the k_z-axis. The situation can be divided into two cases, case A and case B. In case A, the Fermi surface makes the open orbit for the k_z-direction, and there is no Fermi surface perpendicular to its direction. In case B, the Fermi surface has sections perpendicular to the k_z-axis. The vector connecting two interacting f spins is denoted by $\boldsymbol{R}_{nt}=(R_\perp,0,R_z)$, in which $R_z=2\pi(n+t)/Q$, n is an integer, $0\leqq t<1$ and $2\pi/Q$ is the lattice spacing for the z-direction, and $R_\perp$ takes a continuous value. The RKKY interactions $J(\boldsymbol{R}_{nt}:t)$ are represented by $J(R_z)$ for $R_\perp=0$ and by $J(R_\perp)$ for $R_z=0$. The $J(R_z)$ and $J(R_\perp)$ in case B show the usual oscillatory behavior because the Fermi surface has sections perpendicular to $\boldsymbol{R}_{nt}$. The $J(R_\perp)$ in case A shows the oscillatory character for the same reason, but $J(R_z)$ show the damping with constant sign since there is no Fermi surface perpendicular to $\boldsymbol{R}_{nt}$. Thus, in case A, $J(R_\perp)$ and $J(R_z)$ have the different analytic structures. How are these different structures connected for the middle direction of $\boldsymbol{R}_{nt}$? Furthermore, the damping of $J(R_z)$ is the exponential type for $t=0$ but the power type proportional to R_z^{-2} for $t\neq0$. It is expected that introduction of $R_\perp$ may give the different effect on $J(R_z)$ according to $t=0$ and $t\neq0$.

For the reason mentioned above, the analytic structure of $J(R_\perp,R_z)$ in case A will be considered in this paper, in which $J(R_\perp,R_z)$ is the $J(\boldsymbol{R}_{nt}:t)$ with non-zero $R_\perp$ and R_z, and its calculations will be carried out for the constant matrix element case because they were limited to its case in I. $J(R_\perp,R_z)$ is given by eq. (2) in I, that is,

$$J(R_\perp,R_z)=\frac{C}{16\pi}\sum_\nu\sum_{\nu'}\int d\varepsilon\int d\varepsilon'\,\frac{f(\varepsilon)[1-f(\varepsilon')]}{\varepsilon'-\varepsilon}\,I_{\nu t}(\varepsilon)^*\,I_{\nu' t}(\varepsilon'), \tag{1}$$

$$I_{\nu t}(\varepsilon)=\int dk_z\,\exp(iR_z k_z)\,B_{\nu k_z}(t)\,J_0(R_\perp\sqrt{\varepsilon-\varepsilon_\nu(k_z)}), \tag{2}$$

where same notations as in I are used, and the integral region with respect to k_z is limited to the first zone and is bound by $\varepsilon\geqq\varepsilon_\nu(k_z)$. Since the constant matrix element case is noted and only intraband scattering for $\nu=\nu'=1$ is considered, we can put $B_{\nu k_z}(t)=1$ in eq. (2)

2. Evaluation of $I_{1t}(\varepsilon)$

We will approximately calculate $I_{1t}(\varepsilon)$ ($\nu=1$) here on a basis of the stationary phase method[2]. $I_{1t}(\varepsilon)$ is given by

$$I_{1t}(\varepsilon)=\int dk_z\,\cos R_z k_z\,J_0(R_\perp\sqrt{\varepsilon-\varepsilon_1(k_z)}). \tag{3}$$

The large contributions to this come from vicinities of the belly(1) and neck(1) on the Fermi surface, in which (1) means the first zone.

2.1 Contribution from belly (1)

The band energy $\varepsilon_1(k_z)$ is expanded up to the second order around belly(1) at $k_z=0$ and it is given by eq.(4). Then $I_{1l}(\varepsilon)$ is given by eq.(5).

$$\varepsilon_1(k_z)=\varepsilon_0+k_z^2/m_0 \quad (\varepsilon_0=\varepsilon_1(0),\ m_0=2/\varepsilon_1''(0)), \tag{4}$$

$$I_{1l}(\varepsilon)=\int_{-k_0}^{k_0} dk_z\ \cos R_z k_z\ J_0\left(R_p\sqrt{k_0^2-k_z^2}\right), \tag{5}$$

where $k_0^2=m_0(\varepsilon-\varepsilon_0)$ and $R_p=R_\perp/\sqrt{m_0}$. This integral can be carried out by use of the integral table for the Bessel functions[3] and we get

$$I_{1l}(\varepsilon)=2\frac{\sin k_0\sqrt{R_z^2+R_p^2}}{\sqrt{R_z^2+R_p^2}} \tag{6}$$

2.2 Contribution from neck (1)

The band energy $\varepsilon_1(k_z)$ is expanded up to the second order around neck(1) at $k_z=Q/2$ and its energy band and $I_{1l}(\varepsilon)$ are given by

$$\varepsilon_1(k_z)=\varepsilon_1-(k_z-Q/2)^2/m_1\ (\varepsilon_1=\varepsilon_1(Q/2),\ m_1=2/|\varepsilon_1''(Q/2)|), \tag{7}$$

$$I_{1l}(\varepsilon)=2\theta(\varepsilon-\varepsilon_1)\int_0^{Q/2} dk_z\ \cos R_z k_z\ J_0(R_s\sqrt{k_1^2+x^2}) + 2\theta(\varepsilon_1-\varepsilon)\int_{k_1'}^{Q/2} dk_z\ \cos R_z k_z\ J_0(R_s\sqrt{x^2-k_1'^2}), \tag{8}$$

where $x=Q/2-k_z$, $k_1^2=m_1(\varepsilon-\varepsilon_1)$, $k_1'^2=m_1(\varepsilon_1-\varepsilon)$, $R_s=R_\perp/\sqrt{m_1}$ and $\theta(x)$ is the step function. The variable change from k_z to x is made, and next the integral regions with respects to x are extended into infinity $(Q/2\to\infty)$. Then we get

$$I_{1l}(\varepsilon)=2\cos(R_z Q/2)[\theta(\varepsilon-\varepsilon_1)\int_0^\infty dx\ \cos R_z x\ J_0(R_s\sqrt{k_1^2+x^2})$$

Table I. Functional form of $I_{1l}(\varepsilon)$ caused from neck (1)

	$R_z > R_s$		$R_z < R_s$	
	$\varepsilon < \varepsilon_1$	$\varepsilon > \varepsilon_1$	$\varepsilon < \varepsilon_1$	$\varepsilon > \varepsilon_1$
$t=0$	$-2(-1)^n\frac{\sin k_1'\sqrt{R_z^2-R_s^2}}{\sqrt{R_z^2-R_s^2}}$ (10a)	0 (10b)	$2(-1)^n\frac{\exp[-k_1'\sqrt{R_s^2-R_z^2}]}{\sqrt{R_s^2-R_z^2}}$ (11a)	$2(-1)^n\frac{\cos k_1\sqrt{R_s^2-R_z^2}}{\sqrt{R_s^2-R_z^2}}$ (11b)
$t=1/2$	$2(-1)^n\frac{\cos k_1'\sqrt{R_z^2-R_s^2}}{\sqrt{R_z^2-R_s^2}}$ (12a)	$2(-1)^n\frac{J_0(R_s k_1)}{\sqrt{R_z^2-R_s^2}}$ (12b)	0 (13a)	$2(-1)^n I(R_s,R_z,\varepsilon)$ (13b)

$$I(R_s,R_z,\varepsilon)=\frac{2}{\sqrt{R_s^2-R_z^2}}\sum_{n=1}^{\infty}(-1)^n\ \sin 2n\phi\, J_{2n}(R_s k_1)\ (\phi=\sin^{-1}(R_z/R_s))$$

$$+\theta(\varepsilon_1-\varepsilon)\int_{k_1'}^{\infty}dx\ \cos R_z x\, J_0(R_s\sqrt{x^2-k_1'^2})]$$

$$+2\sin(R_zQ/2)[\,\theta(\varepsilon-\varepsilon_1)\int_0^{\infty}dx\ \sin R_z x\, J_0(R_s\sqrt{k_1^2+x^2})$$

$$+\theta(\varepsilon_1-\varepsilon)\int_{k_1'}^{\infty}dx\ \sin R_z x\, J_0(R_s\sqrt{x^2-k_1'^2})]. \qquad (9)$$

For the integrals containing Bessel functions, see ref.[3] and Appendix. Because of $R_zQ/2=\pi(n+t)$, $\cos(R_zQ/2)=0$ for $t=1/2$ and $\sin(R_zQ/2)=0$ for $t=0$. Hereafter, we notice both cases of $t=0$ and $t=1/2$. For these t, the results of integrations in eq.(9) are summarized in Table I.

3. Meaning of structures of $I_{1t}(\varepsilon)$ and its validities

As easily seen from eqs.(10)−(13) in Table I, the analytic structures of $I_{1t}(\varepsilon)$ caused from neck(1) are distinguished by the inequalities of $R_z \gtrless R_s$ for both cases of t. This can be related to geometry of the equal energy surfaces in the following way. The band energy for the first band is given by $k_\perp^2+\varepsilon_1(k_z)$. When $\varepsilon_1(k_z)$ is approximated by eq.(7), its equal energy surface is given by $\varepsilon=\varepsilon_1+k_\perp^2-x^2/m_1$ $(x=k_z-Q/2)$, in which only surfaces in the first zone are noted, that is, its zone can be denoted by $-Q/2<x<0$ and $k_\perp>0$. This shape is the hyperbola in the $k_\perp-x$ plane and its asymptotic line is $x=-\sqrt{m_1}k_\perp$. When $R_z=R_\perp/\sqrt{m_1}(=R_s)$, the vector $\boldsymbol{R}_{nt}=(R_\perp,R_z)$ is perpendicular to the asymptotic line, in which $\boldsymbol{R}_{nt}$ can be taken as the two dimensional vector because the energy surfaces are symmetrical around the z−axis. For the equal energy surfaces with larger energy than ε_1 $(\varepsilon>\varepsilon_1)$, there is no section on its surface perpendicular to $\boldsymbol{R}_{nt}$ with $R_z>R_s$, and there is section perpendicular to $\boldsymbol{R}_{nt}$ with $R_z<R_s$ at vicinity of neck(1). However, for the surfaces of $\varepsilon<\varepsilon_1$, the situatuation is opposite. Thus the inequalities of $R_z \gtrless R_s$ distinguishing the structures of $I_{1t}(\varepsilon)$ are equivalent to condition that the equal energy surfaces have sections perpendicular to $\boldsymbol{R}_{nt}$ or not. On the other hand, for $I_{1t}(\varepsilon)$ caused from belly(1), the structure is simple as seen from eq.(6), and $I_{1t}(\varepsilon)$ consists of the single term. The reason is that the equal energy surfaces are elliptic and have sections perpendicular to $\boldsymbol{R}_{nt}$ with an arbitrary direction.

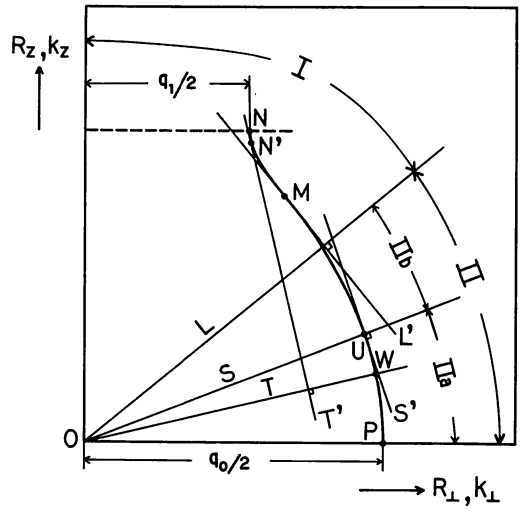

Fig.1. The Fermi surface in case A is shown. The representative points, tangential planes and their normals on its surface are also indicated. The tangential lines at W and N' are parallel and have the common normal.

Next let us discuss validities of $I_{1t}(\varepsilon)$ since they were derived using the approximated band energies expanded at belly(1) and neck(1). As easily seen from eq.(1), the large contribution to $J(R_\perp,R_z)$ is caused from vicinity of $\varepsilon=\varepsilon'=\varepsilon_F$, that is, Fermi surface. For this reason, we show the Fermi surface for case A in Fig.1. The curve $PWUMN'N$ denotes its surface. The M is inflection point on its surface, and the line L' is the tangential one at M, and the line L is its normal, in which really L' is the plane not line because the Fermi surface is symmetrical around the k_z−axis. The $R_\perp-R_z$ plane is divided into two regions by the line L, I and II. Perhaps, the approximated band

energy given by eq.(7) can represent the part *NM* well. Therefore, eqs.(10) and (12) are valid in the region I, and eq.(11) and (13) in the region II. On the other hand, let us assume that the part *PU* can be well represented by the approximated band energy given by eq.(4) and the part *UM* cannot well, in which the boundary point *U* is roughly marked in Fig.1. Eq.(6) is valid in the region IIa. We summarize the valid equations of $I_{lt}(\epsilon)$ for each region immediately below.

I : *eq.(10) and eq.(12)* (14a)
IIa : *eq.(6), eq.(11) and eq.(13)* (14b)
IIb : *eq.(11) and eq.(13)* (14c)

4. $J(R_\perp, R_z)$

In this section, we will consider $J(R_\perp, R_z)$ in case A ($\epsilon_F > \epsilon_1$) caused from the intraband scattering ($\nu=\nu'=1$). Its $J(R_\perp, R_z)$ is denoted by $J_{11}(R_\perp, R_z)$.

4.1 Case of $t=0$

4.1.1 Region I

Eq.(10) is inserted into eq.(1). Because of $I_{lt}(\epsilon)=0$ for $\epsilon > \epsilon_1$, we get

$$J_{11}(R_\perp, R_z)=0. \tag{15}$$

$J(R_\perp, R_z)$ is caused from the interband scattering ($\nu=1, \nu'=2$) and indicates the exponential damping since a electron flies the band gap in its scattering.

4.1.2 Region IIa

We insert eqs.(6) and (11b) into eq.(1) and perform the energy integrals, and get as the asymptotic form for large R ($R=|\boldsymbol{R}_{nt}|$).

$$J_{11}(R_\perp, R_z)=-\frac{Cm_0q_0}{16}\cdot\frac{\cos q_0R_0}{R_0^3}+\frac{Cm_1q_1}{16}\cdot\frac{\cos q_1R_1}{R_1^3}+\frac{C(m_0m_1)^{\frac{1}{2}}}{4}\left[1-\frac{R_0R_1(R_0+R_1)^2(q_0^2-q_1^2)^2}{4(R_0q_0+R_1q_1)^4}\right]$$
$$\times\frac{R_0q_0+R_1q_1}{R_0R_1(R_0+R_1)^2}\sin\left\{\frac{1}{2}(q_0R_0+q_1R_1)\right\}, \tag{16}$$

where $R_0=(R_\perp^2+m_0R_z^2)^{\frac{1}{2}}$, $R_1=(R_\perp^2-m_1R_z^2)^{\frac{1}{2}}$, and q_0 and q_1 are the diameter of belly(1) and neck(1), respectively (see Fig.1). Eq.(16) agrees with ones given by eqs.(30),(31) and (38) in paper I, in which note that the definitions of m_0 and m_1 in I are different from those in this paper. The periods of oscillations for the first and second terms in eq.(16) are q_0R_0/R and q_1R_1/R, respectively, when we regard them as a function of R. The wave number $q_0R_0/2R$ is equal to the distance in the $k_\perp-k_z$ space from origin to the tangential plane at the point near belly(1). For example, when $\boldsymbol{R}_{nt}$ is in the direction of OW in Fig.1, it is equal to distance from origin to tangential plane at W. Similarly, $(q_1R_1+QR_z)/2R$ is equal to distance from origin to tangential plane at a point near neck(1). However, because of $QR_z=2\pi n$, we must note that $\cos q_1R_1=\cos(q_1R_1+QR_z)$ in eq.(16), in which $q_1R_1/2R$ is the distance from center of neck(1) on the zone boundary ($k_z=Q/2$) to its tangential plane. The period of oscillation for the third term is the average of them. It can be concluded that each period is equal to distance between two tangential planes of the Fermi surface perpendicular to $\boldsymbol{R}_{nt}$, in which they are located opposite with respect to origin.

4.1.3 Region IIb

Although the accurate asymptotic form of $J_{11}(R_\perp, R_z)$ could not derived because of inaccuracy

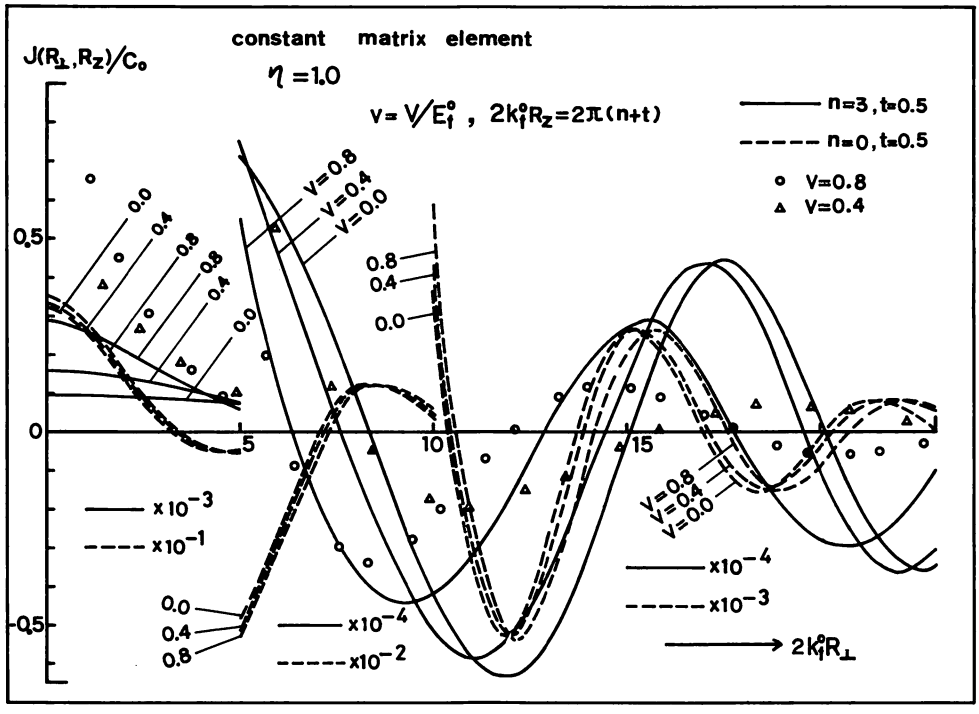

Fig.2. $J(R_\perp,R_z)$ for $t=1/2$ are plotted as a function of $2k_f^0R_\perp$. k_f^0 and E_f^0 are radius of the Fermi sphere and the Fermi energy for $V=0$, in which V is strength of the potential defined in paper I. $2k_f^0R_z$ and $v=V/E_f^0$ are the parameters, and $C_0=Ck_f^{04}$ and $\eta=Q/2k_f^0$. The solid and dashed lines are the numerically calculated results due to eq.(11) in ref.[4], and the former should be compared with eq.(17) and the latter with eq.(19). The results due to the modified eq.(17) are indicated by ○ and △, in which the values of q_1 are calculated using the two wave energy dispersion.

of eq.(6), it consists of three terms similar to eq.(16). But, each period should be modified. When direction of $\boldsymbol{R}_{nt}$ varies from T to L gradually (see Fig.1 for T and L), the two periods corresponding to q_0R_0/R and q_1R_1/R approach each other and finally agrees. For this reason, when $\boldsymbol{R}_{nt}$ is in direction of L, $J_{11}(R_\perp,R_z)$ vanishes since the first and second terms in eq.(16) cancel each other because of opposite sign and there does not exist the scattering process giving the third term. This result connects to one given by eq.(15). But really, because the small contribution from inflection point M exists, it seems that there remains the higher order terms than one of R^{-3}. Accurate evaluation of its contribution is future problem.

4.2 Case of t=1/2

4.2.1 Region I

We perform the energy integrals by inserting eq.(12b) into eq.(1) and by changing variables of $\varepsilon=x^2$ and $\varepsilon'=y^2$, then get

$$J_{11}(R_\perp,R_z)=-\frac{Cq_1^2}{16(R_z^2-R_s^2)}[J_0(u)N_0(u)+J_1(u)N_1(u)] \quad (u=q_1R_\perp/2), \tag{17}$$

where the formulae for integrals including Bessel and Neumann functions[3] are used and $N_n(u)$ is

the Neumann function. We must note that eq.(17) is valid for $R_z >> R_s$ because eq.(12b) is valid for its condition as seen from (A.3) in Appendix. We here take the large $R_\perp$. Then R_z must also become large by the condition $R_z > R_s$. Thus we get the asymptotic form of eq.(17) using those for $J_n(u)$ and $N_n(u)$.

$$J_{11}(R_\perp, R_z) = \frac{C}{4\pi (R_z^2 - R_s^2) R_\perp^2} \sin q_1 R_\perp . \tag{18}$$

This shows that, by introduction of $R_\perp$, $J(R_z)$ derived in paper I ($J(R_z) \propto R_z^{-2}$) begins to oscillate with period equal to diameter of neck(1) toward its radial direction. On the other hand, eq.(17) shows the logarithmic divergence for $R_\perp \to 0$. This divergence can be canceled by one due to the interband scattering as was already shown in I.

The validity of eq.(17) is investigated numerically in Fig.2. Then, we must note that eq.(17) is valid for $R_\perp << \sqrt{m_1} R_z$. The values of the effective mass m_1 calculated by use of the two wave energy dispersion are $m_1 = 1/9$ for $v = 0.4$ and $m_1 = 1/4$ for $v = 0.8$, and are very small. Therefore, the valid region of eq.(17) with respect to $2k_f^0 R_\perp$ is very narrow in Fig.2. The denominator $(R_z^2 - R_s^2)$ in its equation is replaced by R_z^2 in order to consider the period of oscillation rather than the amplitude, and ○ and △ are calculated by use of its modified equation. As easily seen from Fig.2, the period of eq.(17) is in good agreement with the numerical calculations for large v ($v = 0.8$). For large v, q_1 is larger. That is, when a diameter of neck(1) is large, the period of eq.(17) is good. For $v = 0.4$, the first zero point of both $J(R_\perp, R_z)$ is in good agreement.

4.2.2 Region IIa

As easily seen from eq.(13b), the contribution to $I_{11}(\varepsilon)$ due to neck(1) is zero for $R_z = 0$. Therefore, when $R_z << R_s$, $J(R_\perp, R_z)$ can be caused from only belly(1). The result can be derived by insertion of eq.(6) into eq.(1) and is given by

$$J_{11}(R_\perp, R_z) = -\frac{C m_0 q_0}{16} \cdot \frac{\cos q_0 R_0}{R_0^3} \tag{19}$$

This result is consistent with the numerical calculations shown by the dashed lines in Fig.2. That is, the potential dependences for periods and amplitudes of $J(R_\perp, R_z)$ are small because its effect on q_0 and m_0 is proportional to v^2 and is small. This form is very different from eq.(16) for $t = 0$ and means that existence of neck(1) can be ignored for $t = 1/2$ and $R_s >> R_z$.

4.2.3 Region IIb

$J_{11}(R_\perp, R_z)$ in this region cannot be calculated in the present stage by insertions of eqs.(13b) and (6) into eq.(1) because integrations are difficult. Since it is predicted that contribution from neck(1) become large compared to region IIa, it is difficult to understand the analytic structure of $J_{11}(R_\perp, R_z)$. Furthermore, when direction of $\boldsymbol{R}_{nt}$ is in vicinity of L, we cannot also answer how the oscillation form given by eq.(19) is connected to the form given by eq.(17) because the contribution from vicinity of inflection point M is not evaluated.

Appendix

In the integrals in eq.(9), the formula for the following type integral cannot be found in the book[3].

$$I(a, b, c) = \int_0^\infty dx \ \sin ax \ J_0(b\sqrt{x^2 + c^2}). \tag{A.1}$$

Here this integral will be evaluated. By use of addition theorem[3], we get

$$I(a,b,c)=\sum_{n=0}^{\infty}\epsilon_n(-1)^n J_{2n}(bc)\int_0^{\infty}dx\ \sin ax\ J_{2n}(bx), \tag{A.2}$$

where $\epsilon_0=1$ and $\epsilon_n=2(n>0)$. The integral in eq.(A.2) can be easily found[3] and eq.(A.2) becomes to

$$I(a,b,c)=\theta(b-a)(b^2-a^2)^{-1/2}\sum_{n=0}^{\infty}\epsilon_n(-1)^n \sin 2n\phi\ J_{2n}(bc)$$

$$+\theta(a-b)(a^2-b^2)^{-1/2}\sum_{n=0}^{\infty}\epsilon_n \tan^{2n}\xi\ J_{2n}(bc), \tag{A.3}$$

where $\sin\phi=a/b$ and $\sin 2\xi=b/a$. In the second term, because of $\tan\xi<1$, only its leading term $(n=0)$ is remained.

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