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An Integral for Second-Order Multiple Scattering Perturbation Theory

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This paper presents the closed form evaluation of a six-dimensional integral. The integral arises in the application to many-electron systems of a multiple scattering perturbation expansion at second order when formulated in fourier space. The resulting function can be used for the calculation of both the electron density and the effective one-electron potential in an SCF calculation. The closed form expression derived here greatly facilitates these calculations. In addition, the evaluated integral can be used for the computation of second-order corrections to the "optimized Thomas–Fermi theory."

I. INTRODUCTION

This paper presents the closed form evaluation of the function defined by

$$\Lambda(k_F, \mathbf{k}', \mathbf{k}'') = \frac{m^2 k_F^2}{4\pi^4 \hbar^4 (2\pi)^6} \int d^3r' d^3r'' e^{i\mathbf{k}'\cdot\mathbf{r}'} e^{i\mathbf{k}''\cdot\mathbf{r}''} \frac{j_1[k_F(r' + |\mathbf{r}' - \mathbf{r}''| + r'')]}{r'|\mathbf{r}' - \mathbf{r}''|r''}. \tag{1}$$

This function is encountered in the application of multiple scattering perturbation theory [2, 3] at second order when formulated in fourier space. The specific problem in which this arose was the computation of the electron density of the embedded atom [1], although it would arise for any many-electron problem. The use of a closed form expression greatly enhances the speed of the computation. A further use of this function is in the second-order correction to the closely related optimized Thomas–Fermi (OTF) theory [4, 5]. It has been observed [6] that the OTF electron density is noticeably improved with the second-order correction and that routine evaluation would be worthwhile. A closed form expression for Eq. (1) would facilitate the computation of this correction.

An interesting point for further investigation is that the higher order terms in the multiple scattering perturbation theory expansion share some features with the second-order term. A transformation of the entire expansion to fourier space would result in integrals with many of the same features as the one in Eq. (1) and the techniques presented here could be applied to the general higher order term. Although systematic evaluation of higher order terms in a perturbative expansion is not expected to be productive, there is another possible benefit of work in this direction. A general formal expression could be derived for the nth-order term and, after introducing a suitable approximation, a rearrangement and summation to infinite order might be possible. It may be possible to obtain a highly accurate integral expression for the electron density in this way. One can draw an analogy to the work of Gell-Mann and Brueckner [7] in which just such a summation is performed in a perturbative expansion.

For these reasons, a closed form solution of the integrals in Eq. (1) is presented. The integrations are rather complicated and their evaluation is by no means direct. Even with the closed form solution, it is necessary to address some subtle issues that arise due to the multiple-valued nature of the solution. The details are presented in this paper.

II. REDUCTION TO THREE DIMENSIONAL INTEGRALS

As written, Eq. (1) is not amenable to direct integration. However, the introduction of some integral identities leads to a tractable expression. The first identity is for the spherical Bessel function

$$j_1(k_F z) = -\frac{i}{2k_F^2} \int_{\Gamma_x} x e^{ixz}\, dx, \tag{2}$$

where k_F is a positive real number, z is an arbitrary complex number, and Γ_x is a contour in the complex-x plane that begins on the real axis at $-k_F$, goes above the real axis, and ends back on the real axis at k_F (see Fig. 1a). The standard identity for the spherical Bessel function [8] has an integration path that is strictly on the real axis. The

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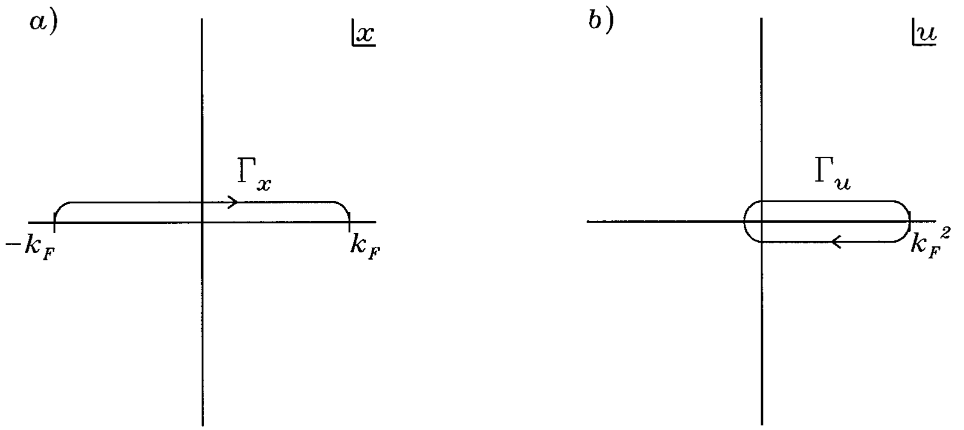

FIG. 1. Contours used in the integrals of Eq. (5): (*a*) Γ_x; (*b*) Γ_u.

deformed path used here, though, has two advantages. First, it allows the introduction of the integral representation

$$\frac{e^{ix|\mathbf{r}'-\mathbf{r}''|}}{|\mathbf{r}'-\mathbf{r}''|} = -\frac{1}{2\pi^2}\int d^3q\,\frac{e^{i\mathbf{q}\cdot(\mathbf{r}'-\mathbf{r}'')}}{x^2-q^2}. \tag{3}$$

The positive imaginary part of x ensures that the correct pole of the integrand is surrounded by the path of integration in q. Second, the radial integrals over r' and r'' become absolutely convergent when the imaginary part of x is positive. Introducing the two integral representations (2) and (3) and performing the resulting integrals over $\mathbf{r}'$ and $\mathbf{r}''$, we obtain

$$\Lambda(k_F,\mathbf{k}',\mathbf{k}'') = \frac{im^2}{\pi^4\hbar^4(2\pi)^6}\int d^3q \int_{\Gamma_x}\frac{x\,dx}{(x^2-q^2)(x^2-|\mathbf{q}+\mathbf{k}'|^2)(x^2-|\mathbf{q}-\mathbf{k}''|^2)}. \tag{4}$$

The integral over x can now be performed by contour integration. We introduce the new integration variable, $u = x^2$. Based on the path specified for x, the path of integration in u begins at $u = k_F^2$ on the positive real axis, continues below the real axis toward the origin, goes around the origin in a clockwise direction, and continues above the positive real axis to $u = k_F^2$ (see Fig. 1b). Denote this closed contour by Γ_u. The theorem of residues can then be used to evaluate the integral. For real α, β, and γ,

$$\begin{aligned}\int_{\Gamma_x}&\frac{x\,dx}{(x^2-\alpha^2)(x^2-\beta^2)(x^2-\gamma^2)}\\ &= \frac{1}{2}\int_{\Gamma_u}\frac{du}{(u-\alpha^2)(u-\beta^2)(u-\gamma^2)}\\ &= -\pi i\left\{\frac{\eta(k_F-|\alpha|)}{(\alpha^2-\beta^2)(\alpha^2-\gamma^2)}+\frac{\eta(k_F-|\beta|)}{(\beta^2-\alpha^2)(\beta^2-\gamma^2)}\right.\\ &\qquad\left.+\frac{\eta(k_F-|\gamma|)}{(\gamma^2-\alpha^2)(\gamma^2-\beta^2)}\right\},\end{aligned} \tag{5}$$

where $\eta(z)$ is the Heaviside function. Applying this to Eq. (4) and performing a little rearrangement,

$$\begin{aligned}\Lambda(k_F,\mathbf{k}',\mathbf{k}'') = \frac{m^2}{\pi^3\hbar^4(2\pi)^6}&\{F(k_F,\mathbf{k}',-\mathbf{k}'')\\ &+F(k_F,\mathbf{k}',\mathbf{k}'+\mathbf{k}'')+F(k_F,\mathbf{k}'',\mathbf{k}'+\mathbf{k}'')\},\end{aligned} \tag{6}$$

where a new function has been introduced:

$$F(k_F,\boldsymbol{\kappa},\boldsymbol{\kappa}') = \int_{q<k_F}\frac{d^3q}{(q^2-|\mathbf{q}+\boldsymbol{\kappa}|^2)(q^2-|\mathbf{q}+\boldsymbol{\kappa}'|^2)}. \tag{7}$$

III. EVALUATION OF $F(k_F, \kappa, \kappa')$

Evaluation of this integral is complicated by the fact that the integrand contains divergences if k_F is larger than either $\kappa/2$ or $\kappa'/2$. Dealing with divergences is generally a straightforward process, but in this case, the singularity structure of the integrand leads to multiple-valued functions after integration. Some care must be exercised in picking out the correct branch to use for the final result.

This three-dimensional integral can be evaluated in two quite different ways. It is possible to perform the integrals directly; the necessary indefinite integrals are all either tabulated or readily worked out. The process is laborious, however. It is necessary to keep track of the relative sizes of the vectors, the signs of certain terms, and the correct limits over which the integration is performed. An alternative approach will be presented here. It is worth mentioning here that both approaches lead to the same result, providing a check on the correctness of the solution.

Equation (7) is more easily evaluated after introducing another integral identity. There is a subtle problem involved, though, that must be addressed. For real, positive a and b, we can write

$$\frac{1}{ab} = \int_0^1 \frac{dz}{[az + b(1-z)]^2}. \tag{8}$$

For the problem at hand, however, we wish to apply this identity to situations where a and b are of arbitrary sign. If a and b are both negative, it is easily seen that Eq. (8) is still valid. If a and b have opposite signs, however, there is a divergence in the integrand that renders the integral undefined. One might consider using the same expression with a replaced by $-a$, for instance, but this would lead to an awkward situation in which the relative signs of the two factors must be monitored. This would lead to great complications, especially when the two factors are integrated over, as they are here.

The solution is to introduce a contour, Γ_z, that begins at 0, ends at 1, and avoids the real axis in between. There can be no objection to this deformation if a and b have the same sign, but there is an immediate ambiguity if they have opposite signs. Going below or above the singularity must lead to different results, since the integral over a closed contour around the singularity does not vanish. However, the ambiguity is in the imaginary part of the result and can be conveniently discarded at the end. The integral representation used is therefore given by

$$\frac{1}{ab} = \int_{\Gamma_z} \frac{dz}{[az + b(1-z)]^2}, \tag{9}$$

where it is understood that the contour does not touch the real axis, except at the end points, and that only the real part of the result is to be retained.

The integrals over $\mathbf{q}$ are easily evaluated after this identity is introduced, and we obtain

$$\begin{aligned} F(k_F, \boldsymbol{\kappa}, \boldsymbol{\kappa}') &= \pi k_F \int_{\Gamma_z} \frac{dz}{|\boldsymbol{\kappa} z + \boldsymbol{\kappa}'(1-z)|^2} \left\{ \frac{(\kappa^2 z + \kappa'^2(1-z))}{4k_F|\boldsymbol{\kappa} z + \boldsymbol{\kappa}'(1-z)|} \right. \\ &\quad \left. \times \ln\left(\frac{\kappa^2 z + \kappa'^2(1-z) + 2k_F|\boldsymbol{\kappa} z + \boldsymbol{\kappa}'(1-z)|}{\kappa^2 z + \kappa'^2(1-z) - 2k_F|\boldsymbol{\kappa} z + \boldsymbol{\kappa}'(1-z)|} \right) - 1 \right\}. \end{aligned} \tag{10}$$

In evaluating the final integral, it is convenient to first reduce some of the clutter by introducing the quantities

$$\begin{aligned} a &= \kappa'^2, & \alpha &= \kappa'^2 \\ b &= \kappa^2 - \kappa'^2, & \beta &= \boldsymbol{\kappa}' \cdot (\boldsymbol{\kappa}' - \boldsymbol{\kappa}) \\ & & \gamma &= |\boldsymbol{\kappa} - \boldsymbol{\kappa}'|^2. \end{aligned} \tag{11}$$

Equation (10) then becomes

$$\begin{aligned} F(k_F, \boldsymbol{\kappa}, \boldsymbol{\kappa}') &= \pi k_F \int_{\Gamma_z} \frac{dz}{(\alpha - 2\beta z + \gamma z^2)} \left\{ \frac{a + bz}{4k_F[\alpha - 2\beta z + \gamma z^2]^{1/2}} \right. \\ &\quad \left. \times \ln\left(\frac{a + bz + 2k_F[\alpha - 2\beta z + \gamma z^2]^{1/2}}{a + bz - 2k_F[\alpha - 2\beta z + \gamma z^2]^{1/2}} \right) - 1 \right\} \\ &= \frac{\pi}{4} \left\{ \frac{(\alpha\gamma + b\beta)z - (\alpha\beta + b\alpha)}{(\alpha\gamma - \beta^2)[\alpha - 2\beta z + \gamma z^2]^{1/2}} \right. \\ &\quad \times \ln\left(\frac{a + bz + 2k_F[\alpha - 2\beta z + \gamma z^2]^{1/2}}{a + bz - 2k_F[\alpha - 2\beta z + \gamma z^2]^{1/2}} \right) \\ &\quad \left. \left. + \frac{H}{\alpha\gamma - \beta^2} \ln\left(\frac{H + G(z)}{H - G(z)} \right) \right\} \right|_{\Gamma_z}, \end{aligned} \tag{12}$$

where

$$\begin{aligned} G(z) &= (ab + 4k_F^2\beta + (b^2 - 4k_F^2\gamma)z) \\ H &= [(a^2\gamma + 2ab\beta + b^2\alpha) - 4k_F^2(\alpha\gamma - \beta^2)]^{1/2}. \end{aligned} \tag{13}$$

That Eq. (12) is the correct indefinite integral can be verified by differentiation of the right-hand side. The right-hand side is then evaluated at the limits and the vector quantities are reintroduced. The final result is

$$F(k_F, \boldsymbol{\kappa}, \boldsymbol{\kappa}') = \frac{\pi}{4|\boldsymbol{\kappa}\times\boldsymbol{\kappa}'|^2}\left\{\kappa\boldsymbol{\kappa}'\cdot(\boldsymbol{\kappa}'-\boldsymbol{\kappa})\ln\left|\frac{\kappa+2k_F}{\kappa-2k_F}\right| + \kappa'\boldsymbol{\kappa}\cdot(\boldsymbol{\kappa}-\boldsymbol{\kappa}')\ln\left|\frac{\kappa'+2k_F}{\kappa'-2k_F}\right| + \Delta^{1/2}\ln\left(\frac{4k_F^2\boldsymbol{\kappa}\cdot\boldsymbol{\kappa}'-\kappa^2\kappa'^2+2k_F\Delta^{1/2}}{4k_F^2\boldsymbol{\kappa}\cdot\boldsymbol{\kappa}'-\kappa^2\kappa'^2-2k_F\Delta^{1/2}}\right)\right\}, \tag{14}$$

where

$$\Delta = \kappa^2\kappa'^2|\boldsymbol{\kappa}-\boldsymbol{\kappa}'|^2 - 4k_F^2|\boldsymbol{\kappa}\times\boldsymbol{\kappa}'|^2. \tag{15}$$

Only the real part of Eq. (14) is to be retained. For this reason, absolute value signs have been placed about the arguments of the logarithms in the first two terms. In the last term, though, this cannot be done since the quantity Δ can be either positive or negative. The logarithm is a multiple valued function, evaluation of which is ambiguous by a multiple of $i\pi$. If Δ is positive, this ambiguous term can be discarded and absolute value signs used around the logarithm's argument. If Δ is negative, however, the argument of the logarithm is complex. Further, the magnitude of the argument is one, so that the logarithm itself is purely imaginary. Multiplication by $\Delta^{1/2}$, which is also purely imaginary, then yields a purely real result. The problem is that the ambiguity in the logarithm makes a real contribution to the result. It cannot be simply dropped and the proper multiple to use in the final expression must be determined based on the physical constraints of the problem at hand. Rather than determine this multiple for $F(k_F, \boldsymbol{\kappa}, \boldsymbol{\kappa}')$, however, the functions will be combined in Eq. (6) and the correct multiple deduced for the overall function.

IV. RECOMBINATION AND CHOICE OF BRANCH

Equation (6) expresses $\Lambda(k_F, \mathbf{k}', \mathbf{k}'')$ as a sum of three terms, each of which can be evaluated using Eq. (14). The recombination of these terms is performed via a straightforward, although tedious, exercise in algebra. Part of this task was performed with a symbolic mathematics program [10]. The result is a function that, aside from k_F, depends on the two vector magnitudes, k' and k'', and the angle between them (or equivalently, its cosine). It turns out that a more symmetrical expression is obtained by replacing the angle between the vectors by a third vector magnitude, given by $k = |\mathbf{k}' + \mathbf{k}''|$. The three vector magnitudes are physically constrained by the triangle inequality, $|k' - k''| \le k \le (k' + k'')$. A further simplification is obtained if the reduced quantities

$$x = k/2k_F \qquad x' = k'/2k_F \qquad x'' = k''/2k_F \tag{16}$$

are introduced. In this way, the dependence of the function on k_F can be explicitly extracted. We then obtain

$$\Lambda(k_F, \mathbf{k}', \mathbf{k}'') = \frac{m^2}{2\pi^3 k_F \hbar^4 (2\pi)^6}\lambda(x, x', x''), \tag{17}$$

where

$$\lambda(x, x', x'') = \frac{\pi}{p}\left\{(-x^2+x'^2+x''^2)x\ln\left|\frac{x+1}{x-1}\right| + (x^2-x'^2+x''^2)x'\ln\left|\frac{x'+1}{x'-1}\right| + (x^2+x'^2-x''^2)x''\ln\left|\frac{x''+1}{x''-1}\right| + d^{1/2}\ln\left(\frac{a-bd^{1/2}}{a+bd^{1/2}}\right)\right\} \tag{18}$$

and

$$\begin{aligned} p &= (x+x'+x'')(-x+x'+x'')(x-x'+x'')(x+x'-x'') \\ d &= x^2x'^2x''^2 - p/4 \\ a &= x^2x'^2x''^2 + \tfrac{1}{2}(x^4+x'^4+x''^4) - (x^2+x'^2+x''^2) + 1 \\ b &= x^2+x'^2+x''^2 - 2. \end{aligned} \tag{19}$$

The physical constraints on the three variables are that they all be nonnegative and satisfy the triangle inequality, $|x' - x''| \le x \le (x' + x'')$.

In certain circumstances, it is convenient to substitute two new variables, u and v, for x' and x''. The old and new variables are related by

$$x' = \tfrac{1}{2}x(u+v). \qquad x'' = \tfrac{1}{2}x(u-v). \tag{20}$$

With the hope that no confusion will occur, the function of the new variables will be denoted by $\lambda(x, u, v)$. The function is given explicitly by

$$\lambda(x, u, v) = \frac{\pi}{2p}\left\{(-2 + u^2 + v^2)x^3 \ln\left|\frac{x+1}{x-1}\right| + (1 - uv)(u + v)x^3 \ln\left|\frac{x(u+v)+2}{x(u+v)-2}\right| + (1 + uv)(u - v)x^3 \ln\left|\frac{x(u-v)+2}{x(u-v)-2}\right| + 2d^{1/2} \ln\left(\frac{a - bd^{1/2}}{a + bd^{1/2}}\right)\right\}, \tag{21}$$

where now

$$\begin{aligned} p &= x^4(u^2 - 1)(1 - v^2) \\ d &= \frac{x^6(u^2 - v^2)^2}{16} - p/4 \\ a &= \frac{x^6(u^2 - v^2)^2}{16} + \frac{x^4(u^4 + 6u^2v^2 + v^4 + 8)}{16} - \frac{x^2(u^2 + v^2 + 2)}{2} + 1 \\ b &= \frac{x^2(u^2 + v^2 + 2)}{2} - 2. \end{aligned} \tag{22}$$

A convenient feature of the new variables is that their physical limits are independent of the other variables: $0 < x$; $1 < u$; and $-1 < v < 1$. Another useful property is that, viewing $\lambda(x, u, v)$ as a purely mathematical function, it is found to be symmetric with respect to interchange of the two variables u and v.

It is now time to consider the proper branch to use for the multiple-valued function. The ultimate criterion will be to require that the function be continuous in all its variables. This seems reasonable in view of the original definition of the function in Eq. (1). Continuous variation of the vectors $\mathbf{k}'$ and $\mathbf{k}''$ should result in a continuous variation of the function itself. This does not require smooth behavior, however, and, indeed, it is impossible to obtain a solution which is everywhere smooth. However, we can determine the behavior of the function for one limiting case and then extend this behavior continuously to all other cases.

The awkwardness is confined to the term

$$s_1 = d^{1/2} \ln\left(\frac{a - bd^{1/2}}{a + bd^{1/2}}\right), \tag{23}$$

where the logarithm can be evaluated up to an arbitrary multiple of $i\pi$. When d is positive, the extra term is imaginary and should be neglected. Since the argument of the logarithm is real in this case, we can obtain an unambiguous result by simply putting absolute value signs around it. When d is negative, however, the extra term is multiplied by an imaginary square root. Which branch is chosen will affect the value of the result. An important task is therefore to identify where d is negative and, further, to investigate the behavior of the other parameters, a and b, in this region.

Suppose x has a given value and we wish to investigate the behavior of s_1 in the (u, v)-plane. If $x > 1$, it is easily shown that d is everywhere positive. The evaluation of s_1 in such cases is straightforward. Therefore, suppose that $x < 1$. For u sufficiently close to 1 and for sufficiently large u, d is positive. In between, there is a region where d is negative, bordered by the two curves.

$$u_d^{\pm} = \left[v^2 + \frac{2(1 - v^2)}{x^2}(1 \pm [1 - x^2]^{1/2})\right]^{1/2}. \tag{24}$$

There is no other region for acceptable values of u and v, where d is negative.

The parameter b is negative for small values of u and positive for larger values. The dividing line is given by the curve

$$u_b = \left[\frac{4}{x^2} - (v^2 + 2)\right]^{1/2}. \tag{25}$$

This can be shown to cross the $u_d^{\pm}$ curve at two points, $(v_s^{\pm}, u_s)$, where

$$\begin{aligned} v_s^{\pm} &= \pm\left[\frac{1 - [1 - x^2]^{1/2}}{1 + [1 - x^2]^{1/2}}\right]^{1/2} \\ u_s &= \frac{[2 - x^2 + 2[1 - x^2]^{1/2}]^{1/2}}{x}. \end{aligned} \tag{26}$$

With a little algebra, a can be shown to be nonnegative everywhere along the border where $d = 0$. Further, it is positive wherever d is positive. In the region where d is negative, though, there is one region where a is negative. region contains the curve where $b = 0$ and touches the curve $u_d^{\pm}$ at precisely the two points $(v_s^{\pm}, u_s)$. A plot of these regions for $x = 0.88$ is given in Fig. 2.

As already mentioned, in the regions where $d > 0$, the computation of s_1 is unambiguous. Further, when $d < 0$, it is a straightforward and unambiguous matter to ensure continuity of the function as the parameters, a and b, change sign. The situation is no longer unambiguous when considering its behavior when crossing the boundary where d changes sign. By definition, s_1 is necessarily continuous when crossing this boundary regardless of which branch is chosen for the logarithm. However, for the function to be smooth as well, only one choice of branch is possible. Unfortunately, it is not possible to ensure smooth behavior along the entire curve where $d = 0$. Although a is necessarily nonnegative along this curve, b may have either sign. Requiring $\lambda(x, u, v)$ to be smooth when crossing the $d = 0$ curve for $b < 0$ and requiring continuity elsewhere leads to a nonsmooth transition when the border is crossed for $b > 0$. A similar situation is encountered when smooth behavior is required for the $b > 0$ portion of the curve. The correct behavior is deduced by considering the $x \to 0$ limit. In this limit, b is nonnegative along the entire $d = 0$ curve. We therefore insist on smooth behavior across the boundary in this limit and extend this behavior to other values of x. The consequence of this is that the function is smooth as d changes sign when $b < 0$. Continuity is then enforced for all other regions of the (u, v)-plane.

Note that the points $(v_s^{\mp}, u_s)$ are special. Going entirely around either point alone, continuous behavior causes the function to return with a different value. On the other hand, going entirely around both points causes the function to return with the same value. Viewing the (u, v)-plane as a complex plane for the variable $z = v + iu$, these two points can be viewed as branch points that are connected to each other by a cut. The branch cut chosen here is the curve $u_d^{\pm}$ between these two points.

With these criteria, the function s_1 is given by

$$s_1 = \sqrt{d}\ln\left|\frac{a - b\sqrt{d}}{a + b\sqrt{d}}\right| \qquad (d > 0) \tag{27a}$$

$$= \sqrt{-d}\left\{2\arctan\left(\frac{b\sqrt{-d}}{a}\right) - \phi\right\} \quad \begin{pmatrix} d < 0, b^2|d| < a^2 & \\ & \\ a > 0, b < 0 & \phi = 0 \\ a < 0 & \phi = 2\pi \\ a > 0, b > 0 & \phi = 4\pi \end{pmatrix} \tag{27b}$$

$$= \sqrt{-d}\left\{-2\arctan\left(\frac{a}{b\sqrt{-d}}\right) - \phi\right\} \quad \begin{pmatrix} d < 0, a^2 < b^2|d| & \\ & \\ b < 0 & \phi = \pi \\ b > 0 & \phi = 3\pi \end{pmatrix}. \tag{27c}$$

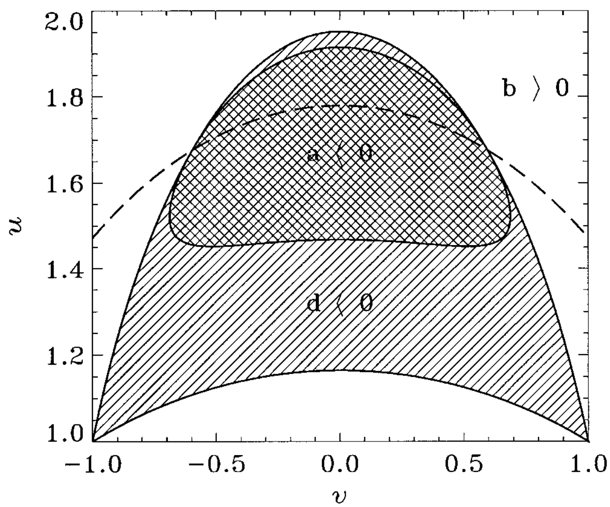

FIG. 2. Behavior of the parameters a, b, and d in the (u, v)-plane for $x = 0.88$. The region where $d < 0$ is represented by the slashed region. The region where $a < 0$ is represented by a cross-hatched region. The curve where $b = 0$ is shown by a dashed line.

V. SPECIAL CASES

Equations (17), (18), and (27) provide the closed form solution of the six-dimensional integral defining $\Lambda(k_F, \mathbf{k}', \mathbf{k}'')$. Although these equations are valid for all values of its variables, there are certain situations which are computationally awkward. Individual terms have divergences which are canceled by divergences in other terms. Also, situations where the numerator and denominator of a term vanish at the same point are encountered. For computational work, it is necessary to identify these situations and to evaluate the function properly when they occur.

Consider the function $\lambda(x, x', x'')$ of Eq. (18). Whenever any of the variables is equal to the sum of the other two, the quantity p appearing in the denominator vanishes. In such cases, the numerator also vanishes and a finite result is obtained by using the L'Hopital rule. For specificity, assume that $x'' = x + x'$. Then

$$\lambda(x, x', x + x') = \frac{\pi}{4xx'(x + x')}\left\{(1 - x^2)\ln\left|\frac{x + 1}{x - 1}\right| + (1 - x'^2)\ln\left|\frac{x' + 1}{x' - 1}\right| - (1 - (x + x')^2)\ln\left|\frac{(x + x') + 1}{(x + x') - 1}\right|\right\}. \tag{28}$$

A similar result holds when x or x' is equal to the sum of the other variables.

This expression must be modified in the special case that one of the variables is equal to zero. Because of the triangle inequality, the other two variables must be equal to each other. Suppose that $x'' = 0$. Then $x' = x$ and we get

$$\lambda(x, x, 0) = \frac{\pi}{2x}\ln\left|\frac{x + 1}{x - 1}\right|. \tag{29}$$

If all three variables are equal to zero, this simplifies to

$$\lambda(0, 0, 0) = \pi. \tag{30}$$

The other awkward situations occur when the logarithms diverge. The first term in Eq. (18) diverges when $x = \pm 1$. Likewise, the second term diverges when $x' = \pm 1$ and the third when $x'' = \pm 1$. The final term is more complicated, but it can be shown to diverge only at the same points. Further, the divergence of the last term precisely cancels any divergence in the first three. For $x = 1$, it is readily worked out that

$$\lambda(1, x', x'') = \frac{\pi}{((x' + x'')^2 - 1)(1 - (x' - x'')^2)}\left\{(x''^2 - x'^2 + 1)x'\ln\left|\frac{x' + 1}{x' - 1}\right| + (x'^2 - x''^2 + 1)x''\ln\left|\frac{x'' + 1}{x'' - 1}\right| + (x'^2 + x''^2 - 1)\ln\left|\frac{4(x'^2 - 1)(x''^2 - 1)}{(x'^2 + x''^2 - 1)^2}\right|\right\}. \tag{31}$$

Analogous relations cover the cases where $x' = 1$ or $x'' = 1$. If two variables are equal to one, for instance if $x = x' = 1$, then

$$\lambda(1, 1, x'') = \frac{\pi}{x''(x''^2 - 4)}\left\{(x'' - 2)\ln\left|\frac{x'' + 1}{x'' - 1}\right| - x''\ln\left|\frac{16(x''^2 - 1)}{x''^4}\right|\right\}. \tag{32}$$

Finally, if all three variables equal one,

$$\lambda(1, 1, 1) = 2\pi \ln 2. \tag{33}$$

VI. CONCLUSIONS

The function defined by Eq. (1) has been evaluated in closed form. The important equations for computational work are Eqs. (17), (18), and (27). Several special cases are enumerated in Eqs. (28)–(33). A program was written to evaluate these quantities and was used for the computation of the electron density of the embedded atom. As expected, the use of this program significantly expedited the computations. The results of these calculations are to be reported in another paper [1].

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