Computation of crystal Green's functions in the complex-energy plane with the use of the analytical tetrahedron method

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The analytical tetrahedron method (ATM) for evaluating perfect-crystal Green's functions is reviewed. It is shown that the ATM allows for computing matrix elements of the resolvent operator in the entire complex-energy plane. These elements are written as a scalar product involving weighting functions of the complex energy, which are computed on a mesh of $\vec{k}$ points in the Brillouin zone. When the usual approximations are made within each tetrahedron, namely linear interpolations for the dispersion relations as well as for the numerator matrix elements, the weighting functions only depend on the perfect-crystal dispersion relations. In addition, the analytical expression obtained for a tetrahedral contribution to the weighting functions is simpler than what is usually expected. Analytical properties of our expressions are discussed and all the limiting forms are worked out. Special attention is paid to the numerical stability of the algorithm producing the Green's-function imaginary part on the real energy axis. Expressions which have been published earlier are subject to computational problems, which are solved in the new formulas reported here.

I. INTRODUCTION

The Green's-function technique has proved extremely efficient when dealing with electronic or vibrational properties of imperfect solids.[1,2] It is especially beneficial for solving problems involving highly localized perturbations, such as point defects[3–5] and questions relating to surfaces or interfaces.[6–8] The Green's-function approach provides a convenient way of handling nonperiodic infinite systems without resorting to a cluster modeling. In this technique the size of the problem is controlled by the degree of localization of the crystal disturbance:[9] the more localized the perturbation, the lighter the computational effort. This simplification requires an explicit computation of the perfect-crystal Green's function in a basis set spanning the impurity space. Many of the limitations of the method issue from the practical difficulty of this computational task. Today such a computation is performed in two steps. The first step is the evaluation of the imaginary part of the Green's function, a problem somewhat analoguous to a perfect-crystal density-of-states calculation. The second step is the Hilbert transformation of this imaginary part to yield the real part of the Green's function. This, of course, requires a preliminary computation of the imaginary part on a wide and dense energy mesh. In this paper we indicate how it is possible to obtain a high-accuracy complex Green's-function matrix in only one step, and on an arbitrary (possibly quite reduced) energy mesh. Furthermore, by contrast with the techniques used previously, the complex Green's function (more exactly, a matrix element of the resolvent operator) is obtained in the form of the simple scalar product

$$G(z)=\sum_{\vec{k}}\sum_{n} w^{n}_{\vec{k}}(z)F_n(\vec{k}) , \tag{1}$$

where z stands for any complex energy, n runs over the retained set of bands, and $\vec{k}$ runs over a specific mesh that samples the Brillouin zone; $F_n(\vec{k})$ denoting the input matrix elements of the spectral projection operator. It must be emphasized that Eq. (1) is valid in the entire complex-energy plane. The approach described below is then directly applicable to problems involving contour integration of the Green's function, like those required by recent summation techniques over occupied states.[10,11] Another advantage of the above formulation [Eq. (1)] lies in the fact that the weight factors $w^{n}_{\vec{k}}(z)$ can be computed once and for all for a given perfect crystal and need not be repeated for different sets of matrix elements $F_n(\vec{k})$. Moreover, repetitive calculations of the scalar product are especially well suited to be handled by a vector processor. In this paper we shall describe basically how to obtain the coefficients $w^{n}_{\vec{k}}(z)$.

In designing this technique we did not find it more desirable to restrict ourselves to highly symmetric problems as in conventional approaches. For instance, the formulas we derive are valid for the most general triclinic lattice. This is especially important because the consideration of low-symmetry situations is needed increasingly in practical applications.[12,13] We use a decomposition of the Brillouin zone into a set of tetrahedra,[14–16] and, contrary to what is sometimes believed,[17,18] the lack of symmetry of these polyhedra do not induce prohibitively complicated expressions, neither for the imaginary part nor for the real part of the scalar product coefficients, even if the $\vec{k}$ dependence of the matrix element $F_n(\vec{k})$ is included to linear order. In this respect, we do not mean that these simple expressions are easily obtained. Intricate algebraic manipulations, which are not reported here in full detail, are needed, and many of them had to be carried out using a symbolic manipulation program.[19] Finally, we benefit here from another practical advantage of the tetrahedron

partitioning: The gradient of the dispersion relations are not explicitly needed.[20] This is particularly valuable in the numerous cases where the analytical gradient is not easily obtained, thus hindering the application of usual extrapolation techniques.[21,22]

II. THE ANALYTICAL TETRAHEDRON METHOD

The computation of most spectral properties of solids involves the evaluation of integrals such as

$$I(E)=\int_{\Omega}F(\vec{k})\,\delta(E(\vec{k})-E)\,d^3k = \int_{E(\vec{k})=E}F(\vec{k})/|\vec{\nabla}E(\vec{k})|\,dS \tag{2}$$

and

$$J(E)=\mathrm{P}\int_{\Omega}\frac{F(\vec{k})}{E-E(\vec{k})}d^3k=\mathrm{P}\int_{-\infty}^{+\infty}\frac{I(x)}{E-x}dx\ . \tag{3}$$

In these equations, $E(\vec{k})$ denotes a dispersion relation in the reciprocal space and $F(\vec{k})$ stands for a matrix element. In Eq. (2), dS is an infinitesimal element of the intersection area of the surface $E(\vec{k})=E$ with the volume Ω where integration has to be performed; the symbol P indicates that the integrals in Eq. (3) have to be understood in terms of a principal value. These integrals are intimately connected with the imaginary part [Eq. (2)] and with the real part [Eq. (3)] of a spectral function.

For twenty years many techniques have been devised to deal with this particular integration problem.[23–26] Among these, the analytical tetrahedron method (ATM) shows a number of advantages. It consists in introducing a decomposition of the $\vec{k}$-space volume Ω into a set of nonoverlapping tetrahedra.[14–18,27–31] $I(E)$ and $J(E)$ are then obtained by accumulating tetrahedral contributions. In this method the spirit of the so-called linear-analytical approach[32] is dominating: A linear interpolation of the dispersion relation is constructed so that the constant-energy surface is approximated by a plane within each tetrahedron.

The analytical determination of a tetrahedral contribution to the imaginary part $I(E)$ of the spectral function is then rather straightforward. In the most recent works devoted to this subject, the $\vec{k}$ dependence of the matrix element $F(\vec{k})$ is taken into account by a linear interpolation similar to that used for the dispersion relation $E(\vec{k})$.[17,29,30,33] In this paper, a slightly different formulation is proposed for the tetrahedral contribution to surface integrals like $I(E)$ [Eq. (2)], because the expressions given elsewhere are not always stable from a numerical point of view. This is made clear in Appendix B.

The analytical calculation of a tetrahedral contribution to principal value integrals like $J(E)$ [Eq. (3)] is much more involved. It was worked out first by Gilat and Bharatiya,[17] and, more recently, for susceptibility calculations.[18] However, the analytical expressions obtained by these authors appear so complicated that it is generally found more convenient to compute the real part $J(E)$ from the imaginary part $I(E)$ by a numerical Hilbert transformation [refer to Eq. (3)].[30] Fortunately, the algebraic expressions obtained previously for a tetrahedral contribution to $J(E)$ (Refs. 17 and 18) can be simplified considerably. This holds true even in more general situations; for instance, when evaluating Fourier elements of the Green function.[31]

The ability of the ATM to approximate a Green's-function matrix element by a scalar product [Eq. (1)], involving well-defined weight factors, has not been emphasized. Also, the ATM expressions are not restricted to the real-energy axis.[34] Once analytical formulations have been obtained for a complex energy z, they of course include both surface and volume integrals $I(E)$ and $J(E)$ for z approaching a real value E. However, the interest of the complex-energy plane extension is not restricted to derive these limits.

III. GREEN'S FUNCTION

Application of the Green's-function technique requires the evaluation of some matrix elements of the resolvent operator

$$(z-H)^{-1}=\sum_{n}\sum_{\vec{k}}|\psi_n(\vec{k})\rangle\langle\psi_n(\vec{k})|/[z-E_n(\vec{k})] \tag{4}$$

in a basis whose size depends on the particular defect potential treated. In Eq. (4), $|\psi_n(\vec{k})\rangle$ denotes an eigenvector of the one-electron perfect-crystal Hamiltonian H associated with the eigenvalue $E_n(\vec{k})$, where n runs over the bands. The number of bands actually included depends either on the perturbation potential, in conventional Green's-function approaches, or on the perfect-crystal orbital content, in the emerging matrix formulation.[10] Any matrix element of the resolvent operator is written as a $\vec{k}$-space integration

$$R(z)=\Omega^{-1}\sum_{n}\int_{\Omega}F_n(\vec{k})/[z-E_n(\vec{k})]\,d^3k\ , \tag{5}$$

where Ω denotes the reciprocal unit cell, or the first Brillouin zone (or an irreducible part of it, when an appropriate symmetrization of the basis has been performed), and $F_n(\vec{k})$ stands for a given matrix element of the spectral projection operator $|\psi_n(\vec{k})\rangle\langle\psi_n(\vec{k})|$.

Using the analytical tetrahedron method, including the $\vec{k}$ dependence for the numerator function $F_n(\vec{k})$ to a linear order, and denoting by $\vec{k}_i$, $i=1$, 2, 3, or 4 the position of the four corners of a given tetrahedron in $\vec{k}$ space, a tetrahedral contribution to $R(z)$ can be written

$$\Omega^{-1}\sum_{n}\int_{v}\{F_n(\vec{k})/[z-E_n(\vec{k})]\}\,d^3k = \sum_{n}\sum_{i=1}^{4}r_i^n(z)F_n(\vec{k}_i)v/\Omega\ , \tag{6}$$

where v stands for the tetrahedron volume and $r_i^n(z)$ is a complex weight factor, depending on z and on the corner energies E_i of the nth band $[E_i=E_n(\vec{k}_i)]$ through the relation

$$r_i^n(z)=\frac{(z-E_i)^2}{\prod_{k(\neq i)}(E_k-E_i)}+\sum_{j(\neq i)}\left[\frac{(z-E_j)^3}{\prod_{k(\neq j)}(E_k-E_j)}\frac{\ln[(z-E_j)/(z-E_i)]}{E_i-E_j}\right] . \tag{7}$$

In this equation, the indices i, j, and k run over the values $1,\ldots,4$. By contrast with the expressions previously proposed,[17,18] the above formulation [Eq. (6)] has the advantage that the corner values of the numerator matrix elements appear in a sum where they are multiplied by weight factors that depend only on the actual value of z and on the energy dispersion relations. In addition, the weight factors $r_i^n(z)$ [Eq. (7)] are surprisingly simple and can be easily constructed. However, attention must be paid to the case where two (or more) corner energies are identical; we shall consider this problem in Appendix A. It must be noted that there is no logarithmic singularity at $z=E_i$ in Eq. (7) owing to the following identity:

$$\sum_{j(\neq i)}\left[\frac{(z-E_j)^3}{\prod_{k(\neq j)}(E_k-E_j)}\frac{1}{E_i-E_j}\right] =-\frac{(z-E_i)^2}{\prod_{k(\neq i)}(E_k-E_i)}\sum_{j(\neq i)}\frac{z-E_j}{E_i-E_j} , \tag{8}$$

which, as the reader will certainly experience, is not trivial to prove by hand. This is an example of a relation we have "proved" with the help of an algebraic-manipulation program.[19] When z is a large complex number, the following asymptotic relation may be used for the computation of the function $r_i^n(z)$:

$$r_i^n(z)=\frac{1}{4}\frac{1}{z-a_i^n-b_i^n/z}+O(z^{-4}) , \tag{9}$$

with

$$a_i^n=\left[E_i+\sum_{j=1}^{4}E_j\right]\Big/5 \tag{10}$$

and

$$b_i^n=\left[\sum_{j(\neq i)}\left[3(E_j-E_i)^2+\sum_{k(\neq j)}(E_k-E_j)^2\right]\right]\Big/300 . \tag{11}$$

Equation (9) starts the continued-fraction expansion of $r_i^n(z)$.

The Green's function for a real argument E is commonly referred to as the limit

$$G(E)=R(E+i0) . \tag{12}$$

Thus, in order to obtain the expression for the Green's function from the resolvent operator matrix elements [Eq. (6)], we have to take the limit of the weight factors $r_i^n(z)$ when z approaches a real energy value E in the upper-half complex plane $\mathrm{Im}z>0$. Let us write

$$r_j^n(E+i0)=d_j^n(E)-i\pi c_j^n(E) , \tag{13}$$

where j denotes one corner of the tetrahedron. The real part of this expression is easily deduced from Eq. (7). By using the above identity [Eq. (8)], we have obtained the following result, in a form identical with that derived recently by Molenaar *et al.*:[31]

$$d_i^n(E)=\frac{(E-E_i)^2}{\prod_{k(\neq i)}(E_k-E_i)}\left[1+\sum_{j(\neq i)}\frac{E-E_j}{E_i-E_j}\ln|E-E_i|\right] +\sum_{j(\neq i)}\left[\frac{(E-E_j)^3}{\prod_{k(\neq j)}(E_k-E_j)}\frac{\ln|E-E_j|}{E_i-E_j}\right] . \tag{14}$$

Remember that the band label "n" enters such a relation through the corner energies E_i. When two (or more) corner energies are identical, Eq. (14) is no longer useful. Appendix A gives the limit values of $d_i^n(E)$ when equalities between the corner energies happen.

As for the imaginary part of Eq. (13), we obtain from Eq. (7) the result

$$c_i^n(E)=\frac{(E-E_i)^2}{\prod_{k(\neq i)}(E_k-E_i)}\sum_{j(\neq i)}\frac{E-E_j}{E_i-E_j}\Theta(E-E_i) +\sum_{j(\neq i)}\left[\frac{(E-E_j)^3}{\prod_{k(\neq j)}(E_k-E_j)}\frac{\Theta(E-E_j)}{E_i-E_j}\right] , \tag{15}$$

where $\Theta(x)$ is the Heaviside unit step function. From this expression and Eq. (8), one sees that $c_i^n(E)$ vanishes outside the interval $(E_{\min},E_{\max})$, where $E_{\min}$ ($E_{\max}$) is the smallest (the largest) corner energy. $c_i^n(E)$ is a positive cubic function of E in each panel bounded by two successive corner energies. When the corner energies differ from each other, $c_i^n(E)$ is a continuous function of E, as well as its first and second derivatives, except that the second derivative has a jump equal to

$$\frac{6}{\prod_{k(\neq i)}(E_k-E_i)}$$

at $E=E_i$. Therefore, $c_i^n(E)$ is close to a cubic spline function. Nevertheless, at this stage, Eq. (15) is not written in a form suitable for numerical computation. It is subject to numerical instabilities that are described in Appendix B, where stable and explicit formulas are given.

Once a tetrahedral contribution to any matrix element of the resolvent operator has been obtained [Eq. (6)], one accumulates all these contributions. We do not dwell too long on the problem of a tetrahedral subdivision of the $\vec{k}$ volume Ω.[30] It is easy to perform when integrating over the full unit cell of the reciprocal space: The unit cell is divided into small parallelepipeds (minizones), whose edges are parallel and commensurable with those of the unit cell. The vertices of the minizones define the $\vec{k}$ mesh of points (usually a few hundred, depending on the desired

accuracy) at which the dispersion relations $E_n(\vec{k})$ and the matrix element $F_n(\vec{k})$ are to be computed. Subsequently, each minizone is divided into six tetrahedra having equal volumes, each being defined by four of the corners of the parallelepiped. When integrating over the first Brillouin zone, or an irreductible part of it, a tetrahedral subdivision is particularly easy to perform when the $\vec{k}$ volume is a prism[33] (hexagonal system), a tetrahedron, or an aggregate of these two kinds of polyhedra;[35] as for the irreductible wedge of cubic crystals, a new tetrahedral subdivision scheme has recently been proposed.[36]

Thus a matrix element of the resolvent operator can be written from Eq. (6) as

$$R(z)=\sum_t \sum_n \sum_{i=1}^{4} r_i^n(z) F_n(\vec{k}_i) v/\Omega \ , \tag{16}$$

where the sum over t means a summation over the whole set of tetrahedra that fill the $\vec{k}$-space volume Ω and $\vec{k}_i$ stands for one of the corners of a tetrahedron, the volume of which being denoted by v as before. This equation can be rewritten in the form given by Eq. (1) where the sum over $\vec{k}$ means a summation over the points of the $\vec{k}$ mesh and where the weight factor $w_{\vec{k}}^n(z)$ is given by

$$w_{\vec{k}}^n(z)=\sum_{t \ni \vec{k}} r_{j(\vec{k})}^n(z) v/\Omega \ . \tag{17}$$

In this equation, we first sum over all the tetrahedra that have the given mesh point $\vec{k}$ as one of their corners; the symbol $j(\vec{k})$ means that the $\vec{k}$ point at hand is the corner j $(=1, 2, 3, \text{or } 4)$ of the tetrahedron t. The calculation of $w_{\vec{k}}^n(z)$ is easily implemented on the computer. The maximum number of tetrahedra which join at a given $\vec{k}$ point is 24.

As for the Green's function for real argument, one has from Eq. (1)

$$G(E)=\sum_{\vec{k}} \sum_n w_{\vec{k}}^n(E+i0) F_n(\vec{k}) \tag{18}$$

with

$$w_{\vec{k}}^n(E+i0)=\sum_{t \ni \vec{k}} [d_{j(\vec{k})}^n(E)-ic_{j(\vec{k})}^n(E)] v/\Omega \ , \tag{19}$$

which can be computed using the expressions we have obtained for the d and c functions. $w_{\vec{k}}^n(z)$ can be computed once and for all for a given perfect crystal: It depends only on the dispersion relation $E_n(\vec{k})$. This Green's-function summation technique has been applied for the first time to study the vibrational effects of an impurity embedded in a semiconductor crystal. The results will be published elsewhere.[37]

IV. DENSITY OF STATES

Earlier ATM works were devoted to the computation of the density of states. For completeness, and because numerical instabilities are sometimes encountered when using formulations published so far, we briefly derive hereafter a tetrahedral contribution to the density of states. This can be obtained by setting $F_n(\vec{k})=1$ in the above equations. A tetrahedral contribution to the density of states then writes

$$(1/\Omega) \sum_n \int_v \delta(E_n(k)-E)\, d^3k = \sum_n C_n(E) v/\Omega \ , \tag{20}$$

where, as before, v denotes the tetrahedron volume, and

$$C_n(E)=\sum_{i=1}^{4} c_i^n(E) \ . \tag{21}$$

From Eq. (15), we obtain

$$C_n(E)=3 \sum_{i=1}^{4} \left[\frac{(E-E_i)^2}{\prod_{k\,(\neq i)} (E_k-E_i)} \Theta(E-E_i) \right] . \tag{22}$$

$C_n(E)$ is a parabolic spline function of E that vanishes outside the interval $(E_{\min}, E_{\max})$, owing to the identity

$$\sum_{i=1}^{4} \frac{(E-E_i)^2}{\prod_{k\,(\neq i)} (E_k-E_i)} = 0 \ , \tag{23}$$

which can be obtained by summing over i both sides of Eq. (8). This recovers earlier results.[27,33] However, we do not recommend the use of the above formula because the expression directly derived from Eq. (15) is ill conditioned for some constant-energy plane orientations. A cure is provided in Appendix B.

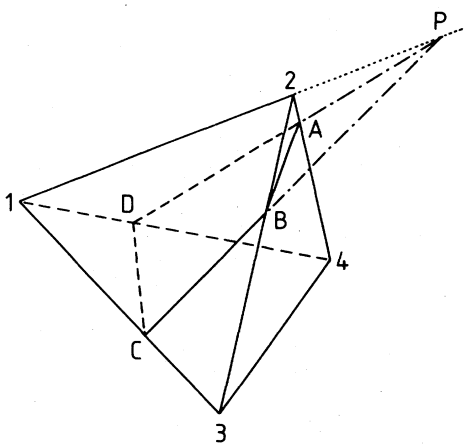

FIG. 1. The intersection area of the constant-energy plane $E_n(\vec{k})=E$ with a tetrahedron is the quadrilateral $ABCD$ when $E_2<E<E_3$. In numerous works devoted to the analytical tetrahedron method, this area has been considered as the difference between the triangles PDC and PAB. This gives rise to numerical instabilities because P goes to infinity when E_1 approaches E_2. In the present paper the quadrilateral $ABCD$ is constructed as the sum of triangles, without extrapolations outside the tetrahedron. This can be done in two ways, depending on which diagonal, AC or BD, is used. Therefore, Eq. (B5), which we have derived analytically, is easily interpreted.

APPENDIX A

When two (or more) corner energies are identical, Eq. (7) is still valid after appropriate limit calculations. In the present appendix, all the cases of degeneracy are reviewed. Let us first assume that no more than two corner energies are identical, let us say $E_l=E_m$ (l and $m=1$, 2, 3, or 4). We obtain in this case

$$r_i^n(z)=\frac{(z-E_i)^2}{(E_i-E_m)^2(E_k-E_i)}\left[1+\left[2\frac{z-E_m}{E_i-E_m}+\frac{z-E_k}{E_i-E_k}\right]\ln(z-E_i)\right]$$
$$+\frac{(z-E_m)^2}{(E_m-E_i)^2(E_k-E_m)}\left[1+\left[2\frac{z-E_i}{E_m-E_i}+\frac{z-E_k}{E_m-E_k}\right]\ln(z-E_m)\right]+\frac{(z-E_k)^3}{(E_k-E_i)^2(E_k-E_m)^2}\ln(z-E_k) \quad \text{(A1)}$$

for the two sites i different from the sites l and m; in this equation k indexes the site different from i, l, and m:

$$r_l^n(z)=r_m^n(z)=\frac{(z-E_j)^3}{(E_j-E_k)(E_j-E_m)^3}\ln(z-E_j)+\frac{(z-E_k)^3}{(E_k-E_j)(E_k-E_m)^3}\ln(z-E_k)$$
$$+\frac{z-E_m}{(E_m-E_j)(E_m-E_k)}\left\{\frac{1}{2}+\frac{z-E_j}{E_m-E_j}+\frac{z-E_k}{E_m-E_k}+\left[\left[\frac{z-E_j}{E_m-E_j}\right]^2\right.\right.$$
$$\left.\left.+\left[\frac{z-E_k}{E_m-E_k}\right]^2+\frac{z-E_j}{E_m-E_j}\,\frac{z-E_k}{E_m-E_k}\right]\ln(z-E_m)\right\}, \quad \text{(A2)}$$

where sites j and k ($j\neq k$) are the two sites different from the sites l and m where equality occurs between the corner energies.

When more than two corner energies are identical, it is more convenient to write explicitly the related expressions, by assuming that the corner energies for the nth band has been labeled in such a way that[17,28,33] $E_1\leq E_2\leq E_3\leq E_4$. The following expressions have been obtained:

$$r_1^n(z)=r_2^n(z)=r_3^n(z)=\frac{(z-E_4)^3}{(E_4-E_3)^4}\ln\left[\frac{z-E_4}{z-E_3}\right]+\frac{6(z-E_4)^2-3(E_4-E_3)(z-E_4)+2(E_4-E_3)^2}{6(E_4-E_3)^3},$$
$$r_4^n(z)=3\frac{(z-E_4)^2(z-E_3)}{(E_4-E_3)^4}\ln\left[\frac{z-E_3}{z-E_4}\right]-\frac{3}{2}(z-E_3)\frac{2(z-E_4)-(E_4-E_3)}{(E_4-E_3)^3}-\frac{1}{E_4-E_3}, \quad \text{(A3)}$$

when $E_1=E_2=E_3<E_4$;

$$r_1^n(z)=r_2^n(z)=3\frac{(z-E_3)^2(z-E_2)}{(E_3-E_2)^4}\ln\left[\frac{z-E_2}{z-E_3}\right]\frac{3}{2}(z-E_2)\frac{2(z-E_3)-(E_3-E_2)}{(E_3-E_2)^3}-\frac{1}{E_3-E_2},$$
$$r_3^n(z)=r_4^n(z)=3\frac{(z-E_2)^2(z-E_3)}{(E_3-E_2)^4}\ln\left[\frac{z-E_3}{z-E_2}\right]\frac{3}{2}(z-E_3)\frac{2(z-E_2)+(E_3-E_2)}{(E_3-E_2)^3}+\frac{1}{E_3-E_2}, \quad \text{(A4)}$$

when $E_1=E_2<E_3=E_4$;

$$r_1^n(z)=3\frac{(z-E_1)^2(z-E_2)}{(E_2-E_1)^4}\ln\left[\frac{z-E_2}{z-E_1}\right]\frac{3}{2}(z-E_2)\frac{2(z-E_1)+(E_2-E_1)}{(E_2-E_1)^3}+\frac{1}{E_2-E_1},$$
$$r_2^n(z)=r_3^n(z)=r_4^n(z)=\frac{(z-E_1)^3}{(E_2-E_1)^4}\ln\left[\frac{z-E_1}{z-E_2}\right]-\frac{6(z-E_1)^2+3(z-E_1)(E_2-E_1)+2(E_2-E_1)^2}{6(E_2-E_1)^3}, \quad \text{(A5)}$$

when $E_1<E_2=E_3=E_4$; and finally

$$r_1^n(z)=r_2^n(z)=r_3^n(z)=r_4^n(z)=\frac{1}{4}\frac{1}{z-E_1} \quad \text{(A6)}$$

when $E_1=E_2=E_3=E_4$.

To obtain the expressions for $d_i^n(E)$ [Eq. (14)], the real part of $r_i^n(z)$ must be taken for a real energy E. This can be done by setting $z=E$ in the above equations and by using absolute value for the argument of all logarithms involved.

APPENDIX B

This appendix is devoted to an explicit formulation of the functions $c_i^n(E)$, first introduced in Eq. (13), and given by Eq. (15). It is assumed here also that the corners $\vec{k}_i$ of the tetrahedron have been labeled in such a way that

$E_1 \le E_2 \le E_3 \le E_4$. We know that $c_i^n(E)$ vanishes outside the interval (E_1,E_4). Inside this interval, we have obtained the expressions

$$c_1^n(E)=\left[\frac{E_2-E}{E_2-E_1}+\frac{E_3-E}{E_3-E_1}+\frac{E_4-E}{E_4-E_1}\right]\frac{(E-E_1)^2}{(E_4-E_1)(E_3-E_1)(E_2-E_1)} \quad \text{if } E_1 \le E \le E_2 ,$$

$$c_1^n(E)=\frac{1}{2}\left[\frac{E_3-E}{(E_3-E_1)^2}\left[\frac{(E_3-E)(E-E_2)}{(E_4-E_2)(E_3-E_2)}+\frac{(E_4-E)(E-E_1)}{(E_4-E_1)(E_4-E_2)}+\frac{(E_3-E)(E-E_1)}{(E_3-E_2)(E_4-E_1)}\right]\right.$$
$$\left.+\frac{E_4-E}{(E_4-E_1)^2}\left[\frac{(E_4-E)(E-E_1)}{(E_4-E_2)(E_3-E_1)}+\frac{(E_4-E)(E-E_2)}{(E_4-E_2)(E_3-E_2)}+\frac{(E_3-E)(E-E_1)}{(E_3-E_1)(E_3-E_2)}\right]\right] \quad \text{if } E_2 \le E \le E_3 , \quad \text{(B1)}$$

$$c_1^n(E)=\frac{(E_4-E)^3}{(E_4-E_1)^2(E_4-E_2)(E_4-E_3)} \quad \text{if } E_3 \le E \le E_4 ,$$

$$c_2^n(E)=\frac{(E-E_1)^3}{(E_2-E_1)^2(E_3-E_1)(E_4-E_1)} \quad \text{if } E_1 \le E \le E_2 ,$$

$$c_2^n(E)=\frac{1}{2}\left[\frac{E_3-E}{(E_3-E_2)^2}\left[\frac{(E_3-E)(E-E_2)}{(E_4-E_2)(E_3-E_1)}+\frac{(E_4-E)(E-E_2)}{(E_4-E_2)(E_4-E_1)}+\frac{(E_3-E)(E-E_1)}{(E_3-E_1)(E_4-E_1)}\right]\right.$$
$$\left.+\frac{E_4-E}{(E_4-E_2)^2}\left[\frac{(E_3-E)(E-E_2)}{(E_3-E_2)(E_3-E_1)}+\frac{(E_4-E)(E-E_1)}{(E_4-E_1)(E_3-E_1)}+\frac{(E_4-E)(E-E_2)}{(E_3-E_2)(E_4-E_1)}\right]\right] \quad \text{if } E_2 \le E \le E_3 , \quad \text{(B2)}$$

$$c_2^n(E)=\frac{(E_4-E)^3}{(E_4-E_1)(E_4-E_2)^2(E_4-E_3)} \quad \text{if } E_3 \le E \le E_4 ,$$

$$c_3^n(E)=\frac{(E-E_1)^3}{(E_2-E_1)(E_3-E_1)^2(E_4-E_1)} \quad \text{if } E_1 \le E \le E_2 ,$$

$$c_3^n(E)=\frac{1}{2}\left[\frac{E-E_2}{(E_3-E_2)^2}\left[\frac{(E_3-E)(E-E_2)}{(E_4-E_2)(E_3-E_1)}+\frac{(E_4-E)(E-E_2)}{(E_4-E_2)(E_4-E_1)}+\frac{(E_3-E)(E-E_1)}{(E_3-E_1)(E_4-E_1)}\right]\right.$$
$$\left.+\frac{E-E_1}{(E_3-E_1)^2}\left[\frac{(E_3-E)(E-E_2)}{(E_4-E_2)(E_3-E_2)}+\frac{(E_4-E)(E-E_1)}{(E_4-E_1)(E_4-E_2)}+\frac{(E_3-E)(E-E_1)}{(E_3-E_2)(E_4-E_1)}\right]\right] \quad \text{if } E_2 \le E \le E_3 , \quad \text{(B3)}$$

$$c_3^n(E)=\frac{(E_4-E)^3}{(E_4-E_1)(E_4-E_2)(E_4-E_3)^2} \quad \text{if } E_3 \le E \le E_4 ,$$

$$c_4^n(E)=\frac{(E-E_1)^3}{(E_2-E_1)(E_3-E_1)(E_4-E_1)^2} \quad \text{if } E_1 \le E \le E_2 ,$$

$$c_4^n(E)=\frac{1}{2}\left[\frac{E-E_2}{(E_4-E_2)^2}\left[\frac{(E_3-E)(E-E_2)}{(E_3-E_2)(E_3-E_1)}+\frac{(E_4-E)(E-E_1)}{(E_4-E_1)(E_3-E_1)}+\frac{(E_4-E)(E-E_2)}{(E_3-E_2)(E_4-E_1)}\right]\right.$$
$$\left.+\frac{E-E_1}{(E_4-E_1)^2}\left[\frac{(E_4-E)(E-E_1)}{(E_4-E_2)(E_3-E_1)}+\frac{(E_4-E)(E-E_2)}{(E_4-E_2)(E_3-E_2)}+\frac{(E_3-E)(E-E_1)}{(E_3-E_1)(E_3-E_2)}\right]\right] \quad \text{if } E_2 \le E \le E_3 , \quad \text{(B4)}$$

$$c_4^n(E)=\left[\frac{E-E_3}{E_4-E_3}+\frac{E-E_2}{E_4-E_2}+\frac{E-E_1}{E_4-E_1}\right]\frac{(E_4-E)^2}{(E_4-E_1)(E_4-E_2)(E_4-E_3)} \quad \text{if } E_3 \le E \le E_4 .$$

These equations differ from analogous results presented elsewhere[17,29,33] when $E_2 \le E \le E_3$. In that case, the intersection area of the constant-energy plane $E_n(\vec{k})=E$ with the tetrahedron is a quadrilateral, which has been considered as the difference between two triangles in all the papers devoted to the analytical tetrahedron method (Fig. 1). This leads to an unfortunate instability in the numerical evaluation of such a contribution. The reason for this is that, when E_1 comes close to E_2, both triangles become extremely large, giving rise to a considerable loss of significant digits when substraction is performed. By contrast, the expressions we give here for $E_2 \le E \le E_3$ are written as a symmetric sum of positive terms; our expression can be interpreted as the result of the following integration formula:

$$\int_{ABCD} F(\vec{k})\,dS=\tfrac{1}{6}[(F_A+F_B+F_C)S_{ABC}+(F_B+F_C+F_D)S_{BCD}+(F_C+F_D+F_A)S_{CDA}+(F_D+F_A+F_B)S_{DAB}] , \quad \text{(B5)}$$

which is exact when $F(\vec{k})$ is a linear function of $\vec{k}$. In Eq. (B5), *ABCD* is a quadrilateral in a given plane of the three-

dimensional $\vec{k}$ space, $F_A, \ldots, F_D$ denotes the value taken by the function $F(\vec{k})$ at the corners $A, \ldots, D$, and $S_{ABC}, \ldots, S_{DAB}$ stand for the area of the four triangles that can be drawn in $ABCD$ without introducing other corners than those of the quadrilateral (Fig. 1). Another advantage of the above formulation resides in the fact that no problem is encountered when two (or more) corner energies are identical, except when $E_1=E_2=E_3=E_4$, in which case the four c functions reduce to

$$\delta(E-E_1)/4 ,$$

where $\delta(x)$ is the Dirac delta function.

The sum over i of the above expression is related to the tetrahedral contribution to the density of states [Eq. (20)]. One obtains

$$C_n(E)=3\frac{(E-E_1)^2}{(E_2-E_1)(E_3-E_1)(E_4-E_1)} \quad \text{if } E_1\le E\le E_2 ,$$

$$C_n(E)=3\left[\frac{(E_3-E)(E-E_2)}{(E_4-E_2)(E_3-E_2)(E_3-E_1)}+\frac{(E_4-E)(E-E_1)}{(E_4-E_1)(E_4-E_2)(E_3-E_1)}\right] \quad \text{if } E_2\le E\le E_3 , \tag{B6}$$

$$C_n(E)=3\frac{(E_4-E)^2}{(E_4-E_1)(E_4-E_2)(E_4-E_3)} \quad \text{if } E_3\le E\le E_4 .$$

Equation (B6) for $E_2\le E\le E_3$ is written as a sum of two positive quantities and differs from an expression commonly used for density of states calculations.[27,33] As said above, the present formulation should be beneficial for reasons of numerical stability.

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