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Simplification of Green's-function calculations through analytic continuation

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A computational scheme is described which simplifies many Green's-function calculations of energy-dependent quantities such as the density of states through a novel use of analytic properties. Calculations are performed at complex energies well above the real axis where the quantities of interest are slowly varying. Physical results are then obtained by analytically continuing Green's-function matrix elements back to real energies using an efficient numerical procedure based on Taylor-series expansions. The approach is simple, versatile, and particularly well suited for evaluating the complicated Brillouin-zone integrals which often appear in Green's-function calculations. In recent coherent-potential-approximation (CPA) calculations for $Hg_{1-x}Cd_xTe$, the use of this technique cut the required computer time by about a factor of 3.

I. INTRODUCTION

Many of the properties of crystalline, imperfect, and disordered solids are conveniently calculated by using Green's-function techniques.[1-3] At present, however, numerical use of these techniques is lengthy and cumbersome. One ingredient contributing to the complexity of such calculations is the singular behavior of the Green's function G on the real energy axis.[4]

Recently, the analytic properties of G for complex energies have been used[5,6] to simplify Green's-function calculations of quantities such as the charge density and total energy, which require a summation over the occupied states of a system. Instead of integrating the appropriate matrix elements of G along the real energy axis up to the Fermi level, as had previously been done, the real energy integrals in Refs. 5 and 6 are replaced by contour integrals in the complex energy plane. The contours are chosen to ensure smooth energy variations of G far from the real axis, thereby eliminating rapid energy variations, and reducing the required numerical work.

In this Brief Report we present a novel computational scheme also based on the use of complex energies which simplifies Green's-function calculations of energy-dependent quantities such as the density of states. This scheme consists of two basic steps. In step one, all numerical calculations (Brillouin-zone integrations, solution of Dyson's equation, etc.) are performed along a line of energies well above the real axis where energy variations are smooth. In step two, the important matrix elements of G are analytically continued back to the real axis using an efficient numerical procedure based on Taylor-series expansions. While this approach may not be superior for extremely-high-resolution results requiring numerical accuracies within a percent or so, its simplicity and versatility have already been demonstrated to yield quantitatively significant physical parameters ($\sim$5–10% accuracy) very efficiently.[7]

II. BRILLOUIN-ZONE INTEGRATION

The analytic continuation procedure described in Sec. III is especially useful in the context of Brillouin-zone integration, which is often the most time-consuming aspect of Green's-function calculations. The most general form of Brillouin-zone integral encountered in such calculations[8] is

$$G(E^+)=\int_{BZ} d^3k\, G(E^+,\vec{k}) = \int_{BZ} d^3k\, f(k)[E^+-E(\vec{k})-\Sigma(E^+,\vec{k})]^{-1} . \quad (1)$$

Here $E^+=E+i0^+$ is an energy infinitesimally close to the real axis, $f(\vec{k})$ is a slowly varying function of $\vec{k}$, $E(\vec{k})$ is a real band energy, and $\Sigma(E^+,\vec{k})$ is a complex self-energy [with $\mathrm{Im}\Sigma(E^+,\vec{k})\leq 0$]. In the special case $\Sigma(E^+,\vec{k})=0$, a variety of efficient Brillouin-zone schemes can often be implemented which exploit the fact that the imaginary part of $G(E^+,\vec{k})$ reduces to a series of δ functions at the band energies.[9] The only sophisticated technique which is also applicable in the presence of a finite self-energy, such as that found in disordered alloy calculations, is the special directions method of Bansil.[10]

In many Green's-function calculations, the matrix element $G(E^+)$ is most conveniently evaluated by adding a small, finite imaginary part to E^+ and directly calculating $G(E^+,\vec{k})$ at a large number of $\vec{k}$ points.[4,11] The drawback to this approach, of course, is that the number of $\vec{k}$ points which must be considered for accurate results is usually enormous due to the rapid $\vec{k}$-space variations of $G(E^+,\vec{k})$ when $|\mathrm{Im}\Sigma(E^+,\vec{k})|$ is small.

If the energy E^+, however, is replaced by a complex energy z in the upper half plane, the integral $G(z,\vec{k})$ is a much more slowly varying function of both z and $\vec{k}$. Only a relatively small number of $\vec{k}$ points is then required to evaluate $G(z)$. Unfortunately, the resulting $G(z)$ is considerably broader[12] than the desired $G(E^+)$. As a result, complex energies have been used previously only in the evaluation of Brillouin-zone integrals requiring low-resolution results.[11] The novel feature of the present scheme, which allows complex energies to be used without significant loss of accuracy, is the elimination of spurious broadening through analytic continuation back to the real axis.

III. NUMERICAL ANALYTIC CONTINUATION PROCEDURE

The procedure for performing the analytic continuation presented in this section is applicable to any function $F(z)$

which is analytic in the entire upper half plane of z.

The proper initial choice of complex energies to be used is specified as follows. Let us suppose that $F(E^+)$ must eventually be determined in the real energy interval $E_{\min} \leq E \leq E_{\max}$ in discrete steps ΔE. ΔE should be chosen such that $E_{\max} = E_{\min} + N\Delta E$, with N an integer. It is then necessary to consider only a discrete set of complex energies of the form

$$z_{n,m} = E_{\min} + n\,\Delta E + im\,\Delta E \quad , \tag{2}$$

where n and m are integers (cf. Fig. 1). The initial calculations of $F(z)$ should be performed along a line of such energies for a particular value of $m = M$. The optimal choice of M depends on ΔE and requires a compromise between ease of numerical computation of $F(z)$ (large M), which often involves integrals such as Eq. (1), and accuracy of the analytic continuation process to the real axis (small M). For reasons that will become clear, the accurate evaluation of the function at the end points $F(E^+_{\min})$ and $F(E^+_{\max})$ of the desired interval is ensured if the range of n to be considered in the initial row of values is $-(M+1) \leq n \leq N+M+1$.

In Fig. 1 the relevant portion of the complex energy plane is shown for a typical starting point $M=5$. The desired values of $F(E^+)$ lie at energies represented by triangles (heavy solid line) along the real axis in the figure. The initial calculations of $F(z)$ should therefore involve the energies $-6 \leq n \leq N+6$ along the line $m=5$, represented by circles.

The extension of $F(z)$ back to the real axis is achieved through repeated use of the Taylor-series expansion of $F(z)$,

$$F(z) = \sum_{j=0}^{\infty} F^{(j)}(z_0)(z-z_0)^j/j! \quad , \tag{3}$$

about a point z_0 for which $F(z_0)$ has already been determined. In each application of Eq. (3) the coefficients of a truncated form of the series are fit to $F(z_0)$ and other known values of the function. The resulting polynomial is then used to generate one new value of $F(z)$ for z closer to the real axis than z_0.

Since the approximation involved in truncating Eq. (3) is only accurate for z close to z_0, the entire analytic continuation process consists of a series of steps, M in all, which lead to $F(E^+)$ on the real axis. Specifically, a given step generates a new row of values $F_{n,m-1} \equiv F(z_{n,m-1})$ from previously determined values in preceding rows. The values of $z_0 = z_{n,m}$ to be considered in each step lie in the range $(-m+1) \leq n \leq (N+m-1)$. The energy configurations which determine the known values of $F(z)$ to be used in each application of Eq. (3) are described below.

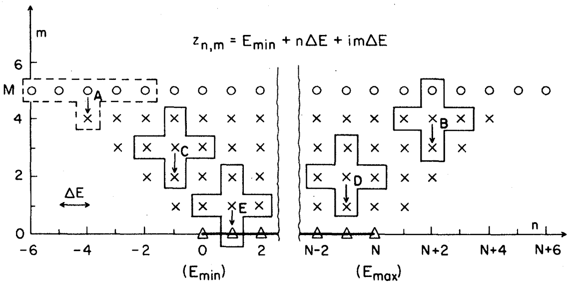

FIG. 1. Schematic illustration of the analytic continuation procedure for the starting point $M=5$. Boxes A–E represent the generation of one new value of the function in each of steps 1–5, respectively. {Dashed box: quartic expansion [cf. Eq. (4)] appropriate for step 1; Solid box: cubic expansion used for remaining steps [cf. Eq. (5)].} ○: energies where function is known initially. Δ: energies where function is ultimately determined. ×: energies where function is evaluated during intermediate steps.

In the example of Fig. 1, the analytic continuation procedure generates values of $F(z)$ for all energies represented by crosses. Examples of the generation of one new value in each of steps 1–5 are presented in boxes A–E, respectively. The figure illustrates how the number of values of z for which $F(z)$ must be evaluated decreases as the real axis is approached.

The first step, corresponding to row $m=M$, differs somewhat from those involving closer rows in that five consecutive values along the row must be considered (box A). These values are used to fit the unknown coefficients $F^{(j)}(z_0)$ of a quartic expansion of $F(z)$ about the central point $z_0 = z_{n,m}$. In the example in box A of Fig. 1, the new value $F_{-4,4}$ is generated from expansion about $z_{-4,5}$ (the central point) using the known values of $F(z)$ at the circled points in the box, $z_{n,5}$ for $-6 \leq n \leq -2$. In general, the value of $F_{n,m-1}$ generated by such a fit for the central point $z_0 = z_{n,m}$ is given explicitly by

$$F_{n,m-1} = 5F_{n,m}/2 + (F_{n-2,m} + F_{n+2,m} - 10F_{n-1,m} - 10F_{n+1,m})/12 + i(F_{n+2,m} - F_{n-2,m} - 5F_{n+1,m} + 5F_{n-1,m})/6 \quad . \tag{4}$$

Once the first two rows $(m = M, M-1)$ of values of $F(z)$ have been determined, a simpler, cubic approximation to Eq. (3) can be used as indicated in boxes B–E. For $z_0 = z_{n,m}$, this fit produces the new value

$$F_{n,m-1} = 4F_{n,m} - F_{n,m+1} - F_{n-1,m} - F_{n+1,m} \quad . \tag{5}$$

The final step yields the desired values of $F(E^+)$. Note that the radius of convergence of Eq. (3) is given by $\operatorname{Im} z_0$. The use of the cubic fit therefore ensures that only values of $z_{n,m}$ within this radius of convergence are required to fit the coefficients of Eq. (3), even as the real axis is reached.

Since only algebraic manipulations are involved, the procedure just described requires a minimal amount of computer time. To illustrate its effectiveness, we now consider the test function

$$h(z) = 2[z - (z^2-1)^{1/2}] + (z + 0.1 + 0.05i)^{-1} + (z - 0.1 + 0.05i)^{-1} \quad , \tag{6}$$

which is analytic in the upper half plane and exhibits many properties similar to those of Green's functions. The dotted curve in Fig. 2 shows $-\operatorname{Im} h(E^+)$. Its appearance is similar to a density of states containing $E^{1/2}$ singularities at $E = \pm 1$ and sharp Lorentzian structure at $E = \pm 0.1$. We use this sharp structure to illustrate the analytic continuation procedure. To begin, we calculate $h(z)$ off the real axis for $\Delta E = 0.02$ and $M=5$ (to give $\operatorname{Im} z = 0.1$). The dashed

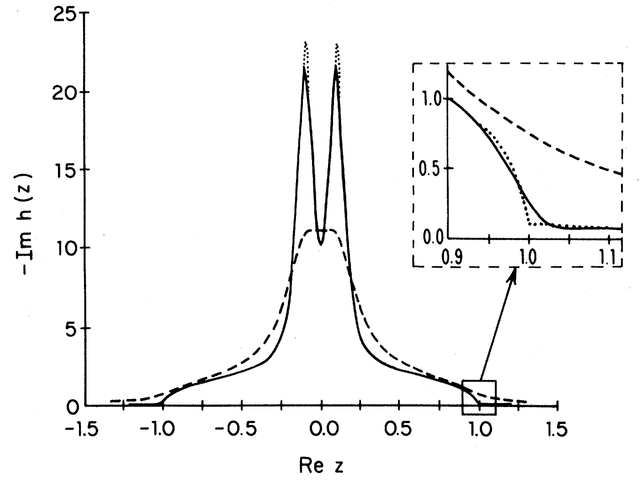

FIG. 2. Negative imaginary part of the test function $h(z)$ [cf. Eq. (6)] vs Rez for Im$z=0^+$ (dotted curve), and Im$z=0.1$ (dashed curve). The solid curve results from the application of the analytic continuation procedure to calculate values of $h(z)$ for $\Delta E=0.02$ and $M=5$.

curve in Fig. 2, $-\text{Im}h(z)$ vs Rez, along this line indicates how much the sharp structure is smoothed. This smearing of the band edges and Lorentizian structure is typical of that found for Green's functions evaluated for complex arguments. Using the values of $h(z)$ for Im$z=0.1$, we analytically continue the function numerically back to the real axis using the procedure described in this section. The result is indicated by the solid curve in Fig. 2. The Lorentzian peaks are again quite prominent, but not quite as sharp as the dotted curve, and the $E^{1/2}$ edges reappear, as seen in the inset. Noticeable discrepancies arise only in the vicinity of structure whose width is on the order of ΔE, as in the tips of the Lorentzian peaks and right at the band edges.

IV. IMPLEMENTATION IN REALISTIC CALCULATIONS

The approach described in this paper is easily implemented and widely applicable. It has been thoroughly tested by the present authors[7] in large-scale coherent-potential-approximation (CPA) calculations for $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$. The solution of the CPA equations[2] in realistic calculations requires several iterations. At each stage of iteration it is necessary to determine matrix elements of the form $G(E^+)$ in Eq. (1) in some range of E. These lead to a new approximation to the CPA self-energy. This process is continued to self-consistency. The present scheme is particularly well suited for such calculations since, in addition to simplifying the Brillouin-zone integrations, the use of complex energies often speeds up the iterative process as well.[13]

Some brief comments about the calculations for $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ in Ref. 7 will be useful to those wishing to use this scheme. These calculations utilized an empirical tight-binding approximation. The required Brillouin-zone integrals were evaluated by dividing the irreducible Brillouin zone into cubes,[14] determining $G(z,\vec{k})$ at each cube center, and multiplying by the fraction of the cube volume contained in the zone. For an energy spacing $\Delta E=0.075$ eV and $M=5$ (i.e., Im$z=0.375$ eV), 444$\vec{k}$ points were required to obtain accurate results.[15] Self-consistency to 0.1% was achieved in 2–4 iterations. As an accuracy check, the HgTe and CdTe densities-of-states calculations were performed for the same ΔE using the brute-force approach of adding a 0.02-eV imaginary part to E^+ and determining $G(E^+,\vec{k})$ at 2135 $\vec{k}$ points. The average root-mean-square difference between these reference results and the densities of states shown in Fig. 5 of Ref. 7 was about 3%.

The reduction in computer time associated with the analytic continuation was tested by performing straightforward CPA calculations for $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ with $x=0.3$, 0.5, and 0.7 using the same ΔE and Im$E^+=0.02$ eV. At least 825 $\vec{k}$ points and up to eight iterations were required to obtain CPA densities of states differing by less than 2% from those in Ref. 7 obtained from the analytic continuation technique. Overall, the computational scheme described here reduced the required computer time by about a factor of 3. A reduction of an order of magnitude could be achieved for numerical accuracies in the 10–20% range.

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[13] The iterative process speeds up because $\Sigma(z,\vec{k})$ becomes a more slowly varying function of z as Imz is increased.

[14] J. F. Janak, in *Computational Methods in Band Theory,* edited by P. M. Marcus, J. F. Janak, and A. R. Williams (Plenum, New York, 1971), p. 323.

[15] Away from the band edges, 203 points suffice.