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Exact solution for the resolvent matrix of a generalized tridiagonal Hamiltonian

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The exact solution for the resolvent matrix of a generalized tridiagonal Hamiltonian whose elements are themselves block matrices is obtained. The capability of the method is demonstrated by applying it to study the electronic structure on the surface of semiconductors. Some interesting insights regarding the difference between the Shockley states and Tamm states are also discussed.

I. INTRODUCTION

The tridiagonal Hamiltonian

$$H=\begin{bmatrix} \cdot & \cdot & \cdot & & & \\ V_{-1\,-2} & h_{-1\,-1} & V_{-1\,0} & & & \\ & V_{0\,-1} & h_{0\,0} & V_{0\,1} & & \\ & & V_{1\,0} & h_{1\,1} & V_{1\,2} & \\ & & & \cdot & \cdot & \cdot \end{bmatrix} \qquad (1)$$

has many applications in physics. For example, it has been used to study the excitations in several one-dimensional systems such as random alloys, biopolymers, and mixed crystals. It has also been used to study surface states, interface states, and defect states in a linear chain of atoms.

The basic calculation involved in these applications is the solution of the eigenvalue problem

$$Hu=Eu\,, \qquad (2)$$

or equivalently, the determination of the resolvent matrix

$$R(z)=(z-H)^{-1}\,. \qquad (3)$$

A simple diagram technique was first formulated by Wu and Taylor[1] and later extended by Wu, Tung, and Schwartz[2] to calcultate exactly the resolvent matrix. In this paper, we shall extend the method to the cases where each of the "elements" V_{ij} and h_{ii} of H are $n\times n$ submatrices. For the most general treatment, we shall neither require that any of these submatrices commute nor require that they be nonsingular. This generalization is of great significance because it increases the applicability of the method tremendously. For example, when applied to calculate the surface electron states of a real solid, the generalization not only opens the door to solving problems in three dimensions, it also allows one to include as many neighbor interactions and as many states per atom as needed for an adequate description of the electronic structure.

II. RESOLVENT MATRIX

In this section, we present the generalization of the diagrammatic techniques of Wu and Taylor[1] to calculate the resolvent matrix $R(z)$. We divide the matrix $R(z)$ into blocks so that each element $R_{nn'}$ of R is a block matrix with the same dimensions as the blocks in H (i.e., V_{ij} or h_{ii}). The elements $R_{nn'}$ can be expressed by the series

$$R_{nn'}=R_0(n)\delta_{nn'}+R_0(n)T_{nn'}R_0(n') + R_0(n)\sum_{n''}T_{nn''}R_0(n'')T_{n''n'}R_0(n')+\cdots\,, \qquad (4)$$

where

$$R_0(n)=(z-h_{nn})^{-1} \qquad (5)$$

and

$$T_{nn'}=V_{n,n+1}\delta_{n+1,n'}+V_{n,n-1}\delta_{n-1,n'}\,. \qquad (6)$$

We shall represent each term in Eq. (4) by a diagram using the basic symbols as defined in Fig. 1(a). It should be noted that here, each of the elements introduced is a matrix. Since these matrices do not commute in general, the order of multiplication must be maintained.

Consider the diagonal elements R_{nn}. These elements can be expressed by a series of diagrams represented in Fig. 1(b). The series contains par-

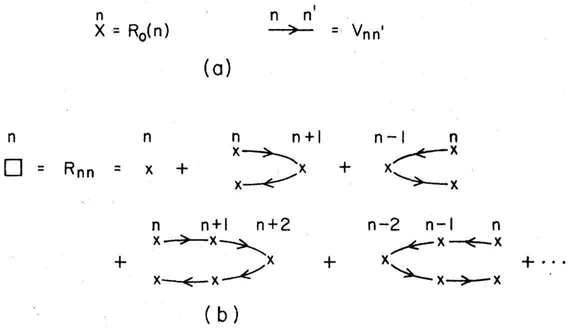

FIG. 1. (a) Diagrams for $R_0(n)$ and $V_{nn'}$. (b) Diagrammatic expansion of R_{nn}.

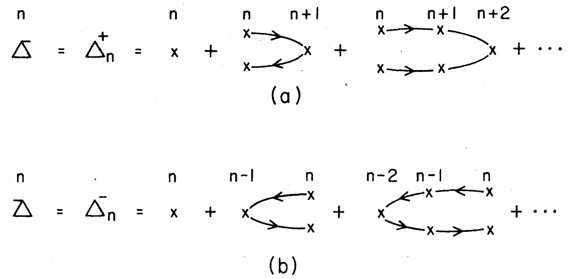

FIG. 2. Diagrammatic expansion of (a) Δ_n^+, (b) Δ_n^-.

tial sums of the type Δ_n^+ and Δ_n^- defined by Figs. 2(a) and 2(b). Δ_n^+ (Δ_n^-) includes all terms that start from n and returning to n after journeys to all $n' \geqslant n (n' \leqslant n)$. The series for R_{nn} can be regrouped in terms of these partial sums as shown in Fig. 3. The series is now a geometric series which can be summed to give

$$R_{nn} = [R_0^{-1}(n) - V_{n,n+1}\Delta^+_{n+1}V_{n+1,n} - V_{n,n-1}\Delta^-_{n-1}V_{n-1,n}]^{-1}\,. \tag{7}$$

The only problem that remains is the solution of $\Delta_n^\pm$. In Fig. 4, we grouped the terms in the series for $\Delta_n^\pm$ in terms of $\Delta^\pm_{n\pm1}$. These series are again geometric and can be summed to give the recursion relations:

$$\Delta_n^\pm = [R_0^{-1}(n) - V_{n,n\pm1}\Delta^\pm_{n\pm1}V_{n\pm1,n}]^{-1}\,. \tag{8}$$

Once a starting $\Delta_n^\pm$ is determined by a boundary conditions imposed on the problem, the rest of the Δ's can be computed using the recursion relations (8).

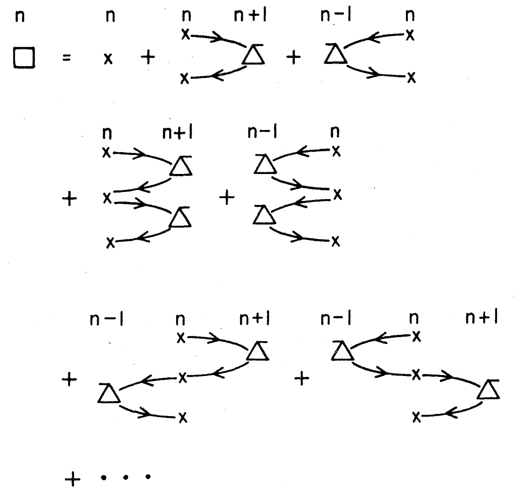

FIG. 3. Diagrammatic expansion of R_{nn} in terms of Δ^+_{n+1} and Δ^-_{n-1}.

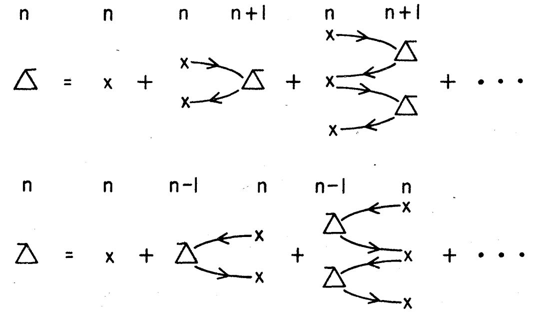

FIG. 4. Diagrammatic expansion of Δ_n^+ and Δ_n^-.

We now consider the off-diagonal elements $R_{nn'}$. These can be expressed in terms of $\Delta_n^\pm$ as illustrated in Fig. 5(a). We have

$$R_{nn'} = R_{nn}V_{n,n\pm1}\Delta^\pm_{n\pm1}\cdots V_{n'\mp1,n'}\Delta^\pm_{n'} \quad (n' \gtrless n)\,. \tag{9}$$

Equations (7)–(10) plus the boundary condition mentioned earlier completely determine R. From the diagram shown in Fig. 5(b), we also derive a useful recursion relation for R_{nn}:

$$R_{nn} = \Delta_n^+ + \Delta_n^+ V_{n,n-1}R_{n-1,n-1}V_{n-1,n}\Delta_n^+ \tag{10}$$

or

$$R_{nn} = \Delta_n^- + \Delta_n^- V_{n,n+1}R_{n+1,n+1}V_{n+1,n}\Delta_n^-\,. \tag{11}$$

III. APPLICATION TO SURFACE PROBLEMS

A. Hamiltonian

As an example of the possible application of our method, we shall study the electronic structure on the surface of semiconductors. We shall base our method on the tight-binding theory partly because of its simplicity and partly because when used in a semiempirical way, it gives bulk band structures in good agreement with those derived from a pseudopotential theory.[3] For a semi-infinite solid, the

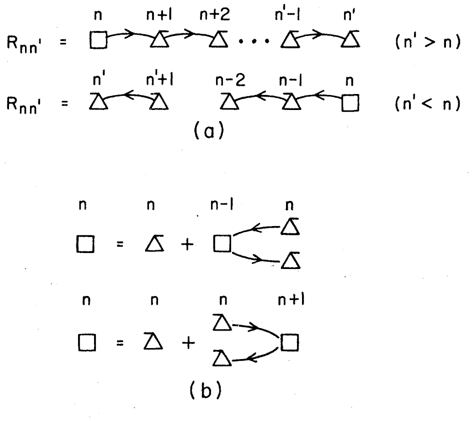

FIG. 5. (a) Diagrammatic expansion of $R_{nn'}$. (b) Diagrammatic expansion of R_{nn} in terms of $R_{n-1,n-1}$ or $R_{n+1,n+1}$.

translational symmetry in the direction parallel to the surface is preserved. Using a set of local orbitals $|\phi_{\alpha,l}\rangle$, where α labels each state at a given site l, we construct a two-dimensional Bloch wave for the nth plane parallel to the surface:

$$|\vec{k}_s,\alpha,n\rangle=(1/\sqrt{N})\sum_l e^{i\vec{k}_s\cdot\vec{R}_{nl}}|\phi_{\alpha,l}\rangle\,. \tag{12}$$

Here $\vec{k}_s$ is a wave vector parallel to the surface, and $\vec{R}_{nl}$ is the position of the atom on the lth site in the nth plane. The Hamiltonian of the system represented by matrix elements $\langle n,\alpha,\vec{k}_s|H|\vec{k}_s,n',\alpha'\rangle$ will in general have the form

$$H=\begin{bmatrix} h_s & \Gamma & & & \\ \Gamma^\dagger & h & C & & \\ & C^\dagger & h & C & \\ & & C^\dagger & h & C \\ & & & \cdot & \cdot\quad\cdot \end{bmatrix}\,, \tag{13}$$

where h_s, h, Γ, and C are submatrices with dimensions determined by the number of orbitals $|\phi_{\alpha,l}\rangle$ per atom. h_s can be interpreted as the Hamiltonian for the surface layer which we labeled by $n=0$. Γ is the coupling of the surface layer to the bulk layer described by the Hamiltonian h, and C is the coupling between bulk layers. More complicated situations can also be described in this spirit by allowing a series of h_s's and/or Γ's different from the bulk h and C.

B. Resolvent matrix

The periodicity of the Hamiltonian (13) beyond $n=1$ suggests further simplification of our method to calculate the resolvent matrix. From Fig. 2(a), we see that $\Delta_1^+=\Delta_2^+=\cdots\equiv\Delta$, because for $n=1,2,\ldots,$

$$R_0(n)=(z-h)^{-1}$$

and

$$\begin{aligned} &V_{n,n+1}=C\\ &V_{n+1,n}=C^\dagger\,. \end{aligned} \tag{14}$$

From Eq. (8), we get therefore,

$$\Delta=(z-h-C\Delta C^\dagger)^{-1}\,. \tag{15}$$

The solution of the above equation for Δ is the most difficult part in the application of our method. We shall discuss a rapid method of solution in Sec. III D. For now, we shall derive the resolvent matrix in terms of Δ. On the surface of the crystal, the boundary condition requires that $V_{n,n+1}=V_{n+1,n}=0$ for n negative. Therefore, from Eq. (7),

$$R_{00}=(z-h_s-\Gamma\Delta\Gamma^\dagger)^{-1}\,. \tag{16}$$

The rest of the diagonal blocks of the resolvent matrix can be calculated using the recursion formula (10) which simplifies to

$$R_{11}=\Delta+\Delta\Gamma^\dagger R_{00}\Gamma\Delta \tag{17}$$

and

$$R_{n+1,n+1}=\Delta+\Delta C^\dagger R_{nn}C\Delta\quad(n\neq 0)\,. \tag{18}$$

Likewise, the off-diagonal elements $R_{nn'}$ are derived from Eq. (9),

$$\begin{aligned} &R_{0n'}=R_{00}\Gamma\Delta(C\Delta)^{n'-1}\quad(n'>0)\,,\\ &R_{nn'}=R_{nn}(C\Delta)^{n'-n}\quad(n'>n\neq 0)\,,\\ &R_{nn'}(z)=R^*_{n'n}(z^*)\quad(n'<n)\,. \end{aligned} \tag{19}$$

Note that the resolvent matrix is completely determined by Δ.

C. Density of states

The density of states can be calculated directly from the diagonal blocks of R. The local density of states is given by

$$D_n(E)=-(\pi)^{-1}\operatorname{Im}\operatorname{Tr}R_{nn}(E+i0^+)\,. \tag{20}$$

The set of recursion formulas (16)–(18) allows one to study how the local density of states changes systematically from the surface into the bulk. Repeated application of the formulas gives

$$\begin{aligned} R_{n+1,n+1}=&\sum_{k=0}^{n}(\Delta C^\dagger)^k\Delta(C\Delta)^k\\ &+(\Delta C^\dagger)^n(\Delta\Gamma^\dagger)R_{00}(\Gamma\Delta)(C\Delta)^n\,. \end{aligned} \tag{21}$$

The last term results from the presence of the surface. It gives rise to a change in the local density of states,

$$\delta D_n(E)=-(\pi)^{-1}\operatorname{Im}\operatorname{Tr}(\Delta C^\dagger)^{n-1}(\Delta\Gamma^\dagger)R_{00}(\Gamma\Delta)(C\Delta)^{n-1}\,. \tag{22}$$

The rest of the terms in Eq. (21) give the bulk contributions to the local density of states, which in the limit $n\to\infty$ becomes the bulk density of states.

$$D_B(E)=-(\pi)^{-1}\operatorname{Im}\operatorname{Tr}\left(\sum_{k=0}^{\infty}(\Delta C^\dagger)^k\Delta(C\Delta)^k\right)\,. \tag{23}$$

Using the cyclic invariance of the trace, we can rewrite this equation as

$$D_B(E)=-(\pi)^{-1}\operatorname{Im}\operatorname{Tr}A\Delta\,, \tag{24}$$

where

$$A\equiv\sum_{k=0}^{\infty}(C\Delta)^k(\Delta C^\dagger)^k\,. \tag{25}$$

The series for A is trivially summed if $C\Delta$ and $\Delta C^\dagger$ commute. Otherwise, the summation is only slightly more complicated as A satisfies

$$A-(C\Delta)A(\Delta C^{\dagger})=1\,. \tag{26}$$

We can also calculate the total surface correction to the density of states:

$$D_S(E)\equiv[D_0(E)-D_B(E)]+\sum_{n=1}^{\infty}\delta D_n(E)\,. \tag{27}$$

Again using the cyclic invariance of the trace the summation can be carried out:

$$D_S(E)=-(\pi)^{-1}\operatorname{Im}\operatorname{Tr}[(1+\Gamma\Delta A\Delta\Gamma^{\dagger})R_{00}]-D_B(E)\,. \tag{28}$$

Equation (28) gives for the first time, an exact closed form solution to the total surface correction. The factor $1+\Gamma\Delta A\Delta\Gamma^{\dagger}$ normalizes the surface states, i.e., if E_S is the energy of the surface state, $D_S(E)$ becomes $\delta(E-E_S)$. [Note $D_B(E)=0$ outside the band where E_S occurs.] More important, this factor enables one to calculate the exact shape of resonances when energies in the bulk band region are considered. Finally the poles of R_{00}, calculated using Eq. (16), give the energies of the surface states. The position of the poles can be determined from

$$\|E-h_s-\Gamma\Delta\Gamma^{\dagger}\|=0\,. \tag{29}$$

The term $\Gamma\Delta\Gamma^{\dagger}$ can be considered as an effective or coherent potential arising from the coupling of the surface to the bulk.

D. Solution of Δ

As noted previously, Δ plays a central role in the determination of the resolvent matrix. The solution of Eq. (15) for Δ can best be done by defining $Y=\Delta C^{\dagger}$ so that

$$\Delta=(z-h-CY)^{-1}\,. \tag{30}$$

Multiplication by $C^{\dagger}$ on the right-hand side and $z-h-CY$ on the left-hand side gives

$$CY^2+(h-z)Y+C^{\dagger}=0\,. \tag{31}$$

Equation (31) belongs to a class of mathematical equations known as the unilateral equations and their solutions were reviewed by Roth.[4] It turns out that Eq. (31) has many solutions among which only one is a physically acceptable solution. We outline below the method for finding the solution.

Using a similarity transformation Q, we can write Y as $Y=Q\overline{Y}Q^{-1}$, where $\overline{Y}$ is diagonal. Then substitution into Eq. (31) and multiplication on the right-hand side by Q gives

$$CQ\overline{Y}^2+(h-z)Q\overline{Y}+C^{\dagger}Q=0\,. \tag{32}$$

Expressing Q in terms of its columns q_n, i.e., $Q=(q_1\cdots q_n)$ and $\overline{Y}_{ij}=y_i\delta_{ij}$, we get

$$[Cy_i^2+(h-z)y_i+C^{\dagger}]q_i=0\,. \tag{33}$$

Equation (33) is a λ-matrix problem,[5] defined in general by

$$(C_r\lambda^r+C_{r-1}\lambda^{r-1}+\cdots+C_1\lambda+C_0)x=0\,, \tag{34}$$

where the C's are $n\times n$ matrices and x is a column vector. The equation can be solved by forming the generalized block companion matrices. This procedure transforms Eq. (33) into the form

$$Ax=\lambda Bx\,, \tag{35}$$

where

$$A=\begin{pmatrix}0 & I\\ -C^{\dagger} & 0\end{pmatrix}\quad\text{and}\quad B=\begin{pmatrix}I & 0\\ h-z & C\end{pmatrix}.$$

Equation (35) is a generalized eigenvalue problem which can be solved by standard programs in the computer. y_i is simply the eigenvalue of this equation and q_i is simply the first n component of the corresponding eigenvector x. In general, Eq. (33) will have a solution only if

$$\|Cy^2+(h-z)y+C^{\dagger}\|=0\,. \tag{36}$$

If C is a $n\times n$ matrix, Eq. (36) gives $2n$ solutions for y out of which only n are physically allowed. It turns out that the solutions for y have a unique form which simplified the selection of the appropriate value. Equation (36) has the symmetrical form

$$\begin{aligned}&a_ny^{2n}+a_{n-1}y^{2n-1}+\cdots+a_0y^n\\&\quad+a_{-1}y^{n-1}+\cdots+a_{-n}=0\,,\end{aligned} \tag{37}$$

where $a_{-i}=a_i^*$ and a_0 is real. If all the a_i's are real, the equation is a reciprocal equation. In general, if y_i is a solution of Eq. (37), $1/y_i^*$ is also a solution. Thus, Eq. (37) factors as

$$\prod_{i=1}^{n}(A_iy^2+2B_iy+A_i^*)=0\,. \tag{38}$$

Consider the solutions of

$$Ay^2+2By+A^*=0\,.$$

Let $A=|A|e^{i\theta}$ and $\beta=-B/|A|$, then

$$e^{i\theta}y^2-2\beta y+e^{i\theta}=0\,. \tag{39}$$

The typical solutions for y are therefore

$$y_{\pm}=[\beta\pm(\beta^2-1)^{1/2}]e^{i\theta}\,. \tag{40}$$

For $z=E+i0^{+}$, one of the solutions will be inside a unit circle in the complex y plane and the other will be outside the unit circle. Convergence of the series from which Eq. (30) is derived requires that only solutions inside the unit circle be allowed. The trajectories of the allowed values of y_i in the complex y plane as a function of E provides valuable information about the bulk bands. For energies in the bulk bands, the trajectory of one or more of the y_i falls on the unit circle ($|y_i| = 1 - 0^+$). For energies in the band gap, all the trajectories are inside the unit circle ($|y_i| < 1$). These facts are best presented by a simple one-dimensional example which we shall publish shortly.

E. Silicon (111) surface

For the purpose of demonstrating the applicability of our method, we consider a nontrivial example, the unrelaxed (111) surface of silicon. For convenience, we shall use Hirabayashi's Hamiltonian.[6] We calculated the density of states $D_{S,B}(E)$ for a specific wave vector $\vec{k}_s$ parallel to the surface. We present here only the $\vec{k}_s = 0$ results because this result can be compared directly with the bulk band structure in the (111) direction. For $\vec{k}_s = 0$, h_s, h, Γ, and C are the following matrices in Hirabayashi's model:

$$h_s = h = -\begin{bmatrix} 8.40 & 0.90 & 0.90 & 0.90 & 0.889 & 0.889 & 0.889 & 0.228 \\ 0.90 & 8.40 & 0.90 & 0.90 & 1.10 & 1.10 & 2.35 & 0.889 \\ 0.90 & 0.90 & 8.40 & 0.90 & 1.10 & 2.35 & 1.10 & 0.889 \\ 0.90 & 0.90 & 0.90 & 8.40 & 2.35 & 1.10 & 1.10 & 0.889 \\ 0.889 & 1.10 & 1.10 & 2.35 & 8.40 & 0.90 & 0.90 & 0.90 \\ 0.889 & 1.10 & 2.35 & 1.10 & 0.90 & 8.40 & 0.90 & 0.90 \\ 0.889 & 2.35 & 1.10 & 1.10 & 0.90 & 0.90 & 8.40 & 0.90 \\ 0.228 & 0.889 & 0.889 & 0.889 & 0.90 & 0.90 & 0.90 & 8.40 \end{bmatrix} \quad (10^{-1}\ \mathrm{Ry})$$

and

$$\Gamma = C = -\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.437 & 0.226 & 0.226 & 0.076 & 0 & 0 & 0 & 0 \\ 0.437 & 0.226 & 0.076 & 0.226 & 0 & 0 & 0 & 0 \\ 0.437 & 0.076 & 0.226 & 0.226 & 0 & 0 & 0 & 0 \\ 2.198 & 0.437 & 0.437 & 0.437 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (10^{-1}\ \mathrm{Ry}).$$

In Fig. 6, we show the density-of-states curve as well as the bulk band structure from Γ to L in the neighborhood of the fundamental gap. The bulk band structure was calculated by the direct diagonalization of the bulk Hamiltonian. It can be seen that the band edges and the band gaps calculated with our method agree exactly with the band-structure calculation. The effect of the overlapping bands shows up clearly in the bulk density of states. The result for the surface state at −0.766 Ry also agrees with Hirabayashi's result. Actually our method determines the energy much more accurately as we do not truncate the Hamiltonian like Hirabayashi. A major portion of the computer time went into the solution of Y. For each value of the energy, the solution takes about 0.1 CPU (central processor unit) seconds on an IBM 370/165 computer.

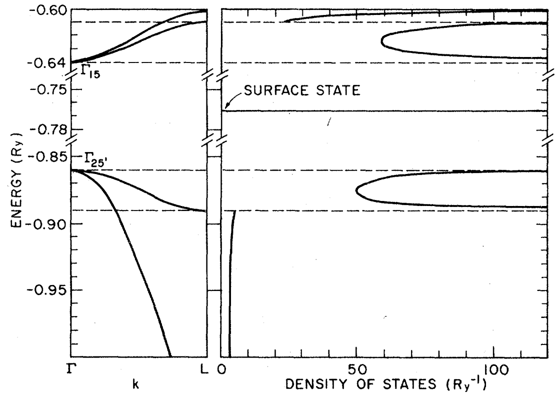

FIG. 6. Bulk band structure and density of states for $\vec{k}_s = 0$ along the (111) direction of Si. The δ function at −0.766 Ry is the surface state and the rest are the bulk density of states.

The surface state derived in this example was first suggested by Shockley.[7] For some time there has been some confusion regarding the precise definition[8] of the Shockley states and another type of surface states known as the Tamn states.[9] Shockley states are said to appear when there is no surface perturbation, i.e., $h_s = h$ and $\Gamma = C$, and when the energy bands cross. From Eqs. (16), (26), and (28) we see that $D_S(E) = 0$ when $h_s = h$ and $\Gamma = C$, i.e., there are no surface states. The nonexistence of the surface states seems to contradict Shockley's theorem. One explanation of the disappearance of the surface states is that Shockley based his theory on a finite system; as the system becomes semi-infinite, the surface states move to infinity. This explanation is only partly correct because only one of the surfaces has moved to infinity. To resolve the paradox, we study the condition for the surface states [Eq. (29)]:

$$S(E) \equiv \| E - h_s - \Gamma \Delta \Gamma^\dagger \| = 0 .$$

Consider the $S(E)$ curve for Hirabayashi's Hamiltonian. In Fig. (7) we show $S(E)$ with $h_s = h$ and $\Gamma = C$ (dashed line). This curve has no zero, so there should be no surface state. However, if we perturb one of the values in h_s very slightly (say from $h_{11} = -0.84$ to $h_{11} = -0.8399$ in h_s) so that $h_s \neq h$, we then find the other set of curves (solid line) for $S(E)$. It is seen that now a surface state is recovered at energy E_s'. In addition there is an isolated but nonsimple singularity at $E = E_s$. It was found that in the limit $h_s = h$, the surface-state energy $E_s' = E_s$. The nonanalytical nature of $S(E)$ is a result of treating the solid as semi-infinite from the very outset. The singularity can be avoided if we redefine the blocks in the Hamiltonian by adding a row and column of null matrices,

$$H' = \begin{bmatrix} 0 & 0 & 0 & 0 & \\ 0 & h & C & 0 & \\ 0 & C^\dagger & h & C & \\ 0 & 0 & C^\dagger & h & \\ & & & & \ddots \end{bmatrix} , \quad \text{etc.},$$

so that

$$h_s' = \begin{pmatrix} 0 & 0 \\ 0 & h \end{pmatrix}, \quad h' = \begin{pmatrix} h & C \\ C^\dagger & h \end{pmatrix},$$

and $h_s' \neq h'$. This procedure, however, would double the size of the block matrices. Whichever method one chooses is mainly a matter of preference.

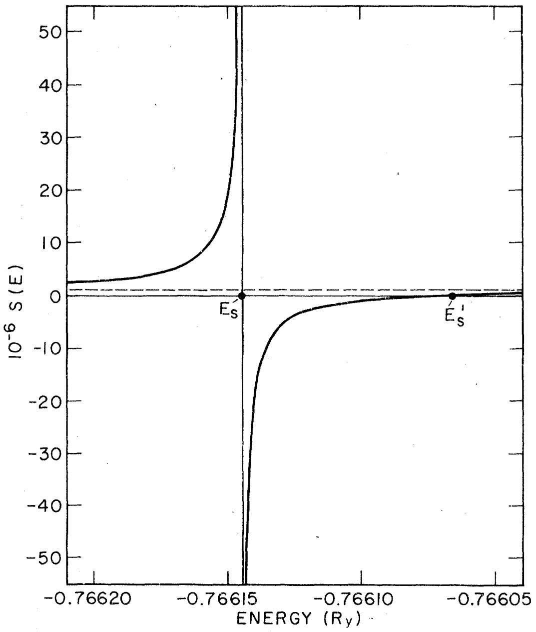

FIG. 7. $S(E)$ curve defining the Shockley state at E_s.

IV. CONCLUSION

In this work, we have developed a method for calculating the resolvent matrix of a generalized block tridiagonal matrix. The method has the following important features.

(i) The method allows one to calculate the resolvent matrix exactly without the need to truncate the Hamiltonian or set other arbitrary boundary conditions.

(ii) The method allows one to calculate both "local" density of states as well as total density of states.

(iii) The method allows one to calculate the exact shape of resonances.

(iv) The method allows one to incorporate as many neighbor interactions and as many states per atom as needed for an adequate description of the system.

(v) The method is computationally simple. In many cases, the solution has simple mathematical form so that it can be studied analytically.

As a demonstration of the capability of this method, we have applied the method to study the electronic structure on the surface of semiconductors. There exist a large body of references in the field of surface physics for solving Hamiltonians of the type given by Eq. (13). We have not attempted to review them here, instead we cite a few references[3,6,10-14] mainly to point out that in these works the methods of computation are very inefficient because many bulk states have to be included in the calculations. In contrast, the present method incorporates all the bulk information into Δ, which can be solved rapidly. The speed and accuracy of this method, we hope, would provide a better handle in solving the more difficult problems of reconstruction and many-body effects on solid surfaces.

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