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Calculation of ballistic conductance through Tamm surface states

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Ballistic conduction through Tamm surface states is studied theoretically. We calculate the conductance in systems of scanning tunneling microscopy (STM) with double tips as well as a single tip. Conductance spectra of flat surfaces containing surface states are qualitatively proportional to the density of states at the first layer of surfaces if we calculate on boundary conditions that allow net current to flow parallel to surfaces. The potential difference between the first layer and inner layers enhances the conduction through Tamm states. When a STM tip is put on an island of a surface, the conductance varies as a function of the step height of the island. The variation is explained by the difference in the step-height dependence between surface-state and bulk-state conduction. The tunneling between the surface states of islands and substrates is the main path of the surface-state conduction at low step heights. The study of the conduction in islands demonstrates the importance of the conduction path in surfaces to electrodes. The ballistic conductance spectra between two tips in double-tip systems show one-dimensional features, which suggests high conductance when the Fermi energy is located near band edges of surface states.

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I. INTRODUCTION

Surface states are formed at interfaces of the vacuum and materials and are intrinsic to surfaces of materials. Until now they have been observed using various experimental techniques in surface science. However, very recently, conduction through surface states has attracted much attention[1] and its properties have been studied directly using microscopic methods such as scanning tunneling microscopy (STM).[2–4]

On the other hand, surface states have been extensively studied theoretically[5,6] since the early works by Tamm[7] and Shockley.[8] But, the number of theoretical works that studied directly the transport properties through surface states is not so large. In particular, little is known about ballistic transport through surface states, despite its importantance in microscopic measurements. For example, how large is the contribution of the surface-state conduction to the total conduction when both surface and bulk states coexist? How sensitive is the surface-state conduction to irregularities such as steps or defects? What information about surface states is obtained from conduction measurements? These questions are important for analyzing experimental data, but they remain unanswered, mainly due to lack of quantitative calculations of conduction through surface states. In earlier theoretical works, conduction though surface states was studied using such approximations as the neglect of bulk states or the perturbative approach of tunneling.

In this paper we present numerical calculations of the ballistic conduction through surface states and clarify the properties theoretically. The model for surfaces used in this paper is very simple. But, since it describes both surface and bulk states within a single Hamiltonian and we do not use such approximations as tunneling, we can determine without ambiguity the magnitude of the conduction through surface states. This is a starting point for more realistic calculations.

In this paper we discuss three topics on the surface-state conduction. One is the mechanism of the observation of surface states in STM. In the early stage of development of STM surface states were observed on semiconductor surfaces.[9–11] Peaks corresponding to surface states were clearly seen in the spectra obtained by scanning tunneling spectroscopy (STS). So far, the STS spectra have been explained qualitatively in terms of the local density of states (LDOS) of sample surfaces using the Tersoff-Hamann theory.[12] Since the component of surface states is finite in the LDOS at surfaces, it seems that the surface states observed in STS can also be explained by the Tersoff-Hamann theory. However, the observation of surface states in STM is not trivial, as shown below.

Using scattering theory, Noguera pointed out that surface states may not be observed in STM because the group velocity of surface states is zero in the direction perpendicular to surfaces.[13,14] The reason for the seeming success of the theory of Tersoff and Hamann in explaining the observation of surface states is that it takes account of only the tunneling process between a tip and a surface, and the paths of the tunneling electrons to the electrodes in contact with surfaces are not explicitly considered. If we consider that surface states decay into the bulk, it is not clear why the electrons in surface states travel to the electrodes. Furthermore, Noguera showed that Bardeen's perturbative approach is not valid for surface states. Since the Tersoff-Hamann theory is based on Bardeen's formalism, there are no grounds for its application to STS spectra of surface states. The reason for the observation of surface states in STM is not clear.

Noguera mentioned two possibilities for the surface-state observation. One is the current flowing parallel to surfaces. The other is the effect of inelastic scattering or temperature in surfaces. Makoshi made a similar argument and showed other possibilities.[15] For example, surface states and bulk states may mix due to irregularities such as defects. Electrons in surface-state bands may tunnel to bulk bands due to the band bending. Though there are several possibilities, it has not yet been settled which is dominant for the surface-state observation, due to the lack of concrete calculations of the surface-state conduction.

In this paper we calculate the conductance in a STM system containing surface states and discuss a possibility that the observation of surface states in STS is explained by the lateral current. In the calculations of conductance we do not use the periodic boundary condition for the directions parallel to the surface. The periodic boundary condition is useful in the case for which only bulk states exist in surfaces, and is widely used. However it cannot be used to calculate the conductance through surface states, because only the channels propagating perpendicular to surfaces contribute to the conductance calculated on the periodic boundary condition, and the contribution of surfaces states is not taken into account. Therefore, in this paper we calculate the conductance on a boundary condition that allows net current to flow laterally, and we determine the magnitudes of the conductions though bulk and surface states. We find that in the case of flat surfaces without surface defects and steps the ratio of the surface-state component in conductance to the bulk-state component is qualitatively reproduced by the density of states (DOS) at the outermost layer of the surface. This result suggests that the observation of surface states in STS is explained by the lateral current and supports partially the use of LDOS for analyzing STS spectra of surface states.

The second topic of the present paper is to investigate the surface-state conduction in islands on surfaces. Hasegawa, Lyo, and Avouris performed point-contact measurement on silicon surfaces using STM.[2] They compared the electrical conductances between when an STM tip is put on flat terraces and when on islands and found that the conductance of the latter is lower than that of the former by about one order of magnitude. This result suggests that the electrical current flows mainly through surface states in their experiment. In this paper we present calculations of the conductance when a tip is put on an island and investigate properties of the conduction in islands.

So far, the reduction of electrical conduction in islands has usually been explained by the scattering of electrons at the steps of islands in the diffusive regime. However, since the lateral size of the islands in the experiment by Hasegawa, Lyo, and Avouris is about $100 \times 100\,\text{Å}^2$, the electrical conduction in the islands can be assumed to be ballistic. We show that in such a ballistic regime the tunneling from the surface states of islands to those of substrates rather than the scattering at steps is a good picture for explaining the reduction of conductance in islands.

The third topic of this paper is to simulate the conductance measurement using the double-tip STM. Recently the electrical conduction of surfaces was directly measured using micro-four-point probes,[4,16] where the contribution of surface states to surface conduction was discussed. The distance between probes in these experiments is of micrometer order and the electrical conduction is not ballistic. But it is a promising tool for measuring directly the electrical transport on the nanometer scale, and in the future it may become possible to study directly the ballistic conduction of surfaces by decreasing the distance between probes. In this paper we present calculations of ballistic conductance in the double-tip STM and discuss the role of surface states in the conduction of this system.

Theoretical studies on the two-probe measurement have been performed by two groups.[17,18] They assumed that the conduction between probes and sample surfaces is through tunneling and derived expressions for tunneling current by using the perturbation theory similar to Bardeen's approach. In the present paper we use the Landauer formula[19] for calculating conductance. The Landauer formalism allows us to calculate the ballistic conductance exactly without the approximation of tunneling and can be used even when probes are in close contact with sample surfaces. In this formalism it is easy to take account of minute atomic structures of tip-surface contacts and to extend to calculations of the conductance of realistic surfaces. We discuss the surface-state conduction from an atomistic point of view.

The surface state studied in this paper is the Tamm state.[7] Tamm states exist when the potential of the outermost layer of surfaces is different from that of inner layers by a certain amount.[5,6] Tamm states were experimentally observed on Cu(100) and Cu(111) surfaces[20] and superlattices.[21] Different from the Shockley state,[8] Tamm states exist in single-band systems without band gaps. The reason for studying the Tamm state in this paper is that the system of Tamm states is very simple, though there is no difficulty in principle in calculating the conductance through Shockley states. In Sec. II, we present the model studied in this paper and the method of calculation. Results calculated for flat surfaces, islands, and double-tip systems are shown in Sec. III.

II. METHOD OF CALCULATION

A. Model

Figure 1 shows the schematic of the models studied in this paper. We calculate the conductance for three systems. One is a system consisting of a single STM tip and a flat surface, which corresponds to Fig. 1(a) with neglect of the second tip. The second is an island on a substrate surface with a single tip as shown in Fig. 1(b). The third is a system of double tips on a flat surface as shown in Fig. 1(a).

In single-tip systems we assume chemical potentials respective for the tip and sample surface and consider the situation in which a current flows from the tip to the sample surface by the difference of the chemical potentials. In double -tip systems we can assume three independent chemical potentials for the first tip, the second tip, and the sample surface, if we connect the third electrode to the sample surface. In this paper we consider a situation in which the chemical potential of the first tip is higher than that of the sample surface, and the chemical potential of the second tip is equal to that of the sample surface. Therefore a part of electrons injected from the first tip into the sample surface is ejected through the second tip, and the remaining electrons go out through the electrode contacted with the sample surface. This is similar to the setup assumed in the earlier theoretical works of two-probe measurements[17,18] except for the absence of the bias voltage between the second tip and sample surface. Note that this is different from the setup for the two-probe measurement where sample surfaces are not connected with the third electrode and the current flows only between the two probes.

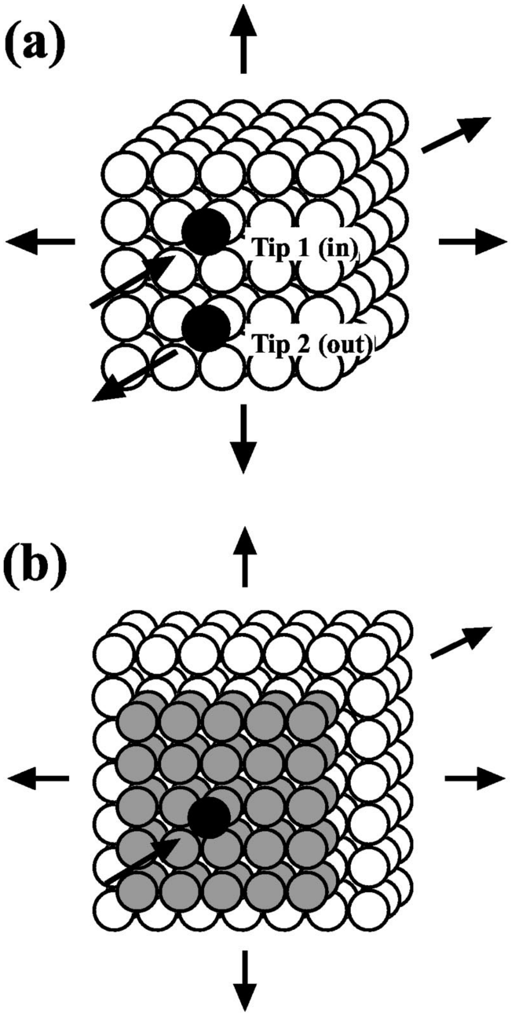

FIG. 1. Schematic of the models studied in this paper. Surfaces are (a) a flat surface and (b) an island on a flat substrate. In the case of the flat surface we study the configuration with double tips as well as with a single tip. Open and closed circles show the surface atoms and the atoms at the apexes of the tips, respectively. Gray circles show the atoms of the island.

The surface atoms including the part of the island are arranged in the simple-cubic lattice. We use a tight-binding method with only a single s orbital for each atomic site and the transfer energy $-t_S$ ($t_S>0$) between nearest-neighbor atoms. We neglect the overlap integral. The on-site energy is zero except for the outermost layer where the on-site energy is U. When $|U|$ is greater than t_S, a Tamm state exists.[5,6] The energy dispersion of this state is given by

$$E(\mathbf{k}_\parallel)=U+\frac{t_S^2}{U}-2t_S(\cos k_xa+\cos k_ya), \tag{2.1}$$

where $\mathbf{k}_\parallel=(k_x,k_y)$ is a wave vector parallel to the surface and a is the lattice constant. The wave function of this state decays exponentially into the surface by a ratio of $-t_S/U$ for every layer.

We assume that the apex of the tips is a single atom and electrons always pass through the single apical atom. It is conjectured based on theoretical calculations that this situation is realized when normal STM images are observed in experiments.[22] In such a situation we expect that the conduction between a tip and a surface does not depend much on the minute atomic structure of the tip. Therefore, instead of taking realistic atomic structures of tips into account, we substitute a semi-infinite one-dimensional chain for the structure of the tips in this paper for simplicity. It is not so difficult to extend the present calculations using more realistic models for the tips. But, since our interest in this paper is concentrated on the transport in surfaces, we think this simple model enough for the purposes of the present paper.

We calculate the conductance on the condition that the transfer energy $-t_T$ between neighboring atoms in the tips is equal to $-t_S$ or $-2t_S$. As long as t_T is not smaller than the energy range concerned, results do not qualitatively depend on t_T. The on-site energy of the tips is zero. Since we discuss the transport in the contact condition rather than the tunneling condition in this paper, calculations are performed on the condition that the transfer energy $-t_{TS}$ between the tip and surface is the same as $-t_S$.

B. Calculation of conductance

In this paper we calculate the conductance of systems from the atomic scale to the nanometer scale where the electrical transport is ballistic. Therefore we use the Landauer formula[19] for calculating conductance. In the Landauer formalism, conductance G is expressed as

$$G=G_0\sum_{\mu\nu} T_{\mu\nu}, \tag{2.2}$$

where $T_{\mu\nu}$ is the transmission probability from the μth incident channel to the νth scattered channel. G_0 is the units of the quantized conductance given by $2e^2/h$. Since we use a one-dimensional chain for the tip-injecting electrons in the present paper, the number of the incident channel is one.

In order to obtain transmission probability, we solve the Schrödinger equation on appropriate boundary conditions. A simple boundary condition used widely is the periodic boundary condition on the directions parallel to surfaces in the supercell geometry. This reduces the three-dimensional problem to the essentially one-dimensional problem with plural channels, and the methods for solving the latter problem are well established. However, the periodic boundary condition is inadequate to calculate the conduction through surface states, because surface states decay into bulk and propagate only parallel to surfaces. Actually the conductance calculated on the periodic boundary condition does not contain the component of the conduction though surface states, as shown in the next section. Therefore we impose the outgoing boundary condition on the directions parallel to the surface, as illustrated in Fig. 1.

In order to impose this boundary condition on the surface we consider an artificial box consisting of $N_x\times N_y\times N_z$ atomic sites in the semi-infinite surface, where the z direction is perpendicular to the surface. We impose the boundary condition of only outgoing waves on the five sides of the box except for one side facing the vacuum. The outgoing Bloch states for each side are obtained by diagonalizing the transfer matrix defined for each side.[23] Different from imposing hemispherically outgoing waves in the surface, this boundary condition produces artificial scattering at the edges of the box. But, as the size of the box increases, the effect of the scattering becomes small. We use typically a box consisting of 21×21×15 atomic sites in this paper. For the directions parallel to the surface, this size is not large enough to eliminate perfectly the effect of the scattering, especially on the conduction through surface states. However, we verified that calculated results are qualitatively unchanged by increasing the size of the box. In the double-tip case we use a larger box in order to discuss the transport between two tips on surfaces.

The wave function of the tip which injects electrons into the surface is written as a linear combination of the incident and reflected waves. In the double-tip case, the wave function of the second tip is composed of only the outgoing wave.

The transmission probability is calculated by the standard method.[23] In the tight-binding method, the Schrödinger equation is written as

$$\mathcal{H}\mathbf{C}=E\mathbf{C}, \tag{2.3}$$

where the *mn* component of $\mathcal{H}$ is the transfer energy between the m and n sites and the nth component of $\mathbf{C}$ is the amplitude of the wave function at n site.

The coefficient of the nth atom belonging to the tip which injects electrons into the surface is written as

$$C_n=e^{ik_Tan}+re^{-ik_Tan}, \tag{2.4}$$

where r is the reflection coefficient and k_T is the Bloch wave number in the tip. Here we take the same lattice constant for the tips as the surface in this paper. In the double-tip case, the coefficient of the second tip is written as

$$C_n=s_Te^{ik_Tan}, \tag{2.5}$$

where s_T is the transmission coefficient to the second tip.

Out of each side of the box in the surface, the coefficients of the atoms in the lth layer are written as

$$\mathbf{C}_l=\sum_m (\lambda_m)^l\mathbf{u}_m s_m, \tag{2.6}$$

where λ_m and $\mathbf{u}_m$ are, respectively, the mth eigenvalue and eigenvector of the transfer matrix defined for each side of the box. s_m is the transmission coefficient of the mth channel. $\mathbf{C}_l$ is a vector consisting of the same number of components as the atomic sites on the plane of each side of the box. The layer number l is defined along the direction perpendicular to each side of the box. The summation m runs over only the outgoing waves. Here the outgoing Bloch states are defined by that the group velocity is directed toward the outside of the box.

On the boundary conditions above, the matrix equation in infinite dimensions in Eq. (2.3) is reduced to a finite-dimensional coupled linear equation in the form of

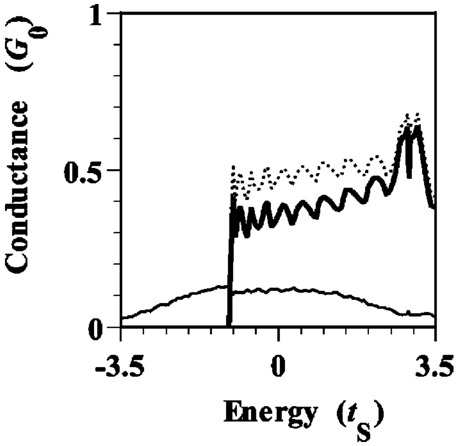

FIG. 2. Conductance of the flat surface as a function of E. U, t_T, and t_{TS} are $2.5t_S$, $2t_S$, and t_S, respectively. Thick and thin solid lines show the surface-state and bulk-state components, respectively. The dotted line is the total conductance.

$$(\tilde{\mathcal{H}}-E)\tilde{\mathbf{C}}=\mathbf{D}, \tag{2.7}$$

where $\tilde{\mathbf{C}}$ is a vector composed of r, s_T, s_m, and the components of $\mathbf{C}$ inside the system, namely, the scattering region. $\mathbf{D}$ is a constant vector, the components of which are zero except for one corresponding to the apex atom of the tip which injects electrons. Different from the usual one-dimensional problems with plural channels, $\tilde{\mathcal{H}}$ is not a block-tridiagonal matrix and the recursive method[23] cannot directly be applied to solving the equation. But, since the major part in $\tilde{\mathcal{H}}$ is block tridiagonal, Eq. (2.7) can be solved by applying partially the recursive method. This saves much computational time and memories. Details are shown in the Appendix.

III. RESULT

A. Flat surface

Figure 2 shows the conductance of a flat surface as a function of the energy E. The size of the box in the surface is 21×21×15 atomic sites. The tip is put on the center atom of the surface. The on-site energy U is $2.5t_S$. The transfer energy between the tip and surface t_{TS} is the same as t_S. The transfer energy in the tip t_T is $2t_S$. The dotted line shows the total conductance. The total conductance spectra as a function of E correspond to the shift of the Fermi level of the system or dI/dV spectra in STS, though the change in electronic structures induced by applying finite bias voltages is not taken into account in this paper. The thick and thin solid lines show the components of transmission to surface and bulk states, respectively. In this paper surface states are discriminated from bulk states on a criterion whether the amplitudes of wave functions at the first, second, and third layers of the surface decay exponentially into the surface.

In the case of present parameters surface states exist within the energy range $-1.1t_S<E<6.9t_S$. Outside of this range only the bulk states are conduction channels and the total conductance is much smaller than the conductance unit G_0. There are two main reasons for this low conductance.

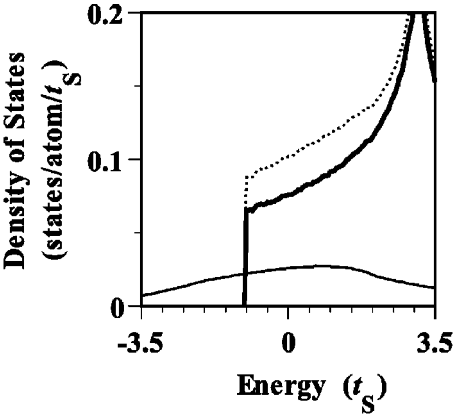

FIG. 3. Density of states at the first layer of the flat surface. U is $2.5t_S$. Thick and thin solid lines show the surface-state and bulk-state components, respectively. The dotted line is the total DOS.

One is that the transfer energy in the tip is different from that in the surface and the matching of waves is not good. The other is that when the on-site energy U is finite, the potential energy at the first layer of the surface is different from those of other sites and it reflects waves. However, when the surface-state channels open, the conductance increases much. In the present case the surface-state component is the major channel of conduction.

Figure 3 shows the DOS at the first layer of the surface. Here the first-layer DOS means the DOS weighted with the square of the absolute values of the coefficients at the first layer in the wave functions. U is $2.5t_S$. The spectra of the first-layer DOS are similar to the conductance spectra shown in Fig. 2. The ratio of the surface component to the bulk one in the conductance spectra is well reproduced by the DOS spectra. This result suggests that STS spectra of flat surfaces containing surface states are approximately proportional to the LDOS at the surface and justifies partially the use of the Tersoff-Hamann theory for a qualitative interpretation of STS spectra of surface states.

Note that this is not always the case for any surface. As shown in the next section the conductance is not proportional to the first-layer DOS in the case of islands on substrates. The first-layer DOS of surface states of islands is finite. But, the conduction through the surface states of islands is negligibly small when the step height of islands is high. This is due to the lack of conduction paths of the surface states of islands to the electrodes connected with substrates, which is similar to the fact that surface states do not propagate perpendicular to surfaces. Therefore, it is conjectured that STS spectra containing surface states are proportional to the first-layer DOS only when the electrons hopping into surface states can readily reach the electrodes connected with surfaces.

The oscillating structures seen in the surface-state component of conductance are due to the finiteness of the box in the surface along the directions parallel to the surface. The amplitude of the oscillation decreases as the lateral size of the box increases. On the other hand, the structures in the bulk-state component are very small. This result means that surface-state conduction is more sensitive to boundaries than bulk-state conduction and we need larger systems in order to discuss theoretically surface-state conduction.

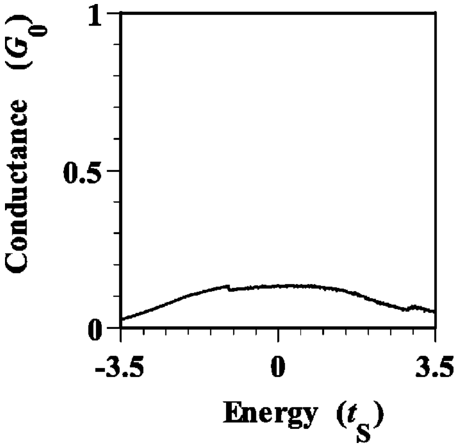

FIG. 4. Conductance of the flat surface calculated on the periodic boundary condition, U, t_T, and t_{TS} are $2.5t_S$, $2t_S$, and t_S, respectively.

In the calculation of the surface-state conductance the boundary condition is crucial. Figure 4 shows the conductance calculated on the periodic boundary condition imposed on the surface. U, t_{TS}, and t_T are the same as those in Fig. 2. The unit cell in the periodic boundary condition is a square consisting of 20×20 atomic sites. The conductance is integrated over the wave vectors parallel to the surface. On the periodic boundary condition each conductance spectrum at a fixed wave vector shows structures: Conductance is close to zero at the energy levels of surface states. These structures are smeared out by the Brillouin-zone integral. The spectrum shown in Fig. 4 is integrated over 50×50 wave vectors in the two-dimensional Brillouin zone of the super cell.

On the periodic boundary condition also surface states exist and the surface-state component in the first-layer DOS is finite. But they are not propagating channels perpendicular to the surface and do not contribute to the conduction on the

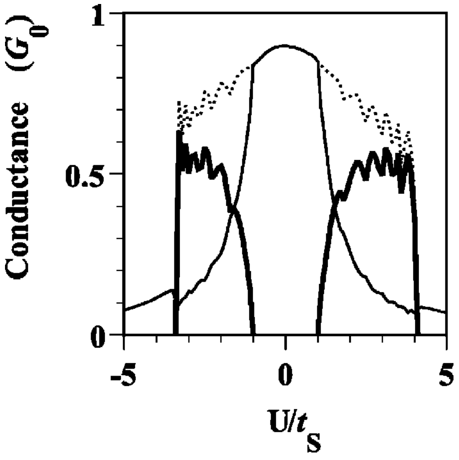

FIG. 5. Conductance of the flat surface as a function of U. E is $0.3t_S$. t_T and t_{TS} are equal to t_S. Thick and thin solid lines show the surface-state and bulk-state components, respectively. The dotted line is the total conductance.

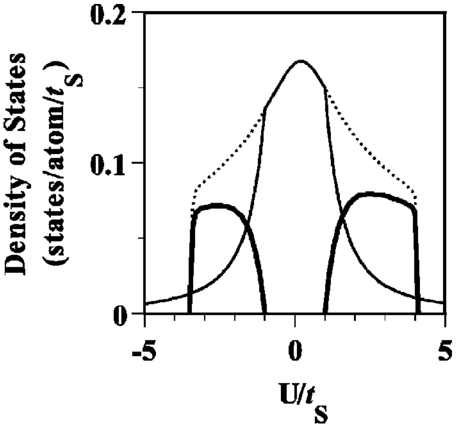

FIG. 6. Density of states at the first layer of the flat surface as a function of U. E is $0.3t_S$. Thick and thin solid lines show the surface-state and bulk-state components, respectively. The dotted line is the total DOS.

periodic boundary condition. Therefore, the conductance calculated on the periodic boundary condition is almost the same as the bulk component on the outgoing boundary condition shown in Fig. 2.

Figure 5 shows the conductance of the flat surface as a function of the on-site energy U. The energy E is fixed at $0.3t_S$. t_{TS} and t_T are equal to t_S. Other conditions are the same as those of Fig. 2. As the absolute value of U increases, the total conductance decreases. But the magnitude of decrease is not very large as long as surface states exist. When the surface states disappear, the conductance decreases abruptly, reflecting the two-dimensional DOS of surface states.

Figures 6 and 7 show the first-layer DOS and the conductance calculated on the periodic boundary condition, respectively, as a function of U. The energy E is $0.3t_S$. t_{TS} and t_T are equal to t_S. Other conditions are the same as those of Figs. 3 and 4. As a function of U also the first-layer DOS qualitatively reproduces the conductance spectra shown in Fig. 5. The ratio of the surface-state component to the bulk-state component is well reproduced by the first-layer DOS. The conductance on the periodic boundary condition agrees fairly well with the bulk component of the outgoing boundary condition shown in Fig. 5.

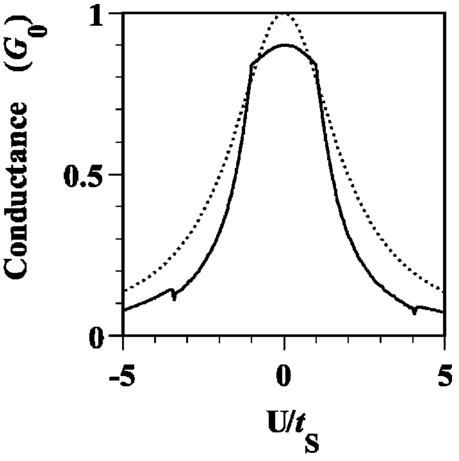

FIG. 7. Conductance of the flat surface calculated on the periodic boundary condition as a function of U. E is $0.3t_S$. t_T and t_{TS} are equal to t_S. The dotted line shows the transmission probability given by Eq. (3.1).

The bulk-state component decreases monotonically as a function of $|U|$. This is due to the scattering at the first layer of the surface. The transmission to bulk states is roughly understood in terms of a one-dimensional chain with a defect. Its transmission probability is given by

$$T=\frac{1}{1+U^2/W^2}, \tag{3.1}$$

where $W=(4t_S^2-E^2)^{1/2}$ and U is the on-site energy of the defect. As shown in Fig. 7 the bulk-state component is qualitatively reproduced by the dotted line given by Eq. (3.1).

In contrast to the bulk-state component, the surface-state component increases with increase of $|U|$ around $|U|\sim t_S$. This means that the stronger the scattering potential at the first layer, the larger the transmission to the Tamm surface states. The reason for this initial increase is that since the wave functions of surface states are more localized with the increase of $|U|$, the amplitude of wave functions at the first layer of the surface also increases. As the amplitude of wave functions at the first layer increases, the hopping probability from the tip to the surface also increases. Once electrons hop into surface states, they travel parallel to the surface and reach the electrode. The conductance is determined mainly by the hopping from the tip to the first layer of the surface. Actually the conductance through surface states shown in Fig. 5 initially increases in proportion to $1-(t_S/U)^2$, which is the square of the amplitude of wave functions at the first layer. With the further increase of $|U|$, the whole of the surface-state band shifts and the DOS at a fixed energy slightly decreases. When the energy goes out of the range of the surface-state band, the surface-state component is discontinuously reduced to zero.

It is probably specific to the Tamm state that the larger the difference in potential between the first layer and inner layers, the higher the conductance of surface states. However, it might generally hold for all surface states that the more strongly wave functions localize at the first layer, the higher the conductance through surface states. In the case of the Shockley state, for example, band gap is an important factor determining the decay of wave functions; the larger the band gap, the more strongly wave functions localize.[5] Therefore it is expected that surface-state conductance is high when Shockley states are formed in midgaps of materials with large band gaps.

B. Island

Figure 8 shows the conductance when an STM tip is put on an island on a surface. In the present paper we use a model for the island surface that the on-site energy at the top layer of the island and at the part facing the vacuum among the first layer of the substrate surface is U and that of other parts is zero. The transfer energy in the island is the same as that in the substrate. Figure 8 shows the case for which U is

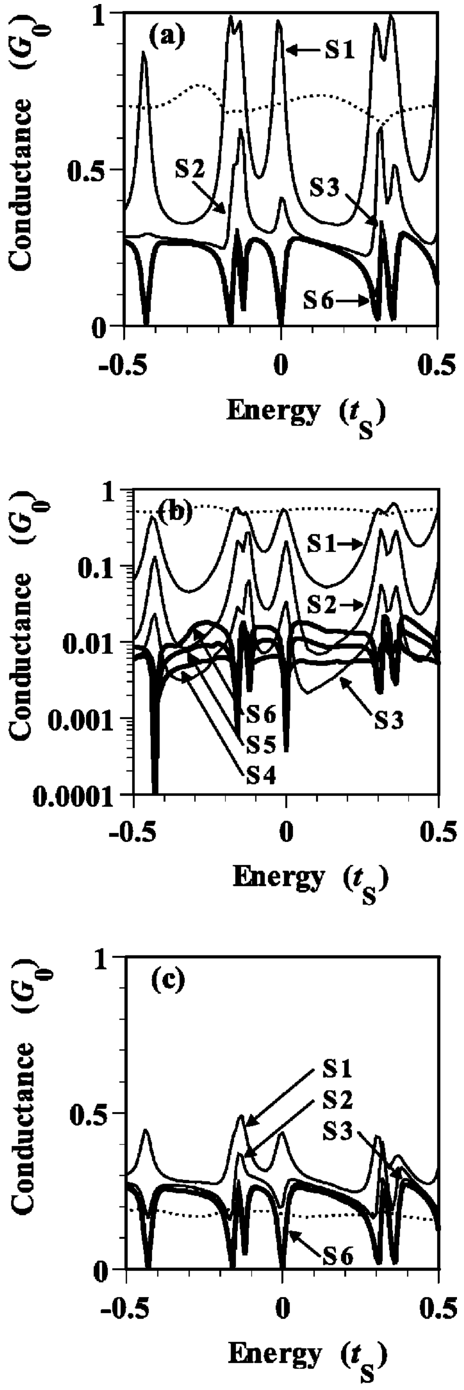

FIG. 8. Conductance when an STM tip is put on an island. The lateral size of the island is 21×21 atomic sites. Each figure shows (a) total conductance, (b) the surface-state component, and (c) the bulk-state component. U is $2.5t_S$. t_T and t_{TS} are equal to t_S. The height of the island varies from 1 to 6 atomic steps. Thin and thick solid lines show the conductances from 1 to 3 and from 4 to 6 step heights, respectively. Label S*n* means the spectrum of the *n*-step height. S4, S5, and S6 are almost the same lines in (a) and (c). Dotted lines show the conductances of the flat surface.

$2.5t_S$. t_{TS} and t_T are equal to t_S. The lateral size of the island is fixed at 21×21 atomic sites. The size of the box in the substrate is 23×23×15 atomic sites. The STM tip is put on the center atom of the island surface. The height of the island varies from 1 to 6 atomic steps. Figures 8(a), 8(b), and 8(c) show the total conductance, surface-state component, and bulk-state component, respectively. Here the surface-state and bulk-state components are defined as the parts transmitting finally to the surface and bulk states of the substrate, respectively. Except for the single-step height, the total conductance tends to decrease as the step height increases. The spectrum almost converges at the three-step height in the case of present parameters. These results are understood from the difference in the step-height dependence between the surface-state and bulk-state components.

Figure 8(b) shows that the surface-state component initially decreases rapidly with increase of the step height and is negligibly small at the three-step height. For heights greater than three steps the surface-state component slightly increases with the step height. This step-height dependence of conductance is qualitatively understood by dividing the surface-state component further into two components. One is the current traveling from the tip to the surface states of the island and then flowing into the surface states of the substrate. The other is the current flowing into the surface states of the substrate through the bulk states of the island. We call the former and latter SS and BS components, respectively. Though we cannot present the strict definition for dividing the surface-state component into these two components, this way of classification helps to understand the step-height dependence as follows.

When the step height is low, the SS component is dominant. But as the step height increases, the SS component decreases rapidly because the wave functions of the surface states decay exponentially into the surface and the probability of tunneling from the surface states of the island to those of the substrate also decay exponentially with increase of the step height.

Contrary to the SS component, the BS component is small at the low-step heights, because the width of the electron beam injected from a single atom of the tip into the bulk states of the island is much narrower than the lateral width of the island and the electron beam does not reach the wave functions of the surface states of the substrate. As the step height increases, the width of the electron beam on the plane at the first layer of the substrate widens and the probability of transmission to the surface states of the substrate increases. Though it is not shown in the figure, the surface-state component as a function of the step height reaches a local maximum at about 10-step height and begins to decrease with the step height. This result might be interpreted as that the electron beam spreads as wide as the lateral size of the island at about 10-step height, and that with further increase of the step height it begins to focus again by the reflection at the sides of the island.

Between the 3- and 4-step heights the SS and BS components are comparable and the major path of conduction is switched from the SS component to the BS component. This switch is reflected in the shapes of the spectra. In the case of lower step heights there are peaks at energy levels corresponding to the surface states of the island that are quantized due to the lateral confinement of the island. But in the higher case these peaks are inverted to dips and the shapes of the spectra are similar to the bulk component shown in Fig. 8(c). The reason for this is as follows. Since the wave functions of surface states have large amplitude at the top layer of the island, a large number of electrons in the tip hop into the surface states of the island at the energy levels of the surface states. When the SS component is major at the low step heights, the probability of transmission to the surface state of the substrate is high at the energy levels of the surface states of the island, which is reflected by the peaks. On the other hand when the step height is high, the electrons hopping into the surface states of the island cannot travel deep into the surface and return to the tip. Therefore the conductance spectra show dips at the energies of the surface states of the island. Though experimentally it is not possible to separate directly the surface-state component from the total conductance, it might be possible to measure the conductance corresponding to the surface-state component by using double tips, because the surface-state conduction is dominant in double-tip measurements as shown in the next section.

In contrast to the surface-state component, the magnitude of the bulk-state component does not change much as the step height increases. The spectra converge on the conductance from the tip to a wire, the cross section of which is the same as that of the island. When the step height of the island is high, the bulk-state component is the dominant channel of conduction and the total conductance is also almost the same as that of the wire.

In the bulk-state component also the peaks in the spectra at the energies of the surface states of the island are inverted to dips as the step height increases. This is also understood by dividing the bulk-state component into two components similarly to the surface-state component. One is the current flowing into the bulk states of the substrate through the surface states of the island and the other is through the bulk states of the island. We call the former and latter SB and BB components, respectively. As the step height increases, the main path of conduction switches from the SB component to the BB component.

In the case of the bulk-state component the magnitudes of these components are comparable between the heights of 1 and 2 steps, which are lower than those of the surface-state component. The reason for this is that the BB component is not small even at low step heights. In the case of the surface-state component the BS component is small at low step heights. It increases as the step height increases and the electron beam spreads in the island. But in the case of the bulk-state component the magnitude of the BB component does not depend much on the step height, and only the SB component decreases as the step height increases. Therefore the peaks are inverted to dips at the lower step height than that of the surface-state component.

Since the surface-state component is finite in the first-layer DOS of islands, the fact that the SS and SB components of the conductance are negligibly small at high step heights means that the conductance is not proportional to the first-layer DOS in the case of islands. This result is in contrast to the case of flat surfaces and demonstrates the importance of the conduction path to electrodes especially in the case of the conduction through surface states, as mentioned in the preceding section.

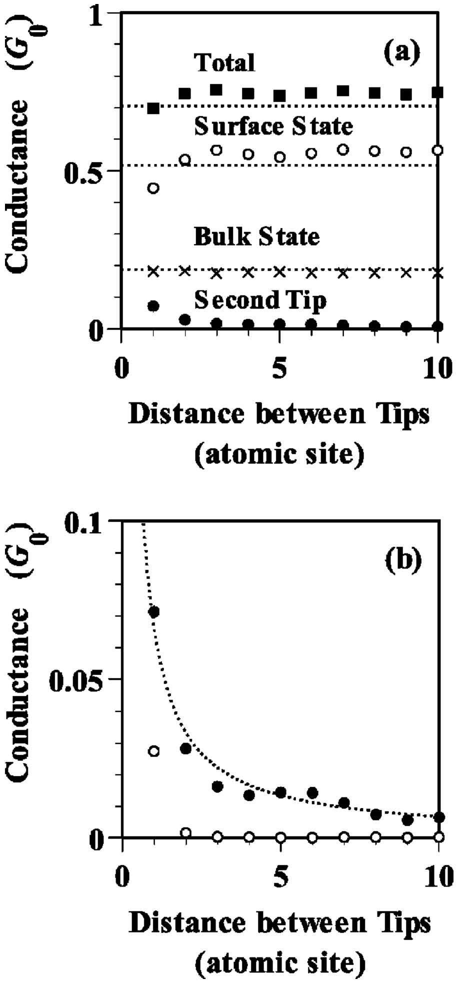

FIG. 9. Conductance in a double-tip system as a function of the distance between two tips. U is $2.5t_S$ t_T and t_{TS} are equal to t_S. E is $-0.5t_S$. (a) Closed squares, open circles, crosses, and closed circles show the total conductance, surface-state component, bulk-state component, and conductance to the second tip, respectively. Dotted lines are the corresponding conductances in the single-tip system. (b) Closed and open circles show the conductance to the second tip in the presence ($U=2.5t_S$) and in the absence ($U=0$) of surface states, respectively. The dotted line shows a curve inversely proportional to the distance.

Though the results of the present calculations cannot be compared directly with the experiment on silicon surfaces by Hasegawa, Lyo, and Avouris,[2] they reproduce the fact experimentally observed that the conductance measured with a STM tip on islands is much lower than that on flat surfaces. According to the present calculation, this result is ascribed to the reduction of the surface-state component in conductance when a STM tip is put on islands. This reduction of the surface-state conduction in the ballistic regime is somewhat different from the usual resistance induced by the scattering of bulk states at step edges. This is because in the case of bulk states, step edges scatter three-dimensionally extended states, whereas in the case of surface states, step heights

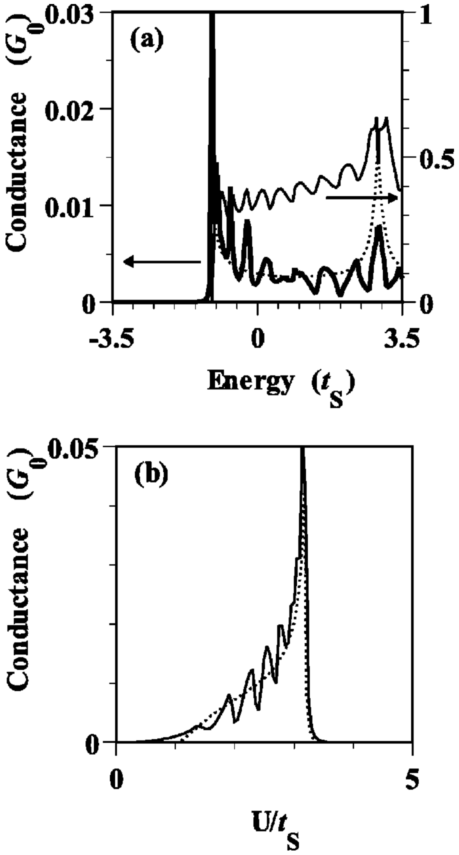

FIG. 10. Conductance between two tips as a function of (a) E and (b) U. The distance between tips is 5 atomic sites. (a) U is $2.5t_S$. t_T and t_{TS} are equal to $2t_S$ and t_S, respectively. Thick and thin solid lines show the conductance between two tips and the surface state component, respectively. The dotted line shows a curve given by Eq. (3.2). (b) E is $-0.5t_S$. t_T and t_{TS} are equal to t_S. Solid and dotted lines show the conductance between two tips and a curve given by Eq. (3.2), respectively.

reduce the tunneling probability between two-dimensionally localized states in islands and substrates.

C. Double tip

Figure 9 shows the conductance of a double-tip system as a function of the distance between the two tips. The surface is a flat surface. The first tip injecting electrons is fixed on the center atom of the surface. The position of the second tip is changed parallel to an axis of the simple square lattice. The size of the box in the surface is $31\times31\times15$ atomic sites. The on-site energy U of the first layer is $2.5t_S$. t_{TS} and t_T are equal to t_S. The energy E is $-0.5t_S$.

Figure 9(a) shows the total conductance, surface-state component, bulk-state component, and conductance for the second tip. The dotted lines are the corresponding conductances in the single-tip case. Except for the nearest-distance case, the surface-state component is slightly enhanced in the presence of the second tip. But as a whole the conductance is not much affected by the second tip. The ballistic current flowing directly to the second tip is very small. It decreases with increase of the distance between the two tips.

Figure 9(b) shows a magnified figure of the ballistic conductance to the second tip. For comparison, the curve in the case without surface states $(U=0)$ is also shown. In the absence of surface states the conductance to the second tip decreases rapidly with distance. But when surface states exist, the decrease is not so fast; the conductance is inversely proportional to the distance between the tips. This result reflects the fact that surface states are two-dimensional states and flux of current conserves. The dependence on the distance is not changed much when the second tip is moved on the surface along the diagonal direction of the simple square lattice. This isotropy is due to the fact that in the present case the energy E is near the bottom of the surface-state band and the energy dispersion is nearly isotropic. When the energy is near the middle of the surface-state band, the energy band is highly anisotropic and the conductance between two tips is also anisotropic as shown by Niu, Chang, and Shih using the effective-mass approximation.[18]

Figure 10 shows spectra of the conductance between two tips as a function of (a) the energy E and (b) the on-site energy U. U and E are fixed at $2.5t_S$ and $-0.5t_S$ in Figs. 10(a) and 10(b), respectively. In both spectra the distance between tips is 5 atomic sites and t_{TS} is equal to t_S. t_T is (a) $2t_S$ and (b) t_S. The size of the box is (a) $21\times21\times15$ and (b) $31\times31\times15$ atomic sites. For comparison the surface-state component is also shown in Fig. 10(a).

Figure 10(a) shows that the shape of the conductance spectrum between two tips is different from that of the surface-state component. The latter reflects the two-dimensional DOS of surface states, but the former is similar to the one-dimensional DOS. Near the bottom energy E_c of the surface-state band the conductance spectrum between two tips diverges proportional to $1/\sqrt{E-E_c}$, reflecting the one-dimensional feature. This result might be interpreted as that among two-dimensional surface states the one-dimensional states parallel to the vector connecting the positions of two tips mainly contributes to the conduction between two tips.

The conductance spectra are roughly explained in terms of the Green's function of the sample surface. Using a perturbation theory Niu, Chang, and Shih showed[18] that the conductance between two tips is proportional to the square of the absolute value of the Green's function as

$$G\propto|g(\mathbf{r}_1,\mathbf{r}_2;E)|^2, \tag{3.2}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the positions of the first and second tips on the surface, respectively. The two-dimensional Green's function at the first layer of the surface is given by

$$g(\mathbf{r}_1,\mathbf{r}_2;E)=\frac{\Omega}{(2\pi)^2}\int\frac{\phi_{\mathbf{k}_\parallel}(\mathbf{r}_1)\phi^*_{\mathbf{k}_\parallel}(\mathbf{r}_2)}{E-E(\mathbf{k}_\parallel)+i\delta}d^2k, \tag{3.3}$$

where Ω is the area of the two-dimensional unit cell and δ is a positive infinitesimal. In the tight-binding model for Tamm states $\phi_{\mathbf{k}_\parallel}(\mathbf{r})$ at an atomic site $\mathbf{r}$ is expressed as

$$\phi_{\mathbf{k}_\parallel}(\mathbf{r})=\left[1-\left(\frac{t_S}{U}\right)^2\right]^{1/2}e^{i\mathbf{k}_\parallel\cdot\mathbf{r}}, \tag{3.4}$$

and the energy dispersion $E(\mathbf{k}_{\parallel})$ is given by Eq. (2.1). Dotted lines in Fig. 10 show curves calculated using Eqs. (3.2)–(3.4). In numerical calculations of the Green's function we used $10^{-2}t_S$ for δ and integrated over 1000×1000 wave vectors in the two-dimensional Brillouin zone.

The approximate curves using the Green's function reproduce well features of the conductance spectra. The oscillations in the conductance spectra are due to the smallness of the box for the directions parallel to the surface. The spectrum in Fig. 10(b) is proportional to $[1-(t_S/U)^2]^2$ near $U \sim t_S$, which reflects the localization strength of wave functions of the surface states.

The distance between tips is very small in the present calculations. When the distance is much greater, the following results are expected. First, since the bulk-state component decreases with distance more rapidly than the surface-state component, most of the double-tip conductance is the conduction through surface states in the ballistic regime. Second, the shapes of the conductance spectra do not qualitatively change with the distance. Third, since the ballistic conductance between two tips decreases inversely proportional to the distance, its magnitude is very small when the distance between tips is large. But since the conductance spectra diverge near the bottom or top of the surface-state bands, it is possible that the ballistic conductance between two tips is high when the Fermi energy is located near band edges.

IV. CONCLUSION

In this paper we have presented the ballistic conductance in STM systems where the Tamm surface states exist. In order to discuss the conduction through surface states, conductances were calculated for the outgoing boundary condition in the surfaces, which allows net current to flow parallel to the surfaces.

In the case of flat surfaces with a single tip, the conductance spectra containing surface states are qualitatively proportional to the DOS at the first layer of the surfaces, which suggests that the surface-state observation in STS is explained by the lateral current and justifies partially the use of the Tersoff-Hamann theory for analyzing STS spectra of surface states. It was found that the conductance through surface states is high when wave functions of surface states are strongly localized at the first layers of surfaces. In the case of Tamm states, wave functions localize strongly when the potential difference between the first layer and inner layers is large. The potential difference scatters waves and usually reduces the bulk-state conduction. In contrast, it increases the conduction through surface states in the case of Tamm states.

Conductances were calculated when a STM tip is put on an island of a surface. The variation in conductance as a function of the step height of the island was explained by the difference in the step-height dependence between the surface-state and bulk-state components. The surface-state component decreases rapidly with increase of the step height. This is because its main conduction path is the tunneling from the surface states of the islands to those of the substrates. In contrast to the flat surfaces the conductance is not proportional to the first-layer DOS at high step heights in the case of islands. This result demonstrates the importance of the conduction path to electrodes connected with sample surfaces especially in discussing the surface-state conduction.

We simulated the ballistic conductance of a double-tip system. In the absence of surface states, the ballistic conductance between two tips decreases rapidly as a function of the distance between the tips. But when surface states exit, the decrease becomes slower and the conductance is inversely proportional to the distance. Therefore, when the distance between tips is large, the surface-state conduction is the dominant channel in the ballistic regime. The ballistic conductance spectra between two tips show one-dimensional features. Therefore the ballistic conductance between two tips might be high when the Fermi energy is located near the edges of surface-state bands.

In the present paper we have studied only the Tamm state. However, it is not difficult to extend the present calculations to the Shockley state. It is also interesting to study the surface-state conduction in more realistic systems such as silicon surfaces. However, in the present paper we used a simple tight-binding method and did not self-consistently calculate the electronic states of the whole system. Therefore effects such as contact resistance were not taken into account. The results in the present paper may be regarded as the case in which the work functions of the tip and surface are the same. In order to discuss the electronic transport in realistic systems it is important to calculate electronic states self-consistently. These are studies left for the future.

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APPENDIX

The coupled linear equation in Eq. (2.7) has a form of

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} = \begin{pmatrix} 0 \\ \mathbf{c} \end{pmatrix}, \tag{A1}$$

where A_{11} is a block-tridiagonal matrix. Using a matrix B defined by $A_{11}B = A_{12}$, the equation is reduced to

$$\tilde{A}_{22}\mathbf{x}_2 = \mathbf{c}, \tag{A2}$$

where $\tilde{A}_{22} \equiv A_{22} - A_{21}B$. Once this coupled linear equation is solved, $\mathbf{x}_1$ is obtained from $\mathbf{x}_1 = -B\mathbf{x}_2$. Therefore, the problem is reduced to solving the equation $A_{11}B = A_{12}$, where A_{11} has a form of

$$A_{11}=\begin{pmatrix} a_{11} & a_{12} & 0 & \cdots & 0\\ a_{21} & a_{22} & a_{23} & \ddots & \vdots \\ 0 & a_{32} & \ddots & \ddots & 0\\ \vdots & \ddots & \ddots & a_{N-1N-1} & a_{N-1N}\\ 0 & \cdots & 0 & a_{NN-1} & a_{NN}\end{pmatrix}, \tag{A3}$$

and a_{ij} is a square matrix. This equation can be solved by the well-known recursive method.[23] If we write

$$B=\begin{pmatrix} b_1\\ \vdots \\ b_N\end{pmatrix}, \quad A_{12}=\begin{pmatrix} d_1\\ \vdots \\ d_N\end{pmatrix}, \tag{A4}$$

the coupled linear equation is reduced to

$$\begin{gathered} a_{11}b_1+a_{12}b_2=d_1, \\ a_{ii-1}b_{i-1}+a_{ii}b_i+a_{ii+1}b_{i+1}=d_i \quad (i=2,...,N-1), \\ a_{NN-1}b_{N-1}+a_{NN}b_N=d_N. \end{gathered} \tag{A5}$$

If we define $\tilde{a}_{ii}$ and $\tilde{d}_i$ by

$$\begin{gathered} \tilde{a}_{i-1i-1}\equiv a_{i-1i-1}-a_{i-1i}\tilde{a}_{ii}^{-1}a_{ii-1}, \\ \tilde{d}_{i-1}\equiv d_{i-1}-a_{i-1i}\tilde{a}_{ii}^{-1}\tilde{d}_i, \end{gathered} \tag{A6}$$

with initial conditions $\tilde{a}_{NN}=a_{NN}$ and $\tilde{d}_N=d_N$, we obtain $\tilde{a}_{11}b_1=\tilde{d}_1$, from which b_1 can be solved. Other b_i are obtained from

$$b_i=\tilde{a}_{ii}^{-1}(\tilde{d}_i-a_{ii-1}b_{i-1}). \tag{A7}$$

In practical calculations it is more efficient to rewrite Eqs. (A6) and (A7) in terms of p_i and q_i defined by $\tilde{a}_{ii}p_i=a_{ii-1}$ and $\tilde{a}_{ii}q_i=\tilde{d}_i$.

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