Transmission of double-impurity atomic switches

Z. L. Mišković,* R. A. English, S. G. Davison,† and F. O. Goodman†
Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1
(Received 18 December 1995)

The electron transmission properties of a molecular-electronic switch, represented by a monatomic chain with two atomic impurities, is studied via the tight-binding model. A method, based on the Lippmann-Schwinger equation, is used to obtain simple expressions for the transmission probability. Impurities, occupying neighboring sites in the chain, interact directly and act as a single diatomic impurity. For remote impurities, there is no direct interaction in the tight-binding model, but interference among the multiply reflected Bloch waves between the impurities leads to oscillations in the transmission probability over the energy band. We find that, in either case, controlling the transmission by the impurity-site energies is feasible in the regime of sufficiently weak impurity-chain couplings. [S0163-1829(96)08926-6]

I. INTRODUCTION

The presence of impurities and defects, in polymeric systems, can influence significantly the transmission properties. Through control of one or more impurity parameters, electron transmission along the polymer can be switched on/off. A convenient description of such systems is provided by the tight-binding (TB) model[1,2] of periodic chains. Describing a polymeric system by a TB Hamiltonian with a single orbital per site is certainly an over-simplified model for a molecular-electronic switch. However, it permits analytical results for transmission coefficient, providing qualitative understanding of modes of switch control in terms of various impurity parameters, which may be related to a realistic polymeric chain through a renormalization approach.[3] Of particular interest is the effect of the impurity-chain coupling strength on controlling the transmission by the impurity-site energies. It has been shown[1,2] that sharp switching is favored by weak coupling, in contrast to minimizing temperature effects, which is favored by strong coupling.

Transmission through a single impurity in a metal-like chain has been studied by Sautet and Joachim,[1] using the transfer-matrix (TM) technique, which was subsequently applied to the single-impurity problem in a semiconducting chain with alternating bonds.[2] In the present article, the problem of *two atomic impurities* in a metal-like chain is investigated by the Koster-Slater (KS) method,[4] based on the Lippmann-Schwinger (LS) equation.[5] While both the TM and KS methods are convenient for compact, molecular-type, impurities, the KS method provides an easier way than TM for handling multiple impurities, the example being two atomic impurities, at remote sites. The advantage of the KS method lies in using the asymptotic form of the Green function for the host chain to obtain the transmission coefficient, while the TM technique would require multiple matrix products of high degree.

Working in the TB model, we have to consider separately two cases, namely, impurities occupying adjacent sites in the chain and impurities separated by at least one host atom. In the former case, the impurities interact directly, thus acting as a diatomic molecule, immersed in the chain. Increasing the direct interimpurity coupling leads to the repulsion of the impurity levels, which may end up outside the band, thus losing the ability to control the switching. It will be shown that, in fact, the interimpurity coupling is an another impurity parameter, suitable for switch control. In the case of separated impurities, even though there is no direct coupling between them in TB model, multiple reflections of Bloch waves between the impurities lead to oscillations in transmission probability, possibly damaging the control mechanism of the switch. We shall examine how these interference effects are affected by the impurity-chain coupling and the interimpurity distance.

II. BASIC FORMULATION

The infinite monatomic chain is described by the TB Hamiltonian, whose projection-operator form is[6]

$$H_0=\sum_{n=-\infty}^{+\infty}[\alpha|n\rangle\langle n|+\beta(|n\rangle\langle n+1|+|n+1\rangle\langle n|)], \quad (1)$$

where α (β) is the site (bond) energy and $|n\rangle$ denotes the nth site orbital. The eigenfunctions of H_0 are

$$|\psi_0(k)\rangle=\sum_n c_n^0(k)|n\rangle, \quad (2)$$

where, without loss of generality, we consider Bloch waves traveling from left to right, so that $c_n^0(k)=e^{in\theta_k}$, with momentum $\theta_k=ka$ (a being the chain period) and energy $E(k)=\alpha+2\beta\cos\theta_k$. For the *reduced* energy $X=\cos\theta=(E-\alpha)/2\beta$ inside the band ($-1\leqslant X\leqslant 1$), the Green function for H_0, with the outgoing-wave asymptotic form, can be expressed as[6]

$$G_0(n,m)\equiv\langle n|G_0|m\rangle=\frac{i}{2\beta}\frac{e^{i|n-m|\theta}}{\sin\theta}. \quad (3)$$

Representing the impurities by a potential V, we seek the scattering eigenfunctions of the Hamiltonian $H=H_0+V$, with energy inside the band, namely,

$$|\psi(k)\rangle=\sum_n c_n(k)|n\rangle, \quad (4)$$

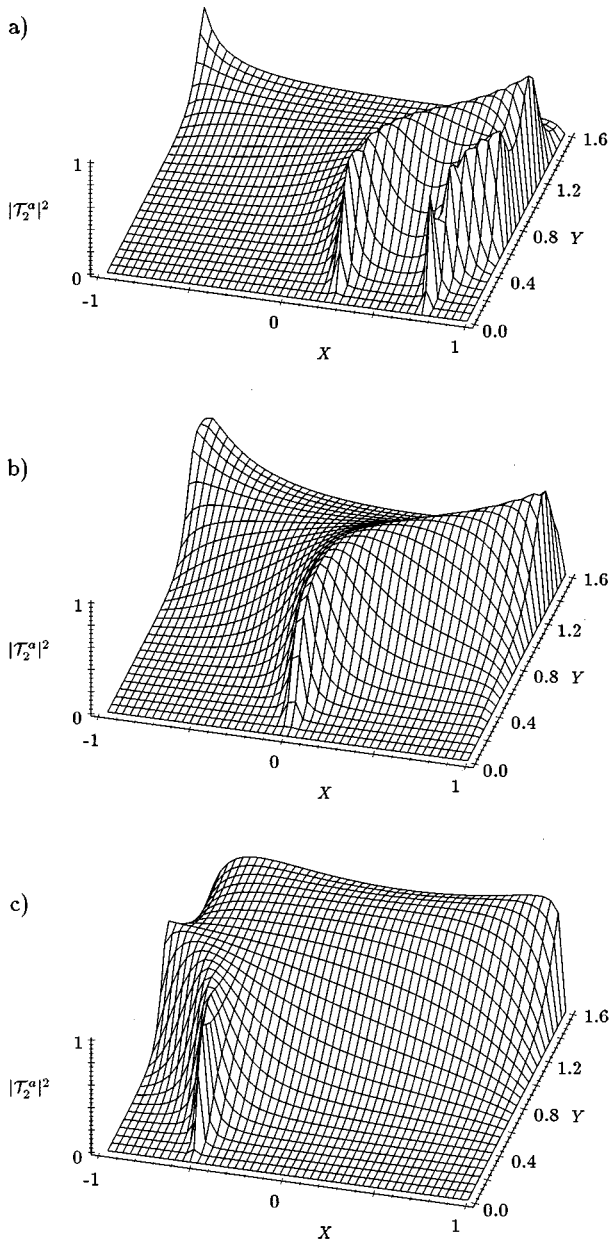

FIG. 1. Dependence of transmission probability for adjacent impurities $|\mathcal{T}_2^a|^2$ on energy X and impurity-chain coupling Y for impurity-site energy $Z=1/2$. Interimpurity couplings Y_h are (a) 0.5, (b) 1, and (c) 2.

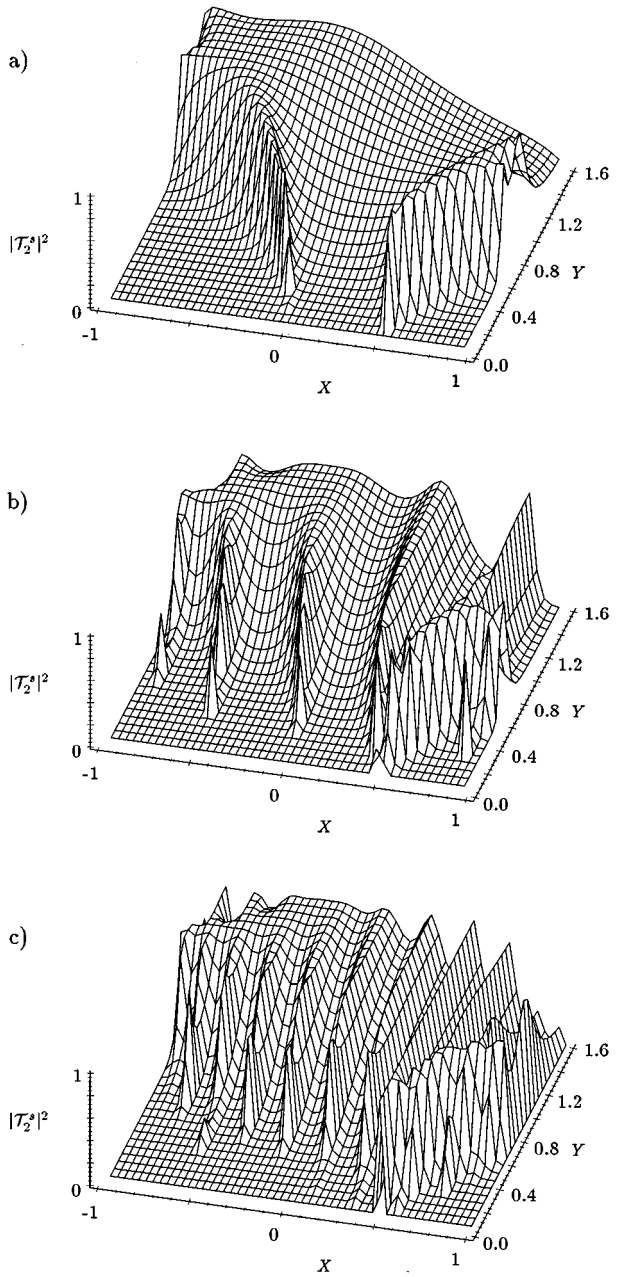

FIG. 2. Dependence of transmission probability for separated impurities $|\mathcal{T}_2^s|^2$ on energy X and impurity coupling Y for impurity-site energy $Z=1/2$. Distances between impurities are (a) $d=2$, (b) $d=6$, and (c) $d=13$.

which are represented, far to the left, by an incoming wave of unit amplitude plus a reflected wave and, far to the right, by a transmitted wave, whence,

$$c_n=\begin{cases} e^{in\theta}+\mathcal{R}_2 e^{-in\theta}, & n\to-\infty, \\ \mathcal{T}_2 e^{in\theta}, & n\to+\infty. \end{cases} \tag{5}$$

In order to determine the *two-impurity transmission coefficient*, $\mathcal{T}_2$, we use the Koster-Slater method,[4] based on the LS equation for the coefficients c_n, viz.,

$$c_n=c_n^0+\sum_{l,m} G_0(n,l)\langle l|V|m\rangle c_m. \tag{6}$$

III. ADJACENT IMPURITIES

Assume that the two host atoms at sites 0 and 1 are replaced by two impurities, which are coupled to each other by β_h. Let their site energies be α_0 and α_1, and their couplings to the neighboring chain atoms β_0 and β_1, respectively. The scattering potential for an electron propagating through the chain with adjacent impurities can now be expressed as

$$\begin{aligned} V_a=2\beta[&Z_0|0\rangle\langle 0|+Z_1|1\rangle\langle 1|+\tfrac{1}{2}(Y_0-1) \\ &\times(|-1\rangle\langle 0|+|0\rangle\langle -1|)+\tfrac{1}{2}(Y_1-1)(|1\rangle\langle 2|+|2\rangle\langle 1|) \\ &+\tfrac{1}{2}(Y_h-1)(|0\rangle\langle 1|+|1\rangle\langle 0|)], \end{aligned} \tag{7}$$

in which

$$Z_j=(\alpha_j-\alpha)/2\beta \tag{8}$$

are the reduced *impurity-site energies* ($j=0,1$), and

$$Y_j=\beta_j/\beta \tag{9}$$

are relative magnitudes of the *impurity-chain coupling* ($j=0,1$), and of the *interimpurity coupling* ($j=h$).

On introducing the notation $t=e^{i\theta}$ and

$$A_j=iZ_j/\sin\theta, \quad B_j=i(Y_j-1)/2\sin\theta, \tag{10}$$

the expressions for G_0 and V_a enable the LS equation (6) to be rewritten as

$$c_n=t^n+B_0t^{|n|}c_{-1}+(A_0t^{|n|}+B_0t^{|n+1|}+B_ht^{|n-1|})c_0 +(A_1t^{|n-1|}+B_1t^{|n-2|}+B_ht^{|n|})c_1+B_1t^{|n-1|}c_2. \tag{11}$$

Taking $n\to+\infty$, the transmission coefficient in (5), for adjacent impurities, is given by

$$\mathcal{T}_2^a=1+B_0c_{-1}+(A_0+tB_0+t^{-1}B_h)c_0 +(t^{-1}A_1+t^{-2}B_1+B_h)c_1+t^{-1}B_1c_2. \tag{12}$$

Utilizing the LS equation (11), the four equations for the coefficients c_{-1}, c_0, c_1 and c_2, required to determine $\mathcal{T}_2^a$ fully, may be generated. In matrix notation, we obtain $MP^T=Q^T$, where $P=[c_{-1},c_0,c_1,c_2]$, $Q=-[t^{-1},1,t,t^2]$ and

$$M=\begin{bmatrix} tB_0-1 & tA_0+B_0+t^2B_h & t^2A_1+t^3B_1+tB_h & t^2B_1 \\ B_0 & A_0+tB_0+tB_h-1 & tA_1+t^2B_1+B_h & tB_1 \\ tB_0 & tA_0+t^2B_0+B_h & A_1+tB_1+tB_h-1 & B_1 \\ t^2B_0 & t^2A_0+t^3B_0+tB_h & tA_1+B_1+t^2B_h & tB_1-1 \end{bmatrix}. \tag{13}$$

The solution for coefficients P is straightforward, yielding

$$\mathcal{T}_2^a=\frac{Y_0Y_hY_1}{C_0^+C_1^+-C_0^-C_1^-t^2}, \tag{14}$$

where

$$C_j^{\pm}=\frac{i}{\sqrt{1-X^2}}\left[Z_j+X\left(\frac{Y_j^2+Y_h}{2}-1\right)\right]-\frac{Y_j^2\pm Y_h}{2}, \quad j=0,1. \tag{15}$$

In order to limit the impurity-parameter space, we restrict ourselves to the case of two identical impurities, having the same site energies ($Z_0=Z_1=Z$) and the same couplings to the chain atoms ($Y_0=Y_1=Y$). We are interested in the effects of the interimpurity coupling Y_h on the transmission, in cases when the impurity level lies inside the band, say, when $Z=1/2$, as in Ref. 1. In Fig. 1, the X and Y dependences of the transmission probability $|\mathcal{T}_2^a|^2$ are displayed for energies inside the band ($-1\leqslant X\leqslant 1$) and for a range of the impurity-chain couplings ($0<Y\leqslant 1.6$), for several values of Y_h (0.5, 1, and 2). It is noteworthy that, for weak impurity-chain coupling ($Y\ll 1$), two peaks occur in the transmission probability at

$$X_{\pm}=\frac{1}{2}[Z_0+Z_1\pm\sqrt{(Z_0-Z_1)^2+Y_h^2}], \tag{16}$$

which are clearly seen in Fig. 1.

IV. SEPARATED IMPURITIES

Let us replace the two host atoms at sites 0 and $d\geqslant 2$ by two impurities, whose site (bond) energies are α_0 (β_0) and α_d (β_d), respectively. Note that, for separated impurities, there is no direct interimpurity coupling, and β_0 and β_d are the impurity couplings to the nearest chain atoms. The scattering potential for an electron propagating through the chain with separated impurities may now be expressed as $V_s=V_0+V_d$, where

$$V_j=2\beta[Z_j|j\rangle\langle j|+\tfrac{1}{2}(Y_j-1)(|j-1\rangle\langle j|+|j\rangle\langle j-1|+|j\rangle \times\langle j+1|+|j+1\rangle\langle j|)], \quad j=0,d \tag{17}$$

in which the reduced *impurity-site energies* Z_j and relative magnitude of the *impurity-chain couplings* Y_j are given by (8) and (9), respectively, for $j=0,d$.

Using the same notation as in (10) with $j=0,d$, the expressions for G_0 and V_s enable the LS equation (6) to be rewritten as

$$c_n=t^n+[A_0t^{|n|}+B_0(t^{|n+1|}+t^{|n-1|})]c_0+B_0t^{|n|}(c_{-1}+c_1) +[A_dt^{|n-d|}+B_d(t^{|n-d+1|}+t^{|n-d-1|})]c_d +B_dt^{|n-d|}(c_{d-1}+c_{d+1}). \tag{18}$$

Taking $n\to+\infty$, the transmission coefficient in (5), for impurities separated by distance d, is given by

$$\mathcal{T}_2^s=1+[A_0+(t+t^{-1})B_0]c_0+[A_d+(t+t^{-1})B_d]t^{-d}c_d +B_0(c_{-1}+c_1)+B_dt^{-d}(c_{d-1}+c_{d+1}). \tag{19}$$

Utilizing the LS equation (18), the four equations for the coefficients c_0, c_d, $b_0\equiv c_{-1}+c_1$, and $b_d\equiv c_{d-1}+c_{d+1}$, required to determine $\mathcal{T}_2^s$ fully, can be generated. In matrix notation, we obtain $NR^T=S^T$, where $R=[c_0,b_0,c_d,b_d]$, $S=-[1,t+t^{-1},1,t+t^{-1}]$, and

$$N=\begin{bmatrix} A_0+2tB_0-1 & B_0 & [A_d+(t+t^{-1})B_d]t^d & B_dt^d \\ 2t[A_0+(t+t^{-1})B_0] & 2tB_0-1 & (t+t^{-1})[A_d+(t+t^{-1})B_d]t^d & (t+t^{-1})B_dt^d \\ A_0+(t+t^{-1})B_0 & B_0 & (A_d+2tB_d-1)t^{-d} & B_dt^{-d} \\ (t+t^{-1})[A_0+(t+t^{-1})B_0] & (t+t^{-1})B_0 & 2t[A_d+(t+t^{-1})B_d]t^{-d} & (2tB_d-1)t^{-d} \end{bmatrix}. \tag{20}$$

The solution for coefficients R is straightforward, yielding

$$\mathcal{T}_2^s=\frac{1}{(1-iC_0)(1-iC_d)+C_0C_dt^{2d}}, \tag{21}$$

where

$$C_j=\frac{Z_j+X(Y_j^2-1)}{Y_j^2\sqrt{1-X^2}}, \quad j=0,d. \tag{22}$$

Interestingly enough, $\mathcal{T}_2^s$ bears a close resemblance to the *single-impurity* transmission coefficient[1]

$$\mathcal{T}_1(j)=\frac{1}{1-iC_j}. \tag{23}$$

Thus, the interference between the two impurities manifests itself in $\mathcal{T}_2^s$ by the presence of the oscillatory term $t^{2d}\equiv e^{i2d\theta}$. In the limit of remote impurities, $d\rightarrow+\infty$, one can take $t^{2d}=0$ on average, and obtain simply $\mathcal{T}_2^s\rightarrow\mathcal{T}_1(0)\mathcal{T}_1(d)$, indicating that there is no interaction between the impurities. In the general case of a finite distance $d\geqslant 2$, we can use the *Chebyshev polynomials* $T_{2d}(X)$ and $U_{2d-1}(X)$ to express the transmission amplitude as

$$|\mathcal{T}_2^s|^2=\frac{1}{\{1+C_0C_d[T_{2d}(X)-1]\}^2+\{C_0+C_d-C_0C_d\sqrt{1-X^2}U_{2d-1}(X)\}^2}. \tag{24}$$

The impurity-parameter space is again limited to the case of two identical impurities, having the same site and bond energies, so that $Z_0=Z_d=Z$ and $Y_0=Y_d=Y$. In optimizing the transmission, (21) and (24) suggest that $|\mathcal{T}_2^s|^2=1$ for all distances d, if one works in the regime $C_0=C_d=0$, that is, $Z+X(Y^2-1)=0$. A slight variation from this condition may introduce an uncontrolled change in transmission, due to interference of multireflected Bloch waves between the impurities. To demonstrate this, we set $Z=1/2$, as in Ref. 1, and display in Fig. 2 the X and Y dependences of $|\mathcal{T}_2^s|^2$ for energies inside the band $(-1\leqslant X\leqslant 1)$ and for a range of the impurity couplings $(0<Y\leqslant 1.6)$, at distances $d=2,6$, and 13 between the impurities. Figure 2 shows that $|\mathcal{T}_2^s|^2$ has an oscillatory behavior over the energy band for wide ranges of d and Y, due to the above-mentioned interference effect.

V. DISCUSSION

The switching property depends on the availability of well-defined on/off regions, where the transmission probability changes between 0 and 1 in a narrow range of the impurity parameters, say, Z and Y. A study of the one-impurity problem reveals that $|\mathcal{T}_1|^2$ develops a *well-defined peak* at the energy $X\simeq Z$, when the impurity site-energy is inside the band $(-1<Z<1)$, for sufficiently weak impurity-chain coupling, $Y\ll 1$ (see Fig. 7 of Ref. 1), which is a desirable feature of the one-impurity model of a molecular switch.[1,2] From Figs. 1 and 2, it is also seen that, in the two-impurity case, controlling the switching by the impurity-site energies remains feasible in the regime of weak impurity-chain coupling.

In designing molecular switches, we are also interested in the transmission at the Fermi level X_F, which we choose at $X=X_F=1/2$, as in Ref. 1. In the case of adjacent impurities, (16) suggests that it is possible to control the switching by changing the interimpurity coupling Y_h, in addition to the above-mentioned control via impurity-site energy. In Fig. 3, we display the Z and Y_h dependence of $|\mathcal{T}_2^a|^2$ at $X=X_F=1/2$, for two identical impurities, and for several values of impurity-chain coupling Y (0.2, 0.5, and 0.8). It is clear from the figure that, for $Y\ll 1$, both Z and Y_h may serve to control the switch on/off operation.

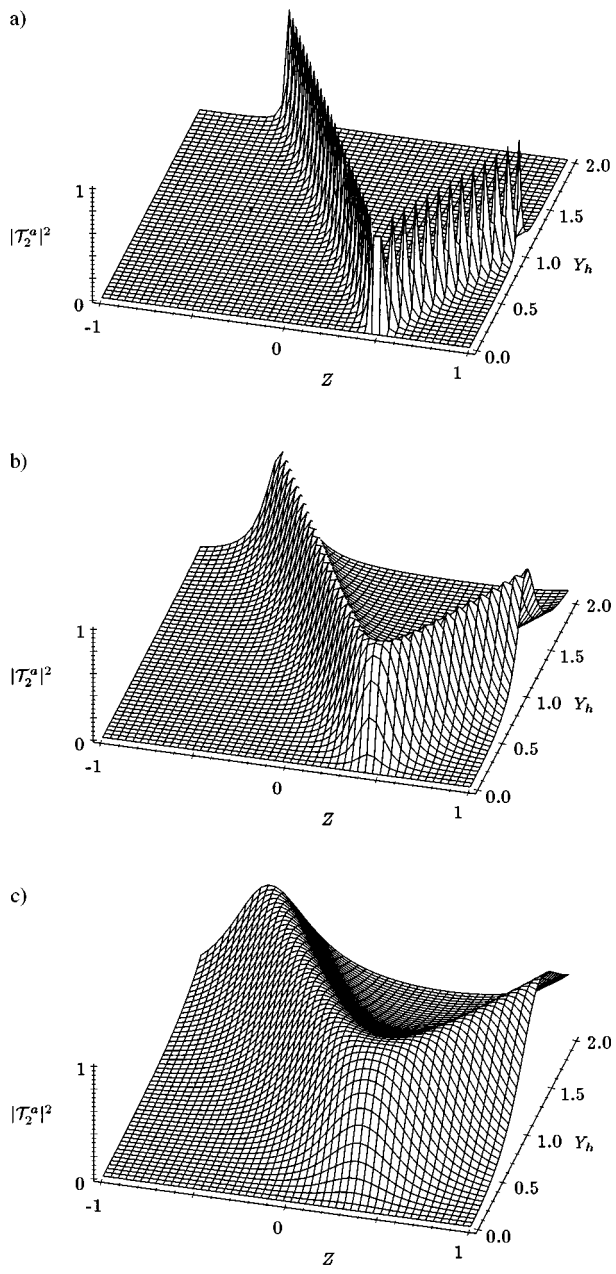

FIG. 3. Dependence of transmission probability for adjacent impurities $|\mathcal{T}_2^a|^2$ on Z and Y_h for $X=1/2$ and (a) $Y=0.2$, (b) $Y=0.5$, and (c) $Y=0.8$.

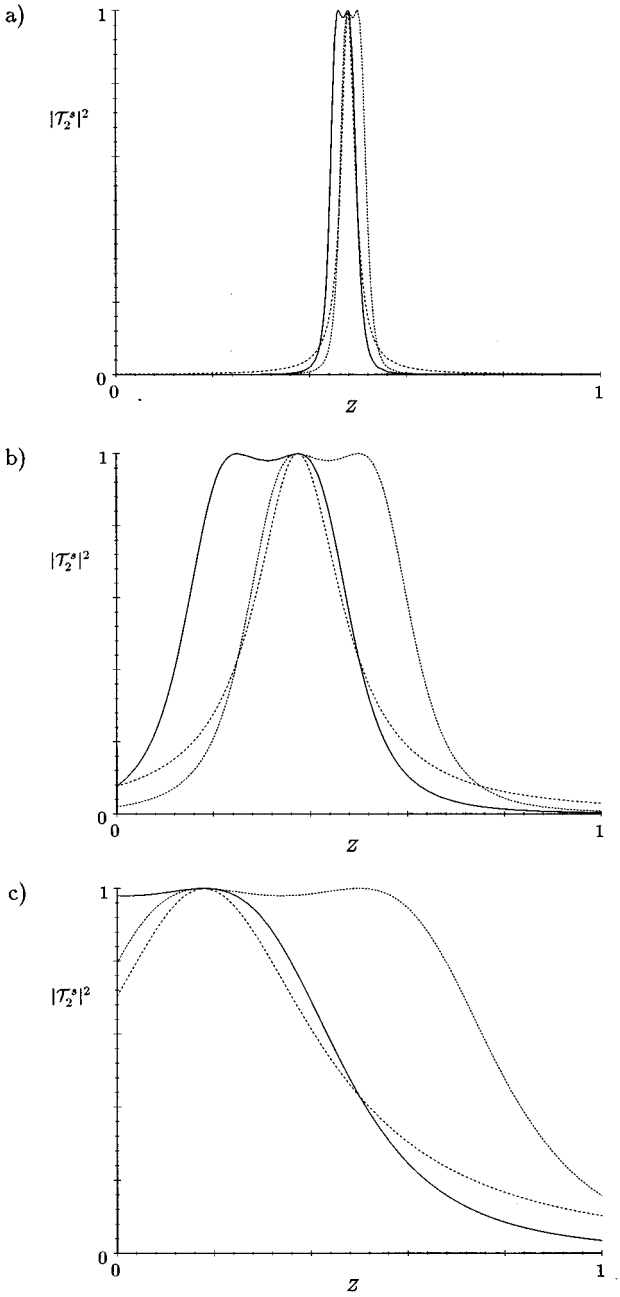

FIG. 4. Dependence of transmission probability for separated impurities $|\mathcal{T}_2^s|^2$ on Z for $X=1/2$ and (a) $Y=0.2$, (b) $Y=0.5$, and (c) $Y=0.8$. The distances $d=2+3n$, $d=3+3n$, and $d=4+3n$ (n being a non-negative integer) are represented in each plot by solid, dashed, and dotted curves, respectively.

In case of separated impurities, the distance d is not a suitable control parameter, so instead we are interested in establishing on/off regions, which are insensitive to the d-dependent interference effects. Figure 2 shows that, for all distances d, the peak at $X \simeq Z$ remains the dominant feature in the transmission probability, for sufficiently small values of Y, which is a suggested regime of operation in the multi-impurity situation. To illustrate the Z control of switching, we consider the transmission at $X=X_F=1/2$ for two identical impurities. In this case, $|\mathcal{T}_2^s|^2$ becomes a triperiodic function of d. In Fig. 4, we display its Z dependence for $d=2+3n$, $d=3+3n$, and $d=4+3n$ (n being a non-negative integer), and for $Y=0.2$, 0.5, and 0.8. Even though the peak at $Z \simeq 1/2$ (for small Y) is spread by the interference effects for the various d values, the Z parameter may well be used as a means of controlling the switch operation. Larger values of Y create a wider dispersion in the Z on-off regions, again because of interference. Consequently, we conclude that a weak impurity-chain coupling reduces interference effects and enables closer packing of multiple switches along the host chain.

ACKNOWLEDGMENTS

The work reported here was supported by the Natural Sciences and Engineering Research Council of Canada. Z.L.M. wishes to thank the Department of Applied Mathematics, University of Waterloo, for its kind support.

*On leave from The Institute of Nuclear Sciences–Vinča, Belgrade, Serbia, Yugoslavia.
†Also with the Department of Physics, University of Waterloo, and the Guelph-Waterloo Program for Graduate Work in Physics.

[1] P. Sautet and C. Joachim, Phys. Rev. B **38**, 12 238 (1988).
[2] R. A. English and S. G. Davison, Phys. Rev. B **49**, 8718 (1994).
[3] R. Farchioni, G. Grosso, and G. Pastori Parravicini, Phys. Rev. B **53**, 4294 (1996).
[4] G. F. Koster and J. C. Slater, Phys. Rev. **95**, 1167 (1954); G. F. Koster, *ibid.* **95**, 1436 (1954); J. Callaway, J. Math. Phys. **5**, 783 (1964).
[5] B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950).
[6] S. G. Davison and M. Steslicka, *Basic Theory of Surface States* (Clarendon, Oxford, 1992).