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LETTER TO THE EDITOR

Control of the quantum path–target state distance: bistable-like characteristic in a small tight-binding system

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Abstract. The control of the distance between the quantum path and a given target state in the state space of an $(N+2)$ tight-binding isolated system prepared in a non-stationary initial state is studied as a function of an asymmetry introduced by a change in only one of the coupling constants. When $N>6$, a bistable-like characteristic is found for the variation of the minimum distance between the path and the target as a function of this asymmetry. Optimised systems are proposed to reach the best control of this distance by the asymmetry.

Let ε be the state space (Davis 1976) of a quantum system modelled by a Hamiltonian $H(\theta)$ with θ one of the control parameters of this system. The path $\rho(t)$, i.e. the density operator of the system belonging to ε, is governed by the von Neumann–Liouville equation (Zwanzig 1964, Bratteli and Robinson 1979). If a target state $\bar{\rho}$ is chosen in ε, a change in θ may induce, for the same initial state $\rho(0)$, a $\rho(t)$ deformation such that the Euclidean distance $d(t)$ between $\rho(t)$ and $\bar{\rho}$ increases.

For non-dissipative systems, i.e. when $\rho(t)$ runs only on the extreme point subset of ε, one example is a three-level isolated tight-binding system (figure 1 with $N=1$)

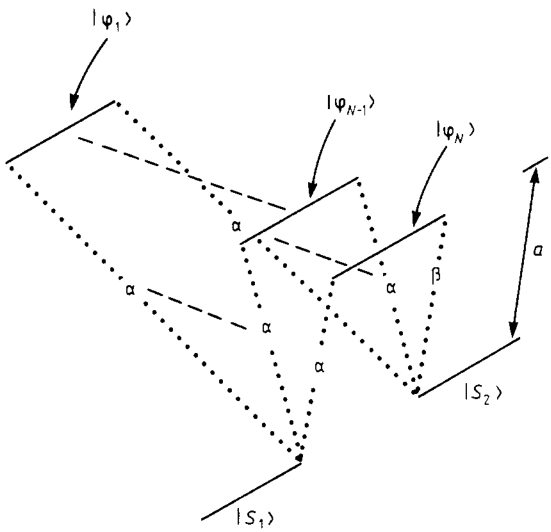

Figure 1. Structure of the $N+2$ tight-binding system studied in this letter. The coupled levels are linked by a point line and the amplitude is labelled on each line. As in the text the energy of the $|s_i\rangle_{i=1,2}$ is e.

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with $\rho(0)=|s_1\rangle\langle s_1|$, $\bar\rho=|s_2\rangle\langle s_2|$ and $\langle s_1|s_2\rangle=0$, $\langle s_i|\varphi_j\rangle=0$. Only $\beta\alpha^{-1}=1$ may lead to $d(t)=0$ (Joachim and Launay 1987). For large and small $\beta\alpha^{-1}$, the minimum distance between $\rho(t)$ and $\bar\rho$ increases to reach the maximum possible distance $\sqrt{2}$ due to the convex structure of ε.

In this letter, we show that a bistable-like characteristic can be obtained with the $(N+2)$-level tight-binding system (figure 1) if $N>1$ and if optimised αa^{-1} are chosen. For these αa^{-1} and when $\beta\alpha^{-1}$ scans the [0, 1] interval, the maximum possible distance between $\rho(t)$ and $|s_2\rangle\langle s_2|$ is close to zero for large N. When $\beta\alpha^{-1}>1$, this distance increases. Compared to the three-level system ($N=1$ in figure 1), the path is stabilised for $\beta\alpha^{-1}\in[0,1]$ because an N increase shadows the perturbation introduced by the coupling β when $\beta\neq\alpha$.

For the purposes of this letter, the $(N+2)$-level system is considered isolated from its surrounding environment. Clearly for bounded quantum systems, the dissipative case is richer in the types of quantum path than is the non-dissipative case (see e.g. Obermayer *et al* 1987) since the Hamiltonian spectrum is no longer discrete, which may lead to chaotic behaviour (Casati and Guarneri 1984, Jose 1986). But isolated quantum systems also lead to interesting paths because they are only controllable in part (Wolovich 1974), i.e. for a given $\rho(0)$, $\rho(t)$ cannot reach all the extreme points of ε even if θ runs over all the control space parameter. Transitions from periodic to almost-periodic paths can dramatically affect $d(t)$ or the speed to go (if possible) from $\rho(0)$ to the vicinity of $\bar\rho$. Hereafter, $|s_1\rangle\langle s_1|$ is the initial state $\rho(0)$ and $|s_2\rangle\langle s_2|$ the target state $\bar\rho$.

It may seem worthless to search for bistable-like characteristics in tight-binding systems more complex than a two-level system since it is well known from the Rabi formula (Rabi 1937, Sukurai 1985) that a two-level system presents such a characteristic. However, firstly, a two-level system has only one control parameter (the ratio between the coupling and the energy difference of the two levels) and one time-scaling parameter (this two-level energy difference). Then there are not enough control parameters to fully optimise the slope of its characteristic. Secondly, if this two-level system is embedded in a periodic tight-binding chain, the control parameter cannot be used to control the low voltage conductance of the overall system as for the $N=3$ system (figure 1) (Sautet and Joachim 1987) since the site energy of half the periodic chain has to change in this case.

When the tight-binding system (figure 1) is not coupled to its environment, $\rho(t)=|\psi(t)\rangle\langle\psi(t)|$, $d(t)=(2-2|\langle s_2|\psi(t)\rangle|^2)^{1/2}$ and $|\psi(t)\rangle$ is a solution of the Schrödinger equation $[\mathrm{i}\hbar\,\partial/\partial t-H(N)]|\psi(t)\rangle=0$ where $H(N)$ is the Hamiltonian of the system in figure 1 given on the tight-binding basis $|s_1\rangle$, $|\varphi_j\rangle_{j=1,N}$ and $|s_2\rangle$ by

$$H(N)=\begin{bmatrix} e & \alpha & \alpha & . & . & . & \alpha & \alpha & 0 \\ \alpha & e+a & 0 & . & . & . & 0 & 0 & \alpha \\ \alpha & 0 & e+a & 0 & . & . & . & 0 & \alpha \\ . & . & 0 & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & 0 & . & . \\ \alpha & 0 & . & . & . & 0 & e+a & 0 & \alpha \\ \alpha & 0 & 0 & . & . & . & 0 & e+a & \beta \\ 0 & \alpha & \alpha & . & . & . & \alpha & \beta & e \end{bmatrix}. \qquad (1)$$

For $|\psi(0)\rangle=|s_1\rangle$, the components $g_j(t)=\langle s_j|\psi(t)\rangle_{j=1,2}$ and $f_j(t)=\langle\varphi_j|\psi(t)\rangle_{j=1,N}$ of $|\psi(t)\rangle$

on this tight-binding basis are solutions of the system:

$$\frac{\mathrm{d}}{\mathrm{d}t}g_1(t)=-\frac{\mathrm{i}}{\hbar}eg_1(t)-\frac{\mathrm{i}}{\hbar}\alpha\sum_{j=1}^{N}f_j(t) \tag{2a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}f_j(t)=-\frac{\mathrm{i}}{\hbar}(e+a)f_j(t)-\frac{\mathrm{i}}{\hbar}\alpha g_1(t)-\frac{\mathrm{i}}{\hbar}\alpha g_2(t) \tag{2b}$$

for all j from $j=1$ to $j=N-1$, and

$$\frac{\mathrm{d}}{\mathrm{d}t}f_N(t)=-\frac{\mathrm{i}}{\hbar}(e+a)f_N(t)-\frac{\mathrm{i}}{\hbar}\alpha g_1(t)-\frac{\mathrm{i}}{\hbar}\beta g_2(t) \tag{2c}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}g_2(t)=-\frac{\mathrm{i}}{\hbar}eg_2(t)-\frac{\mathrm{i}}{\hbar}\beta f_N(t)-\frac{\mathrm{i}}{\hbar}\alpha\sum_{j=1}^{N-1}f_j(t) \tag{2d}$$

where, as usual, the Schrödinger equation has been projected on the preferred tight-binding basis used for (1).

From its definition, the evaluation of $d(t)$ requires only the calculation of $|g_2(t)|^2$ from (2). But the Laplace transforms of $f_j(t)_{j=1,N}$ in (2) are readily expanded from (2b) and (2c) as a function of the $g_j(t)_{j=1,2}$ Laplace transform because there is no coupling between the $|\varphi_j\rangle_{j=1,N}$. Then (2$a$) and (2$d$) can be transformed in a two-equation system with only two unknown functions $g_1(t)$ and $g_2(t)$. After some lengthy expansion, the solution of this simplified system gives for $|g_2(t)|^2$:

$$|g_2(t)|^2=S_N(X)\left[\tfrac{1}{2}+Y_+\left(\frac{\sin(\omega_+t)}{2\hbar\omega_+}\right)^2+Y_-\left(\frac{\sin(\omega_-t)}{2\hbar\omega_-}\right)^2\right.$$
$$\left.-\tfrac{1}{2}\cos(\omega_+t)\cos(\omega_-t)-\tfrac{1}{2}a^2\frac{\sin(\omega_+t)}{2\hbar\omega_+}\frac{\sin(\omega_-t)}{2\hbar\omega_-}\right] \tag{3}$$

with $X=\beta\alpha^{-1}$ the asymmetry parameter and $\omega_\pm=(a/2\hbar)(1-4Y_\pm/a^2)^{1/2}$. The parameter $Y_\pm$ in (3) is given by

$$Y_\pm=\tfrac{1}{2}\alpha^2(-[(2N-1)+X^2]\pm\{[(2N-1)+X^2]^2-4(N-1)(1-X)^2\}^{1/2}) \tag{4}$$

and the time-independent envelope by:

$$S_N(X)=\frac{4(N-1+X)^2}{(2N-1+X^2)^2-4(N-1)(1-X)^2}. \tag{5}$$

Notice that for all N, the $(N+2)$-level system is characterised by the same control parameter αa^{-1}, $\beta\alpha^{-1}$ and the same scaling parameter a.

As already discussed for $N=1$ (Joachim and Launay 1987), the first interesting feature in such a system is the αa^{-1} values which lead for $X=1$ to $d(t)=0$; here we find

$$Z_r(m,p)=\left(\frac{1}{8N}\right)^{1/2}\left[\left(\frac{p}{p-2m-1}\right)^2-1\right]^{1/2} \tag{6}$$

for $p\in\mathbb{N}$, $m\in\mathbb{N}$, $p\geqslant m+1$ and $p\neq 2m+1$.

These 'resonant' αa^{-1} correspond to periodic $\rho(t)$ paths in ε. They come from the solution of the equation $d(t_p)=0$ where t_p is the position of one of the $|g_2(t)|^2$ extremum in time and the unknown in this equation is αa^{-1}.

One consequence of the $1/\sqrt{N}$ law in (6) is the size reduction of the interval where the $Z_r(m, p)$ are found. When N goes to infinity, the only resonant αa^{-1} is zero, i.e. all the $|\varphi_j\rangle$ levels degenerate with $|s_1\rangle$ and $|s_2\rangle$. Another consequence is the $\sqrt{N}$ increase of the speed for the path $\rho(t)$ to go from $|s_1\rangle\langle s_1|$ to $|s_2\rangle\langle s_2|$ because for a given (m, p) in (6), its first time passage at $|s_2\rangle\langle s_2|$ is given from (3) by:

$$t = \frac{2\pi\hbar}{a(1+8NZ_r^2(m, p))^{1/2}}. \tag{7}$$

For an almost-periodic function like (3) with $X = 1$, the existence of the $Z_r(m, p)$ implies that there also exists αa^{-1} leading to destructive interferences, i.e. antiresonant combination of sinusoidals in (3). For a given m in (6), these αa^{-1} must correspond to the $d(t_p)$ cusp points because the passage from one $Z_r(m, p)$ to another comes from a change in p. Each change is a discontinuous process leading to a cusp point between two consecutive $Z_r(m, p)$ for the same m. By the same calculation as for $N = 1$ (Joachim and Lanuay 1987), it is found for the antiresonant αa^{-1} that

$$Z_{ar}(m, p) = \left(\frac{1}{8N}\right)^{1/2}\left[\left(\frac{2p+1}{2p-4m-1}\right)^2 - 1\right]^{1/2} \tag{8}$$

with $p \in \mathbb{N}$, $m \in \mathbb{N}$ and $p > m+1$.

If one tunes α and a to go from a resonant to an antiresonant αa^{-1}, then $\min_j[d(t_j)]$ may increase during this change if t_j is the time position of the $d(t)$ minimum number j. But for antiresonant αa^{-1}, $\min_j[d(t_j)]$ is not so large because $d(t_j)$ is given from (3) and (8) by

$$d(t_j) = \left[1 + \cos\left(j\frac{4m+2}{2p+1}\pi\right)\right]^{1/2}. \tag{9}$$

Then, $\min_j[d(t_j)]$ is independent of N and goes to zero when $Z_r(m, p)$ decreases because such a decrease is given in (7) by an increase of m which pushes the $d(t_j)$ minimum to higher j. For example, for $Z_{ar}(m, m+1)$ the smallest minimum between all the $d(t_j)$ minima is the one number $j = m/2+1$ for odd m and $j = \frac{1}{2}(m+1)+1$ for even m. Even for the worst non-resonant αa^{-1}, i.e. $Z_{ar}(0, 1)$, $\min_j[d(t_j)] = \frac{1}{2}\sqrt{2}$ which is still far from $\sqrt{2}$.

The main interesting feature, however, is the control of $d(t)$ by the asymmetry parameter X when the $(N+2)$-level system is set up in a resonant evolution regime to be sure that $\rho(t)$ coming from $|s_1\rangle\langle s_1|$ pass through $|s_2\rangle\langle s_2|$ for $X = 1$.

Let us first focus on the time-independent envelope term $S_N(X)$ of (3). When N increases, $S_N(X)$ is stabilised on the X interval $[0, 1]$ (figure 2). For small β, the perturbation introduced in the overall system by the state $|\varphi_N\rangle$ (weakly coupled to $|s_2\rangle$ and coupled to $|s_1\rangle$) is shadowed when the number of $|\varphi_j\rangle_{j=2,N}$ states symmetrically coupled on both sides is large (figure 3). When $X > 1$, $S_N(X)$ goes down but the slope of this variation becomes small as N increases. More interestingly, the minimum distance between $\rho(t)$ and $|s_2\rangle\langle s_2|$, calculated with only $S_N(X)$, decreases at $X = 0$ faster than the slope of $S_N(X)$ for $X > 1$ as a function of N (figure 3). Then, already for $N = 6$ a bistable-like control law is obtained by scanning X, for example by slowly changing β for a fixed optimised α corresponding to a resonant αa^{-1} in (6).

However, to obtain the exact ability of X to control $d(t)$, the influence of the time-dependent part $h(t) = |g_2(t)|^2/S_N(X)$ of (3) must be taken into account because for a given $Z_r(m, p)$ and $X \neq 1$ not all the X lead to a periodic $\rho(t)$ path. After the

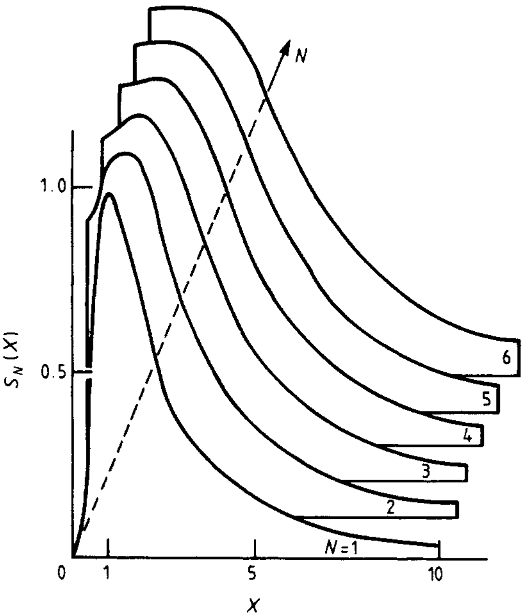

Figure 2. Variation of the time-independent envelope $S_N(X)$ of $|g_2(t)|^2$ as a function of the asymmetry parameter $X = \beta\alpha^{-1}$ for $N \leqslant 6$.

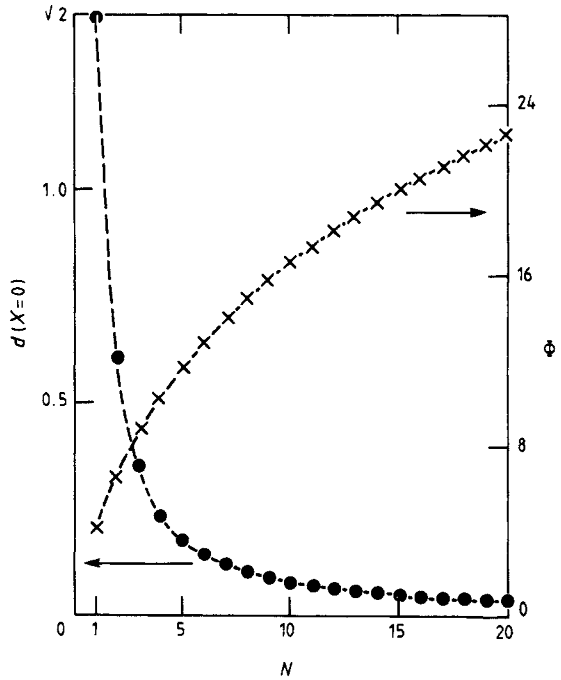

Figure 3. Variation of the minimum distance at $X = 0$ and of the slope of $d(X)$ as a function of N. The distance $d(X = 0)$ and the angle Φ are calculated from the $S_N(X)$ envelope. Φ is the angle between the $d(X)$ ordinate axis and the line tangent to $d(X)$ slope for $X > 1$ near its inflection point.

derivative of (3), the equation obtained to calculate the position of the $d(t)$ extremum in time is given by

$$(Y_-/\omega_-)\sin(\omega_- t) - (Y_+/\omega_+)\sin(\omega_+ t) = 0. \tag{10}$$

Unfortunately when $\beta\alpha^{-1} \neq 1$, this equation which leads to the resonant and anti-resonant X is not analytically solvable for $N > 1$ as it was for $N = 1$ (Sautet and Joachim 1987), i.e. the deformations of $S_N(X)$ due to the time-dependent part $h(t)$ of (3) cannot be found analytically. The numerical solution of (10) shows that for $N > 1$, these deformations are negligible as soon as $Z_r(m, p)$ is chosen small compared to the first resonant αa^{-1} available, i.e. $Z_r(0, 1)$ for the N considered. This comes from the fact that the $(N+2)$-level system evolution reduces to a two-level-like evolution for large a and $X = 1$ because in this case the Fourier spectrum of $|g_2(t)|^2$ is close, aside from the $\omega = 0$ pulsation component, to that of a sinusoidal at a pulsation $\omega = (a/2\hbar)[1 - (1 + 8NZ_r^2(m, p))^{1/2}]$.

The deformations of $S_N(X)$ by $h(t)$ are presented in figure 4(a) for $N = 2$ as a function of the $Z_r(0, p)$ chosen. They are calculated from the maximum possible amplitude reached by $h(t)$ during a time interval which contains at least more than one of its maxima. For figure 4(a) (and also figure 4(b)), the time interval chosen contains the first ten $h(t)$ maxima which corresponds approximately to the first almost period of $h(t)$. When this interval is extended to infinity, the width of each peak in figures 4(a) and 4(b) decreases because $h(t)$ is an almost-periodic function, i.e. it is always possible on a large time interval to find a $h(t)$ maximum as close as desired to one. In this case, in figure 4(a), the $1 - \max_j[h(t_j)]$ function of X tends to be a sum of delta functions. The support of each of these delta functions defines an antiresonant X.

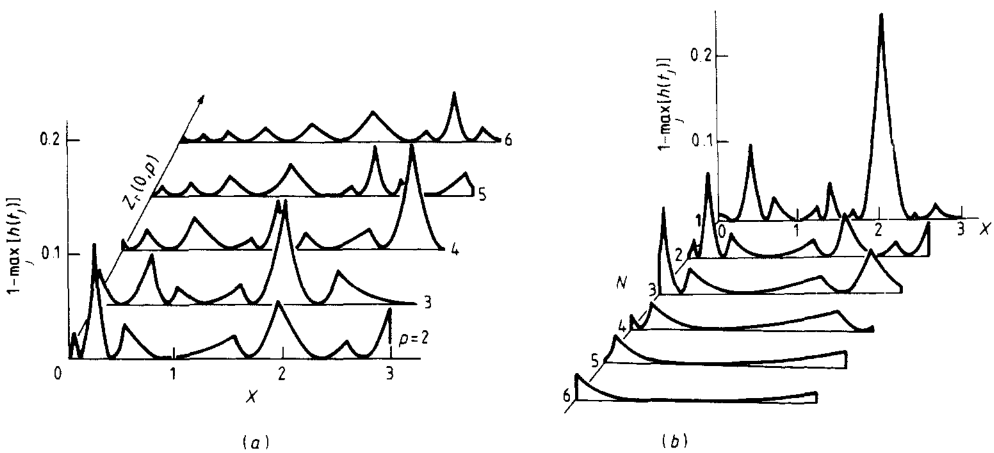

Figure 4. Variation of $1 - \max_j[h(t_j)]$ as a function of X for the first ten $h(t)$ maxima in time with (a) $N = 2$ fixed and (b) $Z_r(0, 1)$ fixed.

In figure 4(b), the deformations induced by $h(t)$ on $S_N(X)$ are presented as a function of N for $Z_r(0, 1)$ at each N. When N increases, $h(t) \propto 1 - \cos(\omega_- t)[2\cos(\omega_+ t) - \cos(\omega_- t)]$ with, in this case and from (4), $\omega_- \gg \omega_+$. Even if ω_- and ω_+ are still incommensurable for $X \neq 1$, ω_+ will play a role in $|g_2(t)|^2$ only on a very long timescale. Then for large N, the antiresonant X peaks are small in amplitude. They are pushed to zero for $X<1$ and to infinity for $X>1$. The deformations of $S_N(X)$ by $h(t)$ can be neglected as soon as $N>5$ even for $Z_r(0,1)$.

In conclusion, it is possible to design a simple quantum system which shows a bistable-like characteristic in controlling, by a small coupling asymmetry, the minimum distance available in time between the path of this system and a given target state in the state space. Contrary to a two-level system, the asymmetry control parameter used to control the path for the isolated case can also be used, in principle, for the control of the low voltage conductance of a periodic chain when the $N+2$ system presented in this letter is embedded in it. Whether or not this control will lead to a bistable-like characteristic for the overall system conductance is currently under investigation.

When N increases, one limitation of the $N+2$ system is the reduction of the interval where resonance αa^{-1} can be chosen to provide a zero minimum distance between the path and the target state when there is no asymmetry in the system. An optimisation between N and αa^{-1} is needed if small $Z_r(m,p)$ cannot be reached for the system considered.

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