

# The Schrödinger's dream: Electronic structure of DNAs and proteins: Quantum automata

Kazumoto Iguchi  
X-Ray Crystallography Laboratory

The concepts of classical and quantum automata are introduced, and it is shown that those play an essential role in order to obtain electronic structures of DNAs and proteins. The classical automata are standard automata that construct a string of symbols. If one wishes to consider the electronic states on the string of symbols, one must regard the symbols as the  $2 \times 2$  transfer matrices and treat their traces. This provides another dimension of automata, that is, quantum automata.

## Introduction

One of dreams of theoreticians is to solve the Schrödinger equation with a potential that is given as a one-dimensional array of the real DNA and protein sequences.<sup>1)</sup> DNAs consist of the four nucleotides and proteins up to the twenty amino acids. They form alphabet to represent the sequences. A string of DNA or that of protein is a very complicated and nonperiodic arrangement of the bases with a very long length. Therefore, one meets a problem of an electron motion in such a nonperiodic potential. This is a crucial and inevitable procedure in order to obtain electronic structures of the DNAs and proteins. This problem has been a main theme in quantum molecular biology, which I would like to call *the Schrödinger's dream*.<sup>2)</sup> However, this has been unsolved for a long time since the discovery of DNA structure - Watson-Crick's double helix. In this paper I would like to pay our attention to recent developments in theoretical and mathematical physics, which seem relevant to solve the above biological problem to my eyes.

## Schrödinger equation with a nonperiodic sequence

Until recently, theoretical and mathematical physicists have been struggling to make a theory for the so-called quasiperiodic systems.<sup>3)</sup> In this problem one wishes to solve the discrete Schrödinger equation with a deterministic potential sequence:  $T_{n+1}\psi_{n+1} + T_n\psi_{n-1} + V_n\psi_n = E\psi_n$ , where  $T_n$  is the hopping integral between the  $n$ th and the  $(n-1)$ th sites and  $V_n$  the on-site potential at site  $n$ , respectively. The potentials  $T_n$  and  $V_n$  take on different values according to the distinct atoms. This enables one to define a nonperiodic potential in the system. One now would like to obtain electronic structure of the system. To do this, it is convenient to map the Schrödinger equation into the transfer matrix form:  $\Psi_{n+1} = \underline{T}(n)\Psi_n$ , where the transfer matrix  $\underline{T}(n)$  is defined by a  $2 \times 2$  matrix  $\underline{T}(n) \equiv ((E - V_n)/T_{n+1}, -T_n/T_{n+1}; 1, 0)$ , and the wave function  $\Psi_n \equiv (\psi_n, \psi_{n-1})$ . If the system consists of  $N$  atoms, then one has to multiply the  $N$  transfer matrices such that  $\Psi_{n+N} = \underline{M}(N)\Psi_n$ , where  $\underline{M}(N) = \underline{T}(n+N-1)\underline{T}(n+N-2) \cdots \underline{T}(n)$ . And from the Bloch theo-

rem  $\Psi_{n+N} = \exp[ikN]\Psi_n$ , one can state a simple approach to obtain energy bands: If  $\text{Tr}[\underline{M}(N)] \leq 2$ , then an energy lies in a band, otherwise it lies in a band gap. In this way, one finds that the trace of a product of the transfer matrices plays an essential role in order to obtain the electronic spectrum of the system.

## Some examples in mathematical physics

Physicists found that if the total number of atoms in the system is developed dynamically and given recursively such as  $N_{k+1} = N_k + N_{k-1}$  with  $N_1 = N_0 = 1$ , then the trace itself is given recursively as well such that  $x_{k+1} = 2x_{k+1}x_k - x_{k-2}$ , where  $x_k = \text{Tr}[\underline{M}(N_k)]/2$ , and this is called the *trace map*. This is a famous example of the Fibonacci lattice given by a deterministic substitution scheme,  $A \rightarrow AB, B \rightarrow A$ .<sup>4)</sup> This provides a sequence of  $A$  and  $B$  such as  $B \rightarrow A \rightarrow AB \rightarrow ABA \rightarrow ABAAB \rightarrow ABAABABA \rightarrow ABAABABAABAAB \rightarrow \cdots$ . So, this system is represented compactly by  $S_{k+1} = S_k S_{k-1}$  with  $S_1 = "A"$  and  $S_0 = "B"$ . This idea has been generalized to the systems with an arbitrary number of letters in the alphabet, say  $r$  letters.<sup>5)</sup> One now finds that if a potential is represented by a deterministic substitution scheme:  $S_{k+1}^{(i)} = W_k^{(i)}[S_k^{(1)}, S_k^{(2)}, \dots, S_k^{(r)}]$  for  $i = 1, \dots, r$ , where  $W_k^{(i)}$  stands for any word made by  $S_k^{(1)}, S_k^{(2)}, \dots, S_k^{(r)}$ , then the dimension of the trace map (i.e., the minimal number of traces representing the trace map) is given by  $r(r+1)/2$ .<sup>5)</sup> This was recently reduced even more to  $3r - 3$ .<sup>6)</sup>

## Mathematical representation of evolution

Consider an evolution of a DNA or a protein chain. At first stage there is only one base, say  $X$ . Next, by synthesis another base,  $Y$ , can be combined to either left or right of the first one such as  $XY$  or  $YX$ . If  $Y = X$ , this represents a duplication of the base. So, a mathematical representation of base evolution can be described by several simple operations: identity,  $\mathbf{I}(X, Y) = (X, Y)$ ; inversion,  $\mathbf{J}(X, Y) = (X^{-1}, Y)$ ;

exchange,  $\mathbf{X}(X, Y) = (Y, X)$ ; left or right multiplication,  $\mathbf{L}(X, Y) = (X, YX)$  or  $\mathbf{R}(X, Y) = (X, XY)$ . For example, a string  $\mathbf{XR}$  provides the Fibonacci evolution such that  $\mathbf{XR}(X, Y) = (XY, X)$ , and by repeatedly using this, one can get the Fibonacci sequence of  $X$  and  $Y$ .<sup>3)</sup> Thus, to me the mathematical structure of DNA and protein evolution process is nothing but that in the theory of quasiperiodic systems. For the  $r$ -letter case this is summarized as in Table 1, and was found that it is equivalent to the concept of Nielsen transformations.<sup>5)</sup>

Table 1. The Nielsen transformations with  $r$  letters. Permutation  $P$  appears only for  $r > 2$ .

	A	B	C	D	...	Z
$J_1$	$A^{-1}$	B	C	D	...	Z
$X_{12}$	B	A	C	D	...	Z
$P$	Z	A	B	C	...	Y
$L_{12}$	BA	B	C	D	...	Z
$R_{12}$	AB	B	C	D	...	Z

### Classical and quantum automata

This type of theory for construction of the system is basically written in the language of automaton,<sup>2,7)</sup> and therefore, so is the mathematical structure of the evolution processes. However, this only describes how to construct the potential in the system, but one has to solve the Schrödinger equation with this potential as discussed before. If one wishes to do this, then one must consider the trace of the product of the transfer matrices even for the system in biology as well. In this way, when an electronic structure is considered, the automaton for the construction of the system is lifted to that of the transfer matrices. The latter provides quantum information of the system while the former provides information of lattice structure of the system. Therefore, one is naturally led to the concepts of *classical and quantum automata*. This is schematically shown in Fig. 1, and I show an example of the electronic structure in Fig. 2. Thus, I would like to conclude that the quantum automaton will play an essential role in order to obtain the electronic structure of very complicated molecules such as DNAs and proteins. This direction is just opened and waiting for you.

This work is supported in part by the Special Researcher's Basic Science Program and the Special Grant for Promotion of Research from the Institute of Physical and Chemical Research (RIKEN).

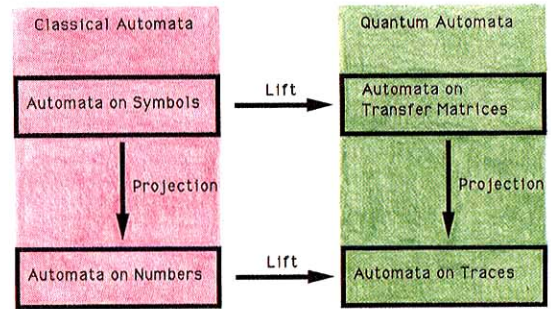


Fig. 1. Classical and quantum automata. Automata on symbols are lifted to automata on transfer matrices. Automata on numbers and on traces are obtained as projection from automata on symbols and on transfer matrices, respectively.

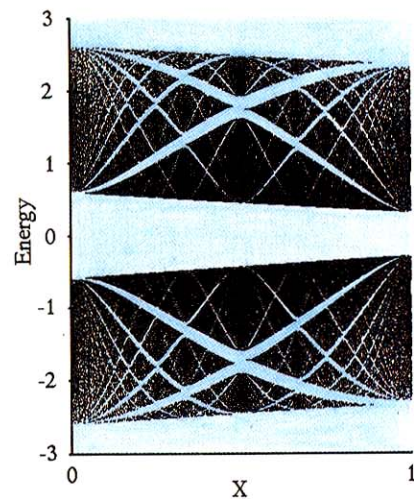


Fig. 2. Electronic structure of quasiperiodic lattices of  $AB_{1-x}C_x$  for  $0 < x < 1$ , where  $x$  is the density of the unit  $AC$  in the chain. The case of  $(T_a, T_b, T_c) = (1, 1.4, 1.2)$  is drawn.

### References

- 1) E. Schrödinger: *What is Life? & Mind and Matter*, (Cambridge University, New York, 1967).
- 2) D. R. Hofstadter: *Gödel, Esher, Bach*, (Vintage, New York, 1979).
- 3) K. Iguchi: Phys. Rev. **B43**, 5915, 5919 (1991); J. Math. Phys. **33**, 3736, 3938 (1992).
- 4) M. Kohmoto et al.: Phys. Rev. Lett. **50**, 1870 (1983).
- 5) K. Iguchi: J. Math. Phys. **34**, 3481 (1993); *ibid.* **35**, 1008 (1994); Phys. Rev. **B49**, 12633 (1994).
- 6) Y. Avishai, D. Berend, and D. Glaubman: Phys. Rev. Lett. **72**, 1842 (1994).
- 7) M. Dekking et al.: Math. Intelligencer **4**, 130, 173, 190 (1982). F. Axel et al.: J. de Phys. **C3**, 181 (1986).