Eigen model as a quantum spin chain: Exact dynamics

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We map the Eigen model of biological evolution [Naturwissenschaften **58**, 465 (1971)] into a quantum spin model with non-Hermitian Hamiltonian. Based on such a connection, we derive exact relaxation periods for the Eigen model to approach static energy landscape from various initial conditions. We also study a simple case of dynamic fitness function.

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The Eigen model of asexual evolution [1,2] is one of the main mathematical models in this field. In this model individuals have offsprings that are subjected to mutation that connects with a selection rule. In his original work Eigen found an error threshold similar to the critical point in critical phenomena such that when the mutation is larger than the error threshold the organism cannot survive. Later, statistical mechanics has been applied to investigate the discrete time version of the original model [3,4]. Franz and Peliti [5] derived another important result in the Eigen model: concentration of individuals around the peak configuration.

In the parallel mutation-selection model, an alternative to the Eigen model, a mutation mechanism and a selection mechanisms are two independent processes that take place concurrently [6]. Baake *et al.* [7] proved that for the parallel mutation-selection scheme, the time evolution equation for the frequencies of different species is equivalent to the Schrödinger equation in imaginary time for quantum spins in a transverse magnetic field. Based on such a connection, recently we used Suzuki-Trotter formalism [8] to study both statics and dynamics of the model with a single peak fitness function [9]. In the present paper, we will extend such study to the Eigen model [1] by reexpressing the Eigen model's dynamics via quantum chain problem, then solving the dynamics to obtain exact relaxation periods for the Eigen model. The dynamic aspects play important role during the evolution in changing environments [10–12]. Thus such aspects in the Eigen model have been considered in recent works [13,14], in which approximate formulas for the relaxation periods have been found and applied to describe a virus-immune system coevolution. Our equations for exact relaxation periods are consistent with approximate formulas in Refs. [13,14] for the case of one mutation per replication.

As in Ref. [9], the genome configuration is specified by a sequence of N spin values $s_k=\pm 1$, $1\leqslant k\leqslant N$. We denote the ith genome configuration by $S_i\equiv(s_1,s_2,\ldots,s_N)$ and the probability of the ith genome at time t is given by $p_{S_i}\equiv p_i(t)$ and the fitness r_i is the average number of offsprings per unit time. In our language, the chosen fitness r_i is a function f that operates on the genome configuration S_i, i.e., $r_i=f(S_i)$.

In the Eigen model, elements of the mutation matrix Q_{ij} represent the probability that an offspring produced by state j changes to state i, and the evolution is given by the set of 2^N coupled equations for 2^N probabilities p_i,

$$\frac{dp_i}{dt}=\sum_{j=1}^{2^N} Q_{ij}r_jp_j-p_i\left(\sum_{j=1}^{2^N} r_jp_j\right). \tag{1}$$

Here p_i satisfies $\Sigma_{i=1}^{2^N}p_i=1$ and $Q_{ij}=q^{N-d(i,j)}(1-q)^{d(i,j)}$ with $d(i,j)\equiv(N-\Sigma_{l=1}^{N}s_i^ls_j^l)/2$ being the Hamming distance between S_i and S_j. The parameter $1-q$ describes the efficiency of mutations. For the parallel mutation-selection model, the dynamics is given by

$$\frac{dp_i}{dt}=\sum_{j=1}^{2^N} m_{ij}p_j+p_ir_i-p_i\left(\sum_{j=1}^{2^N} r_jp_j\right), \tag{2}$$

where m_{ij} are the elements of the mutation matrix $m_{ij}=\gamma_0$ for $d(i,j)=1$, $m_{ij}=-N\gamma_0$ for $i=j$, and $m_{ij}=0$ for $d(i,j)>1$.

Eigen found that it is enough to solve Eq. (1) for only linear parts [1]. Let us decompose the first, linear part of Eq. (1) via mutations to the fixed length $d(i,j)=l$:

$$\frac{dp_i}{dt}=\sum_{l=0}^{N}\sum_{j,d(i,j)=l} Q_{ij}r_jp_j. \tag{3}$$

The second sum is over all configurations having Hamming distance l from the peak configuration. Using the relation $\Sigma_{i=1}^{2^N}Q_{i,j}=1$, we can show that when p_i satisfies Eq. (3), then

$$p_i'(t)\equiv\frac{p_i(t)}{\sum_j p_j(t)} \tag{4}$$

satisfies Eq. (1). We can compare Eq. (3) with Eq. (2) without the last nonlinear term. The terms $l=1$ and $l=0$ in Eq. (3) correspond, respectively, to the first and second terms in Eq. (2). In Eq. (3), there are terms with higher level $l\geqslant 2$ spin flips. Baake *et al.* [7] mapped Eq. (2) into a model of quantum spin chain. Here we will use the same method to

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map the model of Eqs. (1) and (3) into a quantum spin model with additional higher level spin flip terms.

Let us reformulate the system of Eq. (3). As we identify configuration S_j with a collection of spins $s_1^j,\cdots,s_N^j=\pm 1$ and define fitness function f as $r_j=f(s_1^j,\cdots,s_N^j)\equiv f(S_j)$. Let us consider vectors in the Hilbert space of N quantum Pauli spins. With the p_i of Eq. (3), we connect a vector in Hilbert space $\Sigma_{i=1}^{2^N} p_i|S_i\rangle$. Then $r_j\to f(\sigma_1^z,\cdots,\sigma_N^z)$. The l spin flip term Q_{ij} in Eq. (3) can be identified with a matrix element $\langle S_j|D_l|S_i\rangle$ of quantum operator

$$D_l\equiv q^{N-d(i,j)}(1-q)^{d(i,j)}\sum_{1\leqslant i_1<\cdots i_l\leqslant N}\sigma_{i_1}^x\cdots\sigma_{i_l}^x. \tag{5}$$

Thus Eq. (3) is equivalent to Scrödinger equation

$$-H=f(\sigma_1^z\cdots\sigma_N^z)q^N+q^N \times\sum_{l=1}^{N}\left(\frac{1-q}{q}\right)^l\sum_{(1\leqslant i_1<i_2^{2^N}\cdots i_l\leqslant N)}\sigma_{i_1}^x\cdots\sigma_{i_l}^x f(\sigma_1^z\cdots\sigma_N^z),$$

$$\frac{d}{dt}\sum_{j=1}^{2^N}p_j(t)|S_j\rangle=-H\sum_{j=1}^{2^N}p_j(t)|S_j\rangle, \tag{6}$$

and Eq. (4) to

$$Z=\sum_{ij}\langle S_i|e^{-Ht}|S_j\rangle p_j^0,$$

$$p_i=\frac{\sum_j\langle S_i|e^{-Ht}|S_j\rangle p_j^0}{Z}, \tag{7}$$

where σ denotes the spin operator and $|S\rangle$ is the standard notation for the spin state. One can multiply Eq. (6) from the left by $\langle S_i|$ and obtain Eq. (3).

For the single-peaked fitness function, we take

$$f(S_1)=A,$$

and

$$f(S_i)=1 \quad \text{for} \quad i\neq 1, \tag{8}$$

with $S_1\equiv(+1,+1,\ldots,+1)$, which is equivalent to choosing

$$f(S_1)=1+(A-1)\left[\frac{\sum_{i=1}s_i}{N}\right]^p \tag{9}$$

at the limit $p\to\infty$. A careful look at the Hamiltonian of Eq. (6) reveals that it is non-Hermitian. But we will mainly work with the matrix elements between $S_i\neq S_1$ and $S_j\neq S_1$ and for these situations we can miss the multiplier $f(\sigma_1^z\cdots\sigma_N^z)=1$. For that sector of Hilbert space Hamiltonian is Hermitian. To investigate the dynamics, we are using the matrix elements of Hamiltonian

$$-\langle S_1|H|S_1\rangle=Ae^{-\gamma},$$

$$\langle S_i|H|S_j\rangle=\langle S_i|H_{diff}|S_j\rangle, \quad i\neq 1,$$

$$-H_{diff}=\hat{I}e^{-\gamma}+\sum_{l=1}^{N}e^{-\gamma}\left(\frac{1-q}{q}\right)^l\sum_{1\leqslant i_1<i_2^{2^N}\cdots i_l\leqslant N}\sigma_{i_1}^x\cdots\sigma_{i_l}^x, \tag{10}$$

where $\hat{I}$ is identity operator, $\gamma\equiv -N\ln(q)\approx N(1-q)\ll N$. For us only terms $l\ll N$ are relevant, therefore the substitution $q^N[(1-q)/q]^l\to e^{-\gamma}(\gamma/N)^l$ can be applied.

To calculate matrix elements of $T(t)\equiv e^{-Ht}$, one should introduce the Suzuki-Trotter formalism [8]. To perform analytical calculation, it is more convenient to use Eq. (9) for the fitness function then Eq. (10). For any value of p an exact method of Suzuki-Trotter formalism [8] can map the system to the problem in classical statistical mechanics. Moreover, for the large values of p it is well known that the problem is drastically simplified. For the quantum p-spin interactions in a transverse magnetic field, Goldschmidt [15] has found that all the order parameters (magnetizations) are either 1 or 0 and one should take either only transverse interaction terms $(\sigma_{i_1}^x\cdots\sigma_{i_l}^x)$ or only the longitudinal one $(e^{-\gamma}[1+(A-1)(\Sigma_i\sigma_i^z/N)^p])$. Therefore, we can work with system of Eq. (10) using the following trick. With exponential accuracy of order $1/2^N$, it is possible to neglect the σ_i^x terms in Eq. (6) and get

$$\langle S_1|e^{-Ht}|S_1\rangle\sim\exp[(Ae^{-\gamma})t]. \tag{11}$$

Matrix elements $\langle S_i|e^{-Ht}|S_j\rangle$ for $i\neq 1$ can be replaced with exponential accuracy by $\langle S_i|\exp[-H_{diff}t]|S_j\rangle$. Equation

$$\frac{d}{dt}\sum_{i=1}^{2^N}x_i(t)|S_i\rangle=-H_{diff}\sum_{i=2}^{2^N}x_i(t)|S_i\rangle \tag{12}$$

is equivalent to Eq. (3) with $r_j=1$ for $j=2,\ldots,2^N$ and $r_1=0$. Then we derive that

$$\sum_{i=2}^{2^N}x_i(t)=\exp(t)\sum_{i=2}^{2^N}x_i. \tag{13}$$

From Eqs. (11) and (13), we have $p_1\sim\exp[(Ae^{-\gamma})t]$ and $\Sigma_{i=2}^{2^N}p_i\sim e^t$. Therefore, we derive the Eigen's exact formula for the error threshold

$$A>e^{\gamma}. \tag{14}$$

Let us calculate now the transition probabilities $\langle S_j|\exp(-H_{diff}t)|S_i\rangle$ between two states with the total number of M flips between configurations $S_i\equiv\{s_1^i,\ldots,s_N^i\}$ and $S_j\equiv\{s_1^j,\ldots,s_N^j\}$ and define $m=1-2M/N$. We will show below that the model can be solved at

$$\frac{1}{N}\sim(1-q)\ll 1. \tag{15}$$

For the finite $(1-m)$, we guess that the relaxation time t is of order N and define

$$T=te^{-\gamma}/N. \tag{16}$$

There are $N(1+m)/2$ spins without flips $(+1$ spins) and $N(1-m)/2$ flipped spins $(-1$ spins). Let us denote by h_l the term of l spin flip in the Hamiltonian. To calculate the matrix element $\langle S_j|\exp(-H_{diff}t)|S_i\rangle \equiv \langle S_j|\exp(-t\Sigma_l h_l)|S_i\rangle$, let us use an equality $\exp(a\sigma^x_{i_1}\sigma^x_{i_2}\cdots\sigma^x_{i_l}]=\cosh(a)[1+\tanh[a]\sigma^x_{i_1}\sigma^x_{i_2}\cdots\sigma^x_{i_l}]$ and expand the product keeping terms till the Mth degree

$$\langle S_j|e^{-tH_{diff}}|S_i\rangle \approx \sum_{K=1}^{M}\sum_{l_1+\cdots l_K=M}\frac{M!}{l_1!l_2!\cdots}\cosh(\gamma T)^N \times\tanh(\gamma T)^{l_1}\prod_{i>1}\left[\frac{(T\gamma^i)\langle+|\sigma^x_1|-\rangle}{N^{i-1}i!}\right]^{l_i}. \tag{17}$$

We find via the saddle point the principal term in the expression of Eq. (17) among all distributions with different l_i. We keep cosh,tanh only for the one spin flip terms. We calculate also the combinatorics of insertion into M site box combination of l_1 single points, l_2 duplets, $\ldots l_k$ k plets, which satisfy the constraint

$$\sum_{i=1}^{M} il_i=M. \tag{18}$$

We can take the constraint of Eq. (18) into account via a Lagrange parameter λ and write l_i as x_iN. For the logarithm of a typical term for summation in Eq. (17), we have

$$N\phi(T,m,\gamma)\equiv N\Bigg\{\ln\cosh(\gamma T)+x_1\ln[\tanh(\gamma T)]+\frac{1-m}{2}\times\ln\frac{1-m}{2}-\frac{1-m}{2}-\sum_{i=2}[x_i\ln(x_ii!/T)-x_i]+\ln\gamma\sum_{i=2}^{M}ix_i-x_1\ln x_1+x_1+\lambda\left(\sum_i ix_i-\frac{1-m}{2}\right)\Bigg]. \tag{19}$$

The extremum conditions for x_i of Eq. (19) give

$$x_1=\tanh(\gamma T)z/\gamma,\quad i!x_i=Tz^i,\quad i\geqslant 2, \tag{20}$$

where $z\equiv\gamma e^{\lambda}$. Using formulas: $\Sigma_{i=2}^{M}x_i=T\Sigma_{i=2}z^i/i!=T(\exp(z)-z-1)$, $\Sigma_{i=2}^{M}iz^i/i!=\Sigma_{i=1}^{M}iz^i/i!-z=z\exp(z)z-z$, $\Sigma_{i=2}^{M}x_i\ln(x_ii!/T)=T\ln z\Sigma_{i=2}iz^i/i!=Tz\ln z[\exp(z)-1]$, and Eq. (18), we have:

$$zTe^z-Tz+z\tanh(\gamma T)/\gamma=\frac{1-m}{2},$$

$$\phi(T,m,\gamma)=\frac{1-m}{2}\ln\frac{(1-m)\gamma}{2}-\frac{1-m}{2}+\ln\cosh(\gamma T)+z\tanh(\gamma T)[1-\ln z]/\gamma+T[e^z(1-z\ln z)-z(1-\ln z)-1]. \tag{21}$$

Let us now consider an ansatz for $\langle S_1|e^{-Ht}|S_i\rangle$:

$$\langle S_1|\exp[AN(T-T_0)]|S_1\rangle\langle S_1|e^{-H_{diff}t_0}|S_i\rangle=\exp\{N[A(T-T_0)+\phi(T_0,m,\gamma)]\}. \tag{22}$$

While calculating this expression via saddle point, we first find the extremal point $T_0\equiv e^{-\gamma}t_0/N$ from the saddle point condition

$$A=\frac{d\phi(T_0)}{dT}. \tag{23}$$

The transition period $t_1\equiv Ne^{\gamma}T_1$ is defined from the condition that the contribution $\langle S_1|e^{-Ht}|S_i\rangle$ into Z of Eq. (7) is larger than the contributions of other terms $\langle S_j|e^{-Ht}|S_i\rangle$ [equal to e^t according to Eq. (13)]:

$$\exp(N[\phi(T_0,m,\gamma)+A(T_1-T_0)])\geqslant\exp(Ne^{\gamma}T_1),$$

$$T_1=\frac{A}{A-e^{\gamma}}T_0-\frac{\phi(T_0,m,\gamma)}{A-e^{\gamma}}. \tag{24}$$

Thus Eqs. (21), (23), and (24) give the relaxation period $T_1\equiv e^{-\gamma}t_1/N$ under the constraint of Eq. (14) for the fitness A.

There are several phases in dynamics. For $0<t<t_0$, there is a random drift to the peak configuration S_1. For $t_0<t<t_1$, there is a growth in the value of p_1, but the macroscopic majority is still out of the peak configuration. For $t>t_1$, the macroscopic majority is near the peak configuration.

Let us give an explicit expressions for the case

$$\frac{\gamma(1-m)}{A}\ll 1. \tag{25}$$

This is a typical biological situation for observing $1-m\ll 1$. In this case, as we can check later, $T\sim(1-m)\ll 1$, thus one can replace $z\tanh(\gamma T)/\gamma\to zT$ and derive a simplified system of equations:

$$\phi(T,m,\gamma)=\frac{1-m}{2}\left[\ln\gamma\frac{1-m}{2}-(1+\ln z)\right]+T(e^z-1),$$

$$Tze^z=\frac{1-m}{2},$$

$$\frac{d\phi}{dT}=e^z-1=A. \tag{26}$$

Then $T_0=(1-m)/[2(1+A)\ln(1+A)]$. Thus for the relaxation period $t=T_1e^{\gamma}N$, one has an expression

$$t_1=(1-m)N\frac{\ln\dfrac{2e\ln(A+1)}{(1-m)\gamma}}{2(Ae^{-\gamma}-1)}. \tag{27}$$

Equation (27) gives relaxation period from the original distribution, concentrated at the configuration with the overlap Nm with the peak fitness configuration, and mutation per site $1-q=\gamma/N$. The physical meaning of the term $(1-m)N/2$ is trivial (for the case of infinite population): the relaxation period is proportional to the Hamming distance. We can understand also the term $(Ae^{-\gamma}-1)$ in the dominator: it is a natural consequence of the fact that relaxation period should diverge at the error threshold $Ae^{-\gamma}\to 1$. Our derivation is valid when the condition of Eq. (25) is satisfied. An estimate for t_1 has been given in Refs. [13,14].

$$t_1=\frac{\ln\dfrac{1}{1-q}}{Ae^{-N(1-q)}-1}\equiv\frac{\ln\dfrac{N}{\gamma}}{Ae^{-\gamma}-1}. \tag{28}$$

We note that Eq. (28) is qualitatively correct and consistent with Eq. (27) for the case $N(1-m)/2=1$ considered in those works. Our derivation is rigorous only for a large number of flipped spins, i.e. $N(1-m)/2\gg 1$. For a small number of flipped spins considered in Refs. [13,14], we still cannot derive an exact analytical formula.

Let us briefly consider a simple case of a dynamic fitness landscape: a fitness peak $A(t)$ in the first configuration S_1, which changes with the time. Now for the $\langle S_1|e^{-Ht}|S_1\rangle$, we have $\exp[e^{-\gamma}\int_0^t A(\tau)d\tau]$. Equations (23) and (24) transform into

$$A(\tau_0)=\frac{d\phi(T_0)}{dT_0},\quad \phi(T_0,m,\gamma)+\int_{T_0}^{T_1}A(\tau)d\tau>e^{\gamma}T_1. \tag{29}$$

Now this could be a very rich phase structure with different solutions for T_0. For $T_1\equiv t_1e^{-\gamma}/N$, we have

$$\hat{A}=\frac{\int_{T_0}^{T_1}A(\tau)d\tau}{T_1-T_0},\quad T_1=\frac{\hat{A}}{\hat{A}-e^{\gamma}}T_0-\frac{\phi(T_0,m,\gamma)}{\hat{A}-e^{\gamma}}. \tag{30}$$

Now A is replaced with a mean value. For the case of $A\gg\gamma(1-m)$, we again have Eq. (27), only with $A\to\hat{A}$.

For $A\gg 1$, we can calculate the relaxation time from an original uniform distribution on a static landscape: $p_i=1/2^N$. For this purpose, we compare the contribution $\langle S_1|e^{-Ht}|S_1\rangle=2^{-N}\exp[Ae^{-\gamma}t]$ with $\exp(t)$ (sum of other contributions) for their contributions to Z of Eq. (7) and find that

$$t_1=\frac{N\ln 2}{Ae^{-\gamma}-1}. \tag{31}$$

To derive the steady state distributions of p_i, we can set $dp_i/dt=0$ in Eq. (1). For $A\gg 1$ we can derive that $p_i=q^N[(1-q)/q]^{d(1,i)}$ and the result obtained in Ref. [5]: $(1/N)\Sigma_i p_i\Sigma_{l=1}^{N}s_i^l=2q-1$.

Let us briefly consider the case of two isolated flat peaks in fitness landscape with fitness heights A_1 and A_2, and widths g_1 and g_2. The peak of height A_i has g_i one-flip neighbors of the same height. A simple consideration gives for the effective fitness $A_i[1+g_i(1-q)]$. Thus the Svetina-Scuster phenomenon [16] for two peaks appears at $A_1[1+g_1(1-q)]=A_2[1+(1-q)g_2]$.

In 1971, Eigen [1] found an exact error threshold for his model from information theory arguments. After more than 30 years of different approximate or numerical investigations of the Eigen model, we have found the exact dynamics of the model presented in Eqs. (21), (23), and (24). Our Eq. (27) gives the relaxation periods with a high degree of accuracy $O(1-m)^2\sim(d/N)^2$, it is more accurate than Eq. (28) derived in [13,14]. In [9] we compared the accurate result of this work Eq. (27) with the corresponding relaxation period of parallel scheme to conclude that even at the limit of vanishing mutation rates two mutation schemes give a finite (nonvanishing) difference in relaxation periods. Therefore, there is at least one situation in which our exact Eq. (24) or accurate approximation, Eq. (27), gives a new qualitative result. We have also applied the similar method to study a simple case of dynamical environments and obtained Eqs. (29) and (30). The more involved situations with a very rich and interesting phase structure [12] as well as the virus-immune system coevolution [14] can also be investigated by our method. The main open problem is an application of the same method to the finite population case. In this case the search of a peak configuration could be an exponentially large function of N, instead of a linear in Eq. (27). We hope that progress in this direction is possible in the near future, considering funnel-like fitness landscapes. In any case in this work we considered the Eigen model's dynamics as a statistical mechanics problem and exactly solved it.

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