# Quantum mechanics versus classical probability in biological evolution

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We reconsider the mean-field Hamiltonian of the Ising quantum chain as a mutation-selection model of biological evolution. Direct calculation of its Perron-Frobenius eigenvector reveals a fundamental difference between the quantum-mechanical and probabilistic applications, and partially corrects previous results. [S1063-651X(98)07401-7]

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In two recent publications [1,2], we established an equivalence between a mutation-selection model of biological evolution, and an Ising quantum chain. The model in question describes the parallel action of mutation and selection on a population of individuals that are identified with points in binary sequence space, $\{-1,1\}^N$, where $N$ is the length of the sequence. The $n=2^N$ different sequences will be denoted as $A_i := s_1^{(i)} s_2^{(i)} \cdots s_N^{(i)}$, where $s_j^{(i)} \in \{-1,1\}$, $i=1,\ldots,n$, and $j=1,\ldots,N$. It was shown that the corresponding differential equation may be written as the linear system

$$\dot{\boldsymbol{z}} = (\mathcal{H} - N\mu)\boldsymbol{z}, \tag{1}$$

$\boldsymbol{z} \in (\mathbb{R}_{\geqslant 0})^n$, together with the normalization

$$x_i = \frac{z_i}{\sum_{j=1}^n z_j}. \tag{2}$$

Here, $x_i$ is the relative frequency of individuals with sequence $A_i$ $(1 \leqslant i \leqslant n)$, $\mu \geqslant 0$ is the mutation rate, and $\mathcal{H}$ is the Hamiltonian of an Ising quantum chain. Although this equivalence is quite general (it holds for all "fitness landscapes," i.e., assignments of reproduction rates to all $n$ sequences), our focus here is on the case where $\mathcal{H}$ is the mean-field Hamiltonian

$$\mathcal{H} = \mu \sum_{k=1}^N \sigma_k^x + \frac{\gamma}{2N} \sum_{k,\ell=1}^N \sigma_k^z \sigma_\ell^z, \tag{3}$$

where the canonical basis of $\otimes_{i=1}^N \mathbb{C}^2$ has been used. Equation (3) corresponds to Eq. (17) in [1] with $\alpha=0$ and describes the permutation-invariant situation where fitness is a quadratic function (with parameter $\gamma$) of the number of sites with value $+1$, and mutation occurs independently at rate $\mu$ at every site.

The problem is solved when the spectrum of $\mathcal{H}$ is known; in particular, its Perron-Frobenius (PF) eigenvector (or ground state) $\boldsymbol{v}$ determines the equilibrium composition of the population. A quantity suitable to characterize this equilibrium is the average surplus $u$ of sites with value $+1$,

$$u := \frac{\sum_{i=1}^n u_i v_i}{\sum_{j=1}^n v_j}, \quad u_i := \frac{1}{N} \sum_{j=1}^N s_j^{(i)}, \tag{4}$$

cf. Eq. (11) of [1]. In calculating this quantity for $\widetilde{\mathcal{H}} := \mathcal{H} - N\mu$ in the macroscopic limit [1], we implied $\boldsymbol{v}$ to be the infinite tensor product of the Perron-Frobenius (PF) eigenvector, $\tilde{\boldsymbol{v}} \in \mathbb{C}^2$, of the one-site Hamiltonian, normalized so that $\tilde{v}_1 + \tilde{v}_2 = 1$. Further calculations have now revealed the relationship $w = (\gamma/2)u^2$ between the ground state energy per spin, $w$, and the average surplus, $u$, to hold whenever $\boldsymbol{v}$ is a tensor product of the above type. This is so because, in this case, permutation invariance yields

$$u = \sum_{i=1}^{2^N} u_i v_i = \tilde{v}_1 - \tilde{v}_2, \tag{5}$$

$$w = \sum_{i=1}^{2^N} \frac{\gamma}{2} u_i^2 v_i = \frac{\gamma}{2} (\tilde{v}_1^2 - 2\tilde{v}_1 \tilde{v}_2 + \tilde{v}_2^2) = \frac{\gamma}{2} u^2. \tag{6}$$

Since this contradicts our Eqs. (21) and (22) in [1] we must have used $\boldsymbol{v}$ improperly in [1]. Calculations with the *numerical* PF eigenvector of $\widetilde{\mathcal{H}}$ correctly reproduced the rigorous result that $m = \sqrt{1-h^2}$ [Eq. (20) in [1]] and $w = (\gamma/2)(1-h)^2$ [Eq. (21) in [1]] are its quantum-mechanical magnetization and ground state energy, respectively. Here, it is $h = \mu/\gamma$, and we concentrate on the regime $0 \leqslant h \leqslant 1$. The surplus, however, comes out as $u = 1-h$, instead of Eq. (22) in [1], but in line with Eq. (6).

Indeed, our previous calculations had tacitly assumed a change in normalization (from $L^2$ to $L^1$) to commute with the thermodynamic limit. In order to understand the problem, let us now investigate the finite-size equations. Since the PF eigenvector must be contained in the symmetric sector, the number of variables may be reduced from $2^N$ to $N+1$ by defining $y_i$ to be the (equilibrium) frequency of sequences with $i$ sites with value $+1$, i.e., $y_i := \sum_{\{j\}} v_j \geqslant 0$ where $j$ runs through all indices with $Nu_j = i$. Of course, $\sum_i y_i = 1$. The difference equation for the equilibrium of Eq. (1) [and, equivalently, (1) of [1]] then reads

 

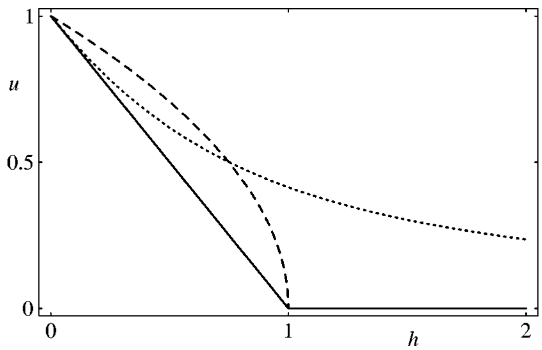


FIG. 1. Average surplus ($u$) of sites with value $+1$ as defined in Eq. (4), in the macroscopic limit. Dotted line: Fujiyama landscape (with $\alpha_j \equiv \alpha = 1$); dashed line: Onsager landscape ($\gamma = 1$); solid line: mean-field landscape ($\alpha = 0$, $\gamma = 2$).

$$2h(N-i+1)y_{i-1}+2h(i+1)y_{i+1}-2hNy_i+\frac{1}{N}(N-2i)^2 y_i = \frac{2}{\gamma}\tilde{\lambda}_{\max} y_i . \tag{7}$$

Here, $\tilde{\lambda}_{\max}$ is the PF eigenvalue of $\tilde{\mathcal{H}}$. In the macroscopic limit [via $i/N \to x$ and $1/N = \Delta x \to 0$, so that $\tilde{\lambda}_{\max}/N \to w$ and $y_i \to f(x)$], one finds that the first three terms of Eq. (7) vanish with $1/N$ with respect to the remaining two. The dominant terms may be read as an equation for a tempered distribution, to be found by Fourier transformation (this is rigorous by Levy's continuity theorem [3]). One gets

$$f(x) = a\,\delta(x-h/2)+(1-a)\,\delta(x-(1-h/2)). \tag{8}$$

The parameter $a$, $0 \leqslant a \leqslant 1$, reflects the $\mathbb{Z}_2$ symmetry of the problem, and the unique symmetric solution is obtained from $a = 1/2$. The extremal states correspond to $a = 0$ and $a = 1$. With $a = 0$, one calculates the surplus

$$u = \int_0^1 (2x-1) f(x)\,dx = \begin{cases} 1-h, & 0 \leqslant h < 1 \\ 0, & h \geqslant 1 \end{cases} \tag{9}$$

in line with the prediction (6) for a pure state.

To explore the reasons for the discrepancy, let us now change the normalization *prior* to taking the thermodynamic limit, i.e., consider basis vectors of the symmetric sector that are unit vectors in the 2-norm, instead of the 1-norm as was the case until now. This corresponds to the change of coordinates

$$\tilde{y}_i := \binom{N}{i}^{-1/2} y_i , \quad \zeta_i := \frac{\tilde{y}_i}{\|\tilde{y}\|_2}, \quad i = 0, \ldots, N. \tag{10}$$

The difference equation is transformed accordingly,

$$2h\sqrt{i(N+1-i)}\,\zeta_{i-1}+2h\sqrt{(i+1)(N-i)}\,\zeta_{i+1}-2hN\zeta_i + \frac{1}{N}(N-2i)^2\zeta_i = \frac{2}{\gamma}\tilde{\lambda}_{\max}\zeta_i . \tag{11}$$

After careful regrouping of the terms according to their scaling, which results in a clear distinction from the previous case (7), one finds, for the macroscopic limit, the solution

$$g(x) = a\,\delta(x-(1-\sqrt{1-h^2})/2) + (1-a)\,\delta(x-(1+\sqrt{1-h^2})/2), \tag{12}$$

which, for $a = 0$, gives the correct magnetization

$$m = \int_0^1 (2x-1) g(x)\,dx = \sqrt{1-h^2}. \tag{13}$$

So, the change of basis, crucial for our (probabilistic rather than quantum-mechanical) application, does not commute with the macroscopic limit. It also changes Fig. 2 of [1] and Fig. 1 of [2], the correct version of which is shown in Fig. 1.

No such problem arises for the Fujiyama or Onsager landscapes, as also treated in [1,2]. In general, however, great care must be exercised when converting quantum-mechanical states to classical probabilities, a problem not unknown to some of the specialists [4].


[1] E. Baake, M. Baake, and H. Wagner, Phys. Rev. Lett. **78**, 559 (1997).

[2] H. Wagner and E. Baake, in *Physical Applications and Mathematical Aspects of Geometry, Groups and Algebras*, edited by H.-D. Doebner, P. Nattermann, and W. Scherer (World Scientific, Singapore, 1997), Vol. II, p. 821.

[3] H. Bauer, *Probability Theory* (de Gruyter, Berlin, 1996).

[4] R. Bürger, J. Math. Biol. **24**, 341 (1986); B. Kümmerer (personal communication).