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.

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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 which 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 $s_j^{(i)} \in \{-1,1\}$, $i = 1,\ldots,n$, $j = 1,\ldots,N$. It was shown that the corresponding differential equation may be written as the linear system

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

$\boldsymbol{z} \in (\mathbb{R}_{\geq 0})^n$, 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 ($1 \leq i \leq n$), $\mu \geq 0$ 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. Eq. (3) corresponds to Eq. (17') with $\alpha = 0$ (primed numbers refer to formulas of [1]), and describes the permutation-invariant situation where fitness is a quadratic function (with parameter γ) of the number of sites with value $+1$, and mutation occurs independently at rate μ 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'). 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 s.t. $\tilde{v}_1 + \tilde{v}_2 = 1$. 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

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

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

Since this contradicts our Eqs. (21') and (22'), 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')) and $w = \frac{\gamma}{2}(1-h)^2$ (Eq. (21')) are its quantum-mechanical magnetization and ground state energy, respectively. Here, $h = \mu/\gamma$, and we concentrate on the regime $0 \leq h \leq 1$. The surplus, however, comes out as $u = 1 - h$, instead of Eq. (22'), 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. $y_i := \sum_{\{j\}} v_j \geq 0$ 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')) then reads

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

Here, $\tilde{\lambda}_{\max}$ is the PF eigenvalue of $\widetilde{\mathcal{H}}$. In the macroscopic limit (via $i/N \to x$ and $1/N = \Delta x \to 0$, s.t. $\tilde{\lambda}_{\max}/N \to w$ and $y_i \to f(x)$), one finds that the first three terms of (7) vanish with $1/N$ w.r.t. 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

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

The parameter a, $0 \le a \le 1$, 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

$$u \;=\; \int_0^1 (2x-1)\, f(x)\, dx \;=\; \begin{cases} 1-h\,, & 0 \le h < 1 \\ 0\,, & h \ge 1 \end{cases} \qquad (9)$$

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

$$\tilde{y}_i \;:=\; \binom{N}{i}^{-\frac{1}{2}} y_i\,, \quad \zeta_i \;:=\; \frac{\tilde{y}_i}{\|\tilde{\boldsymbol{y}}\|_2}\,, \quad i = 0, \ldots, N\,. \qquad (10)$$

The difference equation is transformed accordingly,

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

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

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

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

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

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 below.

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].

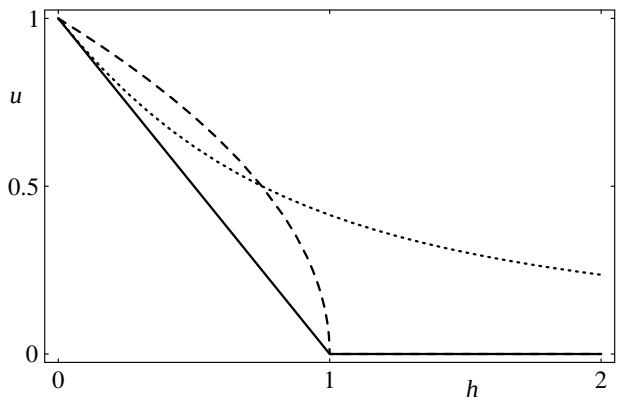

FIG. 1. Average surplus (u) of sites with value +1 as defined in (4), in the macroscopic limit. Dotted: Fujiyama landscape (with $\alpha_j \equiv \alpha = 1$); dashed: Onsager landscape ($\gamma = 1$); solid line: mean-field landscape ($\alpha = 0$, $\gamma = 2$).

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