Thermodynamic behavior of a phase transition in a model for sympatric speciation

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We investigate the macroscopic effects of the ingredients that drive the origin of species through sympatric speciation. In our model, sympatric speciation is obtained as we tune up the strength of competition between individuals with different phenotypes. As a function of this control parameter, we can characterize, through the behavior of a macroscopic order parameter, a phase transition from a non-speciation to a speciation state of the system. The behavior of the first derivative of the order parameter with respect to the control parameter is consistent with a phase transition and exhibits a sharp peak at the transition point. For different resources distribution, the transition point is shifted, an effect similar to pressure in PVT system. The inverse of the parameter related to sexual selection strength behaves like an external field in the system and, as thus, is also a control parameter. The macroscopic effects of the biological parameters used in our model reveal thus fingerprints typical of thermodynamic quantities in a phase transition of an equilibrium physical system.

The branching of a single population into two or more species without prevention of gene flow through geographic segregation is known as sympatric speciation.1–4 Herbivorous insects have long been considered prime candidates for sympatric speciation because of an intimate and frequently highly specialized relationship with their host plants, which serve as habitat, food resource, and, often, mating location.5 The apple maggot fly Rhagoletis pomonella has been considered, since 1966, as the classical example of sympatric speciation in progress.6 R. pomonella shifted from feeding on the unabsced fruit of its native host hawthorn (Crataegus spp.) to utilizing the introduced, domesticated apple (Malus pumila) sometime in the mid-1800s in the Hudson River Valley region of the state of New York. Genetic evidence suggests that the species is in the process of shifting and adapting to this new host plant.7–9

Two ingredients are important for sympatric speciation to happen in a population.10–12 The competition caused by fluctuations in ecology11,12 and assortative mating caused by selective mating13,14. Ecological and sexual selection models have addressed these two aspects of sympatric speciation separately.15 The starting point of ecological models is the assumption that sympatric speciation results from disruptive selection. That is, competition for diverse resources leads to separation in a population, if individuals with intermediate phenotypes are losers when they compete with those with extreme ones. Such selection can cause sympatric speciation because it provides an advantage for reproductive isolation between opposite, well-adapted, extreme phenotypes, and reproductive isolation can be achieved due to evolution of nonrandom mating13,16. Sympatric speciation can also be driven by selective mating, or sexual selection, that is, nonrandom mating leading to differential reproductive successes of different phenotypes. For example if the choice of a mate depends on two traits: male display (e.g. nuptial hue, varying from red to blue through purple) and female preference for variants of display. Some females may prefer red males and others prefer blue males, this can tear the population apart and create a pair of species consisting of red-prefering females and red males and of blue-prefering females and blue males.

To study sympatric speciation by simulations we use the individual-based Penna model.16 In previous work with this model17–20 an abrupt ecological change was the drive that provoked disruptive selection, as in 11,21 which led to speciation through the development of assortative mating. A different strategy was used to simulate sympatric speciation of predators in a food web.20 In this case, three types of intra-specific competition were adopted, depending on the phenotypic group of the predators, and their strength was kept constant during the whole simulation. In particular, a parameter X was introduced, establishing the fraction of the populations of extreme phenotypic predators with which the intermediate phenotypic individuals would compete, besides competing among themselves. In the present paper we adopt the same kind of constant intra-specific competition and study first when speciation is achieved, depending on the value of X, for a uniform resource distribution per phenotype and a sexual selection of constant strength. We show that the competition strength X plays the role of a control parameter in a phase transition, and that the fraction of sexual selective females in the population shows behavior similar to an order parameter. Furthermore, we show that the transition point and its functional form depend on the carrying capacity distributions and sexual selection strengths.
In the present model, competition for food and assortative mating are related to the same phenotypic trait. This trait is represented by a new pair of non age-structured bit-strings, which are crossed and recombined in the breeding process \[21\]. The phenotypic characteristic is measured by counting, in this new pair of bit-strings, the number of bit positions where both bits are set to 1, plus the number of dominant positions (chosen as 16) with at least one of the two bits set. It will therefore be a number \(k\) between 0 and 32, which we will refer to as the individual’s phenotype. We fix the mutation probability per locus, \(0 \approx 1\), of this phenotypic trait at 0.01.

In order to consider intra-specific competition depending on the individual’s phenotype \(k\), we modified the logistic Verhulst factor introducing three intra-specific competition terms, each one related to a given phenotypic group:

\[
V(k, t) = \begin{cases} 
V_1(k, t), & 0 \leq k < n_1; \text{ especialist} \\
V_m(k, t), & n_1 \leq k \leq n_2; \text{ intermediate}.
\end{cases}
\]

\[
V_2(k, t), \quad n_2 < k \leq 32; \text{ especialist}.
\]

As in the original Penna model, at every time step, and for each individual, a random real number uniformly distributed between 0 and 1 is generated; if this number is smaller than \(V(k, t)\), the individual dies. For the extreme phenotype groups the competition is given by:

\[
V_{1(2)}(k, t) = \frac{P_{1(2)}(k, t) + P_m(k, t)}{F},
\]

where \(P_{1(2)}(k, t)\) accounts for the population with phenotype \(k < n_1\) \((k > n_2)\) at time \(t\), respectively, \(P_m(k, t)\) accounts for the population with phenotype \(k \in [n_1, n_2]\), and \(F\) is a constant proportional to the carrying capacity, taken as \(2 \times 10^5\) in our simulations. Individuals with intermediate phenotypes \((P_m)\) compete among themselves and also with a fraction \(X\) of each population presenting an extreme phenotype. The Verhulst factor for them is:

\[
V_m(k, t) = \frac{P_m(k, t) + X \cdot [P_1(k, t) + P_2(k, t)]}{F},
\]

where \(X\) can be thought of as the strength of competition between intermediate and extreme phenotypic populations. Eq. \(2\) means that individuals with extreme phenotypes \((P_1, P_2)\) compete with those belonging to the same phenotypic group and also with the whole intermediate population, but there is no competition between extreme phenotypes of different groups because we are assuming they are specialized to some extent \((0, n_1 = 13), (n_2 = 19, 32))\) on particular resources.

In order to consider assortative mating, we introduce into each female genome a single locus (bit) that codes for this selectiveness, also obeying the general rules of the Penna model for genetic heritage and mutation. If it is set to 0, the female is not selective in mating (panmictic mating). It is selective (assortative mating) if this locus is set to 1. The mutation probability for this locus, which can be in both directions \((0 \approx 1\), is 0.001. Mutated females that are born selective choose mating partners according to the following mating strategy: If a female has phenotype \(k < 16\) \((k > 16)\), it chooses, among \(N_m\) males, the one with the smallest \((\text{largest})\) phenotype value \(k\); if a selective female has \(k = 16\) then it chooses randomly to act as one of the above. Notice that with this strategy all females reproduce every time step from age \(R = 10\) until death.

![FIG. 1: In (a), (b) and (c) the phenotype distributions of the whole population for different \(X\). In the initial steps of the simulations, \(t = 200\), the distribution is, in all cases, a gaussian centered at intermediate phenotypes. For (a) and (b), the distributions at \(t = 200\), the distribution is, in all cases, a gaussian centered at intermediate phenotypes. For (a) and (b), the distributions at \(t = 200\), the distribution is, in all cases, a gaussian centered at intermediate phenotypes. For (a) and (b), the distributions at \(t = 200\), the distribution is, in all cases, a gaussian centered at intermediate phenotypes. For (c) the distribution is not stationary neither at \(4 \times 10^3\) nor at \(4 \times 10^5\) (see text). (d) The time behavior of the selective females density.](image)
extreme phenotypes mate only with males of its same phenotypic group, see Fig. 4(a) upper line. This means that there are two new sympatric species, reproductively isolated. For the competition strength $X = 0.5$, the phenotype distribution is not stationary: in runs that differ by the choice of the seed of the random number generator, the final distribution sometimes has one maximum at $k = 16$, Fig. 4(c) triangles, and some other times it has two maxima at $k = 0$ and $k = 32$, Fig. 4(c) squares. The time behavior of the density of selective females presents large fluctuations, see Fig. 4(d) central line. Fig. 4 shows an important change in the population organization, from a non-speciation state with $\rho_s \approx 0$, to a sympatric speciation state with $\rho_s \approx 1$, as we increase the strength of competition, $X$, for the intermediate phenotypes. To determine the range of values of $X$ for which sympatric speciation may be obtained, we will analyze the behavior of the mean density of selective females, for many different strengths of competition.

The behavior of the mean density $\langle \rho_s \rangle$ as a function of $X$ is shown in Fig. 2(a). The population changes rather abruptly from a non-speciation to a speciation state when $X_c = 0.5$ [22]. Another fingerprint of the macroscopic effect, $X$ on $\langle \rho_s \rangle$, is the peak shown by the logarithm of the first derivative of the order parameter at $X_c$, Fig. 2(b). These behaviors are very similar to what happens to an isolated. For the competition strength $\approx 0.1$, see Fig. 1(a) squares, and has a mean size of $\approx 50 \times 10^3$, or twice the value of the former phase, and the phenotypes in the population cluster around only two distinctively separated values, Fig. 1(b) squares. In the Fig. 2(b), the large values attained by $\rho_s$ just above $X_c$ arise from large fluctuations in the number of individuals.

Ecological conditions have been considered an essential ingredient for divergence and speciation in sympatry [22]. To evaluate its importance in a phase transition context, we simulated different ecological conditions by modifying the carrying capacity of the environment, which has so far been considered as a constant $F$ in the Eqs. 2 and 3. It will now be phenotype-dependent and will drive the population to experience a disruptive selection between the specialist and intermediate phenotypes. Its general functional form is: $F_{rk} = 2 \times 10^3 \times e^{-(k-16)^2/\sigma_k^2}$, where each individual, with phenotype $k$, will feed on a different resource niche: For small values of $\sigma_k^2$, the specialists will have fewer resources than individuals with intermediate phenotype.

In Fig. 3(a) the macroscopic effect of the carrying capacity is the shift suffered by the transition point for different values of $\sigma_k$, which has then an effect similar to pressure in PVT systems. For small value of $\sigma_k^2$ and for $X > X_c$, case I in Figs. 3(a) and (b), the population prefers a non-speciation state, even in the presence of a high competition for intermediate phenotypes. This happens because there are not enough resources for two groups with extreme phenotypes. It is nevertheless important to notice that the population has a large diversity in this case. That is, the phenotype distribution looks

FIG. 2: a) Mean values the selective females density the order parameter of the speciation transition, as function of the control parameter $X$. b) Logarithm scale of the standard deviation versus $X$. For each value of $X$ we have made 10 simulations with the same parameters, but using different initial seeds for the random number generator. In each simulation we calculate the mean value of the density of selective females during the last $10^4$ time steps, and then average the results of the ten runs.

FIG. 3: The figures show the effect of disruptive selection on the speciation transition. The carrying capacity from I to III correspond to $F_{rk}$ with $\sigma_k^2 = 10^3, 5 \times 10^3, 10^4$, respectively. $F_{rk} = F$ correspond to IV.

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like Fig. 11(c) triangles, but it is a stable distribution, see Fig. 3(b) I.

FIG. 4: In (a) and (b) the effect of the sexual selection strength, $N_m$. It is important to point out that the simulation time for $N_m = 3$ was $8 \times 10^5$, 20 times bigger than in the other cases.

Sexual selection in the population is associated to the number of mating choices each female performs before reproduction, the parameter $N_m$. The probability of a selective female with phenotype $k < 16$ to mate with a male of opposite phenotype is $P_{<16} \approx (0.5)^{N_m}$. In the previous section, $N_m = 50$ and this probability is almost zero, meaning that the selective females are highly discriminatory against the opposite phenotype. With $N_m = 3$ the probability becomes $P_{<16} = 0.125$ and it is then possible for a selective female with $k < 16$ to mate with a male of phenotype $k > 16$. When we reduce the number of mating choices per female, we can see that the phase transition is destroyed, Figs. 11(a) and (b). For an equilibrium physical system the phase transition disappears when there is an applied external field, as, for an example, happens to the paramagnetic transition of magnetic materials at the Curie point. A small value for an external field in the system and in a physical system a field is a control parameter like pressure or temperature. Another characteristic of selective mating is related to the relaxation time since it depends on the $N_m$ value, see caption in Figs. 11h and b. These results, for assortative mating are in qualitative agreement with 13, 14.

We believe these analogies between biological and physical parameters will help in the understanding of the sympatric speciation process.

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