

**Thermodynamic behavior of a phase transition in a model for sympatric speciation**K. Luz-Burgoa,<sup>1,\*</sup> S. Moss de Oliveira,<sup>1</sup> Veit Schwämmle,<sup>1,2</sup> and J. S. Sá Martins<sup>1</sup><sup>1</sup>*Instituto de Física, Universidade Federal Fluminense, Campus da Praia Vermelha, Boa Viagem, Niterói, 24210-340, RJ, Brazil*<sup>2</sup>*Institute for Computational Physics Pfaffenwaldring 27, D-70569 Stuttgart, Germany*

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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 nonspeciation 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 a PVT system. The inverse of the parameter related to a 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 are a reminiscent of the behavior of thermodynamic quantities in a phase transition of an equilibrium physical system.

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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 [3]. *R. pomonella* shifted from feeding on the unabsorbed 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 [6,7].

Two ingredients are important for sympatric speciation to happen in a population [8–10]: The competition caused by fluctuations in ecology [11,12] and assortative mating caused by selective mating [13,14]. Ecological and sexual selection models have addressed these two aspects of sympatric speciation separately [9]. The starting point of ecological models is the assumption that sympatric speciation results from disruptive selection. That is, competition for diverse resources leads to a separation in a population, if individuals with intermediate phenotypes are losers when they compete with those specialists, with extreme phenotypes. Such a selection can cause sympatric speciation because it provides an advantage for reproductive isolation between opposite, well-adapted specialists, and reproductive isolation can be achieved due to an evolution of nonrandom mating [15]. Sympatric speciation can also be driven by selective mating, or sexual selection, that is, nonrandom mating leading to differential reproductive successes of different phenotypes. Suppose, for example, that the choice of a mate depends on its color alone in a population where individuals have colors

ranging from blue to red. Some females may prefer red males and others prefer blue males and 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 works with this model [17–20] an abrupt ecological change was the drive that provoked disruptive selection, as in [11], 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 [21]. In this case, three types of intraspecific 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 population of specialist predators with which the intermediate phenotypic individuals would compete, besides competing among themselves. In the present paper we adopt the same kind of constant intraspecific competition and study first when speciation is achieved, depending on the value of  $X$ , for a constant 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 width of the resources distributions and sexual selection strengths.

In the present model, competition for food and assortative mating are related to the same phenotypic trait, e.g., color or size. This trait is represented by a new pair of non-age-structured bitstrings, which are crossed and recombined in the breeding process [21]. The phenotypic characteristic is measured by counting, in this new pair of bitstrings, 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

\*Electronic address: karenluz@if.uff.br

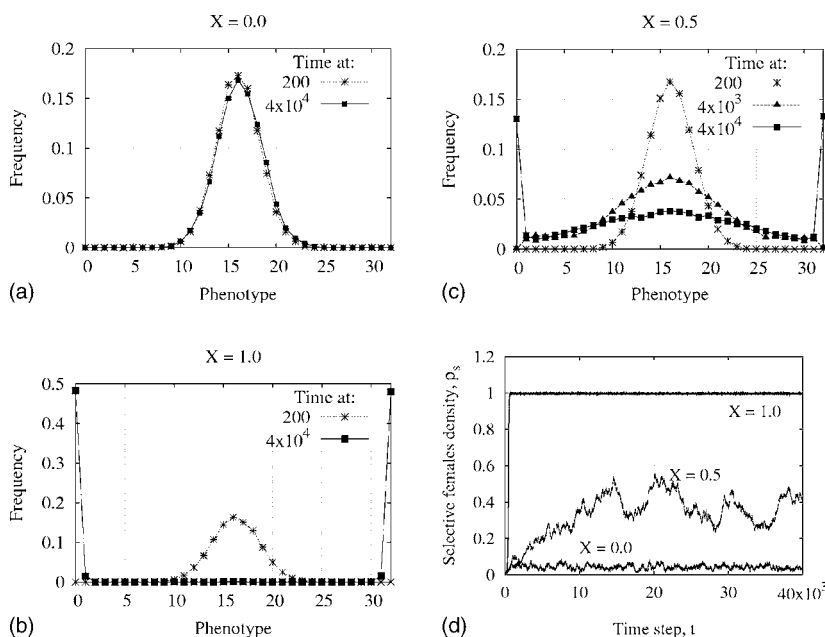


FIG. 1. In (a), (b), and (c) the phenotype distributions of the whole population for different  $X$ . In the initial steps of the simulation,  $t=200$ , the distribution is, in all cases, a Gaussian centered at intermediate phenotypes. For (a) and (b), the distributions at  $t=4 \times 10^3$  are equal to those at  $t=4 \times 10^4$  and are stationary. For (c) the distribution is not stationary either at  $4 \times 10^3$  nor at  $4 \times 10^4$  (see text). (d) The time behavior of the selective females density.

phenotype. We fix the mutation probability per locus,  $0 \rightleftharpoons 1$ , of this phenotypic trait at 0.01.

In the original Penna model the logistic Verhulst factor was introduced in order to keep the population size bounded, albeit not constant. We modified it by introducing three intraspecific competitions depending on the individual's phenotype  $k$ , each one related to a given phenotypic group:

$$V(k,t) = \begin{cases} V_1(k,t), & 0 \leq k < n_1; & \text{specialist} \\ V_m(k,t), & n_1 \leq k \leq n_2; & \text{intermediate.} \\ V_2(k,t), & n_2 < k \leq 32; & \text{specialist.} \end{cases} \quad (1)$$

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 specialist groups the competition is given by

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

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, independent of  $k$ , and 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 specialist population. The Verhulst factor for them is

$$V_m(k,t) = \frac{P_m(k,t) + X[P_1(k,t) + P_2(k,t)]}{F}, \quad (3)$$

where  $X$  can be thought of as the strength of competition between the intermediate population and specialist. Equation (2) means that specialist individuals ( $P_1, P_2$ ) compete with those belonging to the same phenotypic group and also with the whole intermediate population, but there is no competition between specialists of different groups because we are assuming that they are specialized to some extent ( $[0, n_1$

$= 13], [n_2 = 19, 32]$ ) on particular resources, for example, ground and tree Galapagos finches.

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 ( $0 \rightleftharpoons 1$ ), 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 (largest) phenotype value  $k$ ; If a selective female has  $k=16$  then it chooses randomly to act as one of the above. Note that with this strategy all females reproduce every time step from age  $R=10$  until death.

At the beginning of the simulations females are nonselective and all the  $6 \times 10^3$  individuals (half males and half females) have a random phenotype. For the parameter  $X=0$ , the population with intermediate phenotypes does not compete with specialists [Eq. (3)] and, in fact, suffer less competition than the other two [Eq. (2)]. In this case, nearly all females remain nonselective, see Fig. 1(d), lower line, and the phenotype distribution corresponds to a stationary Gaussian function centered at  $k=16$ , Fig. 1(a) squares. As opposed to the situation for  $X=0$ , when we introduce a strong competition for the population with intermediate phenotypes, by setting, say,  $X=1.0$ , only two different specialists survive,  $k=0$  and  $k=32$ , as shown in Fig. 1(b), squares. In this case the density of selective females goes to  $\rho_s \approx 1$  very fast, that is, the specialist females mate only with specialist males of its same phenotypic group, see Fig. 1(d), 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. 1(c), tri-

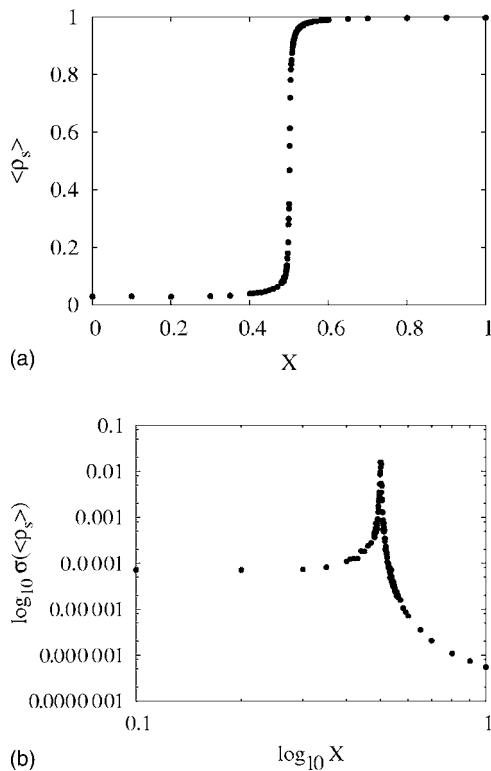


FIG. 2. (a) Mean values of the selective females density, the order parameter of the speciation transition, as function of the control parameter  $X$ . (b) Logarithm scale of the standard deviation versus  $X$ . For each value of  $X$  we have made ten simulations with the same parameters, but using 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.

angles, and some other times it has two maxima at  $k=0$  and  $k=32$ , Fig. 1(c), squares. The time behavior of the density of selective females presents large fluctuations, see Fig. 1(d), central line. Figure 1(d) shows an important change in the population organization, from a nonspeciation 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 nonspeciation to a speciation state when we change slightly the strength of competition, close to  $X_c=0.5$  [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 order parameter as a function of the control parameter in an equilibrium phase transition of a physical system. This transition separates a single-species phase from one in which two species coexist in sympatry. In the single-species phase, Fig. 2(a),  $X < X_c$ , the population presents a high diversity with many different phenotypes in the population, see Fig. 1(a), squares, and has a mean size of

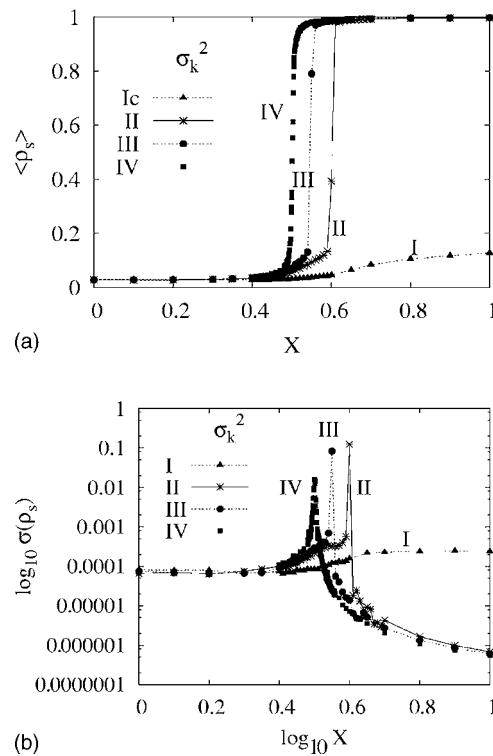


FIG. 3. The figures show the effect of disruptive selection on the speciation transition. The resource distribution for I–III corresponds to  $F_{\sigma_k}$  with  $\sigma_k^2=10^3, 5 \times 10^3, 10^4$ , respectively.  $F_{\sigma_k}=F$  corresponds to IV.

$\approx 25 \times 10^3$ . In the two-species phase, Fig. 2(a),  $X > X_c$ , the mean size of the whole population is  $\approx 50 \times 10^3$ , 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 Fig. 2(b), the large values attained by  $\sigma(\rho_s)$  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 [23]. To evaluate its importance in a phase transition context, we simulated different ecological conditions by modifying the width,  $\sigma_k$ , of the resource distribution of the environment, which has so far been considered as a constant  $F$  in 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  $F_{\sigma_k} = 2 \times 10^5 e^{-(k-16)^2/\sigma_k^2}$ , 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 width of the resource distribution is the shift suffered by the transition point, an effect similar to the shift of the transition point driven by changes in pressure for PVT systems. For small values of  $\sigma_k^2$  and for  $X > X_c$ , case I in Figs. 3(a) and 3(b), the population prefers a nonspeciation state, even in the presence of a high competition for intermediate phenotypes. This happens because there are not enough resources for two groups of specialists. It is nevertheless important to note that the

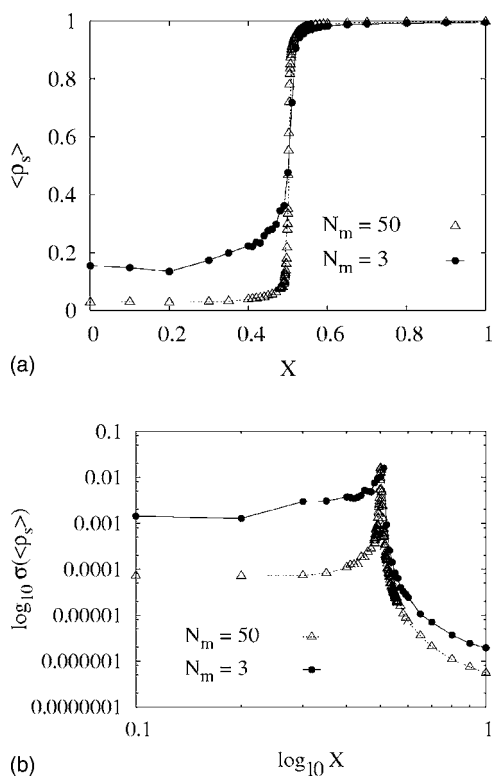


FIG. 4. The effect of the sexual selection strength,  $N_m$ , for  $N_m = 3$  (upper line) and for  $N_m = 50$  (lower line). It is important to point out that the simulation time for  $N_m = 3$  was  $8 \times 10^5$ , 20 times larger than in the other cases.

population has a large diversity in this case. That is, the phenotype distribution looks like Fig. 1(c), triangles, but it is a stable distribution, see Fig. 3(b) I.

Sexual selection in the population is associated with 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 an 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. 4(a) and 4(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 sexual selection strength, equivalent to the application of a magnetic field, produces an increase of the selective female density for  $X < X_c$ , see Fig. 4(a).

In conclusion, we report here an investigation of the macroscopic effects of the parameters ( $X$ ,  $F_{\sigma_k}$ , and  $N_m$ ) on the origin of species by sympatric speciation, characterized by the behavior of  $\langle \rho_s \rangle$ , in a simple model. The behaviors of these biological parameters are similar to the thermodynamical parameters in a phase transition of a physical system. Furthermore, the analogies for  $X$  and  $F_{\sigma_k}$  are in qualitative agreement with other individual-based models that studied the necessary ecological conditions for sympatric speciation [11,12]. The analogy between  $N_m$  and an external field shows that this parameter acts as another control parameter, in addition to  $X$  and  $F_{\sigma_k}$ , since it plays a role analogous to an external field in a physical system. The meaning of this result is that sympatric speciation may be driven by changes in sexual selection strength alone, see Fig. 4(a) for  $X \lesssim X_c$  and  $N_m = 3$ . Again, this result is in qualitative agreement with sympatric speciation by sexual selection found, e.g., in Refs. [13,14].

We emphasize that in our model the population was able to self-organize and eventually speciate without the need of two different resource distributions, for the specialist and intermediate, in contrast with Refs. [11,18,21].

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