(i, j) if and only if diag $(\pi)\Lambda = \Lambda^t \text{diag}(\pi)$ , where diag $(\pi)$  is a diagonal matrix with *i*th diagonal entry  $\pi_i$ . Now suppose  $\Lambda$  is an infinitesimal generator with equilibrium distribution  $\pi$ . If  $P(t) = e^{t\Lambda}$  is its finite-time transition matrix, then show that detailed balance  $\pi_i \lambda_{ij} = \pi_j \lambda_{ji}$  for all pairs (i, j) is equivalent to finite-time detailed balance  $\pi_i p_{ij}(t) = \pi_j p_{ji}(t)$  for all pairs (i, j) and times  $t \geq 0$ .

2. Suppose that  $\Lambda$  is the infinitesimal generator of a continuous-time finite-state Markov chain, and let  $\mu \geq \max_i \lambda_i$ . If  $R = I + \mu^{-1}\Lambda$ , then prove that R has nonnegative entries and that

$$S(t) = \sum_{i=0}^{\infty} e^{-\mu t} \frac{(\mu t)^i}{i!} \mathsf{R}^i$$

coincides with P(t). (Hint: Verify that S(t) satisfies the same defining differential equation and the same initial condition as P(t).)

- 3. Consider a continuous-time Markov chain with infinitesimal generator  $\Lambda$  and equilibrium distribution  $\pi$ . If the chain is at equilibrium at time 0, then show that it experiences  $t \sum_i \pi_i \lambda_i$  transitions on average during the time interval [0, t], where  $\lambda_i = \sum_{j \neq i} \lambda_{ij}$  and  $\lambda_{ij}$  denotes a typical off-diagonal entry of  $\Lambda$ .
- 4. Let  $P(t) = [p_{ij}(t)]$  be the finite-time transition matrix of a finite-state irreducible Markov chain. Show that  $p_{ij}(t) > 0$  for all i, j, and t > 0. Thus, no state displays periodic behavior. (Hint: Use Problem 2.)
- 5. A village with n+1 people suffers an epidemic. Let  $X_t$  be the number of sick people at time t, and suppose that  $X_0 = 1$ . If we model  $X_t$  as a continuous time Markov chain, then a plausible model is to take the infinitesimal transition probability  $\lambda_{i,i+1} = \lambda i(n+1-i)$  to be proportional to the number of encounters between sick and well people. All other  $\lambda_{ij} = 0$ . Now let T be the time at which the last member of the village succumbs to the disease. Since the waiting time to move from state i to state i+1 is exponential with intensity  $\lambda_{i,i+1}$ , show that  $E(T) \approx 2(\ln n + \gamma)/[\lambda(n+1)]$ , where  $\gamma \approx .5772$  is Euler's constant. It is interesting that E(T) decreases with n for large n.
- 6. Let A and B be the  $2 \times 2$  real matrices

$$A = \begin{pmatrix} a & -b \\ b & a \end{pmatrix}, \qquad B = \begin{pmatrix} \lambda & 0 \\ 1 & \lambda \end{pmatrix}.$$

Show that

3

$$e^A = e^a \begin{pmatrix} \cos b & -\sin b \\ \sin b & \cos b \end{pmatrix}, \quad e^B = e^\lambda \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}.$$

11. Ehrenfest's model of diffusion involves a box with n gas molecules. Suppose the box is divided in half by a rigid partition with a very small hole. Molecules drift aimlessly around and occasionally pass through the hole. During a short time interval h, a given molecule changes sides with probability  $\lambda h + o(h)$ . Show that a single molecule at time t > 0 is on the same side of the box as it started at time 0 with probability  $\frac{1}{2}(1 + e^{-2\lambda t})$ . Now consider the continuous-time Markov chain for the number of molecules in the left half of the box. Given that the n molecules behave independently, prove that finitetime transition probability  $p_{ij}(t)$  amounts to

$$p_{ij}(t) = \left(\frac{1}{2}\right)^n \sum_{k=\max\{0,i+j-n\}}^{\min\{i,j\}} {i \choose k} {n-i \choose j-k} \left(1+e^{-2\lambda t}\right)^{n-i-j+2k} \times \left(1-e^{-2\lambda t}\right)^{i+j-2k}.$$

(Hint: The summation index k is the number of molecules initially in the left half that end up in the left half at time t.)

- 12. A chemical solution initially contains n/2 molecules of each of the four types A, B, C, and D. Here n is a positive even integer. Each pair of A and B molecules collides at rate  $\alpha$  to produce one C molecule and one D molecule. Likewise, each pair of C and D molecules collides at rate  $\beta$  to produce one A molecule and one B molecule. In this problem, we model the dynamics of these reactions as a continuous-time Markov chain  $X_t$  and seek the equilibrium distribution. The random variable  $X_t$  tracks the number of A molecules at time t [13].
  - (a) Argue that the infinitesimal transition rates of the chain amount to

$$egin{array}{rcl} \lambda_{i,i-1}&=&i^2lpha\ \lambda_{i,i+1}&=&(n-i)^2eta. \end{array}$$

What about the other rates?

- (b) Show that the chain is irreducible and reversible.
- (c) Use Kolmogorov's formula and calculate the equilibrium distribution

$$\pi_k = \pi_0 \left(rac{eta}{lpha}
ight)^k \left(\! rac{n}{k}\!
ight)^2$$

for k between 0 and n.

## 172 8. Continuous-Time Markov Chains

(d) For the special case  $\alpha = \beta$ , demonstrate that

$$\pi_k = \frac{\binom{n}{k}^2}{\binom{2n}{n}}.$$

To do so first prove the identity

$$\sum_{k=0}^{n} \binom{n}{k}^2 = \binom{2n}{n}.$$

(e) To handle the case  $\alpha \neq \beta$ , we revert to the normal approximation to the binomial distribution. Argue that

$$\binom{n}{k} p^k q^{n-k} = q^n \binom{n}{k} \left(\frac{p}{q}\right)^k \\ \approx \frac{1}{\sqrt{2\pi n p q}} e^{-\frac{(k-np)^2}{2npq}}$$

for p + q = 1. Show that this implies

$$\binom{n}{k}^2 \left(\frac{p^2}{q^2}\right)^k \approx \frac{1}{2\pi n p q^{2n+1}} e^{-\frac{(k-np)^2}{npq}}.$$

Now choose p so that  $p^2/q^2 = \beta/\alpha$  and prove that the equilibrium distribution is approximately normally distributed with mean and variance

$$E(X_{\infty}) = \frac{n\sqrt{\frac{\beta}{\alpha}}}{1+\sqrt{\frac{\beta}{\alpha}}}$$
$$Var(X_{\infty}) = \frac{n\sqrt{\frac{\beta}{\alpha}}}{2\left(1+\sqrt{\frac{\beta}{\alpha}}\right)^{2}}$$

13. Let n indistinguishable particles independently execute the same continuous-time Markov chain with infinitesimal transition probabilities  $\lambda_{ij}$ . Define a new Markov chain called the composition chain for the particles by recording how many of the n total particles are in each of the s possible states. A state of the new chain is a sequence of nonnegative integers  $(k_1, \ldots, k_s)$  such that  $\sum_{i=1}^s k_i = n$ . For instance, with n = 3 particles and s = 2 states, the composition chain has the four states (3,0), (2,1), (1,2), and (0,3). Find the infinitesimal transition probabilities of the composition chain. If the original chain is ergodic with equilibrium distribution  $\pi = (\pi_1, \ldots, \pi_s)$ , find the equilibrium distribution of the composition chain. Finally, show that the composition chain is reversible if the original chain is reversible.

- 14. Apply Problem 13 to the hemoglobin model in Example 8.5.1 with the understanding that the attachment sites operate independently. What are the particles? How many states can each particle occupy? Identify the infinitesimal transition probabilities and the equilibrium distribution based on the results of Problem 13.
- 15. Prove that G(s,t) defined by equation (8.14) satisfies the partial differential equation (8.13) with initial condition G(s,0) = s and  $\nu(t) = 0$ .
- 16. In the homogeneous version of Kendall's process, show that

$$\operatorname{Var}(X_t) = \frac{\nu}{(\alpha - \mu)^2} \Big[ \alpha e^{(\alpha - \mu)t} - \mu \Big] \Big[ e^{(\alpha - \mu)t} - 1 \Big] \\ + \frac{i(\alpha + \mu)e^{(\alpha - \mu)t}}{\alpha - \mu} \Big[ e^{(\alpha - \mu)t} - 1 \Big]$$

when  $X_0 = i$ .

17. Continuing Problem 16, demonstrate that

$$\operatorname{Cov}(X_{t_2}, X_{t_1}) = e^{(\alpha - \mu)(t_2 - t_1)} \operatorname{Var}(X_{t_1})$$

for  $0 \le t_1 \le t_2$ . (Hints: First show that

$$Cov(X_{t_2}, X_{t_1}) = Cov[E(X_{t_2} | X_{t_1}), X_{t_1}).$$

Then apply Problem 16.)

18. In the homogeneous version of Kendall's process, show that the generating function G(s,t) of  $X_t$  satisfies

$$\lim_{t \to \infty} G(s, t) = \frac{\left(1 - \frac{\alpha}{\mu}\right)^{\nu/\alpha}}{\left(1 - \frac{\alpha s}{\mu}\right)^{\nu/\alpha}}$$
(8.18)

when  $\alpha < \mu$ .

19. Continuing Problem 18, prove that the equilibrium distribution  $\pi$  has *j*th component

$$\pi_j = \left(1 - \frac{\alpha}{\mu}\right)^{\nu/\alpha} \left(-\frac{\alpha}{\mu}\right)^j \left(-\frac{\nu}{\alpha}\right)^j$$

Do this by expansion of the generating function on the right-hand side of equation (8.18) and by applying Kolmogorov's method to Kendall's process. Note that the process is reversible.