UNIVERSITÄT ZU KÖLN

Prof. Dr. Joachim Krug
Dr. Su-Chan Park
Institut für Theoretische Physik
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Solutions in Advanced Statistical Physics

Solution 10: Detailed balance and reversibility

Assume that $\gamma_{ij} P_i^* = \gamma_{ji} P_j^*$ for all i, j. Then

$$\pi(\mathcal{L}) \prod_{k=1}^{N} P_{i_k}^* = \prod_{k=1}^{N} \left(\gamma_{i_k i_{k+1}} P_{i_k}^*\right) = \prod_{k=1}^{N} \left(\gamma_{i_{k+1} i_k} P_{i_{k+1}}^*\right) = \pi(\bar{\mathcal{L}}) \prod_{k=1}^{N} P_{i_k}^*, \tag{1}$$

where $i_{N+1} = i_1$ has been used. Hence if no P_i^* is zero, $\pi(\mathcal{L}) = \pi(\bar{\mathcal{L}})$ for all loops, including the case that $\pi(\mathcal{L}) = 0$. Since, from the master equation, $P_i^* = \dfrac{\sum_{j\neq i} \gamma_{ji} P_j^*}{\sum_{j \neq i} \gamma_{ij}}$ for all i, no P_i^* is zero because of the *ergodicity* which implies that the denominator is positive, at least one γ_{ji} in the numerator is positive, and at least one P_k^* is nonzero due to the normalization. [**Short question I**: Construct a simple system which satisfies the detailed balance but $\pi(\mathcal{L}) \neq \pi(\bar{\mathcal{L}})$ for at least one loop. A system with four states will be enough.]

Now assume that $\pi(\mathcal{L}) = \pi(\bar{\mathcal{L}})$ for all loops. First we will prove that $\gamma_{ij} \neq 0$ implies $\gamma_{ji} \neq 0$. Choose an arbitrary state, say k $(\neq i, j)$. Since the system is ergodic, there is a sequence of transitions, or a loop $\mathcal{L}_k$, from k to i and j to k with nonzero transition rates. If $\mathcal{L}_k$ contains $j \to i$, then $\gamma_{ji} \neq 0$ by definition. Otherwise, $\bar{\mathcal{L}}_k$ contains $j \to i$ transition, and since $\pi(\mathcal{L}_k) = \pi(\bar{\mathcal{L}}_k) \neq 0$, $\gamma_{ji} \neq 0$ follows. ¿From the above proof, one can easily see that the totally asymmetric exclusion process (which allows particles to hop only to the, say, right) does not satisfy the detailed balance condition. Now pick up an arbitrary state i_0. Due to the ergodicity, we can always find a path with nonzero rates from i_0 to any $j(\neq i_0)$ $(i_0 \to j_1 \to \cdots \to j_{N_j - 1} \to j)$. Now define

$$P_j^* = P_{i_0}^* \prod_{\ell=1}^{N_j} \frac{\gamma_{j_{\ell-1} j_\ell}}{\gamma_{j_\ell j_{\ell-1}}}, \quad (j_0 \equiv i_0 \text{ and } j_{N_j} \equiv j) \tag{2}$$

for an arbitrary sequence and $P_{i_0}^*$ will be fixed by normalization. The uniqueness of P_j^* is to be proved. Consider two different paths from i_0 to j, say c_1 and c_2 whose corresponding reverse path will be donoted by $\bar{c}_1$ and $\bar{c}_2$, respectively. The path $c_1 \to \bar{c}_2$ form a loop, say $\mathcal{L}$, then reverse loop is $\bar{\mathcal{L}} = c_2 \to \bar{c}_1$. The ratio of two P_j^* along two different paths is $\dfrac{\pi(\mathcal{L})}{\pi(\bar{\mathcal{L}})} = 1$.

If $\gamma_{ij} \neq 0$, then

$$P_j^* = P_i^* \frac{\gamma_{ij}}{\gamma_{ji}} \Rightarrow \gamma_{ij} P_i^* = \gamma_{ji} P_j^*,$$

because P_j^* does not depend on which path you take; in the above equation, we took the path $i_0 \to i \to j$. Not to mention, the final equality is true even if $\gamma_{ji} = 0$.

[**Short question II**: Construct a system which satisfies the detailed balance and the loop identity but is not ergodic. You can find a simplest system having two states.]

[**Short question III**: The ASEP can or cannot satisfy the detailed balance depending on the boundary condition. Convince yourself that the ASEP with fixed (periodic) boundary conditions does (not) satisfy the detailed balance. You can also find the answer of **Short question II** from this example.]

Solution 11: Shocks in the viscous Burgers equation Put the travelling wave solution into the Burgers equation, then

$$-\tilde{V}\Phi' + \Phi\Phi' = \tilde{\nu}\Phi'', \tag{3}$$

where $\tilde{V} = \dfrac{V}{\lambda}$, $\tilde{\nu} = \dfrac{\nu}{\lambda}$, and prime indicates the derivative over $\xi (= x - Vt)$. Operating $\int_{-\infty}^{\xi} d\xi$ on both sides of Eq. (3), we get $-\tilde{V}(\Phi - \phi_L) + \frac{1}{2}\left(\Phi^2 - \phi_L^2\right) = \tilde{\nu}\Phi'$. or

$$(\Phi - \tilde{V})^2 - (\tilde{V} - \phi_L)^2 = 2\tilde{\nu}\Phi'. \tag{4}$$

Putting $\xi = \infty$ in Eq. (4), we get $\tilde{V} = \dfrac{\phi_R + \phi_L}{2}$ or $V = \lambda\dfrac{\phi_R + \phi_L}{2} = \dfrac{J(\phi_R) - J(\phi_L)}{\phi_R - \phi_L}$, because $J(\phi) = \lambda\dfrac{\phi^2}{2}$. Hence

$$-\frac{1}{2\tilde{\nu}}\xi = \int^{\Phi} du \frac{1}{(\tilde{V} - \phi_L)^2 - (u - \tilde{V})^2} = \frac{1}{\tilde{V} - \phi_L}\left(\tanh^{-1}\left(\frac{\Phi - \tilde{V}}{\tilde{V} - \phi_L}\right) - \tilde{C}\right),$$

where $\tilde{C}$ is a constant. So

$$\Phi(\xi) = \frac{\phi_R + \phi_L}{2} - \frac{\phi_L - \phi_R}{2}\tanh\left(\frac{\phi_L - \phi_R}{4\tilde{\nu}}(\xi - c)\right),$$

where $\dfrac{\phi_R - \phi_L}{4\tilde{\nu}}c = \tilde{C}$. If $\phi_L < \phi_R$, the above solution does not satisfy the boundary condition, that is, the shock is unstable. For $\phi_L > \phi_R$, the width of the shock is $\dfrac{\lambda(\phi_L - \phi_R)}{4\nu}d \sim 1$ or $d = \dfrac{4\nu}{\lambda(\phi_L - \phi_R)}$. So as $\nu \to 0$, the solution becomes discontinuous shock.

Solution 12: Cellular automaton rule 184

a.) Since $\ldots 0000\ldots$ and $\ldots 1111\ldots$ should not change the sequence, the conservation requires

$$(000) \to 0, \quad (111) \to 1. \tag{5}$$

Now consider the sequence of repeating (10)'s, that is, $\ldots 10\underline{10}10\ldots$. To conserve the number of 1's, we have only two possibility;

$$(010) \to 1, \quad (101) \to 0, \tag{6}$$

$$(010) \to 0, \quad (101) \to 1. \tag{7}$$

If one consider two sequences of repeating (110) and (100), Eq. (6) should imply the identity rule, or rule number 204. The nontrivial possibility can arise from Eq. (7) with Eq. (5). Considering again two sequences of repeating (110) and (100), the particle number conserving rules are

$$\left\{ \begin{array}{l} (001) \to 1, (100) \to 0 \\ (001) \to 0, (100) \to 1 \end{array} \right\} \quad \text{and} \quad \left\{ \begin{array}{l} (011) \to 1, (110) \to 0 \\ (011) \to 0, (110) \to 1 \end{array} \right\}. \tag{8}$$

Among four possibilities, two are just frame shift, so rules 184 and 226 are the only nontrivial examples.

b.) Let us write down the rule 184 once again.

$$\left\{ \begin{array}{l} (000) \to 0 \\ (111) \to 1 \end{array} \right\}, \left\{ \begin{array}{l} (001) \to 0 \\ (011) \to 1 \end{array} \right\}, \left\{ \begin{array}{l} (010) \to 0 \\ (101) \to 1 \end{array} \right\}, \left\{ \begin{array}{l} (100) \to 1 \\ (110) \to 0 \end{array} \right\}. \tag{9}$$

The rule says that 1 cannot move if its right neighbor is occupied by 1. Otherwise, 1 hops to the right. Hence the stationary state which depends on the initial setting is that without 11 pair. In this case, the current is ρ. The above statement is only true when $\rho \leq \frac{1}{2}$. Since the rule 184 is symmetric under the particle-hole conversion $(1 \leftrightarrow 0)$ followed by the space inversion $[(abc) \leftrightarrow (cba)]$, the stationary state of the system with $\rho > \frac{1}{2}$ should be one without 00 pair. The current for this case is $1-\rho$ because the current of 0's is $-(1-\rho)$. In summary, $J = \min\{\rho, 1-\rho\}$. As the above consideration reveals, the order parameter for this transition can be 11 pair density which is zero for $\rho \leq \frac{1}{2}$ and finite for $\rho > \frac{1}{2}$.

c.)

$$\frac{\partial}{\partial t}\rho(x,t) + \frac{\partial}{\partial x}J(x,t) = 0 \Rightarrow \frac{\partial}{\partial t}\rho(x,t) = -\mathrm{sgn}(1-2\rho)\frac{\partial}{\partial x}\rho(x,t) = -c(\rho)\frac{\partial}{\partial x}\rho(x,t),$$

where $\mathrm{sgn}(x) = 2\Theta(x) - 1$ and $c(\rho) = \mathrm{sgn}(1-2\rho)$. If the initial density is smaller (larger) than $\frac{1}{2}$ at all points, the density profile at t becomes $\rho(x,t) = \rho_0(x \pm t)$ (+ for low density regime). If initial (smooth) density profile crosses $\rho = \frac{1}{2}$ line, the shock starts to form at $\rho_0 = \dfrac{1}{2}$ with $\dfrac{d\rho_0}{dx} > 0$ immediately.