Bethe Ansatz Solution of ASEP with Reflecting Boundaries

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1 Single Particle Solution

To investigate the ASEP model of N particles on L lattice sites with reflecting boundaries. Let us start with one single particle in such a closed lattice. The master equation of the particle can be written as

$$\frac{d}{dt}P(x,t) = \alpha P(x-1,t) + \beta P(x+1,t) - (\alpha+\beta)P(x,t) \tag{1a}$$

$$\frac{d}{dt}P(1,t) = \beta P(2,t) - \alpha P(1,t) \tag{1b}$$

$$\frac{d}{dt}P(L,t) = \alpha P(L-1,t) - \beta P(L,t) \tag{1c}$$

where α and β is hopping rate of particle to left and right, respectively. x denotes the position of the particle is confined to be the integer in the range of $1, 2, \cdots, L$. Eq. (1b) and (1c) are actually the special cases of master equation at the boundaries. By assuming Eq. (1a) is valid for the whole space, we can rewrite Eq. (1b) and (1c) as boundaries condition

$$\alpha P(0,t) = \beta P(1,t) \tag{2a}$$

$$\alpha P(L,t) = \beta P(L+1,t) \tag{2b}$$

The above equations use the technique so called "ghost coordinate", i.e. $x = 0, L+1$. But physically they are essentially the same as the master equation (1b) and (1c), which means the flux of particle are balanced in both direction, thus the reflecting boundaries. The advantage of using Eq. (2) is that it simplifies the calculation a lot.

To solve the case of single particle ASEP, we take the ansatz of separation of variables $P(x,t) = \phi(x)e^{\lambda t}$ and plug into the master equation, obtaining

$$\beta\phi(x+1) - (\alpha+\beta+\lambda)\phi(x) + \alpha\phi(x-1) = 0 \tag{3}$$

Given that x is an integer number, Eq. (3) is essentially a set of liner difference equations with the boundaries by substituting the ansatz of $P_x(t)$ into boundaries of Eq. (2):

$$\alpha\phi(0) = \beta\phi(1) \tag{4a}$$
$$\alpha\phi(L) = \beta\phi(L+1) \tag{4b}$$

The standard method to find the solution is again to take an ansatz $\phi(x) = Az^x$, where z is an arbitrary complex number. We arrive at the characteristic quadratic equation

$$\beta z^2 - (\alpha + \beta + \lambda)z + \alpha = 0 \tag{5}$$

The two roots fulfill $z_1 z_2 = \frac{\alpha}{\beta}$. And the solution of (3) can be written as

$$\phi(x) = C_1 z_1^x + C_2 z_2^x \tag{6}$$

By applying the boundaries Eq. (4) to Eq. (6) we can find all the eigenvalues and corresponding eigenvectors. The results are summarised as following

$$\begin{aligned}
&\lambda_s = 0;\ \phi_s(x) = const.\left(\frac{\alpha}{\beta}\right)^x;\\
&\lambda_k = -(\alpha+\beta) + 2\sqrt{\alpha\beta}\cos(\frac{k\pi}{L});\ k = 1, 2, \ldots, L-1\\
&\phi_k(x) = const.\left(\frac{\alpha}{\beta}\right)^{\frac{x}{2}}\left[\sin\left(\frac{k\pi}{L}x\right) - \sqrt{\frac{\beta}{\alpha}}\sin\left(\frac{k\pi}{L}(x-1)\right)\right].
\end{aligned} \tag{7}$$

The eigenvalue $\lambda_s = 0$ and corresponding eigenvector represent the stationary mode $\phi_s(x)$. Define a scalar product between any two functions by

$$(\phi, \psi) = \int \frac{\phi(x)\psi(x)}{\phi_s(x)}dx \tag{8}$$

Notice that definition Eq. (8) makes $\phi_s(x)$ identical to the stationary distribution $P^e(x)$. By properly choose the constant and when $L \to \infty$, one can check the orthogonality and completeness of the eigenfunctions.

$$\sum_{x=1}^{L} \phi_k(x)\phi_l(x) = \delta_{k,l} \tag{9}$$
$$\sum_{k=1}^{L} \phi_k(x)\phi_k(y) = \delta_{x,y} \tag{10}$$

So for arbitrary initial distribution of $P(x,0)$, we can always decompose it as

$$P(x,0) = \sum_k c_k \phi_k(x) \tag{11}$$

where c_k can be calculated by

$$c_k = \sum_x \phi_k(x) P(x,0) \tag{12}$$

Finally, the solution of single particle on reflecting lattice can be written as

$$P(x,t) = \sum_k \phi_k(x) e^{\lambda_k t} \sum_{x'} \phi_k(x') P(x',0) \tag{13}$$

For the special case that $P(x,0) = \delta_{x,y}$, solution (13) can be simplified to

$$P(x,t) = \sum_k \phi_k(x) \phi_k(y) e^{\lambda_k t} \tag{14}$$

With the complete solution of single particle, we can go further to systems of more than one particle. The idea is that the single particle solution works as building blocks for the N particle solutions. To start with that, we first illustrate the case $N = 2$ and the position of particles are denotes by x_1, x_2 with constraint $x_1 < x_2$.

2 Solution of Two Particles

Firstly, we shall write down the master equation, which looks as following

$$\begin{aligned} \frac{dP(x_1,x_2;t)}{dt} =& \alpha P(x_1-1,x_2;t) + \beta P(x_1+1,x_2;t) \\ &+ \alpha P(x_1,x_2-1;t) + \beta P(x_1,x_2+1;t) \\ &- 2(\alpha+\beta) P(x_1,x_2;t) \end{aligned} \tag{15}$$

And the reflecting boundaries write as

$$\alpha P(0,x_2;t) = \beta P(1,x_2,t) \tag{16a}$$

$$\alpha P(x_1,L;t) = \beta P(x_1,L+1;t) \tag{16b}$$

For the case of more than one particle, we need to take into account the exclusion effect, i.e., one site can be occupied by at most one particle. This can be also written as a boundary condition as

$$\alpha P(x,x;t) + \beta P(x+1,x+1;t) = (\alpha+\beta) P(x,x+1;t) \tag{17}$$

Notice that the exclusive condition must hold for any x. The notation of $P(x, x; t)$ may looks a little bit weird, but keep in mind that it is a boundary condition that denotes the limiting situation $x_1 = x_2$.

The idea to construct the N particle solution is inspired by the standard Coordinate Bethe Ansatz (CBA). However, instead of using the plain plane wave function as building blocks, we use the eigenfunctions of single particle solution. To show that, we need to again do the eigenfunction expansion of the solution, which can be written as

$$P(x_1, x_2, t) = \sum_k \Psi_k(x_1, x_2) e^{\lambda_k t} \tag{18}$$

The key point here is the construction of $\Psi(x_1, x_2)$. We take the Ansatz that the general form of $\Psi(x_1, x_2)$ can be written as

$$\Psi(x_1, x_2) = A_{12}\psi_1(x_1)\psi_2(x_2) + A_{21}\psi_2(x_1)\psi_1(x_2) \tag{19}$$

Plug in to the master equation Eq. (15) we arrive at

$$\alpha\psi_1(x-1) + \beta\psi_1(x+1) - (\alpha+\beta+\lambda)\psi_1(x) = 0 \tag{20a}$$
$$\alpha\psi_2(x-1) + \beta\psi_2(x+1) - (\alpha+\beta+\lambda)\psi_2(x) = 0 \tag{20b}$$

One can readily find $\psi_1(x)$ and $\psi_2(x)$ should be the eigenfunction of single particle master equation, respectively. So we use the solution of section 1 with unfixed coefficients as trial function and keep in mind the exclusive condition should be fulfilled. In the following text, we will discuss several different cases separately.

2.1 Stationary Solution

Let us first check the case $\psi_1(x) = \psi_2(x) = \phi_s(x)$. Namely

$$P^e(x_1, x_2) = \Psi(x_1, x_2) = A\left(\frac{\alpha}{\beta}\right)^{x_1+x_2} \tag{21}$$

This will lead to the stationary solution as one would expected. First, we can easily obtain from Eq. (20) and Eq. (19) that the corresponding eigenvalue $\lambda_k = 0$. And then one can check easily the exclusive condition Eq. (17) is fulfilled.

The prefactor A can be fixed by normalization. However, it is not a trivial work because of the constraint $x_1 < x_2$. We will discuss in detail in general case of N later.

2.2 Non-stationary Modes

We now check the case $\psi_1(x) = \phi_s(x)$, $\psi_2 = \phi_k(x), k = 1, 2, \cdots, L-1$. The exchange of ψ_1 to ψ_2 makes the identical results. So we can write the solution as

$$\Psi(x_1, x_2) = A_{12} \left(\frac{\alpha}{\beta}\right)^{x_1} \phi_k(x_2) + A_{21} \left(\frac{\alpha}{\beta}\right)^{x_2} \phi_k(x_1) \tag{22}$$

We first insert the solution to the master equation Eq. (15), obtaining the corresponding eigenvalue $\lambda_k = -(\alpha+\beta) + 2\sqrt{\alpha\beta}\cos(\frac{k\pi}{L})$.

We now check the exclusive condition Eq. (17). Simply substitute Eq. (22) into the condition. In order to fulfill the exclusive condition, we find that $A_{12}/A_{21} = \alpha/\beta$.

Finally, insert Eq. (2) in to Eq. (16), we can check that $\phi_k(x)$ must choose to be exactly the single particle eigenfunction to fulfill the reflecting boundaries.

Here we summarize the non-stationary eigenvalues and corresponding eigenfunctions for the two particles ASEP.

$$\lambda_k = -(\alpha+\beta) + 2\sqrt{\alpha\beta}\cos(\frac{k\pi}{L});\ k = 1, 2, \ldots, L-1 \tag{23a}$$

$$\Psi(x_1, x_2) = A\left[\frac{\alpha}{\beta}\left(\frac{\alpha}{\beta}\right)^{x_1} \phi_k(x_2) + \left(\frac{\alpha}{\beta}\right)^{x_2} \phi_k(x_1)\right] \tag{23b}$$

Finally, we want remark here, the eigenfunctions listed in Eq. (23) are not the complete set of non-stationary eigenfunctions, we will leave the discussion of this issue to next section.

3 General Solution of N particles ASEP

As before, we first write down the master equation of a N particles system.

$$\begin{aligned}\frac{dP(x_1, \cdots, x_N; t)}{dt} =& \sum_{j=1}^{N} [\alpha P(\cdots, x_j - 1, \cdots; t) + \beta P(\cdots, x_j + 1, \cdots; t) \\ & -(\alpha+\beta) P(\cdots, x_j, \cdots; t)]\end{aligned} \tag{24}$$

Similarly, the reflecting boundaries write as

$$\alpha P(0, x_2, \cdots, x_N; t) = \beta P(1, x_2, \cdots, x_N; t) \tag{25a}$$

$$\alpha P(x_1, \cdots, x_{N-1}, L; t) = \beta P(x_1, \cdots, x_{N-1}, L+1; t) \tag{25b}$$

The exclusive condition for N particles case is more tricky. In principle, one has to consider to case of three body collision and four body collision and

so on. Luckily, in the simple model of ASEP, one can prove that these more than two body exclusive conditions are not new but just linear recombination of two body exclusive condition. So we can write the exclusive condition of a N particles system as

$$\alpha P(\cdots, x, x, \cdots; t) + \beta P(\cdots, x+1, x+1, \cdots; t) = (\alpha+\beta) P(\cdots, x, x+1, \cdots; t) \tag{26}$$

The procedure of searching solution in section 2 can be generalize to N particles case in a straight forward manner. Let us again start with the stationary solution.

3.1 Stationary Solution

Intuitively, we construct the N particles stationary solution as

$$P^e(x_1, x_2, \cdots, x_N) = \Psi(x_1, x_2, \cdots, x_N) = A \prod_{j=1}^{N} \left(\frac{\alpha}{\beta}\right)^{x_j} \tag{27}$$

One can plug in the master equation check that the corresponding eigenvalue $\lambda = 0$, and also verify the exclusive condition as well as the reflecting boundaries are fulfilled by insert the solution in to Eq. (26) and Eq. (25) separately.

We now try to fix the parameter A by normalization. Let us denote $q := \frac{\alpha}{\beta}$, then we can write A as following

$$A^{-1} = \sum_{\Omega} q^{\sum_j x_j} = \sum_{x_1 < x_2 < \cdots < x_N} q^{\sum_j x_j} \tag{28}$$

Let us do a variable change so that

$$\begin{aligned} \sum_j x_j &= E_0 + E \\ E_0 &= 1 + 2 + \cdots + N = \frac{N(N+1)}{2} \end{aligned}$$

We can derive that E is a integer in the range of $0, 1, \cdots, N(L-N)$. So Eq. (28) can be rewrite as

$$A^{-1} = q^{E_0} \sum_{E=0}^{N(L-N)} g(E) q^E \tag{29}$$

where $g(E)$ is the number of partitions of positive integer E to N parts with each of size at most $L-N$. From the number partition theory, we identify

$$\sum_{E=0}^{N(L-N)} g(E)q^E = \binom{L}{N}_q = \frac{[L]_q!}{[L-N]_q![N]_q!} \tag{30}$$

where $[N]_q = 1 + q + q^2 + \cdots + q^{N-1}$ is called a q number, and Eq. (30) is called the q binomial coefficient[]. So we finally arrive at

$$P^e(x_1, x_2, \cdots, x_N) = q^{-\frac{N(N+1)}{2}} \binom{L}{N}_q^{-1} \prod_{j=1}^{N} q^{x_j} \tag{31}$$

In [], G. M. Schütz use a quantum group formalism obtained the same result with a different notation. We emphasize here that our method is much more easily to understand and no prerequisite knowledge of quantum mechanics and group theory is needed.

With the equilibrium N particle distribution, we can readily calculate the equilibrium distribution of any tagged particle. Denote he distribution of the kth particle $p_k(x)$, we have

$$\begin{aligned} p_k(x) &= \sum_{0<x_1<\cdots<x_{k-1}\le x-1} P^e(x_1, x_2, \cdots, x_N) \sum_{x<x_{k+1}<\cdots<x_N\le L} P^e(x_1, x_2, \cdots, x_N) \\ &= q^{(N+1-k)(x-k)} \binom{x-1}{k-1}_q \binom{L-x}{N-k}_q \Big/ \binom{L}{N}_q \end{aligned} \tag{32}$$

Finally, the equilibrium density profile can be obtain by summing up $p_k(x)$

$$\rho(x) = \sum_{k=1}^{N} p_k(x) \tag{33}$$

3.2 Non-stationary Modes

Inspired by the two particle calculation, we start to searching for N particle non-stationary eigenfunctions by taking the following Ansatz

$$\Psi(x_1, x_2, \cdots, x_N) = \sum_{k=1}^{N} A_k \phi_k(x_k) \prod_{j\neq k} \left(\frac{\alpha}{\beta}\right)^{x_j} \tag{34}$$

We again insert the solution to the master equation Eq. (24), obtaining the corresponding eigenvalue $\lambda_k = -(\alpha+\beta) + 2\sqrt{\alpha\beta}\cos(\frac{k\pi}{L})$.

By substitute Eq. (34) into the exclusive condition Eq. (26), we get $A_{k+1}/A_k = \alpha/\beta$.

Finally, the reflecting boundary condition can be checked by choosing $\phi_k(x)$ be exactly the single particle eigenfunctions.

The results are summarized as following:

$$\lambda_k = -(\alpha+\beta) + 2\sqrt{\alpha\beta}\cos(\frac{k\pi}{L});\ k = 1, 2, \ldots, L-1 \tag{35a}$$

$$\Psi(x_1, x_2, \cdots, x_N) = A\sum_{k=1}^{N}\left(\frac{\alpha}{\beta}\right)^{k-1}\phi_k(x_k)\prod_{j\neq k}\left(\frac{\alpha}{\beta}\right)^{x_j} \tag{35b}$$

3.3 Completeness of Eigenfunctions

Although we found some non-stationary eigenmodes listed in Eq. (35). We have to say, this is not a complete set of all eigenmodes. This can be checked by counting the number of independent eigenfunctions. For a discrete system like N particles on L lattice sites, there dimension of the configuration space is $\binom{L}{N}$. So the transition matrix should has $\binom{L}{N}$ independent eigenvectors. However, we only found N instead of $\binom{L}{N}$.

The possible remaining eigenfunctions, as one may expect intuitively, can be constructed by combination of non-stationary single particle eigenfunctions. We can write them as following

$$\Psi(x_1, x_2, \cdots, x_N) = \sum_{\sigma\in S_N} A_{\sigma(k)}\prod_k \phi_k(x_{\sigma(k)}) \tag{36}$$

The expanded example of simple two particles case reads

$$\Psi(x_1, x_2, \cdots, x_N) = A_{12}\phi_k(x_1)\phi_l(x_2) + A_{21}\phi_k(x_2)\phi_l(x_1) \tag{37}$$

Because $\phi_k(x)$ is exactly the eigenfunction of a single particle on the lattice box $[1, L]$, the reflecting boundaries Eq. (25) can be checked being fulfilled easily.

So we only need to tale care of the exclusive condition Eq. (26). We can simply plug in the general form of $\phi_k(x)$ with unfixed parameters

$$\phi_k(x) = A\left(z^x + Bq^x z^{-x}\right) \tag{38}$$

We found the exclusive condition will be satisfied if we choose $A_{\sigma(k)}/A_{\sigma(l)} = 1,\ z_k \neq z_l$ or $z_k = z_l = \pm\sqrt{\alpha/\beta}$. The later case can be eliminated because the reflecting boundaries Eq. (25) will not be satisfied if we resubstitute into the equations.

It looks like all good in the calculations. But the problem is if we assume this is true, then we should expect the corresponding eigenvalue for the N particles system combined by single particle eigenvalues such like $\lambda = \lambda_k + \lambda_l;\ k, l = 1, 2, \cdots, L-1;\ k \neq l$. However, there are at least two contradictions. The First one is we don't see this sort of eigenvalues if we diagonalize the transition matrix numerically, instead we see something else. The second one is the total number of eigenfunctions can not sum up to $\binom{L}{N}$. So either we have missed something here or somewhere is wrong in my calculation, which I checked for many times.

4 Relaxation Time

Although we can not get the complete set of eigenvalues and eigenfunctions analytically, we can still postulate the largest non-zero value is contained in the set we already found. The largest non-zero eigenvalue we found is

$$\lambda_1 = -(\alpha + \beta) + 2\sqrt{\alpha\beta}\cos(\frac{\pi}{L}) \tag{39}$$

If $L \ll 1$, we can expand the cos term, obtain

$$\lambda_1 = -(\sqrt{\beta} - \sqrt{\alpha})^2 + \frac{\sqrt{\alpha\beta}\pi^2}{L^2} \tag{40}$$

And the relaxation time can be calculated as

$$\tau = -\frac{1}{\lambda_1} \tag{41}$$

There are several information we can read form Eq. (40) and (41). Firstly, we can see the scaling $\tau \approx L^2$, which means the dynamical exponent of the system is 2. Secondly, as we can see from Eq. (40), the bigger difference between α and β, the smaller relaxation time we will get. This is also consistent as one would expect. If we map back to the polymer model, the result here can be compared with the prediction of Rouse theory. Unlike the prediction from Rouse theory that relaxation time does not depend on external force, we have here that stronger external force decreases the relaxation time. This point highlight the fundamental difference between the infinite extensible bead spring model and the rigid bead rod model which is of course finite extensible.

We want to remark here that it would be a hard mathematical problem to prove Eq. (39) leads to the correct relaxation time of the system. Even if we can found all the eigenfunctions, the proof might become a problem

of comparing the roots of a polynomial equation to λ_1 listed here. Because the remaining eigenvalues are related to polynomial equations as hinted by the numerical diagonalize of transition matrix. However, we can still show the numerical evidence of the postulate above, e.g. Fig. 1 shows all the eigenvalues of a system with $L = 10$ lattice sites with the number of particles from 1 to 9. The transition matrix was diagonalize numerically here. The difficult to calculate larger lattice size L lies on that the dimension grow as $\binom{L}{N}$, and if we take $N = L/2$, the dimension of the matrix will became a extremely large number very soon.

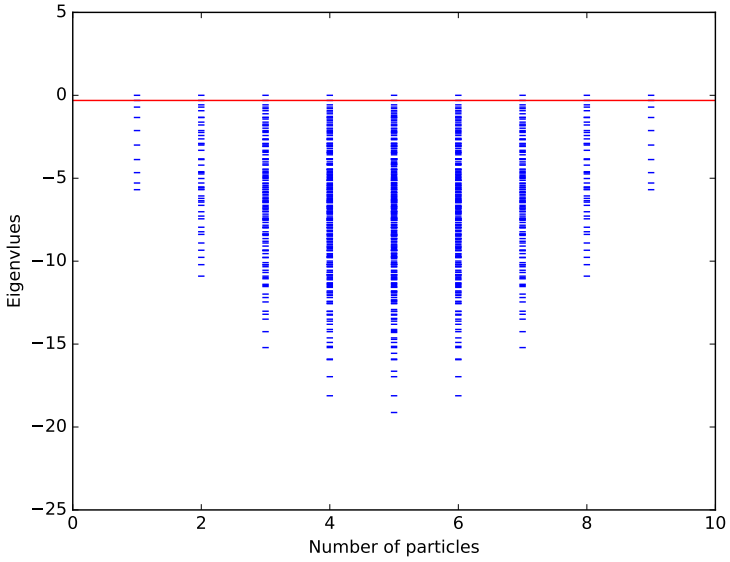

Figure 1: Eigenvalues calculated by numerically diagonalize the transition matrix.

Actually, there are more information hinted by Fig. 1. One can see that all eigenvalues of case $N = 1$ are contained in the set of eigenvalues $N = 2$, and all eigenvalues of case $N = 2$ are contained in the set of $N = 3$ and so on until reach the largest set $N = L/2$. This means the characteristic polynomial of $N = k + 1$ always contains the factor of the characteristic polynomial $N = k$. This is verified by the calculation started from the simplest case $N = 2$ and $L = 4$.

5 Summary

We use the modified Bethe Ansatz methods solve the ASEP model with reflecting boundaries. Although the complete set of eigenvalues and eigenfunctions were not found, the stationary distribution was solved exactly and the one correspond to the relaxation time of the system was postulated. Numerical evidence is provided for later statement.