Solutions to Kinetic models in statistical physics

Min Jae Jo

P1) Show the following: Consider a harmonic motion: $m\frac{d^2x_i}{dt^2} = -k\sum_{j\in\mathbf{n.n. of }i}(x_i - x_j)$, $\lambda x_i = \sum_j V_{i,j}x_j$. Then the eigenvalue i) $\lambda \sim \omega^2$, and ii) the spectral density is $\rho_s(\lambda) \sim \lambda^{\frac{d}{2}-1}$.

 \Rightarrow i) We use the definition of a Laplacian operator V by

$$\sum_{j} V_{i,j} x_j = z x_i - \sum_{j \in \text{n.n. of } i} x_j = \sum_{j \in \text{n.n. of } i} (x_i - x_j),$$

where z is the coordination number of the lattice. Then the original equation can be written as

$$m\frac{d^2x_i}{dt^2} = -k\sum_j V_{i,j}x_j$$

When $V_{i,j}$ is independent of time, this equation can be solved by the method of separation of variables. Inserting the corresponding solution of the form $x_{\ell}(t) = e^{i(\vec{q}\cdot\vec{\ell}-\omega t)}$

$$\sum_{j} V_{i,j} x_j = \frac{m\omega^2}{k} x_i \,.$$

The oscillation frequency is simply related to the eigenvalue $\lambda = \frac{m\omega^2}{k}$.

ii) The spectral dimension is defined as $\rho_s(\omega) \sim \omega^{d_s-1}$. Combining the relation $\rho_s(\omega)d\omega = \rho_s(\lambda)d\lambda$ and the result from i), $\rho_s(\lambda) \sim \lambda^{d_s/2-1}$.

- P2) Show the following: $P_0(n) \sim n^{-d/2} \Rightarrow \mathcal{P}_0(s) \sim (1-s)^{d/2-1} \rightarrow \text{singular when } d < 2 \text{ as } s \rightarrow 1.$
 - \Rightarrow Let us consider the $P_0(n)$ of the spectral density we obtained in P1:

$$P_0(n) = \frac{S_d}{(2\pi)^d} \int_0^\infty e^{-nw\lambda} \lambda^{d/2-1} d\lambda = \frac{S_d}{(2\pi)^d} \int_0^\infty \frac{e^{-x}}{nw} (\frac{x}{nw})^{d/2-1} dx$$
$$= \frac{S_d}{(2\pi)^d} \frac{\Gamma(d/2)}{(nw)^{d/2}} \sim n^{-d/2},$$

where we have used the substitution $x \equiv nw\lambda$. Then the calculation of the generating function becomes

$$\mathcal{P}_{0}(s) = \frac{S_{d}}{(2\pi)^{d}} \int_{0}^{\infty} d\lambda \, \frac{\lambda^{d/2-1}}{1-s+\lambda ws} = \frac{S_{d}}{(2\pi)^{d}(1-s)} \int_{0}^{\infty} d\lambda \, \frac{\lambda^{d/2-1}}{1+\frac{\lambda ws}{1-s}}$$
$$= \frac{S_{d}}{(2\pi)^{d}} \frac{(1-s)^{d/2-1}}{(ws)^{d/2}} \int_{0}^{\infty} dx \, \frac{x^{d/2-1}}{1+x}$$
$$= \frac{S_{d}}{(2\pi)^{d}} \frac{(1-s)^{d/2-1}}{(ws)^{d/2}} \pi \csc(\frac{d\pi}{2}), \quad \text{when } d < 2.$$

Thus $\mathcal{P}_0(s) \sim (1-s)^{d/2-1}$ and singular as $s \to 1$.

P3) Show that i) $F(t) \simeq \frac{1}{\sqrt{\pi}} \frac{1}{t^{3/2}}$ in 1d; ii) $F(t) \simeq \frac{4\pi}{t(\ln t)^2} \frac{1}{t^{3/2}}$ in 2d; and iii) $F(t) \simeq \frac{(1-\mathcal{R})^2}{8\pi^{3/2}} \frac{1}{t^{3/2}}$ in 1d. Find \mathcal{R} in 3d.

 \Rightarrow i) From the Lecture note, the Laplace transform of the occupation probability at the origin is

$$P(s) \simeq \int_0^\infty (4\pi t)^{-d/2} e^{-st} dt = \frac{\Gamma(1 - d/2)s^{d/2 - 1}}{(4\pi)^{d/2}}, \quad \text{when } d/2 < 1.$$
(1)

Thus, $P(s) \simeq (4s)^{-1/2}$ in 1*d*. Then the Laplace transform of the first-passage probability to the origin,

$$F(s) = 1 - \frac{1}{P(s)} \simeq 1 - \sqrt{4s},$$
 (2)

and the eventual return probability R = F(s = 0) = 1. Because F(s) does not diverge for small s, it is not convenient to invert this Laplace transform directly. Instead, we consider the derivative of F(s):

$$-F'(s) = \mathcal{L}(tF(t)) = s^{-1/2},$$

where \mathcal{L} is a notation for the Laplace transform. We can then directly apply Eq. (1) to find that $tF(t) = (\pi t)^{-1/2}$ and thus $F(t) \simeq \frac{1}{\sqrt{\pi}} \frac{1}{t^{3/2}}$.

ii) Firstly, we must cut off the integral for t < 1 to eliminate the spurious singularity that arises from using the long-time form of P(t) for short times. Then we have

$$P(s) \simeq \int_0^\infty (4\pi t)^{-1} e^{-st} dt = \frac{\Gamma(0, x)}{4\pi}$$
$$\simeq -\frac{\ln s}{4\pi}, \quad \text{when } s \to 0.$$

Then the Laplace transform of the first-passage probability to the origin,

$$F(s) \simeq 1 + \frac{4\pi}{\ln s}$$
, when $s \to 0$.

Again, the eventual return probability R = F(s = 0) = 1 and we consider the derivative of F(s):

$$-F'(s) = \mathcal{L}(tF(t)) = \frac{4\pi}{s(\ln s)^2}, \quad \text{when } s \to 0.$$

Since the Laplace transform of a constant function equals 1/s, the function tF(t) must vary weakly in time to give the extra factor of $(\ln s)^{-2}$ and thus $F(t) \simeq \frac{4\pi}{t(\ln t)^2}$. iii) For d = 3,

$$P(s) \simeq \int_0^\infty (4\pi t)^{-3/2} e^{-st} dt$$
,

and it is useful to differentiate to both sides of the above equation:

$$P'(s) \simeq \frac{-1}{(4\pi)^{3/2}} \int_0^\infty t^{-1/2} e^{-st} dt = \frac{-1}{8\pi\sqrt{s}},$$

where we have used Eq. (1). Then $P(s) = P(0) - \frac{\sqrt{s}}{4\pi}$ and F(s) is given by

$$F(s) = 1 - \frac{1}{P(s)} \simeq 1 - \frac{1}{P(0) - \frac{\sqrt{s}}{4\pi}} \simeq 1 - \frac{1}{P(0)} \left(1 + \frac{\sqrt{s}}{4\pi P(0)} \right)$$
$$= 1 - \frac{1}{P(0)} - \frac{\sqrt{s}}{4\pi P(0)^2}.$$

Using $\mathcal{R} = F(s=0) = 1 - P(0)^{-1}$, the above equation is rewritten as follows:

$$F(s) = \mathcal{R} - \frac{(1-\mathcal{R})^2 \sqrt{s}}{4\pi}$$

Note that $\mathcal{R} = 1 - P(0)^{-1} < 1$ and the random walk is transient. By comparing with Eq. (2), the asymptotic form of F(t) is given by

$$F(t) \simeq \frac{(1-\mathcal{R})^2}{8\pi^{3/2}} \frac{1}{t^{3/2}}.$$

P4) Show that i) $F(t) \sim \frac{y_0}{\sqrt{8\pi Dt^3}} e^{-y_0^2/8Dt} \sim t^{-3/2}$ and ii) the survival probability $S(t) = 1 - \frac{2}{\sqrt{\pi}} \int_{y_0/\sqrt{8Dt}}^{\infty} e^{-u^2} du \rightarrow \frac{y_0}{\sqrt{2\pi Dt}}$.

 \Rightarrow i) The first-passage probability to the origin at time t is just the flux to this point with the probability density $c(y,t) = \frac{1}{\sqrt{8\pi Dt}} \left[e^{-(y-y_0)^2/8Dt} - e^{-(y+y_0)^2/8Dt} \right]$:

$$F(t) = 2D \frac{\partial c(y,t)}{\partial y} \Big|_{y=0} = \frac{y_0 e^{-y_0^2/8Dt}}{\sqrt{8\pi D t^{3/2}}} \sim t^{-3/2}, \quad \text{as } t \to \infty$$

ii) The survival probability S(t) of the two particles may be found from $S(t) = 1 - \int_0^t F(0, t') dt'$. Using the substitution $x^2 = y_0^2/8Dt'$ leads to

$$S(t) = 1 - \frac{2}{\sqrt{\pi}} \int_{y_0/\sqrt{8Dt}}^{\infty} e^{-x^2} dx = \operatorname{erf}(y_0/\sqrt{8Dt}) \to \frac{y_0}{\sqrt{2\pi Dt}}, \quad \text{as } t \to \infty$$

P5) Consider a Sierpinski gasket. i) Obtain the fractal dimension. Consider random walks on an infinite Sierpinski gasket. ii) Obtain the spectral dimension and random walk dimension.



Figure 1: Compartment of a Sierpinski gasket.

 \Rightarrow i) Let us consider a Sierpinski gasket in Fig. 1. Observe that it is a triangle, and consists of three smaller triangles with a triangular space between them. These three triangles are identical copies of the entire fractal, so we decide that our value for n will be 3. Now what is the scaling factor? Observation also easily tells us that the edge of the smaller triangles is half the edge of the fractal itself. Thus our scaling factor r is 2. Applying these to formula, we get:

$$d_f = \frac{\ln n}{\ln r} \simeq 1.585 < 2$$

ii) In Fig. 1, some of the equations for the eigenvalue problem are given by

$$\begin{split} \lambda x_1 &= 4x_1 - x_2 - x_3 - x_5 - x_6 \,, \\ \lambda x_2 &= 4x_2 - x_1 - x_3 - x_4 - x_5 \,, \\ \lambda x_3 &= 4x_3 - x_1 - x_2 - x_4 - x_6 \,, \end{split}$$

or equivalently

$$\begin{pmatrix} \lambda - 4 & 1 & 1 \\ 1 & \lambda - 4 & 1 \\ 1 & 1 & \lambda - 4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = - \begin{pmatrix} x_5 + x_6 \\ x_4 + x_5 \\ x_4 + x_6 \end{pmatrix}$$

Solving the equation with respect to x_1 , x_2 , and x_3

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = -\frac{1}{(\lambda - 5)(\lambda - 2)} \begin{pmatrix} \lambda - 3 & -1 & -1 \\ -1 & \lambda - 3 & -1 \\ -1 & -1 & \lambda - 3 \end{pmatrix} \begin{pmatrix} x_5 + x_6 \\ x_4 + x_5 \\ x_4 + x_6 \end{pmatrix}.$$
 (3)

Likewise, x_7 , x_8 , and x_9 can be represented by x_5 , x_{10} , and x_{11} . The equation of x_5 is given by

$$\lambda x_5 = 4x_5 - x_1 - x_2 - x_7 - x_8, \qquad (4)$$

and inserting the solutions x_1, x_2 in Eq. (3) and x_7, x_8 to the right hand side of Eq. (4)

$$(5\lambda - \lambda^2)x_5 = 4x_5 - (x_4 + x_6 + x_{10} + x_{11}).$$

Note that the equation is represented by x_4 , x_6 , x_{10} , and x_{11} . Thus it reduces to the eigenvalue problem with the edge length $2^{k-1}a$, where k is the iteration number and a is the unit length. The renormalized eigenvalue λ' is given by $\lambda' = 5\lambda - \lambda^2$. For $\lambda \to 0$, $\lambda' = 5\lambda$. If we introduce an quantity $D_k(\Lambda)$, the number of eigenvalues in the interval $0 < \lambda < \Lambda$ with the edge length $2^k a$, we obtain $D_k(\Lambda) = D_{k-1}(5\Lambda)$ for $\Lambda \to 0$.

Then spectral density becomes

$$\rho(\lambda) = \frac{d}{d\lambda} \lim_{k \to \infty} \frac{1}{n} D_k(\lambda),$$

and for $\lambda \to 0$

$$\rho(\lambda) = \frac{5}{3}\rho(5\lambda) \,. \tag{5}$$

The spectral dimension d_s is defined as $\rho(b\omega) = b^{d_s-1}\rho(\omega)$. Moreover, the eigenvalue $\lambda = \omega^2/\omega_0^2$ gives the relation $\rho(\omega) = \omega \rho(\omega^2/\omega_0^2)$. Thus we obtained the relation $\rho(b\lambda) = b^{d_s/2-1}\rho(\lambda)$, which gives the spectral dimension by Eq. (5): $d_s \simeq 1.365$ and $d_w = 2d_f/d_s \simeq 2.322$.

P5') Consider a Sierpinski gasket. i) Obtain the fractal dimension. Consider random walks on an infinite Sierpinski gasket. ii) Obtain the spectral dimension and self-avoiding walk dimension ν .

 \Rightarrow i) This is the same problem with the P5-i.

ii) In two dimensional Sierpinski gasket, the partition function is

$$Z = \operatorname{Tr} \prod_{\langle i,j \rangle} [1 + vO_{ij}]$$

= Tr $\prod_{\&} [1 + v(O_{12} + O_{23} + O_{31}) + v^2(O_{12}O_{23} + O_{12}O_{31} + O_{23}O_{31}) + v^3O_{12}O_{23}O_{31}],$

where \prod_{Δ} is the product of the unit triangles and 1, 2, and 3 indicate the vertices of the triangle. Calculating the trace of a, b, c spins in Fig. 2(a), the equation is represented by 1, 2, 3 spins. Then we generally set the factor of Δ as

$$T_{\triangle} = 1 + x(O_{12} + O_{23} + O_{31}) + y(O_{12}O_{23} + O_{12}O_{31} + O_{23}O_{31}) + zO_{12}O_{23}O_{31} + w(O_{12}^2 + O_{23}^2 + O_{31}^2),$$



Figure 2: Renormalization of a Sierpinski gasket.

where we set x, y, z, and w as the independent parameters. The renormalization transformation can be obtained by performing the partial trace. Using the decimation procedure, an exact real space renormalization group transformation for general n can be obtained in the fourdimensional parameter space (x, y, z, w). In the limit $n \to 0$, the transformation reduces as

$$\begin{aligned} x' &= x^2 + x^3 + 2xy + y^2 + 2x^2y ,\\ y' &= x^2y + 2xy^2 ,\\ z' &= w' = 0 . \end{aligned}$$
(6)

Eq. (6) has a fixed point at $x^* = (\sqrt{5} - 1)/2$, $y^* = z^* = w^* = 0$, and the eigenvalue can be found from the linearized transformation. Thus, $\lambda_T = 2^{1/\nu} = (7 - \sqrt{5})/2$ or $\nu = 0.7986 \cdots$.

P6) Show i) and ii). quoted from the Reference below

 \Rightarrow i) We first consider the mean-field equation appropriate to describe the reaction $A_1 + A_2 + \cdots + A_N \rightarrow \phi$

$$rac{\partial
ho_i(t)}{\partial t} = -k
ho_1(t)
ho_2(t)\cdots
ho_N(t)$$

where $\rho_i(t)$ is the density of the *i*th species at time *t* and *k* is a rate constant. When the initial densities of all reactants are equal, the asymptotic form of $\rho_i(t)$ is

$$\rho_i(t) \sim (kt)^{-1/(N-1)}$$
, for $d > d_c$.

We now turn our attention for $d < d_c$. For simplicity, we treat the three-body reaction, but the generalization to the N-body case is immediate. In analogy with the two-body reaction, we write a scaling form for $\rho_i(t)$ by assuming that the decay will be a power-law behavior for t less than the shortest time scale,

$$\rho_i(t) \simeq C_i t^{-\alpha} f_i(x_{23}, x_{13}, x_{12}) \,, \tag{7}$$

where $f_i(x_{23}, x_{13}, x_{12})$ is a scaling function of the dimensionless variables $x_{ij} = t/t_{ij}$, and C_i is a constant which depends on the initial conditions.

To determine α , it is useful to consider the particular initial condition $\rho_1(0) < \rho_2(0) = \rho_3(0)$, so that t_{23} diverges, while $t_{13} = t_{12} = \tau$. Eq. (7) can be written as

$$\rho_i(t) \simeq C_i t^{-\alpha} \bar{f}_i(t/\tau) \,, \tag{8}$$

where $\bar{f}(t/\tau) = f_i(0, t/t_{13}, t/t_{12})$, and α is assumed to be independent of the initial conditions. From the conservation of the particle density difference, $\rho_1(t) - \rho_2(t) = \rho_1(0) - \rho_2(0)$, and from Eq. (8), we have

$$(\rho_1(0) - \rho_2(0))t^{\alpha} = C_1 \bar{f}_1(t/\tau) - C_2 \bar{f}_2(t/\tau)$$

and $\rho_1(0) - \rho_2(0)$ can be rewritten as $(\sqrt{\rho_1(0)} + \sqrt{\rho_2(0)})\tau^{-d/4}$, from which we can immediately determine α and C_i to be

$$\alpha = d/4$$
, $C_1 = C_2 \simeq (\sqrt{\rho_1(0)} + \sqrt{\rho_2(0)})$

In the limit $\rho_1(0) \to \rho_2(0)$, the $t^{-\alpha}$ decay law will be recovered in Eq. (8). Therefor, we find $\rho_i(t) \simeq \sqrt{\rho_i(0)} t^{-d/4}$.

To generalize to the N-body decay for equal initial densities of the reactants, we choose the initial condition $\rho_1(0) < \rho_2(0) = \rho_3(0) = \cdots = \rho_N(0)$, and follow the same steps in 3-body decay. This gives $\rho_i(t) \simeq \sqrt{\rho_i(0)} t^{-d/4}$ for $d < d_c = 4/(N-1)$.

ii) We can apply scaling to the single-species $NA \rightarrow \phi$. The scaling form in Eq. (8) may be written as

$$\rho_A(t) \simeq \rho_A(0) f(t/\tau),$$

and we postulate that $\rho_A(t)$ will be independent of the initial density as $t \to \infty$. This condition immediately fixes the decay law to be $\rho_A(t) \sim t^{-d/2}$ for $d < d_c = 2/(N-1)$, while the mean-field decay of $t^{-1/(N-1)}$ should hold for $d > d_c$.

P7) Suppose that the cluster size dis. at t = 0 is given by $c_k(0) = bk^{-\gamma}$, where $2 < \gamma < 3$. Solve the generating function g(z,t) and $c_k(t)$.

 \Rightarrow In the limit $z \rightarrow 1$, the generating function g(z,0) is asymptotically related by

$$g(z,0) = \sum_{k=1}^{\infty} c_k(0) z^k = \sum_{k=1}^{\infty} b k^{-\gamma} z^k = 1 + b \Gamma (1-\alpha) (1-z)^{\alpha-1}.$$
 (9)

Using Eq. (9), taking the limits $t \to \infty$ and $z \to 1$, and keeping only the leading term, the generating function becomes

$$g(z,t) = (1+t)^{-2} \frac{g(z,0)}{1 - [t/(1+t)]g(z,0)}$$
$$\simeq \frac{t^{-1}}{1 + Ct(1-z)^{\alpha-1}},$$

with $C = -b\Gamma(1 - \alpha)$. From the grouping of variables in the denominator, we identify the scaling variable as $w = k/(Ct)^{1/(\alpha-1)}$, and

$$c_k(t) \simeq t^{-1} (Ct)^{-1/(\alpha-1)} f_\alpha(w) ,$$

as the scaling form of the mass distribution. Indeed,

$$g(z,t) = \sum_{k=1}^{\infty} c_k(t) z^k \simeq t^{-1} \int_0^\infty dw f_\alpha(w) e^{-ws} = \frac{t^{-1}}{1 + s^{\alpha - 1}},$$

where $s = (Ct)^{1/(\alpha-1)}(1-z)$. Hence the scaling function $f_{\alpha}(w)$ is the inverse Laplace transform of $(1+s^{\alpha-1})^{-1}$.

P8)

$$M_1(t) \xrightarrow{t \to \infty} \begin{cases} ? & \text{for } d = 1, \\ ? & \text{for } d = 2, \\ ? & \text{for } d = 3. \end{cases}$$

 \Rightarrow The mass distribution is simply the superposition of Gaussian propagators due to all sources from t = 0 until the present:

$$M_1(\mathbf{r},t) = J \int_0^\infty \frac{dt'}{(4\pi Dt')^{d/2}} e^{-r^2/4Dt'}.$$

Using the substitution $x \equiv r^2/(4Dt')$,

$$M_1(\mathbf{r},t) = \frac{Jr^{2-d}}{4D\pi^{d/2}}\Gamma(\frac{d}{2}-1,\frac{r^2}{4Dt})\,,$$

where Γ is the incomplete gamma function. The solution in the limits $r \ll Dt$ leads to

$$M_{1}(t) \xrightarrow{t \to \infty} \begin{cases} \sqrt{\pi} r \Gamma(-\frac{1}{2}, \frac{r^{2}}{4Dt}) = 4\sqrt{\pi Dt} & \text{for } d = 1, \\ \Gamma(0, \frac{r^{2}}{4Dt}) = -\gamma_{E} - \ln(\frac{r^{2}}{4Dt}) + \mathcal{O}(\frac{r^{2}}{4Dt}) & \text{for } d = 2, \\ r^{-1} \pi^{-1/2} \Gamma(\frac{1}{2}, \frac{r^{2}}{4Dt}) = r^{-1} & \text{for } d = 3, \end{cases}$$

where $\gamma_E \simeq 0.577215$ is Euler's constant.

References

K. Kang, P. Meakin, J. H. Oh, and S. Redner, "Universal behavior of N-body decay processes," J. Phys. A, vol. 17, pp. L665-L670 (1984).