# 6.C.I. Examples

#### (a) One Free Particle on Line of Length L

The phase space is 2-D. "Surface" of constant energy *E* is composed of two line segments of length *L* at  $p = \pm \sqrt{2 m E}$ , where *m* is the mass of the particle.

If we erect an impenetrable wall on each end of the line so that *p* reverses sign at them, the system is ergodic.

If we impose a periodic boundary condition so that the line closes on itself and becomes a circle, p remains unchanged indefinitely. The system is therefore non-ergodic. This is also the case for impenetrable boundaries if  $L = \infty$ .

Boundary conditions are therefore crucial in the determination of ergodicity.

## (b) One Free Particle on Square of Edge L

The phase space ( $\mathbf{x}$ ,  $\mathbf{p}$ ) is 4-D. The surface  $S_E$  of constant energy E is 3-D. The projection of  $S_E$  onto the  $\mathbf{x}$ -space covers the whole square. The projection of  $S_E$  onto the  $\mathbf{p}$ -space is a circle of radius  $\sqrt{2mE}$ .

As in §(a), the system is non-ergodic if  $L \rightarrow \infty$  or periodic boundary conditions are imposed.

For impenetrable walls, the component of the particle momentum perpendicular to the wall reverses sign upon impact, thus allowing the phase point to jump to a different part of the circle in *p*-space. If the ratio  $p_x/p_y$  of the initial momentum is an irrational number, the motion is ergodic. If  $p_x/p_y$  is rational, the motion is periodic and hence non-ergodic. Since the set of rational numbers is a subset of zero measure in the set of real number, the system is ergodic.

## (c) Two Free Particles on Square of Edge L

By free particles we mean

- 1. There is no external forces.
- 2. The particles do not interact except when they collide.

The phase space  $(x_1, p_1, x_2, p_2)$  is 8-D. The surface  $S_E$  of constant energy *E* is 7-D. The projection of  $S_E$  onto the  $x_i$ -space covers the whole square. The projection of  $S_E$  onto the  $(p_1, p_2)$ -space is the 3-D spherical surface  $S^3$  of radius  $\sqrt{2mE}$ .

If we neglect collision effects, each particle will behave as described in §(b). Since each  $p_i$  stays in a fixed circle of radius  $\sqrt{2mE_i}$ , where  $E_1 + E_2 = E$ , the system is non-ergodic.

Collision provides a mechanism for momentum-exchange between the particles and hence ergodic motion.

The effects of collisions on two hard balls on a plane is described in

"TwoBallsOnBoundedPlane.nb"

Denoting a phase point as

 $\boldsymbol{X} = (\boldsymbol{x}_1, \, \boldsymbol{p}_1, \, \boldsymbol{x}_2, \, \boldsymbol{p}_2) = (x_1, \, y_1, \, p_{1x}, \, p_{1y}, \, x_2, \, y_2, \, p_{2x}, \, p_{2y})$ 

 $= (X_1, ..., X_8)$ we study the evolution of a set of  $3^8 = 6561$  phase points with initial coordinates

 $X_i = X_{i0} + j\Delta$  i = 1, ..., 8 j = -1, 0, 1

where  $X_0$  is a phase point depicting two hard balls about to collide and  $\Delta$  is the separation between neighboring phase points.  $\Delta$  is chosen such that some of the phase points correspond to configurations of no collision.

The following graphs are projections of X(t) onto the 3-D sub-spaces  $(x_1, y_1, p_1) \& (p_{1x}, p_{1y}, x_1)$  at 3 different times:

blue dots: initial time. magenta dots: right after collisions begin.

red dots: sometime after.



Note that phase points corresponding to no collision between the balls evolve close to each other and occupy, at all times, a volume of constant size in the sub-space. Those corresponding to collision spread out rapidly after collision occurs.

Reminder: In the 8-D phase space, the size of the volume occupied by any set of phase points is a constant in time.

### (d) Conclusion

The foregoing consideration can be easily generalized to the case of a general system.

Consider an N-particle system with a Hamiltonian

$$H = H_0 + V$$

where  $H_0 = \sum_{i=1}^{N} h_i$  is a sum of non-interacting 1-particle Hamiltonian  $h_i$  and V denotes inter-particle

interactions. Note that *h* contains all external potentials and perhaps the 1-particle average of interparticle interactions.

The straight line trajectories of the free particles can be generalized as follows.

For a given 1-particle energy  $E_i$ , the solutions of  $h_i$  will give trajectories on the constant energy  $(x_i, p_i)$  subspace in the phase space. Since these trajectories (for all possible  $E_i$ ) are solutions of differential equations of single particles, they are unique (non-crossing) and covers the whole  $(x_i, p_i)$  subspace.

The constant energy surface  $S_E$  is covered by these 1-particle solutions in the same manner as the free particle trajectories. Thus, reflective boundary conditions are necessary for the trajectories to cover the configuration sub-space ( $x_1, ..., x_N$ ).

Inter-particle interactions V is the generalization of collisions and allow a phase point to cross between 1-particle trajectories of different  $E_i$ , and hence possible ergodicity.

Consider now the projection of  $\rho(\mathbf{X})$  onto the 1-particle sub-space  $\rho_1(\mathbf{x}_1, \mathbf{p}_1)$ . As can be seen in the two-hard-ball example, the evolution of the exact  $\rho_1(\mathbf{x}_1, \mathbf{p}_1, t)$ , as governed by the Liouville equation, is rather complicated. However, the evolution of  $\rho_1^0(\mathbf{x}_1, \mathbf{p}_1)$  for a set of non-interacting particles is trivial. This suggests another way to derive the equation of motion for  $\rho_1$ .

Thus, instead of following the actual motion of a fixed set of phase points, we can follow a volume  $\Delta \mathbf{X}$  of fixed size that moves according to  $H_0$ . The effect of *V* is then expressed as the scattering of phase points into and out of  $\Delta \mathbf{X}$ . The result is the Boltzmann transport equation [see Chap.11]. Note that ergodicity is no longer an issue in this approach.