Interacting Classical Gas

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September 5, 2016

Contents

1 Preparation

1.1 Scaling behaviour

We investigated the classical gas in harmonic trap with a repulsive interaction. We chose one of the simplest types of interaction:

$$F = \begin{cases} F = F0 & , x < \sigma \\ F = 0 & , x > \sigma \end{cases} \tag{1}$$

$$H = \frac{1}{2} m \omega_0^2 \sum_i x_i^2 + \frac{1}{2} m \sum_i v_i^2 + \sum_{|x_i - x_j| < \sigma} F_0 \left(\sigma - |x_i - x_j| \right) \tag{2}$$

It can be easily shown that eq.2 can be rewrite into the following form:

$$\tilde{H} = \frac{1}{2} \sum_i \tilde{x}_i^2 + \frac{1}{2} \sum_i \left(\frac{d\tilde{x}}{d\tilde{t}} \right)^2 + \sum_{|\tilde{x}_i - \tilde{x}_j| < 1} F_0 \left(1 - |\tilde{x}_i - \tilde{x}_j| \right) \tag{3}$$

with the transformation:

$$\begin{cases} \tilde{H} &= \dfrac{H}{m \omega_0^2 \sigma^2} \\ \tilde{x}_i &= \dfrac{x_i}{\sigma} \\ \tilde{t} &= \omega_0 t \\ \tilde{F}_0 &= \dfrac{F_0}{m \omega_0^2 \sigma} \end{cases} \tag{4}$$

In this manner, we reduced number of the parameters in our model into three: $\tilde{H}$, $\tilde{F}_0$, N. Equivalently, we set σ, ω and m to 1 in our numerical simulation. Throughout, we will use "E" and "F_0" to denote their reduced version $\tilde{H}$, $\tilde{F}_0$.

2 Thermalization

2.1 Dynamics Study

It is natural to think that a many-body system with interaction will be thermalized in "usual" case. To study the condition of thermalization is equivalent to find out the mechanism that prohibits the system from ergodic. In view of this, we begin the study with two-particle motion.
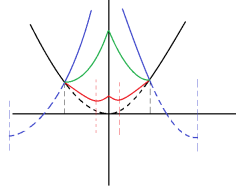
Figure 1: effective potential for two-particle system

two-particle   To see the way interaction change the orbit (energy level) of the particles, we had better start from two-particle case.

We can always think of them in the reference frame of their center of mass "C". In frame C, one can easily show that when there is no interaction, what we will see is that two particles are bound together by a harmonic trap center at C(cf). So their relative motion is also a harmonic oscillation.

In this case, the system has two frequency components. The first one is the frequency of C, which is just ω_0 . The other one is the frequency of their relative motion ω_r, which is slightly deviated from ω_0. The deviation grows with the increase of F_0 and the decrease of internal energy of the pair. As a result, when the F_0 is small and when the E is large, a beat with frequency $\omega_r - \omega_0 = \delta$ will exist.

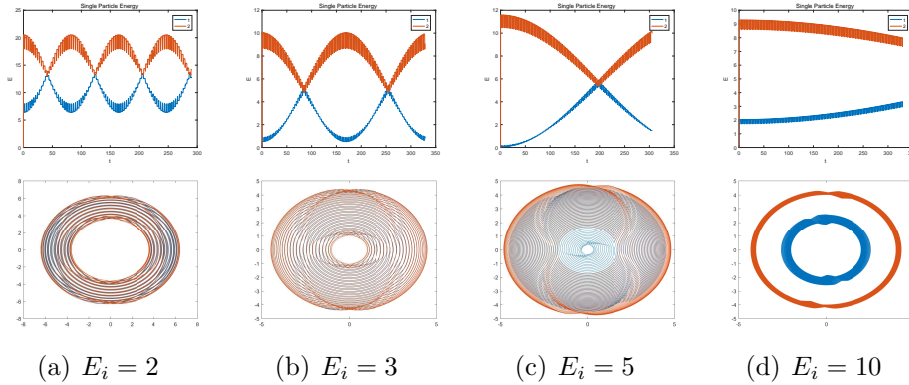(a) $E_i = 2$ (b) $E_i = 3$ (c) $E_i = 5$ (d) $E_i = 10$

Figure 2: the dependence of beat frequency on internal energy
the upper diagram is the energy of every particle, the lower diagram is the orbit in phase-space, where we see quasi-periodic motion clearly. Here, E_i is large(compare to $F_0\sigma$). In this case, the larger E_i is, the lower the beat frequency is. Actually in very low energy, we can retrieve a beat, but that is for different reason – it is a beat between ω_0 and $\frac{\omega_0}{2} + \delta$

More particles Now let's consider the three-particle case. For two parti-
cle, the motion is non-chaotic. On the other hand, intuitively, we will say
that three-body motion is chaotic so that the system could be "thermalized"
soon. However, in some cases, the time scale of thermalizing could still be
very long. Suppose two of them, say, A and B, has small internal energy,
which means their distance and relative velocity are both small. Meanwhile,
suppose particle C has some energy quite different from A & B. In this
case, A & B will often be in the interaction, while C will pass both of them
at a high speed in each period. How will energy transfer between C and
the two-particle system A and B? Since the relative velocity of C and the
two-particle system is usually large, C will pass A-B pair in a short time
τ ($\tau \ll \frac{2\pi}{\omega}$). When C pass A, it gives A a push, and then push A back.
As has been discussed in the two-particle case, this process is equivalent to
giving A a very small speed($\sim O(\tau)$) in the background of a trap. Since the
position and velocity of A and B are both close, the effect of C on A & B are
almost the same (difference$\sim O(\tau\sigma) \sim O(\tau^2)$). In this manner, the passing
of particle C only kicks the center of mass of the A-B pair slightly, leaving
the internal motion of the pair unaffected. In another word, the existence of
C will not have significant effect on the energy transfer between A and B,
but only "dance" with their center of mass. The physics of the "dance" is
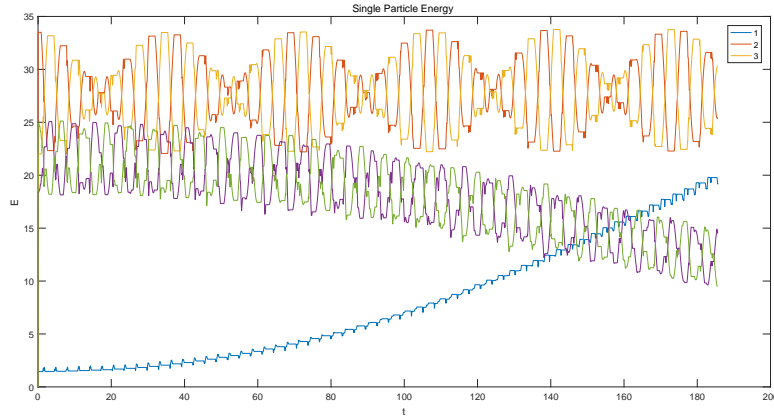similar to the dance between two particle.

Figure 3: evolution of single-particle energy

The argument above still holds in many-particle case. Once we start
from some configuration where n particles have a set of close energy levels
$\{E_n\}$ and another m particles have another set of energy levels close to each
other $\{E_m\}$, and $\{E_n\}$ is quite different from $\{E_n\}$, we will find these two

systems dancing together on the energy level diagram. The discussion above gives us some pictures about the non-ergodic state. For these state, life time is rather long so that once the system reach such configuration (or certain energy distribution), it will take a long time(more than 10^4 periods for N=5 case) to decay.

2.2 Thermalization condition

The main obstruct to get an thermalized state (which can be examined by observing distribution) is the low frequency oscillation mentioned before. Because once these modes are excited, the relaxing time could be very long($>10^4$). As a result, to achieve ergodic state, we have to avoid such low frequency oscillation. According to our discussion before, the solution is to make internal energy of each two-particle pair not "too large". Though it is impossible to express the internal energy of every pair in terms of the total energy E, we can estimate it by the energy interval, which is $\frac{E}{N}$. At least they are of the same order. The thermalization condition could be given by: $F_0\sigma \sim \frac{E}{N}$

As is shown in fig.4 above, the critical point for reaching Boltzmann distribution is $F_0 = 5$ while the energy interval of particles ~ 10, as we expected, they are of the same order. As a supplementary proof of our argument, fig.6 and fig.7 show the great difference of single-particle energy between $F_0 = 2$ & $F_0 = 10$ at $E = 100$, i.e. in the former one there is always some particle maintained at high excitation, while in the latter the system probably goes to ergodic. Till now, we have verified that the criteria of non-ergodic and ergodic state, which is $\frac{NF_0\sigma}{E} \sim 1$, and corresponding feature of their energy distribution.
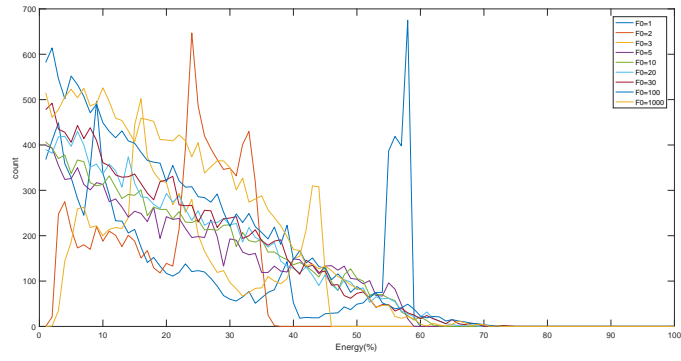
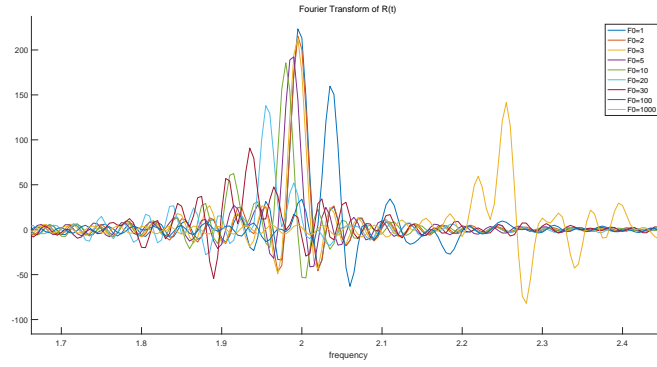Figure 4: Distribution $scanF_0, E = 100, N = 5, \sigma = 1$

Figure 5: Frequency scan F_0, $E = 100$, $N = 5$, $\sigma = 1$
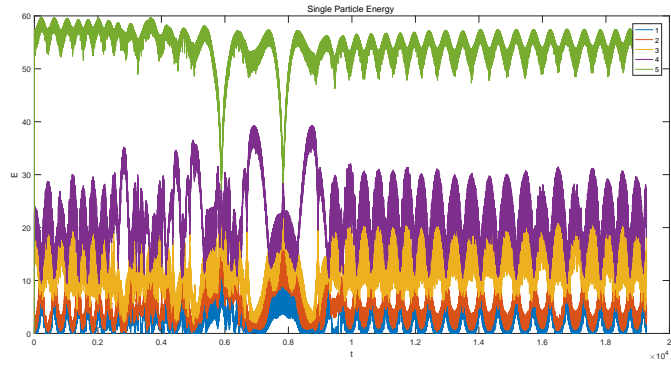
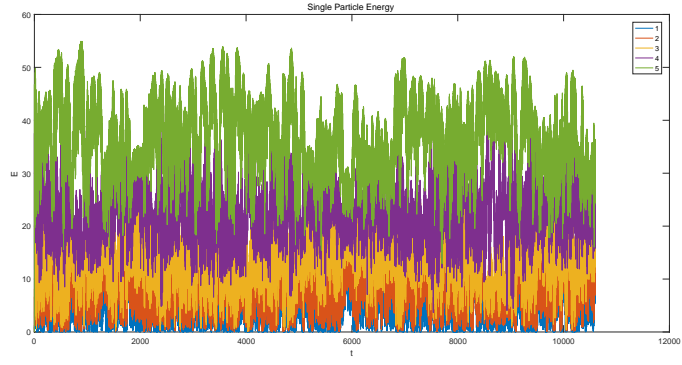Figure 6: energy of each particle, $F_0 = 2$

Figure 7: energy of each particle, $F_0 = 10$

2.3   Verifying Boltzmann distribution

Thermalization could have different definition. In our system, the "thermalization" we want to find means "losing all the memory of initial state". One of the most important information of initial state is energy distribution. We can check whether a system has gone to equilibrium by measuring its energy distribution.

energy distribution   For an isothermal system, the energy distribution of the whole system follows the Boltzmann distribution in equilibrium state. However, for an isolated system where the total energy is conserved, it not obvious to draw some strict conclusion about the distribution.

Intuitively, one will expect that if we measure the energy of a subsystem , e.g. one particle, then we will get a Boltzmann distribution because the rest part of the system serves as a bath for this particle. The temperature of this isolated system is defined according to $Nk_BT = E$. It is evident that this argument only hold when the energy of the single particle is not too big–if one particle has 50% of the total energy, the rest could no longer be think of as a good bath.

In the first picture below, we verify this argument by measuring the energy distribution of every particle at N=10 for different F0 at E=1000 (parameters here satisfy thermalizing condition). In the other two, we tested different N.

To take the first one as an example, Y axis is logarithmically scaled. X axis is the ratio between single particle energy (where half of interaction is taken into account) and total energy of the system. The blue dotted line is the predicted Boltzmann distribution (normalized according to counts). Notice that normalizing of the Boltzmann line only change the intercept, leaving slope untouched, which means the slope is the only thing to compare. In Energy ratio smaller than 30%, the experiment (colourful curves) fits well with the prediction. When energy of a single particle is higher, one can think of the "bath" formed by the remaining part has lower temperature, thus counts decrease faster to zero than Boltzmann law.
It is evident form $Nk_BT = E$ that the slope of Boltzmann distribution in this figure only depend on N. That is the reason why we want to measure at different N below.
In fig.9 and fig.10, the curve is slightly deviated from the standard Boltzmann distribution, which is probably due to the contribution of density of states. Possibility is proportional to Boltzmann exponential factor multiplied by density of states. The reason why we did not take DOS into account previously lies in that the DOS is a constant for simple
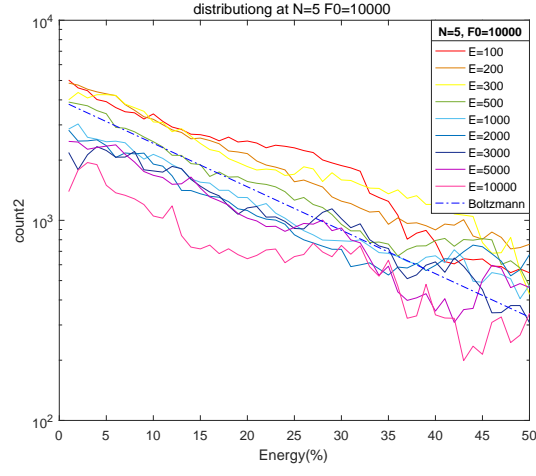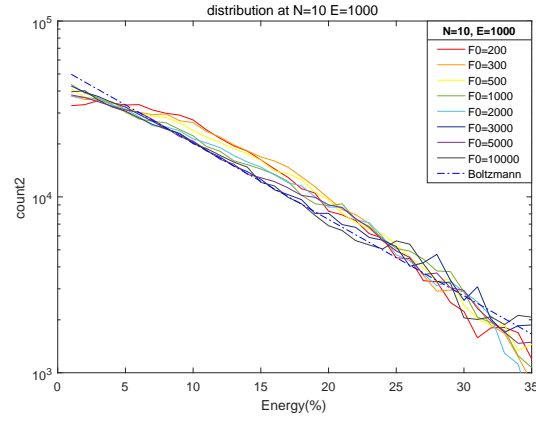
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Figure 8: Energy distribution, N=5, F0=10000

Figure 9: Energy distribution, N=10, E=1000
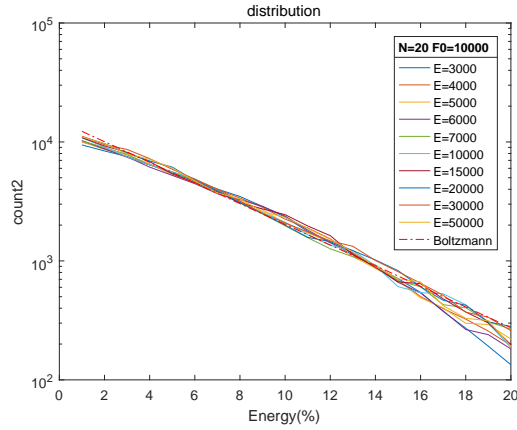

Figure 10: Energy distribution, N=20, F0=10000

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harmonic oscillator. However, for simple harmonic oscillators with short range interaction, the energy shell is deformed in the region of $|x_i - x_j| < \sigma$ so that the DOS is no longer a constant. But since $\sigma << R$, one can think of this as a small modification. Therefore, the tendency of the curve in fig.9 and fig.10 is deviated slightly from Boltzmann distribution.

3 Relaxation in Phase-space (unfinished)

Till now we have verified the energy distribution will go to Boltzmann distribution. However, even if a system have reached Boltzmann distribution, it doesn't mean that the system has completely "forgotten" its initial state. There is other information that could still exist, for instance, the shape of distribution cloud in phase-space. One of the reasons why we care about this quantity is that it has a strong effect on breathing behaviour. For instance, if the distribution cloud is a thin ellipse (all particles oscillate in phase), the amplitude of oscillation of the cloud radius will be very large. On the contrary, if the cloud is a circle (particles phase of oscillation are completely random), we will not see oscillation at all. Going to equilibrium not only require the thermalization mentioned in last section, but also require reaching a stable configuration in phase-space distribution (relaxation).

Shape of Distribution in Phase-space   If the oscillating phases of particles are highly correlated, for example, initial state with zero velocity, the shape of cloud will be a thin ellipse. If the phase of oscillation is completely random, the cloud should be isotropic in phase space. In view of this, we defined a shape factor S:
$S = \frac{a-b}{a+b}$, where a and b are long axis and short axis of inertia ellipse in phase space respectively. a,b can be calculated by diagonalizing the inertia matrices I: $I_{xx} = \sum x^2, I_{xp} = I_{px} = \sum xp, I_{pp} = \sum p^2$ S=1 for line-shape distribution, S=0 for circular distribution. The time evolution of S will probably show how fast the distribution "forget" its initial shape.
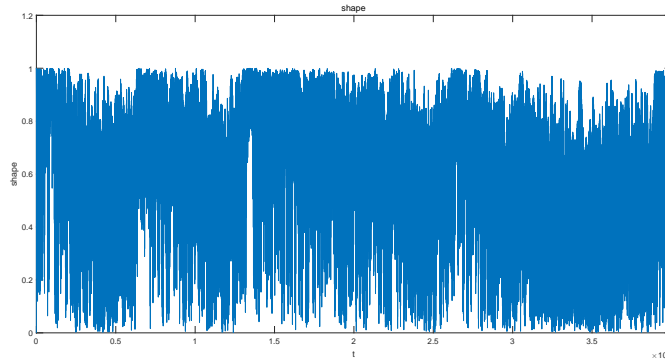

Figure 11: N=5,F0=10000,E=1000, initial S=1

From fig.13, no evidence shows the shape of cloud will converge. Maybe the fluctuation of S is so large that make it hard to identify the convergence
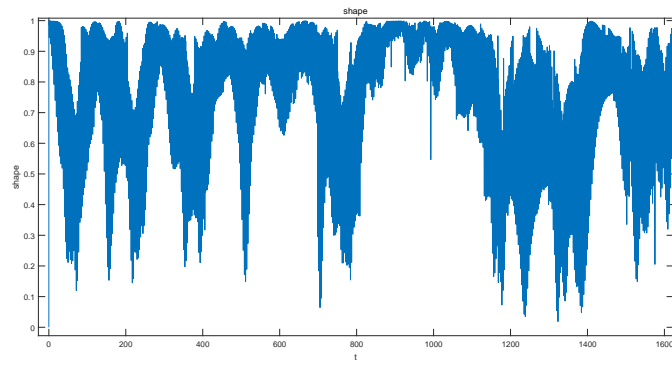
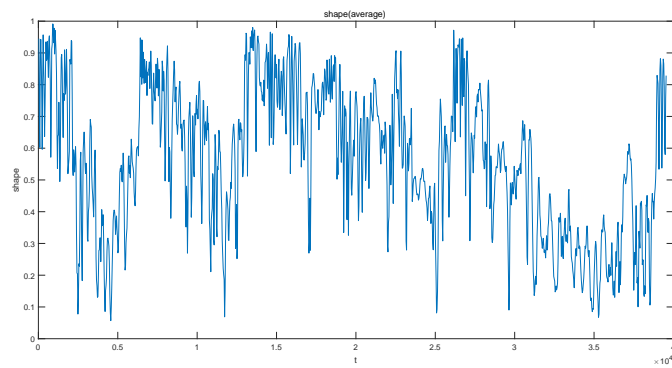Figure 12: Zoom in at the beginning part

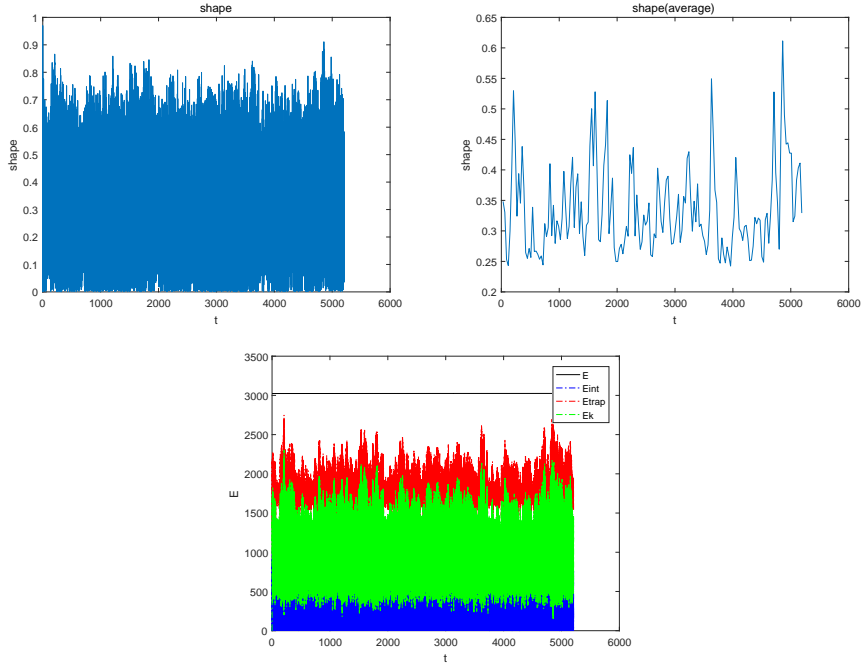Figure 13: average over every 30s to see the main tendency

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Figure 14: N=20, F0=1000, E=3000, initial S=1
Different from N=5 case, this time the fluctuation of S is not that large. In return, with an average over every 30s, the S only fluctuate between 0.5 and 0.2

of S. The only way to solve this problem is using more particle simulation to suppress the fluctuation, while the cost is that the simulation time will be limited.

For N=20(fig.15), the S start evolving from 1 will soon decay and start fluctuating around some lower value(0.1-0.5, perhaps dependent on temperature). To tell whether this value correspond to a stable state of the system, we can set the initial state S to be other value (e.g. zero) to see whether it will come back to the same stable value(see fig.??).

We may zoom in to understand how the distribution cloud is deforming. in fig.17, we can see some peaks and dips. The peaks are generated by particle "bumping" (collision process discribed in Breathing frequency, see fig.20) along the short axis of the cloud, while the dips are generated by "bumping" along the long axis. Since these bumping only means momentum exchange, after a whole bumping process, the distribution should almost come back. So these peaks and dips will not affect the plateau value, as is shown in fig.17

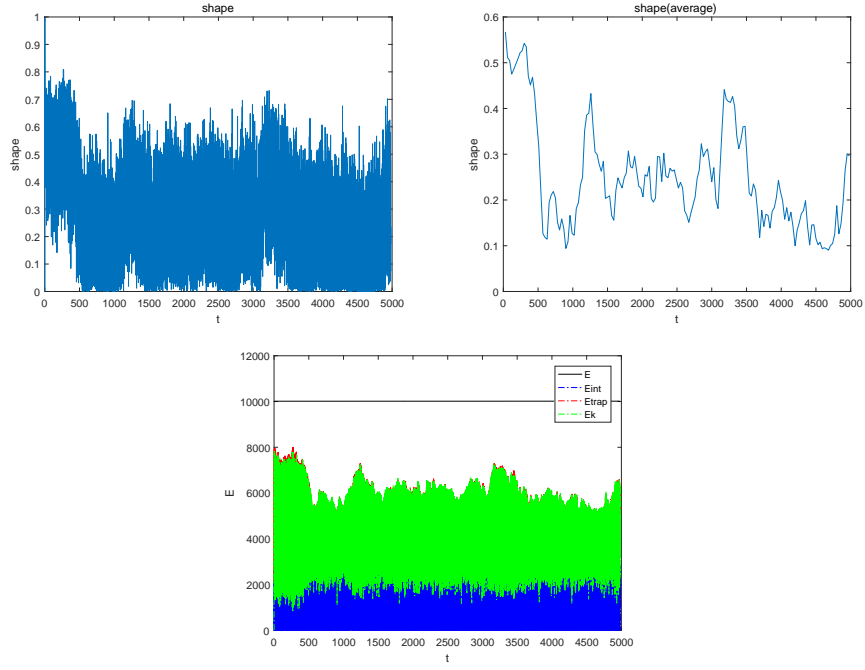In view of this, we take average of a short time to clear this peaks and
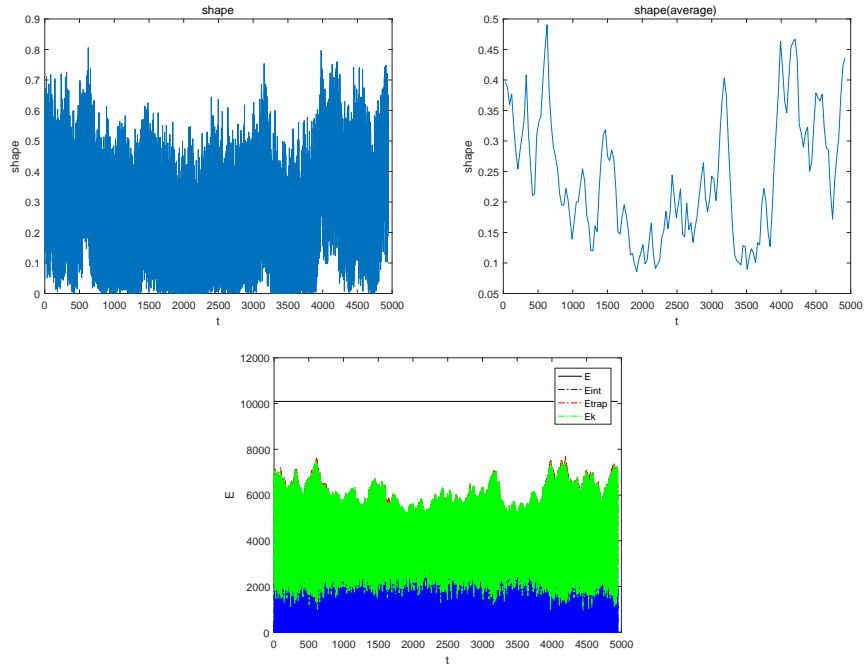
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Figure 15: N=20, F0=1000, E=10000, initial S=1

Figure 16: N=20, F0=1000, E=10000, Initial S=0.05
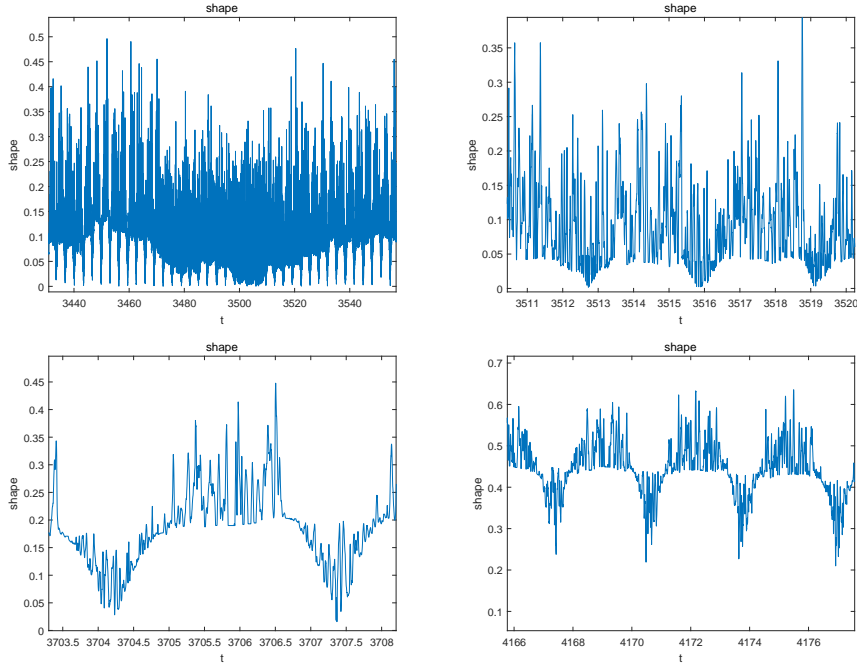
Figure 17: t=5E3, N=20, F=1000, E=10000, initial S=0, zoom in

dips in order to see the time evolution of the overall value of S (the second picture in fig.14,15,**??**).

However, there is still no sufficient evidence of convergence for the overall value of S for N=20.

3.1 Correspondence between energy distribution, behaviour of shape-factor and oscillation of R(t)

3.2 Lyapunov Exponents(unfinished)

Lyapunov exponents describes how fast one orbit diverge from its nearby orbits in phase-space. The largest LE reflects the time scale that system lose its memory in phase-space. We will measure the largest LE along our trajectory and plot its distribution.
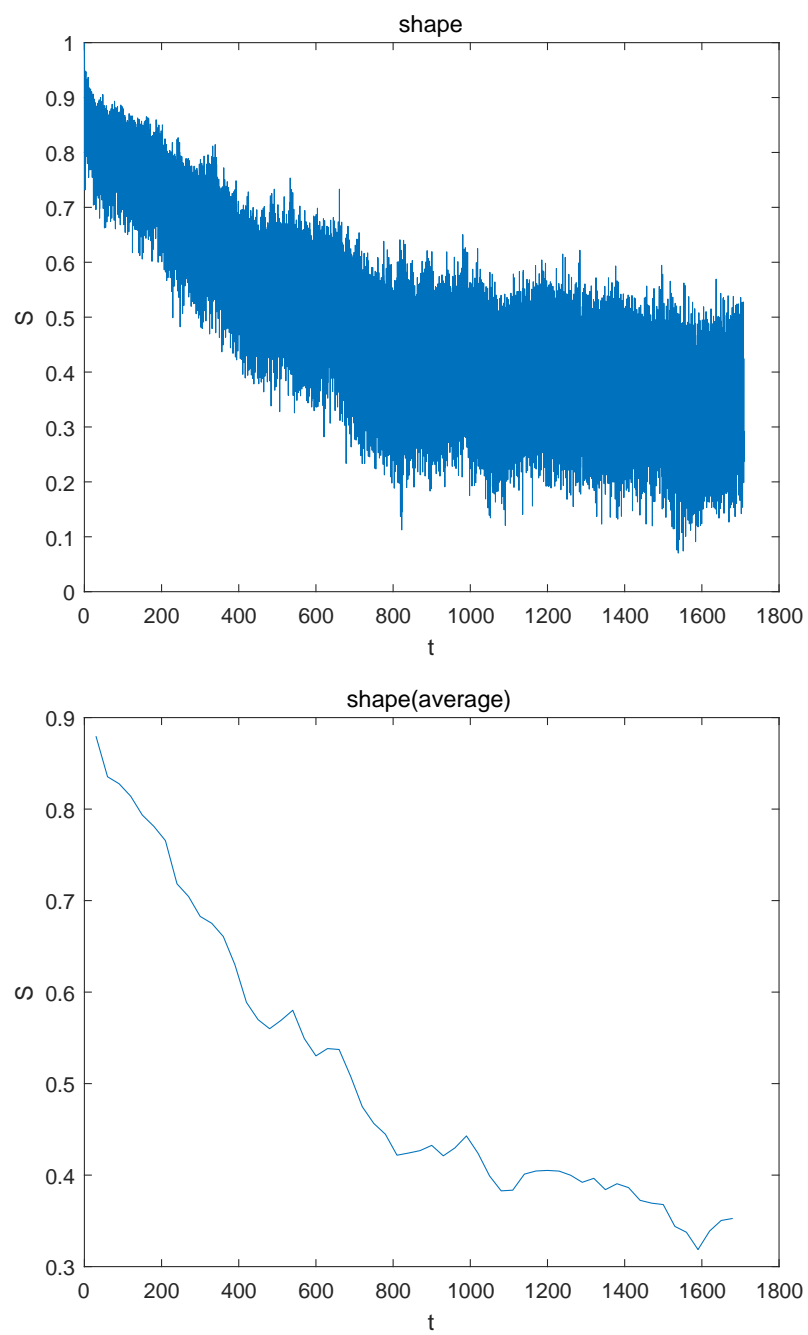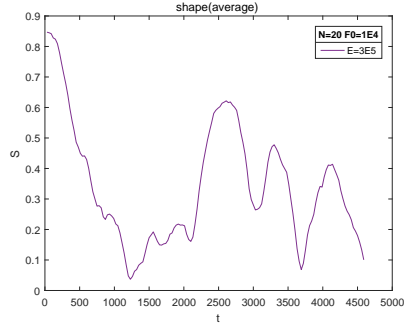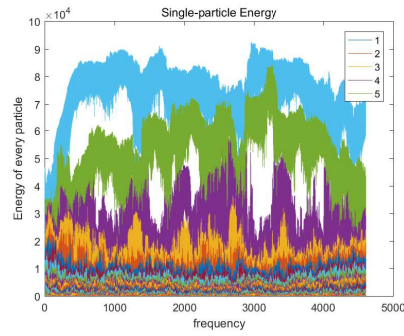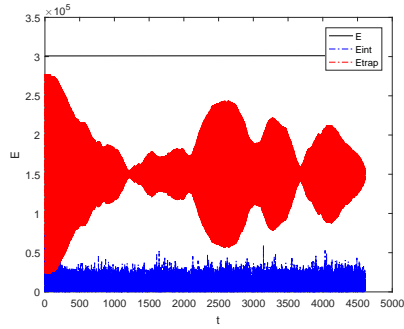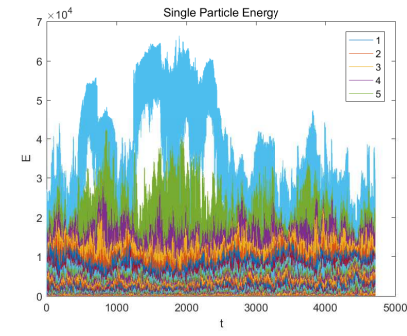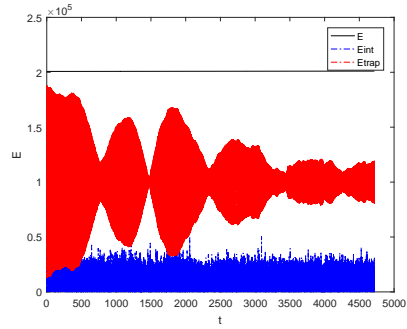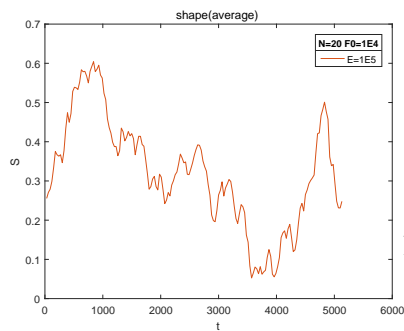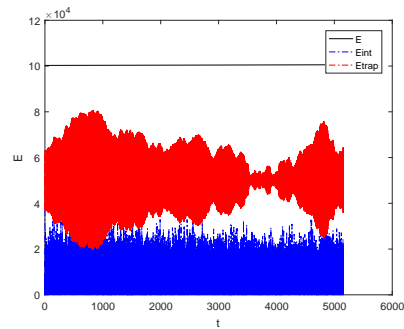
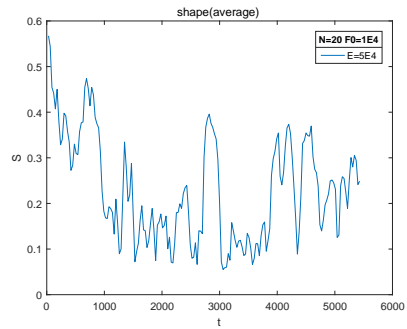Figure 18: N=50, E=20000, F0=10000 ,t=1500

(a) $E = 3E5$

(b) $E = 2E5$

(c) $E = 1E5$

(d) $E = 5E4$

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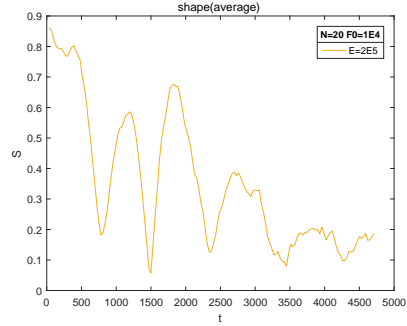
4 Breathing Frequency

Usually, to see the response of a quantum gas to a quench, one start from the ground state and suddenly vary some parameter by a little, for instance, $\omega_0' \to \omega_0 = \omega_0' + \Delta\omega$. In that case, one will observe the radius R oscillating at a certain frequency, which is usually called "breathing mode". In classical version, the ground state may be meaningless–since classical limit is $\bar{h} \to 0$, no matter how low the kT is, $kT/\bar{h}$ is always zero so that classical ground state is quite different from the quantum one. Instead, one will expect that the thermalized high temperature classical gas may have something in common with the high excited state of quantum gas. In view of this, if we want to do a quench similar to quantum case, we should begin with a thermalized distribution at ω_0' and evolve to a new thermalized state at varied ω_0. Furthermore, notice that X and P (normalized) are symmetric for harmonic oscillator. If there is no spontaneous symmetry breaking in phase-space, the distribution cloud should be circular when the gas is completely thermalized. The difference between thermalized cloud before and after quench is circular under different normalization of phase-space. If we look at both of them in the phase-space normalized according to ω_0, we will find the former one is an ellipse while the latter one is a circle. If the ellipse is only slightly deviated from circle, the oscillating amplitude will be too small to be distinguished from noise. Therefore, we start from an extreme case – line distribution (random x, zero p) and observe the oscillation of R(t).

Without interaction, the breathing mode frequency is exactly 2. When there is interaction, the frequency will drift to some other value near 2. We measure the radius of the cloud $R(t)$ and get the frequency spectrum of its oscillation behaviour by Fourier transform. Then we take the peak frequency near 2 as the breathing mode frequency. The frequency measured in different E and F_0 is shown in the Fig.19.

Before discussion about the mechanism of δ, let us first introduce a approach to simplify this problem:

4.1 Rotating frame in Phase-space

Traditionally, we think of there is a distribution cloud in phase space, and due to harmonic trap, the cloud will rotate at frequency ω_0. When there is interaction, we may think there is a small modification of the frequency $\omega = \omega_0 + \delta$. Now we want to understand how δ is dependent on parameters, so it is better to stand in the rotating frame in the phase space. In this frame, the picture we will see is as follow:
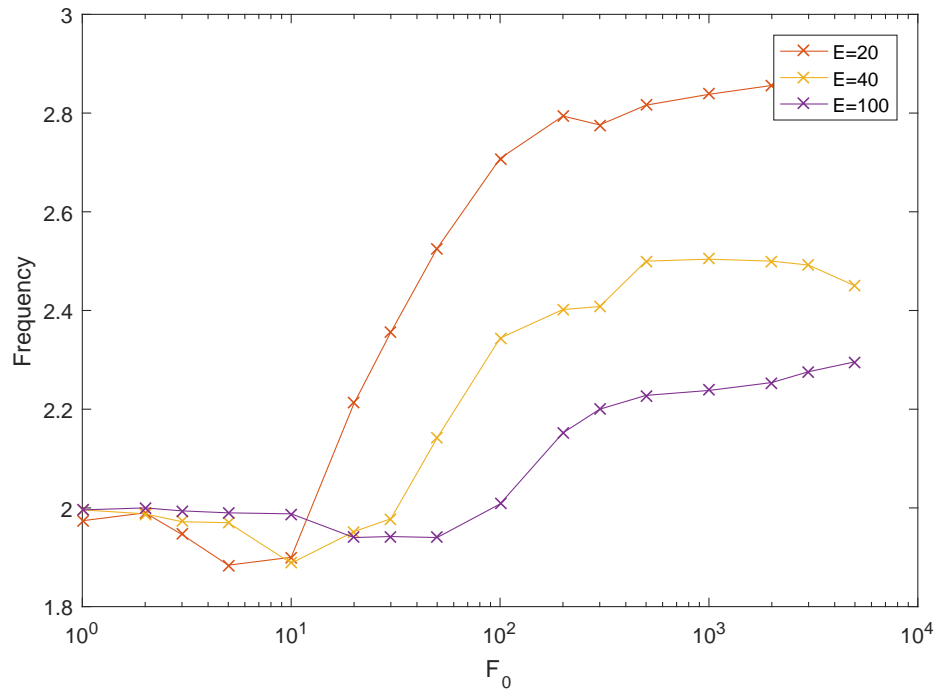
Figure 19: breathing mode frequency measured at different E and F_0

* All particles are stationary when there is no interaction.

* The real X and P axis are rotating counter-clockwise, using real X axis to measure distance between particles to determine the interaction at each moment.

* When there is interaction, particles will gain a "velocity" in phase space: $\dot{P} = F/m$. Other effects are all cancelled by frame rotation.

This picture is actually a classical version of the interaction picture. With this picture, we will soon find the dynamic analysis greatly simplified.

In our system, we choose initial velocity to be zero, which means, the particles are aligned on $X|_{t=0}$ axis in phase-space at the beginning. If the breathing frequency of the system is $\omega = \omega_0 + \delta$, we will expect to see a line (which may gradually deform into an oval cloud or even an isotropic cloud) rotating at δ in rotating frame. If we plot x-p with t, we expect to see a spiral motion. Since the motion we see is an additional rotation in rotating frame, we will call it precession. This precession directly leads to the δ.
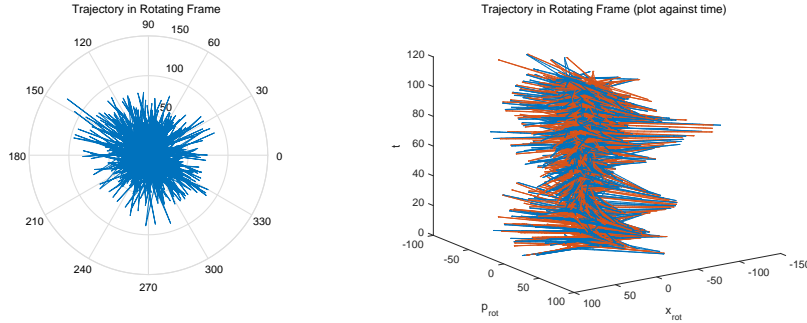

Figure 20: precession motion in phase-space observed in rotating frame (only show one or two particles' trajectory for clarity)

4.2 Estimating Breathing Frequency

What mechanism leads to the precession motion? To answer this question we may turn to two-particle case first. When interaction is very strong, the effect of interaction is equivalent to exchanging momentum when two particles approach each other at distance σ. In the rotating frame in phase-space, this process can be interpret as follows:

Two particles flip to another line(thick gray line) which deviate a small angle α away from original configuration. Similar process happen when there
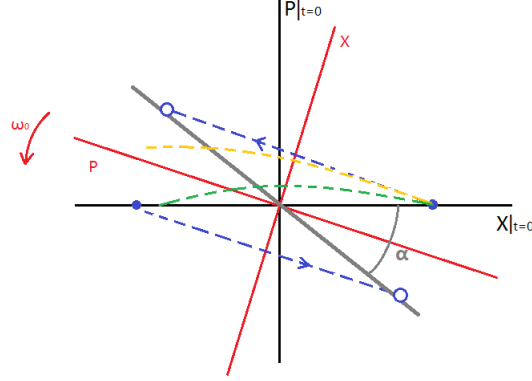
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Figure 21: a schematic diagram of the collision process

are more particles. In every period of harmonic oscillation, each particle meet N particles and collide 2N times, while half of the collisions (N times) are between particles with huge difference in momentum, which is just the process shown in figure21. (As for the remaining half of collisions, colliding particles have small difference in their momentum. Let us say, both particles have positive momentum. In fig.21, it can be shown that two particles on the same half of the P-axis cannot have strong effect on the rotation of distribution.)

Let us estimate the precession angle α with $\frac{\sigma}{R}$, which follows from the two-particle analysis. Radius of the cloud R can be estimated according to $E = Nm\omega_0^2 R^2$ We will get the precession angular velocity

$$\delta = 2\omega_0 \frac{N^{\frac{3}{2}} m^{\frac{1}{2}} E^{-\frac{1}{2}} \sigma \omega_0}{2\pi} \tag{5}$$

When F0 is not that large, the frequency behaviour seems complicated (see fig.19). Usually, when F0 increase, frequency goes down below 2 first and then rise up and converge to some value higher than 2. The reason could also be well understood with the mechanism described before. In the former discussion, we goes to high F0 limit, which means particles exchange momentum in infinitesimal time. For F0 is not very big, the finite interaction time should be taken into consideration. During this time, the behaviour of each particle in phase space is exactly moving along the direction of the real P axis at 'velocity' $F0/m$. Since the real P axis is rotating counter-clockwise, the particle will follow the circular trajectory(orange and green dashed line
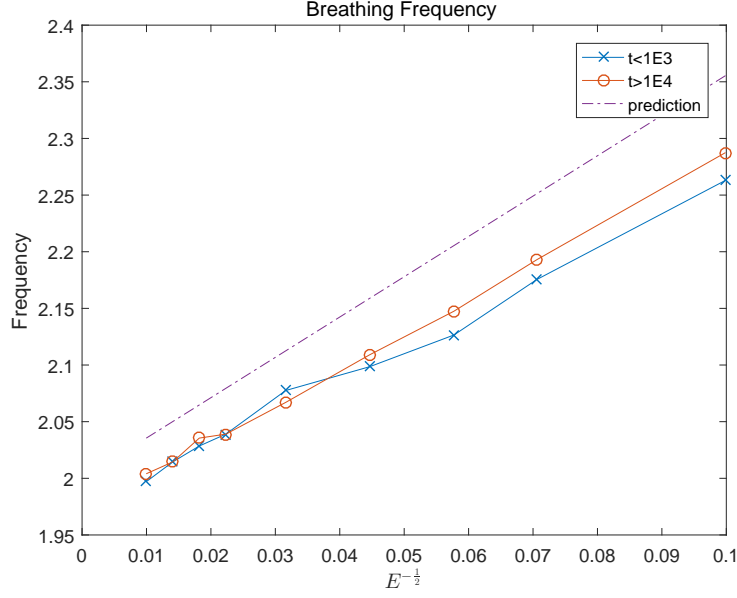
Figure 22: Frequency measured at N=5

Since the prediction is only an estimation by order, which means there could be some extra effective coefficient before the R. In view of this, the result is satisfying.
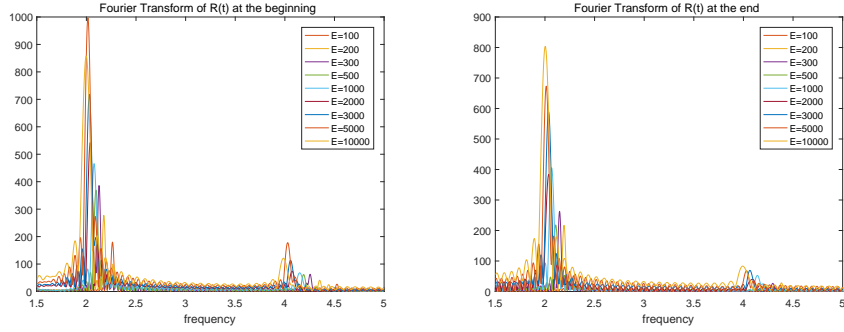

Figure 23: Spectrum at the beginning and the end of measurement

Two spectrum above show the error of our frequency measurement. The line width of the peak is significant compared with the δ. The peak width comes from FT in finite time.
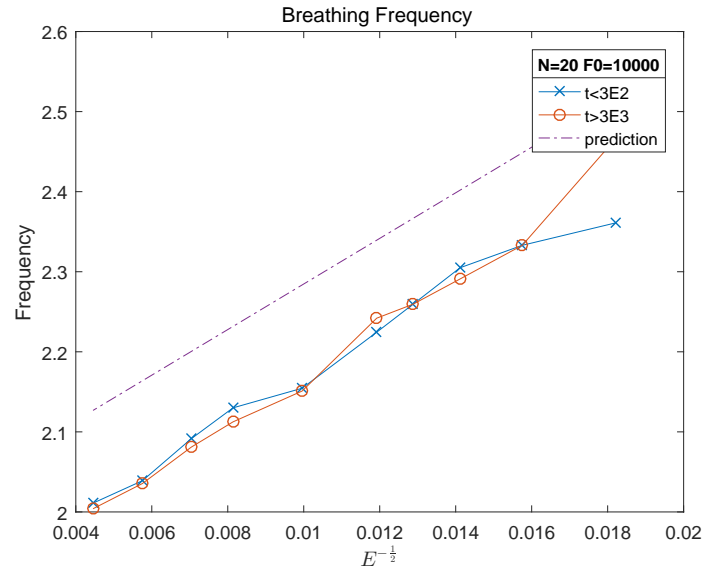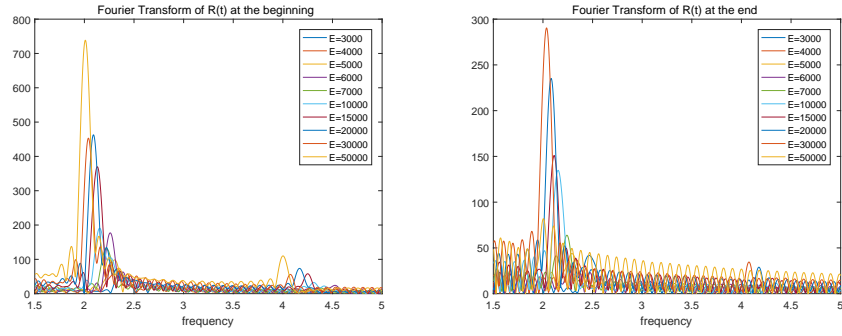
Figure 24: N=20

in fig.21) the α that we once use to estimate the precession motion should decrease with the increase of interaction time. There should be some "critical point" where α goes from plus to minus (dashed green line). At this point, we will see the precession stop so that the frequency is 2. Thus the relation between frequency and F0 shown in fig.19 is well explained.
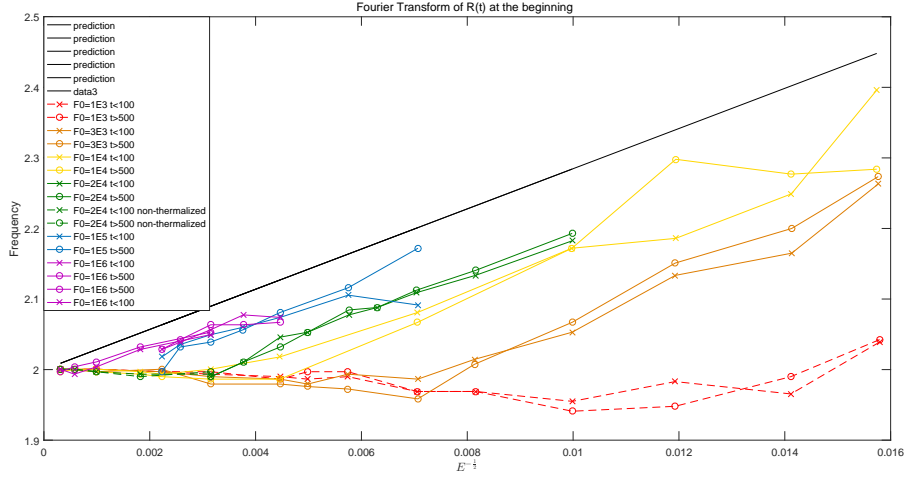

Figure 25: frequency for N=20

Before completing the discussion, it is necessary to point out that none of the argument here require "energy thermalization". In addition, if the system is completely thermalized in terms of their phase of orbit in phase space, the argument will no longer work – there is a stable isotropic distribution in phase space, no matter how the cloud rotate, no oscillation can be observed.

5   Supplement

The picture of breathing frequency is simple in real space. When two particle bounce, they exchange momentum immediately. It can be interpret as particle A carries its momentum P_A and jump σ to the right, while particle B carries its momentum P_B and jump σ to the left. In this manner, every collision will save a particle some time $\frac{\sigma}{v}$. Since v is proportional to R while the number of collision each particle experiences in one period of harmonic oscillation can be estimated by N, we will retrieve $\delta \sim N^{\frac{3}{2}}E^{-\frac{1}{2}}$.

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