Senior Research Project Final Report: Quantum Simulations of a Particle in a Time-Dependent Ratchet Potential

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A particle in a time-dependent ratchet potential is analyzed in this work. The potential is periodic and changes with time. In particular, a broken spatial-temporal symmetry is implemented on the particle to achieve direct transport. As shown by recent experiments [1], cold atoms in optical lattices in a ratchet potential driven by laser fields have successfully demonstrated the transportation of the relevant particles. This is usually achieved by a bi-harmonic AC force that generates a uniform directed motion of the confined particle. However, so far, the theoretical background is usually explained with classical particles. With this work, we explain the ratchet effect with quantum particles using numerical simulations, including dissipative effects.

1. Introduction

The transport phenomena of microscopic particles has been the subject of many studies [2]. In the case of the ratchet potentials, given a bi-harmonic AC driving field, it is shown that the subjected particles display directed motion [1]. This is also called a Brownian motor for classical particles since it favors motion in one direction using the free diffusion supplied by a thermal bath[4]. Although most of the work done is for classical particles, there have been some studies covering quantum particles inside the ratchet potential. It has been shown that it is not possible to observe the ratchet effect in equilibrium systems, and thus the equilibrium must be disturbed by an external perturbation to the system in order to sustain a net flow of the particle in one direction[3].

In this work, we implement a solution for a quantum particle. The particle is under the influence of a spatially asymmetric periodic potential, that fluctuates with time. The overall aim is to generate a net flow in the direction that the ratchet favors, which is to the left in our case. Several methods of oscillation have been tested and will be introduced in this work. First, in order to break the symmetries in the system, we chose a compatible ratchet oscillating with a cosine function so that the amplitude of the potential changes with time, allowing for the particle to move in one direction. Second, a "drift (gliding)" modeling is tested by shifting the ratchet to the desired direction of motion. Then, by shaking the ratchet in opposite directions back and forth, the particle's movement is recorded. Additionally, in previous studies [2][3], it has been shown that the delta-kicked ratchet, where the ratchet potential is only applied as a kick at certain time steps can also be utilized. For this purpose, we utilize the delta-kicked ratchet modeling as a last method.

One thing that separates our solution from the classical ones, is the matter of energy dissipation of the particle. In classical mechanics, the energy of the particle dissipates, and thus one has to give energy into the system in order to keep it moving. For example, a freely diffused particle in a ratchet potential in its off cycle will need further energy to move "uphill" since it is now all the way down. However, for a quantum particle, the problem changes since there is no energy dissipation, and the ratchet oscillating back and forth can actually sustain the directed motion of the particle, without adding extra energy into the system, which is the main goal of our work. However, for a quantum mechanical system, this also makes the possibility of finding the particle at some fixed point very low, meaning that the wave function of the particle scatters over space after some time. Therefore, adding a term of dissipation helps to keep the wave function of the particle more compact, allowing for the particle to localize in the minima of the potential function just like a classical particle would do. In this work, these dissipative effects are introduced by a local and time-dependent potential term.

This ratchet effect has been observed in optical lattices where ultra-cold atoms are trapped. The effect is generated using the interference of two-counter propa-

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gating laser fields that are orthogonally polarized (for a 2-dimensional lattice) creating a dissipative optical lattice [5]. Thus, recent experimental work is the root of our numerical simulations, proving the existence of such an effect in optical lattices.

2. The Model

The single particle obeys the time-dependent Schrodinger's Equation given as,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\cdot\psi(x,t)$$

In order to numerically solve this differential equation, we implement a central difference method which gives out the equation,

$$i\hbar\frac{\partial\psi_j}{\partial t} = -\frac{\hbar^2}{2m}\frac{1}{\Delta x^2}[-2\psi_j + \psi_{j+1} + \psi_{j-1}] + V_j\cdot\psi_j$$

For the discrete spatial steps of the wavefunction in the form ψ_j where j is the index set such that $0 \leq j \leq N-1$, and N is chosen to be a power of 2 ($2^8 = 128$ in this case). Then let us make the substitution,

$$\frac{\hbar^2}{2m(\Delta x)^2} = \epsilon$$

Diving the whole equation by ϵ, we get the following.

$$i\frac{\hbar}{\epsilon}\frac{\partial\psi_j}{\partial t} = [2\psi_j - \psi_{j+1} - \psi_{j-1}] + \frac{V_j}{\epsilon}\cdot\psi_j$$

Now, making the substitution $\frac{\epsilon}{\hbar}t = \tau$, we get

$$i\frac{\partial\psi_j}{\partial t} = [2\psi_j - \psi_{j+1} - \psi_{j-1}] + \frac{V_i}{\epsilon}\cdot\psi_j \qquad (1)$$

Then the Hamiltonian of the system can be expressed as the kinetic and potential energies in the following form.

$$i\frac{\partial\psi_j}{\partial t} = \mathbf{K}\psi_j + \frac{V_j}{\epsilon}\psi_j = \tilde{H}\psi_j$$

For this equation, we utilize the solution in the form,

$$\psi_j(\tau) = e^{-i\tilde{H}\tau}\psi_j(0) \approx e^{-i\mathbf{K}\tau}e^{-i\frac{V_j}{\epsilon}\tau}\psi_j(0)$$

This approximation allows us to evaluate the two operators separately ($\mathbf{K}$ and V_j/ϵ). Then for the $\mathbf{K}$ operator, we implement a FFT (Fast Fourier Transform Method) in order to solve the time-dependent equation. The idea is to go to k-space and express the wavefunctions in terms of the momentum states of the particle. And then we go back to the real space. As we are doing this transformation and going back, we move each increment ($\psi_j(\tau)$) of the wavefunction one step forward, by $\Delta\tau$. Ultimately we arrive at the wavefunction at the next time step ($\psi_j(\tau + \Delta\tau)$), and so forth. Expressing the wavefunctions in the real space in terms of momentum states for the first part of the FFT, we plug in the following expression inside equation 1.

$$\psi_j = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}\phi_k e^{i\frac{2\pi}{N}kj}$$

Then, just evaluating the kinetic term with that we have the following.

$$i\frac{\partial\psi_j}{\partial\tau} = 2\psi_j - \psi_{i+1} - \psi_{i-1}$$

$$\Rightarrow i\frac{\partial}{\partial\tau}[\frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}\phi_k e^{i\frac{2\pi}{N}kj}]$$

$$= \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}(2 - e^{i\frac{2\pi}{N}k} - e^{-i\frac{2\pi}{N}k})e^{i\frac{2\pi}{N}kj}\phi_k$$

$$= \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}4sin^2(\frac{\pi k}{N})e^{i\frac{2\pi}{N}kj}\phi_k$$

$$\Rightarrow \frac{i}{\sqrt{N}}[\sum_{k=0}^{N-1}\frac{\partial}{\partial\tau}\phi_k e^{i\frac{2\pi}{N}kj}] = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}4sin^2(\frac{\pi k}{N})e^{i\frac{2\pi}{N}kj}\phi_k$$

$$\Rightarrow \frac{\partial\phi_k}{\partial\tau} = 4sin^2(\frac{\pi k}{N})\phi_k$$

This gives the time-dependent momentum states of the particle as,

$$\phi(\tau) = e^{-i(4sin^2(\frac{\pi k}{N}))\tau}\phi_k(0) \qquad (2)$$

Similarly, with the reverse Fourier Transform we arrive back at the spatial wavefunctions of the particle (using equation 3). We then move the wavefunction by a small time $\Delta\tau$ to arrive at the wavefunction at the next time step. And through this procedure the algorithm calculates the wave function with respect to position at each time step. The limit of the time steps, i.e. how many time steps the algorithm calculates and plots, is given as an input to the system. But, mostly we have analyzed the motion of the particle until one, two or three periods of oscillation is completed.

$$\phi_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \psi_j e^{-i\frac{2\pi}{N}kj} \tag{3}$$

3. Methods

For the purpose of creating effective directed motion, also known as ratchet current, we have tried different approaches to apply the potential to the system. Mainly, the used methods involve the sinusoidal oscillation, the gliding potential, the shaking potential, and the kicked potential. Each of these methods are presented in the results since they all gave out different evolutions for the particle in the potential.

3A. The Ratchet Potential

The potential that we used in this work is a saw-tooth potential 1, where the slopes of the ratchets favor only one direction of motion.

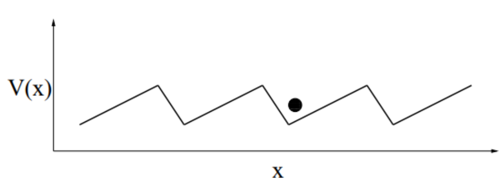


FIG. 1: The periodic ratchet potential shown for a fixed moment in time. The particle is displayed as a classical particle for the sake of simplicity. In reality, we use a Gaussian wave function rather than a point particle.[4]

For the sinusoidal oscillation case, the spatial potential changes with time. For the oscillations in the potential, first, we used a single cosine function.

$$V(x,t) = U(x) \cdot c \cdot (1 + cos(\omega t))$$

Where $U(x)$ is the ratchet potential in one unit cell in the periodic potential, that is a single "tooth", ω is the angular frequency driving the system, and c is some constant. As a second choice, we implemented a bi-harmonic potential, i.e,

$$V(x,t) = U(x) \cdot [c + cos(\omega t) + b \cdot cos(2\omega t + \theta)]$$

Where c is some constant that takes the minima to be 0 (this is to ensure that the potential is never negative), b is some constant, and θ is the relative phase between the two cosine dependencies. The choice of the phase value is extremely important since it changes the movement of the potential drastically.

For the gliding potential, the initial ratchet, as in Figure 1, glides to the left. The main idea is to find a velocity in this direction, that keeps the wave function of the particle compact without too much distortion. For the shaking potential, the ratchet is shaken to the left and right with some fixed frequency ω. Lastly, for the kicked potential, the ratchet is only applied at some time points, as a kick.

3B. Energy Dissipation

The energy dissipation is added to the potential function driving the system as $V \rightarrow V + V_{diss}(t)$. And the term $V_{diss}(t)$ is chosen accordingly so it is likely to lower the energy [6]. This dissipative term adds a phase of $\theta(x)$ to the wave function as it evolves with time. Then the energy of the system varies by the following relation.

$$\frac{\delta E}{\delta\theta(x)} = 2\ \mathbf{Im}\ \psi^*(x)\nabla^2\psi(x)$$

Then a choice of the following form makes sense in order to reduce the local contribution of the phase to the energy.

$$V_{diss} = \alpha\ \mathbf{Im}\ \psi^*(x)\nabla^2\psi(x)$$

By adding this term to the existing potential at each time step, the energy of the wavefunction is minimized. Thus, the wave function has a more compact form as it is evolving with time, and scatters less over space. This can even be seen as getting closer to the classical regime of the particle, where it tends to localize in the minima of the potential, just like a classical particle would do.

4. Results

Using the FFT solution with the given ratchet potentials, we were able to plot both the wave function and the potential function as a stop-motion movie with respect to adjacent time steps. For this solution, the wave function was given the initial condition of a Gaussian function. For a trial solution, it was given that,

$$\psi(x) = e^{-\frac{x^2}{400}}$$

One other measurement that we have considered is the average momentum of the particle, given in Equation 4, along with its expected position. The average momentum tells us about the optimal frequency at which the ratchet should be operating. For a suitable choice of frequency, we plotted the momentum of the particle after several periods of oscillation.

$$\langle p\rangle = \langle \lim_{t\to\infty} \frac{1}{t}\int_0^t p(t)dt\rangle \tag{4}$$

Additionally, in order to have a more realistic simulation, we have plotted 4 units cells of the ratchet in one simulation. Compared to plotting a single saw-tooth in real space, this has allowed us to omit the factors that come from the overlap of the shifted and the rebounded fractions of the wave function. When we plot multiple units at a time, it is ensured that the transported wave function do not interfere with the initial Gaussian itself, thus allowing for a more accurate simulation.

4A. Sinusoidal Potential

For this case, the potential's amplitude oscillates at each time step with a cosine dependency. First, a simple cosine function is tried. Then, since it is used commonly in optical lattices, a bi-harmonic dependence is applied to the system.

For the harmonically driven potential, we have given the system the time dependency of $V(x,t) = U(x)\cdot 0.8\cdot (1+cos(\omega t))$. For the bi-harmonic potential, we have defined the time-dependent potential as $V(x,t) = U(x)\cdot [1.129 + cos(\omega t) + 0.7\cdot cos(2\omega t + 12)]$. For different values of ω, we have plotted the final momentum of the particle after 1 and 2 periods of oscillation.

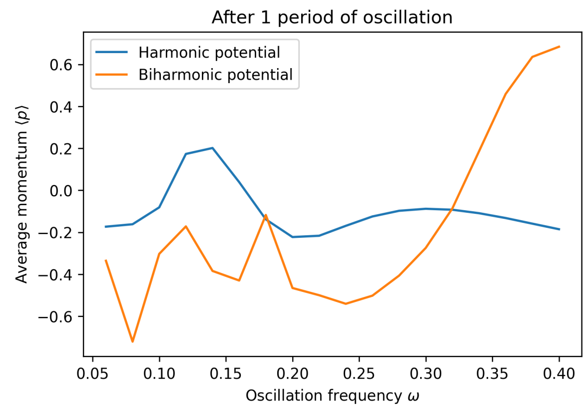


FIG. 2: The average momentum of the particle after one period for the harmonic and bi-harmonic potentials.

Seemingly, for the harmonic potential, after a single period of oscillation, for frequency values above 0.15, the particle has an average momentum in the $-x$ direction, which is the intended direction of the particle. The ratchet should favor motion to the left, which is the $-x$ direction. Then, it seems that either a choice of $\omega \approx 0.06$ or $\omega \geq 0.20$ makes sense in order to sustain the directed motion to the left. For the bi-harmonic case, up to $\omega \approx 0.32$, the momentum is negative. But the negativity is maximized when $0.20 \leq \omega \leq 0.32$, then we again observe a directed motion along the $-x$ direction in Figure 3. This analysis of the frequency values allows us to choose a suitable value so that the ratchet current is generated in the -x direction in the optical lattice.

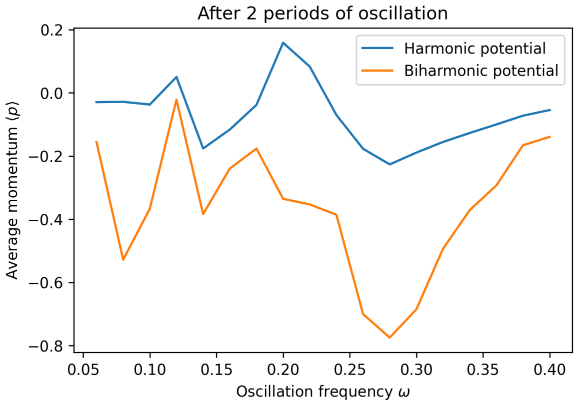


FIG. 3: The average momentum of the particle after two periods for harmonic and bi-harmonic potentials.

Analyzing the momentum after two periods, we see that for the harmonic case the motion along the $-x$ direction is sustained for $\omega \approx 0.06$ or $\omega \geq 0.25$ in figure 2, where the latter is a safer choice since after that value the momentum is always negative. However, as the oscillation frequency gets bigger, it gets harder to keep the initial Gaussian wave function compact, and thus, it disperses. Therefore, for the harmonic case, a choice of around $\omega = 0.26$ looks sensible. After two periods with the bi-harmonic potential, one can see that it looks almost like the harmonic case for $\omega \geq 0.25$, but with bigger absolute values for the momentum. It has a directed motion along the negative x direction as the ratchet favors when $\omega \geq 0.25$, and in any other region, it is mostly unpredictable. Then, for the bi-harmonic potential, a choice of $\omega = 0.27$ can be used to sustain directed motion in the negative direction in the lattice.

4B. Gliding Potential

The gliding potential works by shifting the ratchet to the left directly. With an appropriate choice for the velocity of this shift, the wave function actually keeps compact and moves very nicely in space. In order to find this ideal velocity, we have plotted the final momentum of the particle after some time has passed with changing shifting velocity values for the potential. The maximum of the absolute value of the average momentum is observed at around $c \approx 2.1$ for the constant. The plotted average momentum is calculated at the end of each time evolution cycle, so it is the final average momentum of the particle. Although the criticality is observed at around $c \approx 2.1$, this is actually not the best-case scenario to move the particle in the "-x" direction.

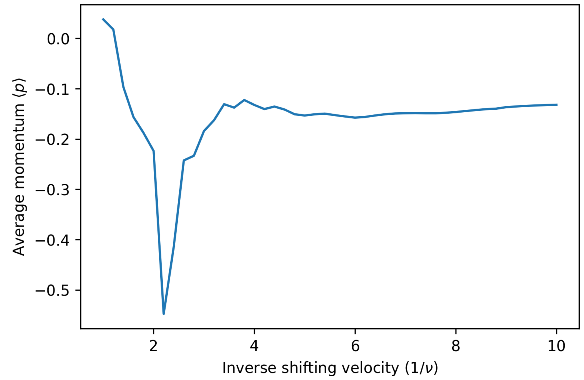


FIG. 4: The average final momentum after one fixed period versus the inverse shifting velocity constant. The constant is referred to as inverse since we divide the shifting amount by this constant. The maximum amount of momentum is observed around $c \approx 2.1$ for this case.

Although the criticality is observed at around $c \approx 2.1$, this is actually not the best-case scenario to move the particle in the "-x" direction. As the time evolution of the particle with the gliding potential is observed, one can see that for this value, the wave function actually scatters a little. If the simulation is given a value of $c \approx 4.8$, then the wave function keeps quite compact while still exhibiting uniform motion in the negative direction, reaching a final average momentum of $\langle p \rangle \approx -0.15$. In Figure 7a, the average momentum of the particle is plotted during the whole time evolution that is captured.

4C. Shaking Potential

The shaking potential works similarly to the gliding potential. But instead of a linear displacement, rather, it shakes with some radial frequency ω associated with a cosine in the form: $-\beta \cdot cos(\omega \cdot t)$, which determines the amount of shift enforced on the potential. In simpler terms, it goes left to right periodically.

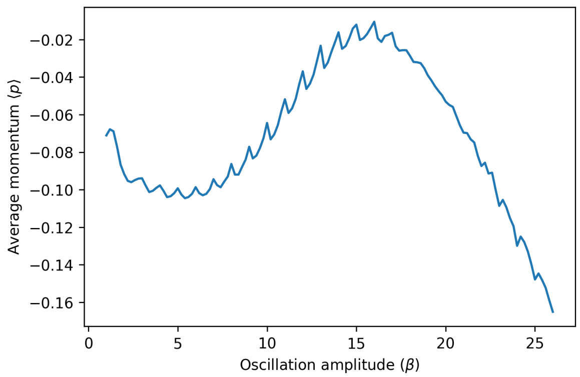


FIG. 5: The average final momentum after one fixed period versus the oscillation amplitude β. The oscillation amplitude determines the amount of shift directly. A maximum value for the (absolute) average momentum is reached at around $\beta = 26$. The oscillation frequency is fixated at $\omega = 2\pi/80$.

Altering the amplitude of oscillation, the optimal value for which the average final momentum gives out the maximum absolute value is determined as $\beta = 26$. This value is used in future simulations of the particle, since it gives out the best result for the motion in the aimed direction. For this value, the wave function holds compact and moves nicely in space. Increasing this amplitude further, higher momentum values in the -x direction are achieved. However, these values are not taken into account since as we increase this amplitude, and we are only capturing for a limited amount of time, the system looks like the gliding potential case. Therefore, it makes sense to take this value since the oscillation is distinctly observable throughout the whole time evolution of the particle that is captured.

4D. Kicked Potential

For the kicked potential, the following form is followed [7].

$$V(x,t) = V_{ratchet}(x,t)\sum_{n=0}^{\infty}(t-n)$$

Where $V_{ratchet}(x,t)$ is the formerly defined saw-tooth-shaped potential. By the integration of the delta function, it is only applied at certain times, as a "kick". In this case, the Gaussian wave function tends to relax and spread over space. However, for some kicking period (the frequency that the delta function is applied), the wave function keeps compact.

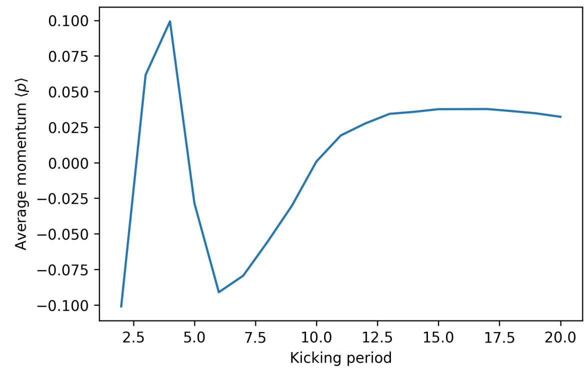


FIG. 6: The average final momentum after a fixed time versus the kicking period.

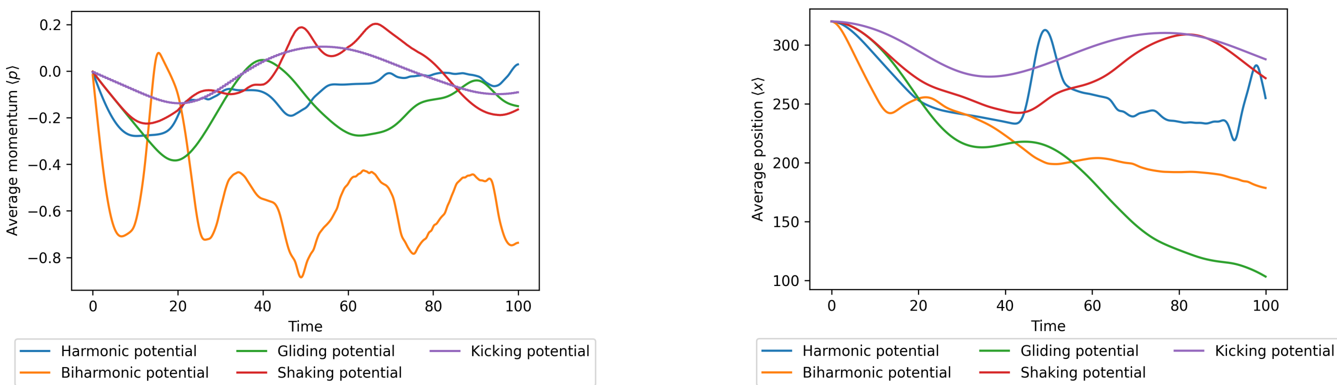
In figure 6, we see that a choice of $n = 6$ yields the best results. It should be noted that, compared to our previous methods, the kicking method ensures a visible less amount of momentum generated in either direction. Although it is not as effective as the previous methods, it can still be used to generate some ratchet current in the -x direction in the lattice.

4E. Motion of the Particle

The motion of the wave function associated with the particle can also be analyzed with the simulations conducted in this work. This tells us about how much the wave function disperses as it travels along the ratchet. For example, with the sinusoidal potentials, we see some dispersion of the wavefunction even before the potential has completed its first period. That is partially due to our assumption that the ϵ is small enough and that we can take the operators $\mathbf{K}$ and V_j/ϵ as commuting operators so that we can separate them as two steps in our code. However as mentioned, the addition of dissipative factors has enabled for better time-evolution of the particle, keeping the wave function more compact.

With the sinusoidal potentials, the main difficulty is finding a suitable and almost perfect choice of the phase and constants that determine the oscillation of the ratchet potential. If the ratchet is too fast then the particle has no time gap to pass to the next unit cell. If it is too slow, then the particle is pushed to the next unit cell, but cannot get through since it collides with the very steep potential in the next unit cell and thus bounces back to its initial position. If it crashes into the potential directly, then it scatters in space, which is also a problem since we need to keep the shape of the initial Gaussian function.

Using our analysis for each method, and choosing the constants accordingly for that purpose, the simulations of the motion of the particle are done. The methods tried for the applied ratchet potential all yield different time evolution scenarios associated with the particle. The average momentum of the particle during some fixed amount of time steps can be seen in Figure 7a. Although the bi-harmonic potential yielded the maximum momentum generated in the -x direction, it was actually the one that dispersed the wave function the most. In general, all potentials, except for the harmonic one, generated a final negative momentum as intended. However, throughout most of the duration of the measurement, the gliding potential has been seen to be keeping the momentum in the negative direction in a more stable way than other methods.



(a) The average momentum of the particle at each time step.

(b) The average position of the particle at each time step.

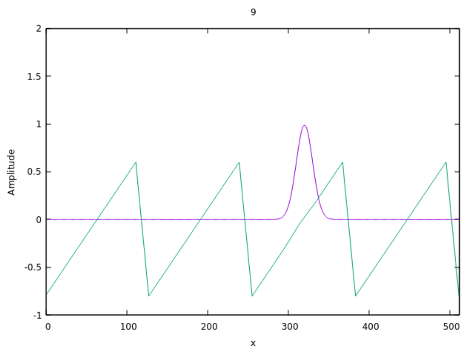
FIG. 7: Average momentum and position of the particle with different methods governing the time-dependency of the ratchet potential. The gliding potential has yielded to be the most stable driving potential for the ratchet. It also moved to particle further to the left compared to other methods. The bi-harmonic potential was used to achieve the highest value for the average momentum in the negative direction.

We can also analyze the average position of the particle in order to get a sense of where it starts and ends its motion in the 1-dimensional lattice. Since a motion along the negative x direction is wanted, all potentials have seemingly succeeded in that, since they all take the particle at a position where $x < 300$. However, the gliding potential has shown the best results in terms of moving the particle further in the -x direction, nearly moving it by 2-unit cells (saw-tooth) to the left. The shaking and kicking potentials did not achieve that much of transport but they were useful in keeping the wave function at a fixed location without disturbing the Gaussian too much.

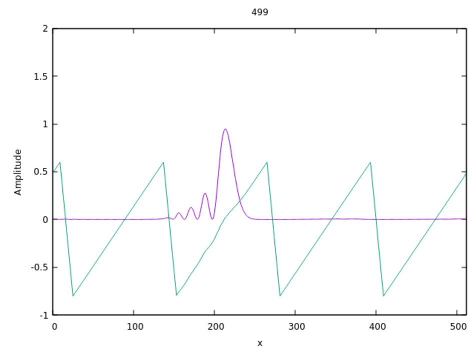
In order to watch the particle's time evolution, a stop-motion-like plotting method is used. The method involves plotting the potential and the wave function at each time step consecutively, so it looks like the wave function is moving in space in real time. Out analysis and commentary on the compactness of the initial Gaussian wave function is based on those observations. One can see a sample of the time evolution of a single particle under the influence of a gliding ratchet potential in Figure 8.

5. Conclusion

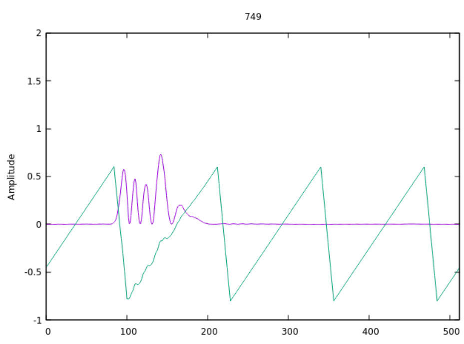
We have found that with different methods and with the use of certain constants at each method, one can actually sustain the directed motion of a single particle inside a time-dependent ratchet potential. However, it is fairly hard to keep the particle from dispersing in space. Since the potential is always moving, at some times there happens to be superposition and clashing in between the potential and the wave-function. Therefore, a suitable choice for a ratchet potential function is of vital importance in order to hold the particle together. We have achieved the best results using the "gliding" potential. It evidently held the wave function together while sustaining the motion along the -x direction in the lattice. For other methods, the predictability and the ability to keep the wave function without dispersing over space were hard to reach. It has also been shown that with the addition of dissipative effects, our results were much enhanced. The addition of energy dissipation helped the wave function go to a classical regime, allowing for the minimization of the particle's energy. Overall, the ratchet potential yielded convenient and promising results for future applications in particles in optical lattices and their transport phenomena. In the case that a suitable ratchet is applied to the particle, one can indeed sustain the directed motion of the particle, observing the ratchet effect.



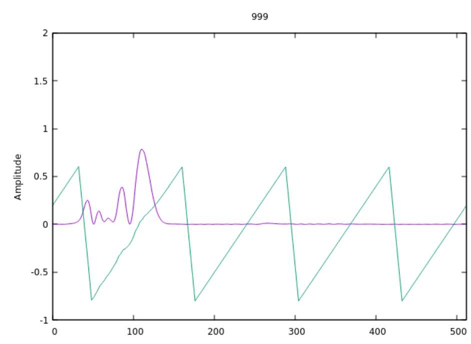
(a) At the starting position of the wave function and the potential.



(b) The second position where the wave function has passed to the next unit cell.



(c) The third position where it has just passed to the second next unit cell.



(d) The last position where it has completed its uniform motion arriving to the left-hand side of the lattice.

FIG. 8: The motion of the wave function under fluctuating ratchet potential at different time steps. The title of each plot represents the discrete time step that the picture is taken in. The ratchet potential (in the green line) glides to the left at each time point, also moving the wave function (in the purple line).

References

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6. Appendix

```
#include <stdio.h>
#include <math.h>
#include <unistd.h>
#include <unistd.h>
#include <complex.h>

#define N 512

static double pi,avx,avp,norm,omega,period,phase,alpha;
static complex buf[N];

int main(nfile,filenames)
int nfile; char *filenames[];
{
  int i,j,k,n,nn,a;
  long it;
  double delta_t,xk,pot[N],cmag(),tpot[N];
  complex cfou[N+1],psi[N],cpot[N],cmom[N];
  void fft();

  FILE * temp = fopen("data.temp", "w");
  FILE * time = fopen("data.time", "w");

  //FILE * pott = fopen("data.pot", "w");
  FILE * psif = fopen("data.psi", "w");
  FILE * gnuplotPipe = popen ("gnuplot -persistent", "w");
  unsigned int usecs;
  usecs = 10000/2.;

  n=N/4;
  nn=n/8;
  pi=4.*atan((double)1.0);

  delta_t = 0.1;
  period = 80.;
  omega = 2.*pi/period;
  phase = 12.;
  alpha = -1.5;

  for(i=0;i<N+1;i++){
    cfou[i]=cos(2.*pi*i/N) +I*sin(2.*pi*i/N);
```

```c
 }

 for(i=0;i<N;i++){
   int j = i % n; // Repeat every 128 steps
     if (i >= N/2 && i < N/2 + n) { // Only initialize psi in the middle unit cell
     psi[i]= exp(-(j-n/2)*(j-n/2)/400.);
   } else {
     psi[i] = 0;
   }
   pot[i] = (j-n/2)/32.;
   if(j > n-nn){ pot[i] = pot[n-nn]-(j-(n-nn))*(pot[n-nn] - pot[0])/(nn);}
   xk = 2.*sin(i*pi/n);
   cmom[i] =  cos(delta_t*xk*xk) -I*sin(delta_t*xk*xk);
 }


for(it=0;it<1*100./delta_t;it++){
   int shift = it/4.8;
   //int shift = (-26.) * cos(omega*it*delta_t);
   for(i=0;i<N;i++){
     int j = (i + shift + N) % N;
     tpot[i]=pot[j]*0.4;
     tpot[i]= tpot[i]+ alpha* cimag(conj(psi[i])*(psi[i+1]-2*psi[i]+psi[i-1]));

     cpot[i] = cos(delta_t*tpot[i])/N -I*sin(delta_t*tpot[i])/N;
     psi[i] = psi[i]*cpot[i];
   }

   fft(N,cfou,psi,1);

   for(i=0;i<N;i++){
     psi[i] = psi[i]*cmom[i];
   }

   fft(N,cfou,psi,-1);

   avx = 0; avp=0.;
   norm =0;
   for(i=0;i<N;i++){
     avx += cmag(psi[i])*i;
     if(i != 0 && i!= N-1) avp += cimag(conj(psi[i])*(psi[i+1]-psi[i-1]));
     norm += cmag(psi[i]);
   }
   avx = avx/norm;
   avp = avp/norm;
   fprintf(time,"%f %f %f\n",it*delta_t,avx,avp);
   fflush(time);

   for(i=0;i<N;i++){
     fprintf(psif,"%d %f %f\n",i,cmag(psi[i]), tpot[i]);

   }
   fflush(psif);
   fprintf(gnuplotPipe, "set xrange [0:512]\n");
   fprintf(gnuplotPipe, "set yrange [-1:2]\n");
   fprintf(gnuplotPipe, "set xlabel 'x'\n");
```

```
    fprintf(gnuplotPipe, "set ylabel 'Amplitude'\n");
    fprintf(gnuplotPipe, "set key off\n");
    fprintf(gnuplotPipe, "%s%ld%s \n", "set title \"",it,"\" ; plot \"data.psi\" u 1:2 w l, \"data.
    psi\" u 1:3 w l");
    fflush(gnuplotPipe);
    for(i=0;i<5;i++) usleep(usecs);
    rewind(psif);

  }

  fprintf(temp,"#average x = %f average p = %f\n",avx,avp);

  for(i=0;i<N;i++){
    fprintf(temp,"%d %f %f\n",i,cmag(psi[i]),tpot[i]);
  }

}

double cmag(cc) complex cc; {return creal(cc)*creal(cc) + cimag(cc)*cimag(cc);}

void fft(n,cfou,vect,mode) int n; complex cfou[]; complex vect[]; int mode;
{
  int i,j,k,nn,J,J0,K,L,L0,M,length,index,index_0,index_incr;
  int no2;
  complex cf,buf1,buf2;

  for(i=0;i<n;i++){
    buf[i]=vect[i];
  }

  if(mode == 1){
    index_0=0;
    index_incr=n;
  }
  else{
    index_0=n;
    index_incr= -n;
  }
  length=1;
  no2=n/2;

  for(nn=no2;nn>0;nn=nn/2){  //   nn = no of ft to be computed at this step
    index_incr/=2;
    index=index_0;
    J0=0;
    L0=0;
    for(k=0;k<length;k++){   //   length = length of the ft at this step
      cf=cfou[index];
      for(j=0;j<nn;j++){     //   go over all the ft's at this step
        J=j+J0;
        K=J+no2;
        L=j+L0;
        M=L+nn;
        buf1=buf[L];
        buf2=buf[M];
        vect[J] = buf1 + cf*buf2;
```

```c
        vect[K] = buf1 - cf*buf2;
      }   // for - j

      index+=index_incr;
      J0=J0+nn;
      L0=L0+nn+nn;
    }    //  for - k

    length=length+length;

    if(nn != 1){
      for(i=0;i<n;i++){
        buf[i]=vect[i];
      }
    }

  }   //  for - nn
  return;
}
```

Listing 1: C code for the time evolution of the particle under a gliding ratchet potential.