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Wave Packet Clustering of Self-focusing Free Particle

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Abstract – We consider free particle wave packets. We introduce the concept of wave packet clustering. We cluster solutions of self-focusing free particles. We apply machine learning algorithm to cluster these solutions. We show that solutions of self-focusing free particle can be clustered with *k*-means clustering.

Keywords – Free Particle, Machine Learning, Self-Focusing, K-Means Clustering, Inverted Harmonic Oscillator.

I. INTRODUCTION

The harmonic oscillator issue in quantum theory is an exact solution that may be used to simulate a variety of physical systems. The inverted harmonic potential, a lesser-known parabolic potential, has received significant attention throughout the years [1-12] due to its wide variety of applications in many fields of physics. A model with an effective inverted harmonic potential [13] describes an LC circuit with negative inductance and capacitance in a quantum mesoscopic environment. The inverted harmonic potential is also utilized to investigate the quick frictionless cooling of ultracold atomic mixtures [14-16] and light propagation in heterogeneous environments [17]. In condensed matter, transition layer states in type-I and type-II Weyl semimetals are controlled by an effective inverted harmonic potential [18].

Although the harmonic oscillator issue is widely known and covered in every basic quantum mechanics textbook, the quantum mechanical system with an inverted harmonic potential is still not completely understood. In [19], the inverted harmonic potential issue is investigated, and non-stationary orthogonal states are calculated analytically. In [19], a new free particle wave packet is produced by exploiting the inverted harmonic potential eigenstates with specified limitations. The new wave packets have a unique self-focusing property and may be employed as a focusing beam when employing the paraxial wave equation rather than the Schrodinger equation.

In this study, we suggest an idea of that new wave packets clustering. These new free particle solutions are non-stationary and non-square integrable odd and even solutions for free particle. Additionally, we numerically investigate clustering of wave packets for free particle with high energy eigenvalues which have huge density values. We show that after adding these wave packets to our data, wave packets clustering cannot be seen explicitly for the small values of densities. We suggested that new wave packets can be clustered around odd and even solutions. Here, we establish the concept of classifying distinct density values into groups, where density values in the same group are related to each other. In other words, densities in the same group have similar values. We demonstrate our concept by studying clustering systematically using the *k*-means clustering method.

II. SELF-FOCUSING FREE PARTICLE WAVE PACKETS

In section 2, the general solution for the inverted harmonic potential using free particle solution is presented. In [19], the problem is studied the other way around. In other words, a new free particle solution using the eigenstates of the inverted harmonic potential is obtained. The newly discovered solution, unlike plane waves, is not square integrable and exhibits a mysterious self-focusing property. In other words, the system experiences a singularity at a critical time [19]. At the unique point, the wave packet's width reaches zero. When the widths come to zero the intensities of these wave packets expand to infinity (similar to the Dirac-delta function).

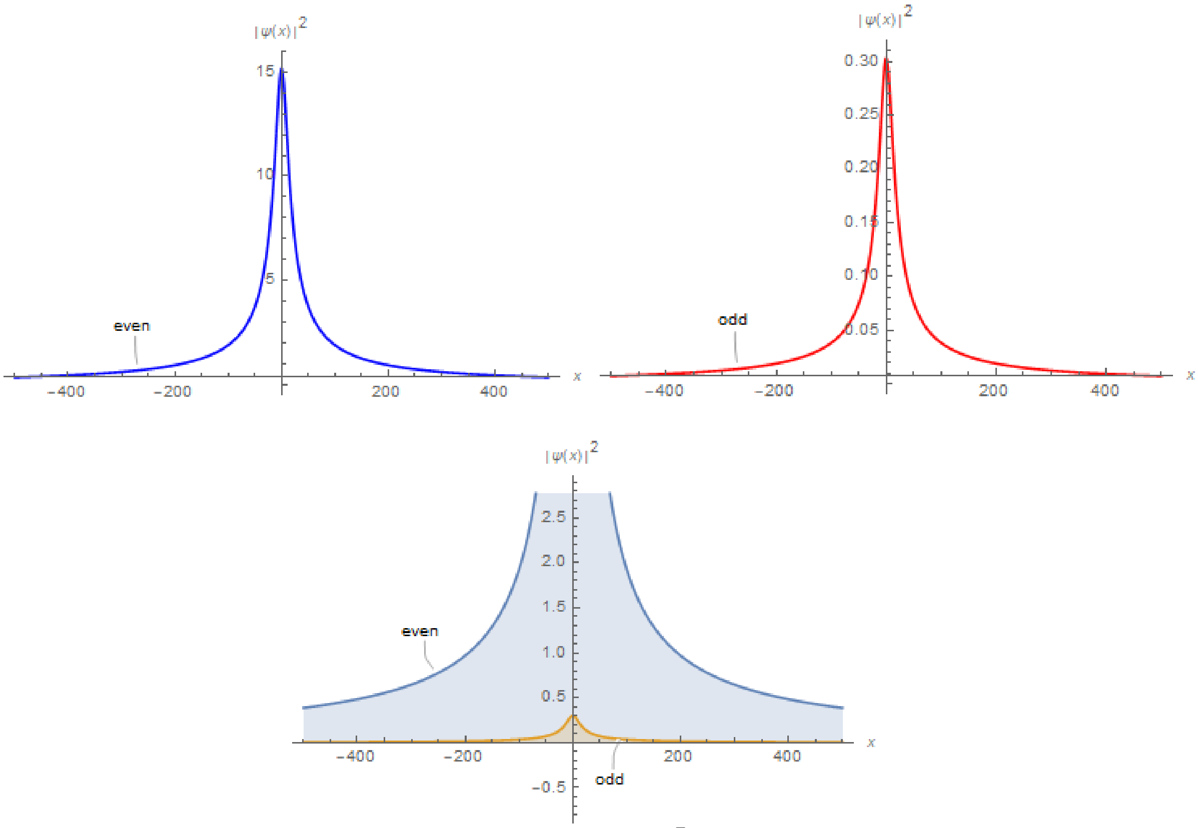


Fig. 1 Wave packets for even and odd solutions for energy parameter $\frac{E}{h\omega}$ = 4.6. We plot even and odd wave packets together at lower panel.

Here we use two non-stationary and non-square integrable odd and even solutions for free particle

$$\Psi_E^- = \frac{x\, e^{-i\frac{m\,\omega\,B\,x^2}{2\,h}-i\frac{E}{h}\tau}}{\sqrt{L^3}} F\left(\frac{iE}{2h\omega}+\frac{3}{4},\frac{3}{2},i\frac{m\omega}{h}\frac{x^2}{L^2}\right)$$

$$\Psi_E^+ = \frac{e^{-i\frac{m\,\omega\,B\,x^2}{2\,h}-i\frac{E}{h}\tau}}{\sqrt{L}} F\left(\frac{iE}{2h\omega}+\frac{1}{4},\frac{1}{2},i\frac{m\omega}{h}\frac{x^2}{L^2}\right) \tag{1}$$

where $\ddot{L} = -\frac{\omega^2}{L^3}$, $B = \frac{\dot{L}}{L} - \frac{\omega}{L^2}$ and $\frac{d\tau}{dt} = L^{-2}$.

These unique free particle solutions are fascinating because of the steady reduction in their widths until the wave packets are all focused at x=0 and then grow infinitely. We can easily see this case in Fig. 1.

The solutions shown above may be applied in the area of electron microscopy, particularly in the optics community, where the paraxial wave equation (a Schrodinger-like equation) is utilized. In optics, self-focusing waves may be created in nonlinear optical systems and have certain practical uses. Finding self-focusing light beams in free space is a critical issue in the optics community. Diffraction happens when a light beam propagates across open space and its peak intensity value reduces. The method obtained in [19] is a feasible candidate for self-focusing light beams in free space (beams that focus without a lens and diffract fast beyond the focal point) and may be employed in a range of applications.

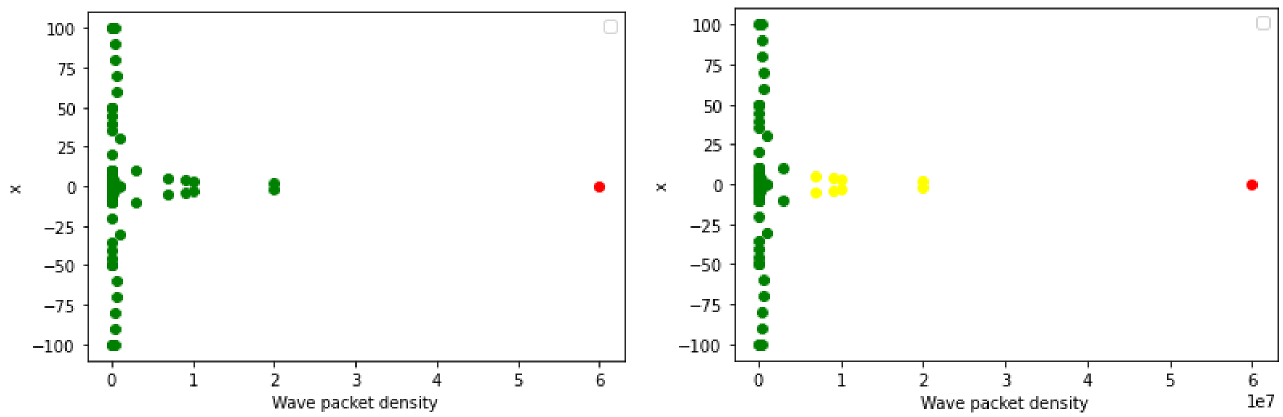
We use (1) to obtain density figures. In Figure 1, we carry out numerical calculations and we plot some odd and even solutions for parameters $\frac{E}{h\omega}$ and width of the non-stationary wave packet L. With the help of these figures, we can easily see the continuously decrease of the wave packets. We plot wave packets with using same parameters ($\frac{E}{h\omega} = 4.6 \; and \; L = 30$) to see similarities of odd and even solutions. Our goal is clustering different wave packets of free particle according to their density values. In other words, with the help of clustering algorithm we will show that densities can be categorized according to whether they are odd or even.

III. WAVE PACKET CLUSTERING

After discussing self-focusing wave packet, let us continue with cluster algorithm. Clustering is widely used in machine learning as a statistical data processing technique. We do not have to categorize data points while learning, hence it's an unsupervised technique. A clustering method can be used to categorize each unlabelled dataset into a certain group based on their similarity and dissimilarity. The qualities of data values which are similar each other are considered to be identical. Data points in various groups, on the other hand, should have diverse attributes.

The notion of density clustering has been described in detail above. The following step is to cluster the densities into groups based on their relationships. To do this, we need a parameter. Here we use the energy eigenvalues $\frac{E}{h\omega}$ and width of the non-stationary wave packet L as a parameter to evaluate closeness of different self-focusing wave packets to each other.

Wave packet clustering as a function of different parameters of a specific self-focusing free particle solutions can be numerically studied by computing densities and then applying a clustering method. There are many other clustering methods available in the literature, many of which have already been used to artificial intelligence [20]. In this study, the k-means clustering technique is used, here k is the number of classes which can be determine manually [20]. The k-means clustering technique has been used by physicists [21, 22]. In comparison to other clustering methods, k-means clustering is a reasonably basic, convergence-guaranteed, computationally quick and efficient methodology. After generating a collection of data, we group the densities using the traditional k-means clustering method.



(a) (b)

Fig. 2 Plot demonstrate wave packet classification in *k* groups using the *k*-means clustering method. We obtain clustering density in other words for different free particle solutions when number of clusters is *k*=2 in (a) and *k*=3 in (b).

Let us start with the definition of the data structure. As we mentioned before the max point of the wave packets is defined by the parameters $\frac{E}{h\omega}$ and L. We use (1) to obtain odd and even solutions. Density of wave packets are calculated with $|\Psi_E^-|^2$ and $|\Psi_E^+|^2$. We perform some numerical calculations for various $\frac{E}{h\omega}$ and L values and produce our data. Values of energy parameter $\frac{E}{h\omega}$ are 5.6, 10.6, 17.6. The dimension of data is 138 rows x 7 columns.

In Figure 2, we plot all the wave packets with respect to position x and using the usual k- means clustering approach, divide them into groups. In the plots, distinct groups are represented by various colors. We choose the number of classes k = 2 and k=3. Indeed, due to their similarity, the densities are grouped together in k = 2. The densities in different groups are distinct, yet the densities in the same group are extremely similar. For instance, the densities of beams in the same class are nearly identical and have similar value, and their densities are barely distinct.

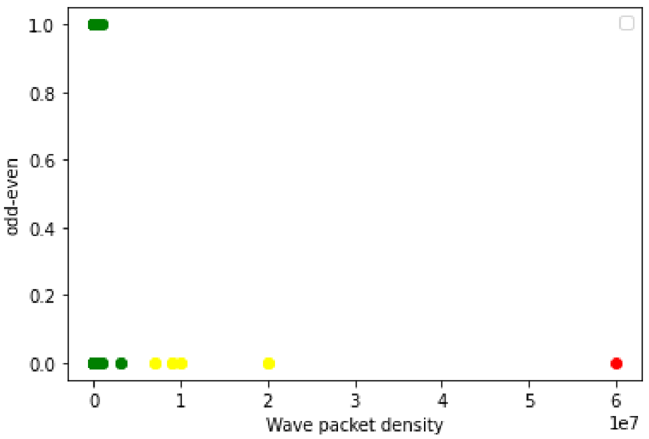


Fig. 3 We cluster wave packets for *k*=3 respect to parameter odd-even.

The densities of self-focusing free particle are clustered in this study. We can cluster where densities based on their odd and even types using machine learning algorithms. In this paper, we classify these wave packets according to their energy parameters and L parameter. We show that using wave packets having greater energy parameter values in our data, we obtain wave packets class which is densely packed in Fig. 2.

We show that the E and L indices have a significant influence in wave packet clustering. We classify the densities of free particle solutions in different parameters according to their odd and even types. In

Figure 2, we show that different densities of free particle solutions have similar density values at specific points and hence they are clustered.

In Figure 3, we plot all the wave packets with respect to their odd or even types with using the usual *k*-means clustering approach, divide them into groups. From green dots in the Fig 3., we show that the wave packets which has similar density values can be clustered in same group. In this green cluster we can see different solutions (odd and even) at same group because of their density values similarity.

IV. CONCLUSION

To summarize, we predicted wave packet clustering and extensively investigated self-focusing free particle solution clustering. In this work, a machine learning clustering algorithm is used in self-focusing free particle solutions. We utilized the energy parameter E and L, as well as the k-means clustering technique, which is usually applied in machine learning, to categorize clustered densities into groups based on their similar features. We believe that this study will lead researchers to study free particle solutions with using clustering and classification methods, as well as machine learning.

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