Quaternionic representation of a one-dimensional wave packet

R. Deepika\textsuperscript{1} and K. Muthunagai\textsuperscript{1}

\textsuperscript{1}Vellore Institute of Technology - Chennai Campus

June 06, 2024

Abstract

The introduction of complex numbers marked a significant leap in mathematics, introducing the imaginary unit $i$ to represent the square root of $-1$. This innovative concept proved invaluable in solving equations involving square roots of negative numbers. The extension to quaternions involved introducing additional imaginary units denoted as $j$ and $k$. A quaternion in an interesting concept that extends complex numbers to 4-D. The manuscript is about using quaternions to calculate wave packets in one-dimension, and anti-hermitian operators to obtain the results in quaternionic form including expectation values of position, momentum and energy. The results are compared to the existing results on complex wave packets in one-dimension.
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R. Deepika K. Muthunagai*

R. Deepika K.Muthunagai*
Address:1,* School of Advanced Sciences,VIT University,Chennai 600 127, Tamil Nadu, India
Email Address: 1deepika.r2021a@vitstudent.ac.in, 2muthunagai@vit.ac.in

Keywords: Quaternions,Wave packets,Quantum Mechanics

The introduction of complex numbers marked a significant leap in mathematics, introducing the imaginary unit \( i \) to represent the square root of \(-1\). This innovative concept proved invaluable in solving equations involving square roots of negative numbers. The extension to quaternions involved introducing additional imaginary units denoted as \( j \) and \( k \). A quaternion in an interesting concept that extends complex numbers to 4-D. The manuscript is about using quaternions to calculate wave packets in one-dimension, and anti-hermitian operators to obtain the results in quaternionic form including expectation values of position, momentum and energy. The results are compared to the existing results on complex wave packets in one-dimension.

1 Introduction

1.1 What are quaternions?

Quaternions are a type of number that exists in four-dimensional space. They were first proposed by W.R. Hamilton in 1843 as a way to extend complex numbers. Complex numbers are like points on a plane, and we can do operations on them that relate to simple transformations of that plane. However, when trying to extend this idea to three or more dimensions, it’s not possible to create a system like the real or complex numbers. But if we take-off the rule that multiplication must be commutative, we can create a number system using points in four-dimensional space.

**Representation of a quaternion:** A quaternion is typically expressed in the form: \( q = p + qi + rj + sk \), where:

- \( p, q, r, \) and \( s \) are real numbers.
- \( i, j, \) and \( k \) are the basis vectors or basis elements or imaginary units.

**Algebraic properties of a quaternion**

- **Noncommutativity:** Quaternion multiplication is noncommutative. In other words, the order matters: “ab” is not necessarily equal to “ba.”
- **Conjugation and Norm:** The conjugate of a quaternion “q” is represented as “\( \bar{q} \)” and is given by: \( \bar{q} = p - qi - rj - sk \). The norm of a quaternion “q” is given by: \( N(q) = q \cdot \bar{q} = p^2 + q^2 + r^2 + s^2 \)
- **Inverse:** The reciprocal (or inverse) of a nonzero quaternion “q” is given by: \( q^{-1} = \frac{\bar{q}}{N(q)} \)
- **Geometric Representation:** Geometrically, quaternions can be visualized as rotors in a four-dimensional space. The coordinates “\( i \),” “\( j \),” and “\( k \)” of a quaternion represent the coordinates of the bivector part of the rotor. The bivector part encodes the rotation plane (often depicted as a yellow disc).

1.2 About Quantum Physics

Quantum physics, or quantum mechanics, is a foundational area of physics concerning the actions of subatomic particles and their interactions. Here are some descriptions about quantum physics:

- **Wave-Particle Duality:** Quantum physics challenges classical notions by revealing that particles (such as electrons and photons) exhibit both wave-like and particle-like behavior. Particles can exist in a superposition of states until measured or observed.
1.3 Quaternions in Quantum Physics

- **Quantization**: Refers to the discrete nature of certain physical quantities, such as energy levels in an atom. Energy levels are quantized, meaning they only take specific allowed values.

- **Uncertainty Principle**: Proposed by Werner Heisenberg, this principle states that there is an inherent limit to precision in simultaneously measuring certain pairs of properties (e.g., position and momentum) of a particle. It is defined as \( \sigma_x \cdot \sigma_p \geq \frac{\hbar}{2} \), where \( \sigma_x \) and \( \sigma_p \) are the standard deviation in 'x' and 'p' respectively.

- **Quantum States and Wavefunctions**: In quantum physics, particles are described using wavefunctions, which tell us about their quantum states. The square of these wavefunctions shows us the likelihood of finding a particle in a specific state at a given time and place. (i.e., \( |\psi(x,t)|^2 \) is the probability density for finding the particle at point x, at time t.

- **Entanglement**: When two particles get entangled their traits become linked even if they’re far apart. Charges in one particle immediately affects the other one no matter how far they are from each other.

- **Quantum Mechanics Equations**: The famous equation in quantum mechanics is the Schrödinger equation, which connects a particle’s energy to its wave function:

  \[
  i\hbar \frac{\partial \phi}{\partial t} = \hat{H}\phi
  \]

  Here, \( \hbar \) denotes the reduced Planck’s constant, and \( \hat{H} \) represents the Hamiltonian operator, describing the total energy of the system.

- **Applications**: Quantum physics underpins technologies like semiconductors, lasers, and MRI machines. It is essential for understanding quantum computing and quantum cryptography.

In summary, quantum physics provides a deeper understanding of the microscopic world, challenging classical intuitions and leading to groundbreaking technological advancements.

1.3 Quaternions in Quantum Physics

Quantum mechanics using quaternions is a variation of standard quantum mechanics. Rather than using complex numbers, it uses quaternions to describe wave functions and operators. Quaternions are four-dimensional objects that can handle spin and have noncommutative multiplication. In this approach, we use an anti-Hermitian Hamiltonian operator. Stephen Adler has explored many solutions using this method [7]. However, using anti-Hermitian principles in quaternionic quantum mechanics has some issues, like not being able to define the classical limit well. Several studies have explored Quaternionic quantum mechanics (\( \mathbb{H} \)QM), with references [2][4][5][8][9][10]. For usage of quaternionic numbers in quantum mechanics, see [1][3]. A recent method in \( \mathbb{H} \)QM eliminated the need for anti-Hermiticity in the Hamiltonian [12] leading to the proof of viral theorem [13] and a well-defined classical limit [11]. Ongoing research focuses on studying fundamental quantum systems in \( \mathbb{H} \)QM, such as the square-well potential and angular momenta [14][4] respectively. Understanding these solutions is crucial as they bridge complex quantum mechanics (\( \mathbb{C} \)QM) and \( \mathbb{H} \)QM, serving as benchmarks for future complex quaternionic systems. This article investigates one-dimensional wave packets, presenting results in quaternionic form.

2 Quaternionic wave packets

De Broglie proposed that particles have associated matter waves, linking particle energy and momentum to wave frequency and wavelength respectively through these equations:

\[
E = \hbar \omega; \quad p = \frac{\hbar}{\lambda}
\]
This concept allows us to describe localized particles of matter and photons using concentrated wave bunches. The quaternionic representation of a particle’s plane wave associated with this theory can be expressed as

$$\Phi(x, t) = C \cos(k) e^{i[kx - \omega t]} + jD \sin(k) e^{i[kx - \omega t]}$$  \hspace{1cm} (1)

The constants $C$ and $D$ are present, where the wave number $k$ is defined as

$$k = \frac{p_x}{\hbar} = \frac{2\pi}{\lambda}.$$  

Here $p_x$ is the momentum operator. This wave function represents a plane wave for all feasible $k$ values, enabling the combination of plane waves having two distinct amplitudes, denoted as $C(k)$ and $D(k)$. The quaternionic form of a one dimension, a localized wave function known as a wave packet $\Phi(x, t)$ can be formulated by combining various plane waves propagating along the $x$-axis, each having different wave-lengths.

$$\Phi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} C(k) \cos(k) e^{i[kx - \omega(k)t]} + jD(k) \sin(k) e^{i[kx - \omega(k)t]} dk$$ \hspace{1cm} (2)

The significance of weighing factors $C(k)$ and $D(k)$ is evident only within a narrow $\Delta k$ interval that encapsulates the wave number $k$ for each corresponding plane wave. At time $t=0$ \( \Phi(x, t) = \Phi(x, 0) = \Phi_0 \) and (2) can be written as

$$\Phi_0(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} C(k) \cos(k) e^{-ikx} + jD(k) \sin(k) e^{-ikx} dk$$ \hspace{1cm} (3)

The wave packet described by equation (3), determined by the $x$-dependent nature of $\Phi_0(x)$, exhibits the essential attribute of localization. The absolute value $|\Phi_0(x)|$ peaks at $x = 0$ and diminishes significantly as $|x|$ increases. As $x$ approaches 0, $e^{ikx}$ tends towards 1, facilitating constructive interference among waves of varying frequencies. However, at considerable distances from $x = 0$ (where $|x|$ is notably large), $e^{ikx}$ undergoes numerous phase changes, leading to rapid oscillations and destructive interference. This circumstance results in a higher likelihood of locating the particle near $x = 0$ with a minimal probability of detection far from $x = 0$. Correspondingly, $C(k)$ and $D(k)$ reach their peaks around $k = 0$ and diminish as $k$ deviates from zero. The quaternionic wave packet at any later time $t$ can be obtained by calculating

$$\int_{-\infty}^{\infty} C(k) \cos(k) e^{i[kx - \omega(k)t]} + jD(k) \sin(k) e^{i[kx - \omega(k)t]} dk$$ \hspace{1cm} (4)

The specifications for the angular frequency $\omega$ and the amplitudes $C(k)$ and $D(k)$ are essential. In a non-dispersive medium, the connection between $\omega$ and the wave number $k$ is expressed as $\omega = c k$ in vacuum and $\omega = \nu_0 k$ in a material medium. The construction of the wave packet for a non-dispersive medium is represented by:

$$\Phi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} C(k) \cos(k) e^{i[kx - \nu_0(k)t]} + jD(k) \sin(k) e^{i[kx - \nu_0(k)t]} dk$$ \hspace{1cm} (5)

$$\Phi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} C(k) \cos(k) e^{ik[x - \nu_0 t]} + jD(k) \sin(k) e^{ik[x - \nu_0 t]} dk$$ \hspace{1cm} (6)

Equation (6) having the same structure as that of (2), shows that $\Phi(x, t)$ is identical with $\Phi(x - \nu_0 t)$, i.e., $\Phi(x, t) = \Phi_0(x - \nu_0 t)$ as the wave packet progresses at a constant velocity $\nu_0$, without any distortion, it moves through a non-dispersive medium. However, in dispersive media, the propagation of harmonic waves at different frequencies involves varied velocities owing to $\omega$ being a function of $k$ (\( \omega = \omega(k) \)). When $\omega(k)$ demonstrates gradual changes relative to $k$ and the range of $k$ values remains restricted within a narrow interval $\Delta k$, it becomes feasible to expand $\omega(k)$ using a Taylor series centered at a specific point $k_0$ within the range of $\Delta k$. 
\[
\omega(k) = \omega + (k - k_0)(d\omega\over dk)_{k_0} + (k - k_0)^2 \frac{1}{2}(d^2\omega\over dk^2)_{k_0} + \ldots
\]  
(7)

\[
\omega(k) = \omega + (k - k_0)V_g + (k - k_0)^2 \beta,
\]  
where \(\omega_0\) is the value of \(\omega(k)\) at \(k_0\) and the derivatives \(V_G = (d\omega\over dk)_0\) and \(\beta = \frac{1}{2}(d^2\omega\over dk^2)_0\) are also evaluated at \(k_0\) ignoring the quadratic and higher order terms in Taylor expansion as \(k - k_0\) terms are small we have from (7),

\[
kx - \omega t \approx (k_0x - \omega_0 t) + \left[ x - \frac{(d\omega\over dk)}{0} t \right] (k - k_0)
\]  
(8)

Substituting (8) in (2)

\[
\Phi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} C(k) \cos(k)e^{i(k_0x - \omega_0 t)}e^{i x - \left( \frac{d\omega}{dk} \right)_0 t} + jD(k) \sin(k)e^{i(k_0x - \omega_0 t)}e^{i x - \left( \frac{d\omega}{dk} \right)_0 t}
\]  
(9)

\[
\Phi(x, t) = g(x, t)e^{i[k_0x - \omega_0 t]} + f(x, t)e^{i[k_0x - \omega_0 t]}
\]  
where, \(g(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} C(k) \cos(k)e^{i x - \left( \frac{d\omega}{dk} \right)_0 t} \)

\[
f(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} D(k) \sin(k)e^{i x - \left( \frac{d\omega}{dk} \right)_0 t}
\]  
The equation (9) can be expressed as a plane wave characterized by wave numbers \(k_0\) and angular frequency \(\omega_0\). The amplitude of the wave is modulated by the factors \(g\) and \(f(x, t)\), where \(f\) depends on \(x\) and \(t\) through the relationship

\[
x = \left( \frac{d\omega}{dk} \right)_0 t
\]

. The modulated functions \(g(x, t)\) and \(f(x, t)\) propagates in the positive \(x\)-direction with the group velocity

\[
V_g = \left( \frac{d\omega}{dk} \right)_0
\]  
(10)

The (9) can be written as

\[
\Phi(x, t) = \frac{1}{\sqrt{2\pi}} e^{ik_0} \int_{-\infty}^{\infty} C(k) \cos(k)e^{i x - \left( \frac{d\omega}{dk} \right)_0 t} + jD(k) \sin(k)e^{i x - \left( \frac{d\omega}{dk} \right)_0 t} \)
\[
\Phi(x, t) = \frac{1}{\sqrt{2\pi}} e^{ik_0} \int_{-\infty}^{\infty} C(k) \cos(k)e^{i x - \left( \frac{d\omega}{dk} \right)_0 t} + jD(k) \sin(k)e^{i x - \left( \frac{d\omega}{dk} \right)_0 t}
\]  
where, \(V_g = \frac{(\omega_0/k)}{0}\) is the phase velocity The phase velocity describes the speed of propagation of the phase within an individual harmonic wave, whereas the group velocity (10) indicates the velocity at which the ensemble of waves comprising the packet moves. Each constituent wave forming the packet advances at a unique pace, with each wave moving in accordance with its individual phase velocity.

3 Quaternionic form of Gaussian Wave Packet

We can define Gaussian wave packet in quaternionic form by

\[
C(k) = 2e^{-\sigma|k-k_0|^2} \quad D(k) = 2je^{-\sigma|k-k_0|^2}
\]  
(11)

\[
\Phi(x, t) = \int_{-\infty}^{\infty} C(k) \cos(k)e^{i[kx - \omega(k)t]} + D(k) \sin(k)e^{i[kx - \omega(k)t]} dk
\]  
(12)

At \(t=0\), the integration can be done by writing \(k' = k - k_0\), i.e.

\[
\Phi(x, 0) = 2e^{-\sigma(k')^2} \int_{-\infty}^{\infty} \cos(k)e^{ikx} + j \sin(k)e^{ikx} dk
\]

\[
= 2e^{-\sigma(k-k_0)^2} \int_{-\infty}^{\infty} \cos(k)e^{i(k-k_0)x} e^{ik_0x} + j \sin(k)e^{i(k-k_0)x} e^{ik_0x} dk
\]
\[ \Phi(x, 0) = \int C(p) \cos(p) \ e^{ipx} + D(p) \sin(p) \ e^{-ipx} \ dp \]
\[ \Delta x \Delta p \geq \hbar \]

4 Complex form of expectation values of position, momentum and energy using complex wave packets

(1) The expectation value of position ‘x’ at given time ‘t’ for the given complex wave packets \( \Phi(x, t) = Ce^{i(kx - \omega t)} \) is expressed as
\[ \langle \hat{X} \rangle = \int \Phi^* \hat{p} \Phi \, dx \]
\[ \langle \hat{X} \rangle = \int (C^* e^{-i[kx - \omega t]}) x(C e^{i[kx - \omega t]}) \, dx \]
\[ \langle \hat{X} \rangle = \int |C|^2 x e^{i[kx - \omega t]} e^{-i[kx - \omega t]} \, dx \]
\[ \langle \hat{X} \rangle = |C|^2 \int x \, dx \]

2. The expectation value of momentum ‘x’ at given time ‘t’ for the given complex wave packets \( \Phi(x, t) = C e^{i[kx - \omega t]} \) is calculated by
\[ \langle \hat{P} \rangle = \int \Phi^* \hat{p} \Phi \, dx \]
\[ \langle \hat{P} \rangle = \int C^* e^{-i[kx - \omega t]} (-i\hbar \frac{d}{dx}) (C e^{i[kx - \omega t]}) \, dx \]
\[ \langle \hat{P} \rangle = -i\hbar \int C^* e^{-i[kx - \omega t]} \left( \frac{d}{dx} \right) (C e^{i[kx - \omega t]}) \, dx \]
\[ \langle \hat{P} \rangle = -i\hbar \int |C|^2 \, dx \]

3. The expectation value of energy ‘x’ at given time ‘t’ for the given complex wave packets \( \Phi(x, t) = C e^{i[kx - \omega t]} \) is evaluated using
\[ \langle \hat{H} \rangle = \int \Phi^* \hat{H} \Phi \, dx \]
\[ \langle \hat{H} \rangle = \int (C^* e^{-i[kx - \omega t]}) \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) (C e^{i[kx - \omega t]}) \, dx \]
\[ \langle \hat{H} \rangle = -\frac{\hbar^2}{2m} \int C^* e^{-i[kx - \omega t]} \frac{d^2}{dx^2} (C e^{i[kx - \omega t]}) \, dx \]
\[ \langle \hat{H} \rangle = -\frac{\hbar^2}{2m} \int |C|^2 e^{i[kx - \omega t]} (-\hbar^2) e^{-i[kx - \omega t]} \, dx \]
\[ \langle \hat{H} \rangle = \frac{\hbar^2 k^2}{2m} \int |C|^2 \, dx \]

5. Quaternionic form of expectation values of position, momentum and energy using quaternionic wave packets

Adler’s anti-hermitian operators is used to formulate these results:

1. The expectation value of position ‘x’ at given time ‘t’ for the given quaternionic wave packets \( \Phi(x, t) = C \cos(k) e^{i[kx - \omega t]} + jD \sin(k) e^{i[kx - \omega t]} \) is computed by
\[ \langle \hat{X} \rangle = \int_{-\infty}^{\infty} \Phi^*(x, t) |x| \Phi(x, t) \, dx \]
\[ \langle \hat{X} \rangle = \int_{-\infty}^{\infty} x (C^2 \cos^2 k + D^2 \sin^2 k) \, dx \]

2. The expectation value of momentum ‘x’ at given time ‘t’ for the given quaternionic wave packets \( \Phi(x, t) = C \cos(k) e^{i[kx - \omega t]} + jD \sin(k) e^{i[kx - \omega t]} \) is obtained by
\[ \langle \hat{P} \rangle = \int_{-\infty}^{\infty} \Phi^* (x, t) \left( -\hbar \frac{\partial}{\partial x} \right) \Phi(x, t) \, dx \]
\[ \langle \hat{P} \rangle = \int_{-\infty}^{\infty} \Phi^* (x, t) [-i\hbar (-Ck \sin(k) e^{i[kx - \omega t]} + jDk \cos(k) e^{i[kx - \omega t]})] \, dx \]
\[ \langle \hat{P} \rangle = \int_{-\infty}^{\infty} C \cos(k) e^{-i[kx - \omega t]} - jD \sin(k) e^{-i[kx - \omega t]} [-i\hbar (-Ck \sin(k) e^{i[kx - \omega t]} + jDk \cos(k) e^{i[kx - \omega t]})] \, dx \]
\[ \langle \hat{P} \rangle = -i\hbar \int_{-\infty}^{\infty} (D^2 - C^2) \cos k \sin k + j(\cdot)(Dk \cos(k) e^{i[kx - \omega t]}) \, dx \]
where \(( -\hbar \frac{\partial}{\partial x} )\) is the anti-hermitian operator and \(j\) is the imaginary part.

3. The expectation value of energy ‘x’ at given time ‘t’ for the given quaternionic wave packets \( \Phi(x, t) = C \cos(k) e^{i[kx - \omega t]} + jD \sin(k) e^{i[kx - \omega t]} \) is found by using
\[ \langle \hat{H} \rangle = \int \left( C \cos(k) e^{-i[kx - \omega t]} - jD \sin(k) e^{-i[kx - \omega t]} \right) \left( -\frac{\hbar^2 k^2}{2m} \right) \left( C \cos(k) e^{i[kx - \omega t]} + jD \sin(k) e^{i[kx - \omega t]} \right) \, dx \]
\[ \langle \hat{H} \rangle = \left( -\frac{\hbar^2 k^2}{2m} \right) \int (C^2 \cos^2(k) + D^2 \sin^2(k)) \, dx \]
when the amplitudes ‘C’ and ‘D’ are equal, the complex solution of the expectation values of the above operators are obtained.

6. Conclusion

The above work describes the quaternionic representation of wave packet using a single wave function with two different amplitudes. Section 2 comprises of quaternionic wave packets in one-dimension, Section 3 describes the quaternionic form of Gaussian wave packets, Section 4 and Section 5 are all about
the expectation values of Position, Momentum and Energy operators in complex and quaternionic form respectively.

Acknowledgement: We thank Assistant Professor Sergio Giardino for his helpful suggestions.

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