# PRELIMINARIES

Quaternion waves in symplectic components

$|n|=1 \qquad n^2=-1 \Rightarrow$

$$e^{n\omega t} = \cos\omega t + n \sin\omega t$$

$$= \cos\omega t + (n_\alpha + j\, n_\beta) \sin\omega t$$

$$= \cos\omega t + n_\alpha \sin\omega t + j\, n_\beta \sin\omega t$$

$$\Rightarrow \quad (e^{n\omega t})_\alpha = \cos\omega t + n_\alpha \sin\omega t$$

$$(e^{n\omega t})_\beta = n_\beta \sin\omega t$$

So symplectic components will always be complex linear combination of complex waves $e^{\pm i\omega t}$

Do not need general unit quaternion in the phase exponents

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Right side Fourier analysis for a quaternion wave function $\phi$

$$\phi(\vec{x},t) = \int dt'\, \phi(\vec{x},t')\, \delta(t-t') = \int dt'\, \phi(\vec{x},t') \frac{1}{2\pi}\int d\omega\, e^{i\omega(t'-t)}$$

$$= \int d\omega\, \phi(\vec{x},\omega)\, e^{-i\omega t} \qquad \phi(\vec{x},\omega) = \frac{1}{2\pi}\int \phi(\vec{x},t')\, e^{i\omega t'}$$

If $L$ is a time-independent wave operator,

$$L\,\phi(\vec{x},t) = \int d\omega\, L\left[\phi(\vec{x},\omega)\, e^{-i\omega t}\right]$$

$$= \int d\omega\, \Phi(\vec{x},\omega)\, e^{-i\omega t}$$ , so different $\omega$ pieces do not couple (no "cross-talk")

## $m=0$ case of quaternion KG wave operator

√ (2)

$$\left[\left(\frac{\partial}{\partial t}+B_0\right)^2-\vec{\nabla}^2\right]\phi=0$$

ansatz $\quad \phi = \Psi(\vec{x})\, e^{-i\omega t} \qquad (\Psi(\vec{x}) \sim \phi(\vec{x},\omega)$ of page ①$)$

$$\left(\frac{\partial}{\partial t}+B_0\right)^2\phi=\left(\frac{\partial^2}{\partial t^2}+2B_0\frac{\partial}{\partial t}+B_0^2\right)\Psi(\vec{x})e^{-i\omega t}$$

$$=\left[B_0^2\Psi-2B_0\Psi i\omega-\Psi\omega^2\right]e^{-i\omega t}$$

So spatial equation is

✓ $$\boxed{B_0^2\Psi-2B_0\Psi i\omega-\Psi\omega^2-\vec{\nabla}^2\Psi=0}$$

$\Psi=\Psi_\alpha+j\Psi_\beta \quad \Psi_{\alpha/\beta}$ are $\mathbb{C}$

$B_0=0, \qquad (\vec{\nabla}^2+\omega^2)\Psi(\vec{x})=0 \qquad (\vec{\nabla}^2+\omega^2)\Psi_\alpha=(\vec{\nabla}^2+\omega^2)\Psi_\beta=0$

$\Rightarrow \Psi_\alpha=C_\alpha e^{\pm i\vec{k}\cdot\vec{x}} \quad \Psi_\beta=C_\beta e^{\pm i\vec{k}\cdot\vec{x}}$

$|\vec{k}|=\omega$

$B_0=nV_0 \qquad B_0^2=-V_0^2$

✓ $$\boxed{(\vec{\nabla}^2+V_0^2+\omega^2)\Psi+2V_0\omega\, n\Psi i=0}$$

$n=in_1+j(n_2-in_3)=in_1+jn_2+kn_3$

$\Psi=\Psi_\alpha+j\Psi_\beta \qquad \Psi_\alpha,\Psi_\beta$ are $\mathbb{C}(1,i)$

$\Psi i=i\Psi_\alpha-ij\Psi_\beta=i(\Psi_\alpha-j\Psi_\beta)$

$$(\vec{\nabla}^2+V_0^2+\omega^2)(\Psi_\alpha+j\Psi_\beta)+2V_0\omega\underbrace{[in_1+j(n_2-in_3)]i(\Psi_\alpha-j\Psi_\beta)}_{-n_1\Psi_\alpha-i(n_2+in_3)\Psi_\beta+j[(n_2-in_3)i\Psi_\alpha+n_1\Psi_\beta]}=0$$

So the pair of coupled equations

✓ $$(\vec{\nabla}^2+V_0^2+\omega^2)\Psi_\alpha+2V_0\omega\left[n_1\Psi_\alpha+i(n_2+in_3)\Psi_\beta\right]=0$$

✓ $$(\vec{\nabla}^2+V_0^2+\omega^2)\Psi_\beta+2V_0\omega\left[(n_2-in_3)i\Psi_\alpha+n_1\Psi_\beta\right]=0$$

③

Write these as

$$\left(\vec{\nabla}^2 + V_0^2 + \omega^2 - 2V_0\omega n_1\right)\Psi_\alpha = 2V_0\omega\, i\,(n_2 + i n_3)\,\Psi_\beta$$

$$\left(\vec{\nabla}^2 + V_0^2 + \omega^2 + 2V_0\omega n_1\right)\Psi_\beta = -2V_0\omega\, i\,(n_2 - i n_3)\,\Psi_\alpha$$

$\Psi_{\alpha,\beta}$ are complex, so can use the Fourier ansatz

$\Psi_\alpha = C_\alpha e^{i\vec{k}\cdot\vec{x}}$ $\quad\Psi_\beta = C_\beta e^{i\vec{k}\cdot\vec{x}}$ $\quad\vec{k}$ to be determined

$$\left(-\vec{k}^2 + V_0^2 + \omega^2 - 2V_0\omega n_1\right)C_\alpha = 2V_0\omega\, i\,(n_2 + i n_3)\,C_\beta$$
$$\left(-\vec{k}^2 + V_0^2 + \omega^2 + 2V_0\omega n_1\right)C_\beta = -2V_0\omega\, i\,(n_2 - i n_3)\,C_\alpha$$

$$\Rightarrow \boxed{\frac{C_\beta}{C_\alpha} = \frac{-2V_0\omega i\,(n_2 + i n_3)}{-\vec{k}^2 + V_0^2 + \omega^2 + 2V_0\omega n_1} = \frac{-\vec{k}^2 + V_0^2 + \omega^2 - 2V_0\omega n_1}{2V_0\omega i\,(n_2 + i n_3)} \equiv R(k) = R(-k)}$$

with $\vec{k}^2$ obey

$$4V_0^2\omega^2\left(n_2^2 + n_3^2\right) = \left(-\vec{k}^2 + V_0^2 + \omega^2\right)^2 - 4V_0^2\omega^2 n_1^2$$

$$\left(-\vec{k}^2 + V_0^2 + \omega^2\right)^2 = 4V_0^2\omega^2\left[n_1^2 + n_2^2 + n_3^2\right] = 4V_0^2\omega^2$$

$$\vec{k}^2 = V_0^2 + \omega^2 \pm 2V_0\omega = (V_0 \pm \omega)^2$$

for 1 dimension, $\vec{k}$ becomes $k_z \equiv k$

independent $\pm$ signs

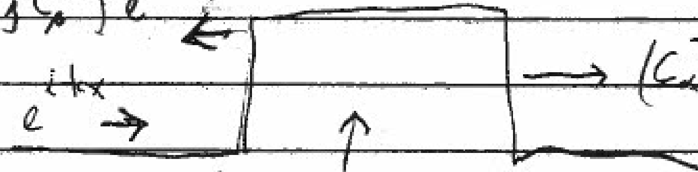
$$k = \pm\left(\omega \pm V_0\right)^2 = \pm k_\pm \qquad k_\pm = \omega \pm V_0$$

2 allowed wave numbers in the interior region, which can propagate right ($r$) or left ($\ell$)

$k_\pm$ are both real

reflected wave $(C_\alpha^R + j C_\beta^R) e^{-ikx}$

incident wave $e^{ikx}$



$(C_\alpha^T + j C_\beta^T) e^{ikx}$ transmitted wave

$x=0$ $x=a$

$$\underbrace{(1+jR(k_+))C_\alpha^{+r} e^{ik_+x} + (1+jR(k_+))C_\alpha^{+l} e^{-ik_+x} + (1+jR(k_-))C_\alpha^{-r} e^{ik_-x} + (1+jR(k_-))C_\alpha^{-l} e^{-ik_-x}}$$

r = right moving
l = left moving

8 unknowns $C_\alpha^R$ $C_\beta^R$ $C_\alpha^T$ $C_\beta^T$ exterior

$C_\alpha^{+r}$ $C_\alpha^{+l}$ $C_\alpha^{-r}$ $C_\alpha^{-l}$ interior

8 matching conditions:
left side $(1, j) \otimes (f_n, \partial_x f_n) = 4$
right side $(1, j) \otimes (f_n, \partial_x f_n) = 4$

So problem is well posed

If $C_\beta^R$ and/or $C_\beta^T \neq 0$ it will give a counter-example to the S-matrix theorem

If $C_\beta^R = 0$ and $C_\beta^T = 0$ it will agree with the S-matrix theorem

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Matching conditions

$x=0$

$$1 + C_\alpha^R = C_\alpha^{+r} + C_\alpha^{+l} + C_\alpha^{-r} + C_\alpha^{-l}$$

$$C_\beta^R = R(k_+) C_\alpha^{+r} + R(k_+) C_\alpha^{+l} + R(k_-) C_\alpha^{-r} + R(k_-) C_\alpha^{-l}$$

$$ik - ik C_\alpha^R = ik_+ C_\alpha^{+r} - ik_+ C_\alpha^{+l} + ik_- C_\alpha^{-r} - ik_- C_\alpha^{-l}$$

$$-ik C_\beta^R = ik_+ R(k_+) C_\alpha^{+r} - ik_+ R(k_+) C_\alpha^{+l} + ik_- R(k_-) C_\alpha^{-r} - ik_- R(k_-) C_\alpha^{-l}$$

$x=a$

$$C_\alpha^T e^{ika} = C_\alpha^{+r} e^{ik_+a} + C_\alpha^{+l} e^{-ik_+a} + C_\alpha^{-r} e^{ik_-a} + C_\alpha^{-l} e^{-ik_-a}$$

$$C_\beta^T e^{ika} = R(k_+) C_\alpha^{+r} e^{ik_+a} + R(k_+) C_\alpha^{+l} e^{-ik_+a} + R(k_-) C_\alpha^{-r} e^{ik_-a} + R(k_-) C_\alpha^{-l} e^{-ik_-a}$$

$$ik C_\alpha^T e^{ika} = ik_+ C_\alpha^{+r} e^{ik_+a} - ik_+ C_\alpha^{+l} e^{-ik_+a} + ik_- C_\alpha^{-r} e^{ik_-a} - ik_- C_\alpha^{-l} e^{-ik_-a}$$

$$ik C_\beta^T e^{ika} = ik_+ R(k_+) C_\alpha^{+r} e^{ik_+a} - ik_+ R(k_+) C_\alpha^{+l} e^{-ik_+a} + ik_- R(k_-) C_\alpha^{-r} e^{ik_-a} - ik_- R(k_-) C_\alpha^{-l} e^{-ik_-a}$$

Now abbreviate $R(k_+) \equiv R_+$ $\quad R(k_-) \equiv R_-$

and see if we can force a contradiction when we make the Ansatz $C_\beta^R = C_\beta^T = 0$

This requires

$$0 = R_+(C_\alpha^{+r} + C_\alpha^{+l}) + R_-(C_\alpha^{-r} + C_\alpha^{-l})$$

$$0 = ik_+ R_+ (C_\alpha^{+r} - C_\alpha^{+l}) + ik_- R_- (C_\alpha^{-r} - C_\alpha^{-l})$$

$$0 = R_+ (C_\alpha^{+r} e^{ik_+a} + C_\alpha^{+l} e^{-ik_+a}) + R_- (C_\alpha^{-r} e^{ik_-a} + C_\alpha^{-l} e^{-ik_-a})$$

$$0 = ik_+ R_+ (C_\alpha^{+r} e^{ik_+a} - C_\alpha^{+l} e^{-ik_+a}) + ik_- R_- (C_\alpha^{-r} e^{ik_-a} - C_\alpha^{-l} e^{-ik_-a})$$

If the determinant of coefficients $\neq 0$, then must have $C_\alpha^{+r} = C_\alpha^{+l} = C_\alpha^{-r} = C_\alpha^{-l} = 0$

But this contradicts the $x=0$ conditions

$$\left.\begin{array}{l} 1 + C_\alpha^R = 0 \\ ik(1 - C_\alpha^R) = 0 \end{array}\right\} \Rightarrow 2 = 0 \quad \text{contradiction}$$

So the determinant must vanish to have the possibility of non quaternionic reflected and transmitted wave

$$M = \begin{bmatrix} R_+ & R_+ & R_- & R_- \\ ik_+R_+ & -ik_+R_+ & ik_-R_- & -ik_-R_- \\ R_+e^{ik_+d} & R_+e^{-ik_+d} & R_-e^{ik_-d} & R_-e^{-ik_-d} \\ ik_+R_+e^{ik_+d} & -ik_+R_+e^{-ik_+d} & ik_-R_-e^{ik_-d} & -ik_-R_-e^{-ik_-d} \end{bmatrix}$$

need $\det M$, using $k_\pm = \omega \pm V_0$

$$R_-/R_+ \equiv R = \frac{-k_-^2 + V_0^2 + \omega^2 - 2V_0\omega h_1}{-k_+^2 + V_0^2 + \omega^2 - 2V_0\omega h_1} =$$

$$= \frac{-(\omega - V_0)^2 + V_0^2 + \omega^2 - 2V_0\omega h_1}{-(\omega + V_0)^2 + V_0^2 + \omega^2 - 2V_0\omega h_1} = -\frac{(1-h_1)}{(1+h_1)}$$

$$ik_-/ik_+ \equiv U = \frac{\omega - V_0}{\omega + V_0}$$

$$e^{ik_\pm d} = \phi_\pm \qquad e^{-ik_\pm d} = \phi_\pm^{-1}$$

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$$\frac{\det(M)}{R_+^4 (ik_\parallel)^2}$$

$$= \det \begin{bmatrix} 1 & 1 & R & R \\ 1 & -1 & UR & -UR \\ \phi_+ & \phi_+^{-1} & R\phi_- & R\phi_-^{-1} \\ \phi_+ & -\phi_+^{-1} & UR\phi_- & -UR\phi_-^{-1} \end{bmatrix}$$ ✓

$$= \det \begin{bmatrix} 2 & 0 & (1+U)R & (1-U)R \\ 1 & -1 & UR & -UR \\ 2\phi_+ & 0 & (1+U)R\phi_- & (1-U)R\phi_-^{-1} \\ \phi_+ & -\phi_+^{-1} & UR\phi_- & -UR\phi_-^{-1} \end{bmatrix}$$ ✓

$$= \det \begin{bmatrix} 2 & 0 & (1+U)R & (1-U)R \\ 1 & -1 & UR & -UR \\ 0 & 0 & (1+U)R(\phi_- - \phi_+) & (1-U)R(\phi_-^{-1} - \phi_+) \\ \phi_+ & -\phi_+^{-1} & UR\phi_- & -UR\phi_-^{-1} \end{bmatrix}$$ ✓

Expanding around the third row we get (back to general case)

$$\frac{\det(M)}{R_+^4 (ik_+)^2} = (1+U)R(\phi_- - \phi_+) \det\begin{pmatrix} 2 & 0 & (1-U)R \\ 1 & -1 & -UR \\ \phi_+ & -\phi_+^{-1} & -UR\phi_-^{-1} \end{pmatrix}$$

$$- (1-U)R(\phi_-^{-1} - \phi_+) \det\begin{pmatrix} 2 & 0 & (1+U)R \\ 1 & -1 & UR \\ \phi_+ & -\phi_+^{-1} & UR\phi_- \end{pmatrix}$$

$$\det\begin{pmatrix} 2 & 0 & (1-U)R \\ 1 & -1 & -UR \\ \phi_+ & -\phi_+^{-1} & -UR\phi_-^{-1} \end{pmatrix} = 2(UR\phi_-^{-1} - UR\phi_+^{-1}) + (1-U)R(\phi_+ - \phi_+^{-1})$$

$$= 2UR(\phi_-^{-1} - \phi_+^{-1}) + (1-U)R(\phi_+ - \phi_+^{-1}) \quad ✓$$

$$\det\begin{pmatrix} 2 & 0 & (1+U)R \\ 1 & -1 & UR \\ \phi_+ & -\phi_+^{-1} & UR\phi_- \end{pmatrix} = 2UR(\phi_+^{-1} - \phi_-) + (1+U)R(\phi_+ - \phi_+^{-1}) \quad ✓$$

So
$$\frac{\det(M)}{R_+^4 (ik_+)^2} = (1+U)R(\phi_- - \phi_+)\left[2UR(\phi_-^{-1} - \phi_+^{-1}) + (1-U)R(\phi_+ - \phi_+^{-1})\right]$$

$$- (1-U)R(\phi_-^{-1} - \phi_+)\left[2UR(\phi_+^{-1} - \phi_-) + (1+U)R(\phi_+ - \phi_+^{-1})\right]$$

$$= R^2\Big[2U(1+U)(\phi_- - \phi_+)(\phi_-^{-1} - \phi_+^{-1}) + (1-U^2)(\phi_- - \phi_+)(\phi_+ - \phi_+^{-1})$$

$$- 2U(1-U)(\phi_-^{-1} - \phi_+)(\phi_+^{-1} - \phi_-) - (1-U^2)(\phi_-^{-1} - \phi_+)(\phi_+ - \phi_+^{-1})\Big] \quad ✓$$

$$\frac{\det M}{(R_+R_-)^2 (ik_+)^2} = 2U\Big[\overbrace{(\phi_- - \phi_+)(\phi_-^{-1} - \phi_+^{-1})}^{2 - \phi_+\phi_-^{-1} - \phi_-\phi_+^{-1}} - \overbrace{(\phi_-^{-1} - \phi_+)(\phi_+^{-1} - \phi_-)}^{-2 + \phi_-^{-1}\phi_+^{-1} + \phi_+\phi_-}\Big]$$

$$+ 2U^2\Big[\overbrace{(\phi_- - \phi_+)(\phi_-^{-1} - \phi_+^{-1})}^{2 - \phi_+\phi_-^{-1} - \phi_-\phi_+^{-1}} + \overbrace{(\phi_-^{-1} - \phi_+)(\phi_+^{-1} - \phi_-)}^{-2 + \phi_-^{-1}\phi_+^{-1} + \phi_+\phi_-}\Big] \quad ✓$$

$$+ (1-U^2)(\phi_+ - \phi_+^{-1})(\phi_- - \phi_-^{-1})$$

$$= 2U\left[4 - (\phi_+ + \phi_+^{-1})(\phi_- + \phi_-^{-1})\right]$$

$$+2U^2(\phi_+ - \phi_+^{-1})(\phi_- - \phi_-^{-1}) + (1-U^2)(\phi_+ - \phi_+^{-1})(\phi_- - \phi_-^{-1})$$

So

$$\boxed{\frac{\det(M)}{(R_+ R_-)^2 (ik_+)^2} = 2U\left[4 - (\phi_+ + \phi_+^{-1})(\phi_- + \phi_-^{-1})\right] + (1+U^2)(\phi_+ - \phi_+^{-1})(\phi_- - \phi_-^{-1})}$$ ✓

This is not identically zero. For example, with $V_0 = \frac{1}{2}\omega$, $\omega a = \pi$

$$U = \frac{\omega - \frac{1}{2}\omega}{\omega + \frac{1}{2}\omega} = \frac{1}{3} \qquad k_+ = \frac{3}{2}\omega \qquad k_- = \frac{1}{2}\omega$$

$$\phi_+ = e^{i\frac{3}{2}\omega a} = e^{i\frac{3\pi}{2}} = -i \qquad \phi_- = e^{i\frac{1}{2}\omega a} = e^{i\frac{\pi}{2}} = i$$

$$\frac{\det(M)}{(R_+ R_-)^2 (ik_+)^2} = \frac{2}{3}\left[4 - 0\cdot 0\right] + \left(1 + \frac{1}{9}\right)(-2i)\,2i = \frac{24}{9} + \frac{40}{9} = \frac{64}{9} \neq 0$$

So cannot have $C_\beta^R = C_\beta^T \equiv 0$

Remarks:

(1) If $n_2 = n_3 = 0$, $n_1 = 1$, then $R_- = R = 0$, $\det(M) = 0$, and $C_\beta^R = C_\beta^T = 0$ This recovers the simple QM limit

(2) Wave velocity inside the potential barrier: $e^{i(k_\pm x - \omega t)}$

wave phase velocity $= \; V = \frac{x}{t} = \frac{\omega}{k_\pm} = \frac{\omega}{\omega \pm V_0}$

For $0 < V_0 < \omega$, the $k_-$ wave has $V > 1$ superluminal