H Operator on Non Eigen States & Wave Packets

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Special note: The material (a bit later into this document) on non-eigenstates and wave packets was developed solely by the author, who was unable to find such material in the literature (though it probably exists somewhere.) Its accuracy has not been checked by others.

The following Wholeness Chart was originally completed on November 21, 2011. The material following it was originally done as of March 13, 2010, and was never fully completed (although almost). That material may have some errors in it, i.e., it may not exactly parallel the chart below (although it should be close.) Note that corrections have been made as of June 1, 2016 to the ½ energy vacuum terms in the continuous solutions. They had been missing a factor of $\delta(0)$.

Wholeness Chart 10-3. Discrete vs Continuous Versions of QFT
(Only Scalars Shown)

	Discrete	**Continuous**
Field Equations Solutions	$\phi(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}\left(a(\mathbf{k})e^{-ikx} + b^{\dagger}(\mathbf{k})e^{ikx}\right)$ $\phi^{\dagger}(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}\left(b(\mathbf{k})e^{-ikx} + a^{\dagger}(\mathbf{k})e^{ikx}\right)$	$\phi(x) = \int \frac{d^3k}{\sqrt{2(2\pi)^3\,\omega_{\mathbf{k}}}}\left(a(\mathbf{k})e^{-ikx} + b^{\dagger}(\mathbf{k})e^{ikx}\right)$ $\phi^{\dagger}(x) = \int \frac{d^3k}{\sqrt{2(2\pi)^3\,\omega_{\mathbf{k}}}}\left(b(\mathbf{k})e^{-ikx} + a^{\dagger}(\mathbf{k})e^{ikx}\right)$
Coefficient commutators	$\left[a(\mathbf{k}),a^{\dagger}(\mathbf{k}')\right] = \left[b(\mathbf{k}),b^{\dagger}(\mathbf{k}')\right] = \delta_{\mathbf{k}\mathbf{k}'}$	$\left[a(\mathbf{k}),a^{\dagger}(\mathbf{k}')\right] = \left[b(\mathbf{k}),b^{\dagger}(\mathbf{k}')\right] = \delta(\mathbf{k}-\mathbf{k}')$
$\mathcal{H}_0^0$	$\pi_0^0\dot{\phi} + \pi_0^{0\dagger}\dot{\phi}^{\dagger} - \mathcal{L}_0^0 = \left(\dot{\phi}\dot{\phi}^{\dagger} + \nabla\phi^{\dagger}\cdot\nabla\phi + \mu^2\phi^{\dagger}\phi\right)$	as at left
H_0^0	$\sum_{\mathbf{k}} \omega_{\mathbf{k}}\left(N_a(\mathbf{k}) + \frac{1}{2} + N_b(\mathbf{k}) + \frac{1}{2}\right)$ $N_a(\mathbf{k}) = a^{\dagger}(\mathbf{k})\,a(\mathbf{k})$, $N_b(\mathbf{k}) = b^{\dagger}(\mathbf{k})\,b(\mathbf{k})$	$\int \omega_{\mathbf{k}}\left(N_a(\mathbf{k}) + \frac{1}{2}\delta(0) + N_b(\mathbf{k}) + \frac{1}{2}\delta(0)\right)d^3k$ $N_a(\mathbf{k}) = a^{\dagger}(\mathbf{k})\,a(\mathbf{k})$, $N_b(\mathbf{k}) = b^{\dagger}(\mathbf{k})\,b(\mathbf{k})$
Operator Units	$N_a(\mathbf{k})$, number of real particles, unitless, M^0 ½ , number of vacuum particles, unitless $a(\mathbf{k})$, $a^{\dagger}(\mathbf{k})$, unitless Similar for $N_b(\mathbf{k})$, $b(\mathbf{k})$, $b^{\dagger}(\mathbf{k})$,	$N_a(\mathbf{k})$, (num real particles)/(**k** space vol), M^{-3} ½ , (num vacuum particles)/(**k** space vol), M^{-3} $a(\mathbf{k})$, $a^{\dagger}(\mathbf{k})$, $M^{-3/2}$ Similar for $N_b(\mathbf{k})$, $b(\mathbf{k})$, $b^{\dagger}(\mathbf{k})$,
	Single Particle State Relations (Only particles, not anti-particles shown)	
Eigenstate Creation	$a^{\dagger}(\mathbf{k})\lvert 0\rangle = \lvert\phi_{\mathbf{k}}\rangle = \left\lvert \frac{e^{-ikx}}{\sqrt{V}}\right\rangle$ Eigenstate at one point in **k** space, spread over volume V in **x** space.	$a^{\dagger}(\mathbf{k})\lvert 0\rangle = \lvert\phi(\mathbf{k})\rangle = \left\lvert \frac{e^{-ikx}}{\sqrt{(2\pi)^3}}\right\rangle$ Eigenstate at one point in **k** space, spread over universe in **x** space. $V \to \infty$

General State Creation, ***C* is General State Creation Operator**	$\vert\phi\rangle = C\vert 0\rangle = \sum_{\mathbf{k}} A_{\mathbf{k}} a^\dagger(\mathbf{k})\vert 0\rangle$ $= \left\vert \frac{1}{\sqrt{V}}\left(A_{\mathbf{k}_1} e^{-ik_1x} + A_{\mathbf{k}_2} e^{-ik_2x} + ..\right)\right\rangle = \left\vert \sum_{\mathbf{k}} A_{\mathbf{k}} \frac{e^{-ikx}}{\sqrt{V}}\right\rangle$ Coefficient $A_{\mathbf{k}}$ unitless. State units $l^{-3/2} = M^{3/2}$	$\vert\phi\rangle = C\vert 0\rangle = \int A(\mathbf{k}) a^\dagger(\mathbf{k}) d^3k\vert 0\rangle$ $= \left\vert \int A(\mathbf{k}) \frac{e^{-ikx}}{\sqrt{(2\pi)^3}} d^3k \right\rangle$ Coefficient $A(\mathbf{k})$ units $l^{3/2} = M^{-3/2}$. State units $l^{-3/2} = M^{3/2}$
Creation Operator *C*	$C = \sum_{\mathbf{k}} A_{\mathbf{k}} a^\dagger(\mathbf{k})$	$C = \int A(\mathbf{k}) a^\dagger(\mathbf{k}) d^3k$
State Norms	$\langle\phi\vert\phi\rangle = 1$	$\langle\phi\vert\phi\rangle = 1$
Coefficient Properties	$\sum_{\mathbf{k}} \vert A_{\mathbf{k}}\vert^2 = 1$	$\int \vert A(\mathbf{k})\vert^2 d^3k = 1$
For an Eigenstate	Only one $A_{\mathbf{k}}$, with $\vert A_{\mathbf{k}}\vert = 1$. $\vert A_{\mathbf{k}}\vert / \sqrt{V} \to 1/\sqrt{V}$	Not very meaningful.
N_a (k) Acting on General State	$N_a(\mathbf{k}) \left\vert \sum_{\mathbf{k}'} A_{\mathbf{k}'} \frac{e^{-ik'x}}{\sqrt{V}} \right\rangle$ $= \vert A_{\mathbf{k}'}\vert^2 \delta_{\mathbf{k}\mathbf{k}'} \left\vert \sum_{\mathbf{k}'} A_{\mathbf{k}'} \frac{e^{-ik'x}}{\sqrt{V}} \right\rangle = \vert A_{\mathbf{k}}\vert^2 \left\vert \sum_{\mathbf{k}'} A_{\mathbf{k}'} \frac{e^{-ik'x}}{\sqrt{V}} \right\rangle$	$N_a(\mathbf{k}) \left\vert \int A(\mathbf{k}') \frac{e^{-ik'x}}{\sqrt{(2\pi)^3}} d^3k' \right\rangle$ $= \vert A(\mathbf{k}')\vert^2 \delta(\mathbf{k}-\mathbf{k}') \left\vert \int A(\mathbf{k}') \frac{e^{-ik'x}}{\sqrt{(2\pi)^3}} d^3k' \right\rangle$
Eigenstate Energy Expectation Value	$\bar{E} = \langle\phi_{\mathbf{k}'}\vert \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(N_a(\mathbf{k}) + \tfrac{1}{2} + N_b(\mathbf{k}) + \tfrac{1}{2}\right)\vert\phi_{\mathbf{k}'}\rangle$ $= \left(\omega_{\mathbf{k}'} + \tfrac{1}{2}\sum_{\mathbf{k}} \omega_{\mathbf{k}} + \tfrac{1}{2}\sum_{\mathbf{k}} \omega_{\mathbf{k}}\right)\langle\phi_{\mathbf{k}'}\vert\vert\phi_{\mathbf{k}'}\rangle$ $= \omega_{\mathbf{k}'} + \sum_{\mathbf{k}} \omega_{\mathbf{k}}$	$\bar{E} = \langle\phi(\mathbf{k}')\vert \int \omega_{\mathbf{k}} (N_a(\mathbf{k}) + \tfrac{1}{2}\delta(0)$ $+ N_b(\mathbf{k}) + \tfrac{1}{2}\delta(0)) d^3k \vert\phi(\mathbf{k}')\rangle$ $= \int \omega_{\mathbf{k}} \left(\delta(\mathbf{k}-\mathbf{k}') + \tfrac{1}{2}\delta(0) + \tfrac{1}{2}\delta(0)\right) d^3k \langle\phi\vert\vert\phi\rangle$ $= \omega_{\mathbf{k}'} + \int \omega_{\mathbf{k}} \delta(0) d^3k$
General State Energy Expectation Value	$\bar{E} = \left\langle \sum_{\mathbf{k}'} A^\dagger_{\mathbf{k}'} \frac{e^{ik'x}}{\sqrt{V}} \right\vert \sum_{\mathbf{k}} \omega_{\mathbf{k}} (N_a(\mathbf{k}) + \tfrac{1}{2}$ $+ N_b(\mathbf{k}) + \tfrac{1}{2}) \left\vert \sum_{\mathbf{k}'} A_{\mathbf{k}'} \frac{e^{-ik'x}}{\sqrt{V}} \right\rangle$ $= \left(\sum_{\mathbf{k}'} \omega_{\mathbf{k}'} A^\dagger_{\mathbf{k}'} A_{\mathbf{k}'} \delta_{\mathbf{k}\mathbf{k}'} + \tfrac{1}{2}\sum_{\mathbf{k}} \omega_{\mathbf{k}} + \tfrac{1}{2}\sum_{\mathbf{k}} \omega_{\mathbf{k}}\right)\langle\phi\vert\phi\rangle$ $= \sum_{\mathbf{k}} \vert A_{\mathbf{k}}\vert^2 \omega_{\mathbf{k}} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} = \bar{\omega} + \sum_{\mathbf{k}} \omega_{\mathbf{k}}$	$\bar{E} = \left\langle \int A(\mathbf{k}') \frac{e^{-ik'x}}{\sqrt{(2\pi)^3}} d^3k' \right\vert \int \omega_{\mathbf{k}} (N_a(\mathbf{k}) + \tfrac{1}{2}\delta(0)$ $+ N_b(\mathbf{k}) + \tfrac{1}{2}\delta(0)) d^3k \left\vert \int A(\mathbf{k}') \frac{e^{-ik'x}}{\sqrt{(2\pi)^3}} d^3k' \right\rangle$ $= \int \omega_{\mathbf{k}} \left(\vert A(\mathbf{k}')\vert^2 \delta(\mathbf{k}-\mathbf{k}') + \tfrac{1}{2}\delta(0) + \tfrac{1}{2}\delta(0)\right) d^3k \langle\phi\vert\vert\phi$ $= \int \vert A(\mathbf{k})\vert^2 \omega_{\mathbf{k}} d^3k + \int \omega_{\mathbf{k}} \delta(0) d^3k = \bar{\omega} + \int \omega_{\mathbf{k}} \delta(0) d^3k$
	<u>**Multi-particle State Relations**</u> (Only particles, not anti-particles shown)	
Multi Eigen Particles Creation	$a^\dagger(\mathbf{k}_1) a^\dagger(\mathbf{k}_2) ... \vert 0\rangle = \vert\phi_{\mathbf{k}_1}, \phi_{\mathbf{k}_2}, ..\rangle$	$a^\dagger(\mathbf{k}_1) a^\dagger(\mathbf{k}_2) ... \vert 0\rangle = \vert\phi(\mathbf{k}_1), \phi(\mathbf{k}_2), ..\rangle$

Multi General Particles Creation, **C_q is qth Particle Creation Operator**	$\lvert\phi_q,\phi_r,...\rangle=\left(C_q C_r ..\right)\lvert 0\rangle$ $=\left(\sum_{\mathbf{k}} A_{q\mathbf{k}} a^\dagger(\mathbf{k})\right)\left(\sum_{\mathbf{k}} A_{r\mathbf{k}} a^\dagger(\mathbf{k})\right)(...)\lvert 0\rangle$ $=\left\lvert\sum_{\mathbf{k}} A_{q\mathbf{k}}\frac{e^{-ikx_q}}{\sqrt{V}},\sum_{\mathbf{k}} A_{r\mathbf{k}}\frac{e^{-ikx_r}}{\sqrt{V}},..\right\rangle$	$\lvert\phi_q,\phi_r,...\rangle=\left(C_q C_r ..\right)\lvert 0\rangle$ $=\left(\int A_q(\mathbf{k}) a^\dagger(\mathbf{k}) d^3k\right)\left(\int A_r(\mathbf{k}) a^\dagger(\mathbf{k}) d^3k\right)(..)\lvert 0\rangle$ $=\left\lvert\int A_q(\mathbf{k})\frac{e^{-ikx_q}}{\sqrt{(2\pi)^3}}d^3k,\int A_r(\mathbf{k})\frac{e^{-ikx_r}}{\sqrt{(2\pi)^3}}d^3k,..\right\rangle$
Normalized Operator C_q	$C_q=\sum_{\mathbf{k}} A_{q\mathbf{k}} a^\dagger(\mathbf{k})$	$C_q=\int A_q(\mathbf{k}) a^\dagger(\mathbf{k}) d^3k$
State Norms	$\langle\phi\vert\phi\rangle=\langle\phi_q,\phi_r,...\vert\phi_q,\phi_r,...\rangle=1$	$\langle\phi\vert\phi\rangle=\langle\phi_q,\phi_r,...\vert\phi_q,\phi_r,...\rangle=1$
Coefficient Properties	$\sum_{\mathbf{k}}\lvert A_{q\mathbf{k}}\rvert^2=1,\quad\sum_{\mathbf{k}}\lvert A_{r\mathbf{k}}\rvert^2=1,$ etc.	$\int\lvert A_q(\mathbf{k})\rvert^2 d^3k=1,\quad\int\lvert A_r(\mathbf{k})\rvert^2 d^3k=1,$ etc.
N_a (k) Acting on Multi General Particles State	$N_a(\mathbf{k})\lvert\phi_q,2\phi_r,..\rangle$ $=N_a(\mathbf{k})\left\lvert\sum_{\mathbf{k}'} A_{q\mathbf{k}'}\frac{e^{-ik'x_q}}{\sqrt{V}},2\sum_{\mathbf{k}'} A_{r\mathbf{k}'}\frac{e^{-ik'x_r}}{\sqrt{V}},..\right\rangle$ $=\left(\lvert A_{q\mathbf{k}'}\rvert^2\delta_{\mathbf{k}\mathbf{k}'}+2\lvert A_{r\mathbf{k}'}\rvert^2\delta_{\mathbf{k}\mathbf{k}'}+..\right)\lvert\phi_r,2\phi_r,..\rangle$ $=\left(\lvert A_{q\mathbf{k}}\rvert^2+2\lvert A_{r\mathbf{k}}\rvert^2+..\right)\lvert\phi_r,2\phi_r,..\rangle$	$N_a(\mathbf{k})\lvert\phi_q,2\phi_r,..\rangle=N_a(\mathbf{k})\times$ $\left\lvert\int A_q(\mathbf{k}')\frac{e^{-ik'x_q}}{\sqrt{(2\pi)^3}}d^3k',2\int A_r(\mathbf{k}')\frac{e^{-ik'x_r}}{\sqrt{(2\pi)^3}}d^3k',..\right\rangle$ $=(\lvert A_q(\mathbf{k}')\rvert^2\delta(\mathbf{k}-\mathbf{k}')$ $+2\lvert A_r(\mathbf{k}')\rvert^2\delta(\mathbf{k}-\mathbf{k}')+..)\lvert\phi_r,2\phi_r,..\rangle$
Multi Eigen Particles Energy Expectation Value	$\bar{E}=\langle\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},..\lvert\sum_{\mathbf{k}}\omega_{\mathbf{k}}(N_a(\mathbf{k})+\tfrac{1}{2}+$ $N_b(\mathbf{k})+\tfrac{1}{2})\rvert\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},..\rangle$ $=(\omega_{\mathbf{k}_1}+2\omega_{\mathbf{k}_2}+..$ $+\tfrac{1}{2}\sum_{\mathbf{k}}\omega_{\mathbf{k}}+\tfrac{1}{2}\sum_{\mathbf{k}}\omega_{\mathbf{k}})\langle\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},..\vert\phi_{\mathbf{k}_1},2\phi_{\mathbf{k}_2},..\rangle$ $=\omega_{\mathbf{k}_1}+2\omega_{\mathbf{k}_2}+...+\sum_{\mathbf{k}}\omega_{\mathbf{k}}$	$\bar{E}=\langle\phi(\mathbf{k}_1),2\phi(\mathbf{k}_2),..\lvert\int\omega_{\mathbf{k}}(N_a(\mathbf{k})+\tfrac{1}{2}\delta(0)$ $+N_b(\mathbf{k})+\tfrac{1}{2}\delta(0))d^3k\rvert\phi(\mathbf{k}_1),2\phi(\mathbf{k}_2),..\rangle$ $=(\omega_{\mathbf{k}_1}+2\omega_{\mathbf{k}_2}+...+\tfrac{1}{2}\delta(0)\int\omega_{\mathbf{k}}d^3k+$ $\tfrac{1}{2}\delta(0)\int\omega_{\mathbf{k}}d^3k)\langle\phi(\mathbf{k}_1),2\phi(\mathbf{k}_2),.\vert\phi(\mathbf{k}_1),2\phi(\mathbf{k}_2),.\rangle$ $=\omega_{\mathbf{k}_1}+2\omega_{\mathbf{k}_2}+...+\delta(0)\int\omega_{\mathbf{k}}d^3k$
Multi General Particles Energy Expectation Value	$\bar{E}=\langle\phi_q,2\phi_r,..\lvert\sum_{\mathbf{k}}\omega_{\mathbf{k}}(N_a(\mathbf{k})+\tfrac{1}{2}$ $+N_b(\mathbf{k})+\tfrac{1}{2})\rvert\phi_q,2\phi_r,..\rangle$ $=(\sum_{\mathbf{k}}\lvert A_{q\mathbf{k}}\rvert^2\omega_{\mathbf{k}}+2\sum_{\mathbf{k}}\lvert A_{r\mathbf{k}}\rvert^2\omega_{\mathbf{k}}+...$ $+\tfrac{1}{2}\sum_{\mathbf{k}}\omega_{\mathbf{k}}+\tfrac{1}{2}\sum_{\mathbf{k}}\omega_{\mathbf{k}})\langle\phi_q,2\phi_r,..\vert\phi_q,2\phi_r,..\rangle$ $=\bar{\omega}_q+\bar{\omega}_r+...+\sum_{\mathbf{k}}\omega_{\mathbf{k}}$	$\bar{E}=\langle\phi_q,2\phi_r,..\lvert\int\omega_{\mathbf{k}}(N_a(\mathbf{k})+\tfrac{1}{2}\delta(0)$ $+N_b(\mathbf{k})+\tfrac{1}{2}\delta(0))d^3k\rvert\phi_q,2\phi_r,..\rangle$ $=(\int\omega_{\mathbf{k}}\lvert A_q(\mathbf{k})\rvert^2 d^3k+2\int\omega_{\mathbf{k}}\lvert A_r(\mathbf{k})\rvert^2 d^3k+..$ $+\tfrac{1}{2}\delta(0)\int\omega_{\mathbf{k}}d^3k+\tfrac{1}{2}\delta(0)\int\omega_{\mathbf{k}}d^3k)\langle\phi_q,2\phi_r,.\vert\phi_q,2\phi_r,.\rangle$ $=\bar{\omega}_q+2\bar{\omega}_r+...+\delta(0)\int\omega_{\mathbf{k}}d^3k$
Note	In the energy expectation derivation for the continuous case, one finds a delta function squared in the vacuum energy part. This is undefined mathematically. By some perspectives, its evaluation leaves a vacuum term of energy $\omega(\mathbf{k}=0)$ which equals μ (one particle mass). An alternative perspective is shown above.	

1. Solutions to Free Field Equations

For a scalar, we have

1.1 Free field solutions

$$\begin{aligned} \phi &= \phi^{+} + \phi^{-} \\ \phi^{\dagger} &= \phi^{\dagger +} + \phi^{\dagger -} \end{aligned} \tag{1}$$

1.1.1 Discrete eigenstates (finite volume B.C.'s or periodic B.C.'s)

$$\begin{aligned} \phi(x) &= \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} \left[a(\mathbf{k}) e^{-ikx} + b^{\dagger}(\mathbf{k}) e^{ikx} \right] \\ \phi^{\dagger}(x) &= \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} \left[b(\mathbf{k}) e^{-ikx} + a^{\dagger}(\mathbf{k}) e^{ikx} \right] \end{aligned} \tag{2}$$

where the summation is from infinite **k** in the negative x direction to infinite **k** in the positive x direction plus similar summations for the y and z directions.

1.1.2 Continuous eigenstates (no B.C.'s over all space)

$$\begin{aligned} \phi(x) &= \frac{1}{\sqrt{(2\pi)^3}} \int \frac{d\boldsymbol{k}}{\sqrt{2\omega_{\mathbf{k}}}} \left[a(\mathbf{k}) e^{-ikx} + b^{\dagger}(\mathbf{k}) e^{ikx} \right] \\ \phi^{\dagger}(x) &= \frac{1}{\sqrt{(2\pi)^3}} \int \frac{d\boldsymbol{k}}{\sqrt{2\omega_{\mathbf{k}}}} \left[b(\mathbf{k}) e^{-ikx} + a^{\dagger}(\mathbf{k}) e^{ikx} \right] \end{aligned} \tag{3}$$

where the integration ranges as the summation in (2) except that here **k** is a continuous variable.

2. Relativistic Quantum Mechanics (RQM)

In relativistic quantum mechanics (RQM) $\phi(x)$ of (2) represents a single particle general state that is a sum of discrete momentum eigenstates of that single particle. The coefficients $a(\mathbf{k})$ and $b^{\dagger}(\mathbf{k})$ are numbers, amplitudes which, when squared, equal the probability of finding the single particle in that discrete eigenstate.

In RQM, $\phi(x)$ of (3) represents a single particle wave packet comprising an integral over momentum eigenstates that are continuous. The coefficients $a(\mathbf{k})$ and $b^{\dagger}(\mathbf{k})$ are numbers which represent the Fourier transform amplitudes of the eigenstates in the continuous momentum space.

In quantum field theory (QFT) these coefficients are not numbers but operators that each create or destroy single particle eigenstates. Commonly in QFT one employs one term in (2) to create or destroy a single particle discrete momentum eigenstate (having no uncertainty in its momentum, but infinite uncertainty in its spatial location.)

2.1 Discrete Solutions

The solutions (2) in RQM are single particle general (sum of eigenstates) states, not operators, of form (where we substitute numerical $A_{\mathbf{k}}$ in RQM for operator $a(\mathbf{k})$ in QFT, etc.)

$$\left|\phi\right\rangle = \sum_{\mathbf{k}} \frac{A_{\mathbf{k}}}{\sqrt{2\omega_{\mathbf{k}}}} \frac{e^{-ikx}}{\sqrt{V}} = \sum_{\mathbf{k}} \frac{A_{\mathbf{k}}}{\sqrt{2\omega_{\mathbf{k}}}} \left|\phi_{\mathbf{k}}\right\rangle \tag{4}$$

where $\left|\phi_{\mathbf{k}}\right\rangle$ has unit norm. That is,

$$\left|\phi_{\mathbf{k}}\right\rangle = \frac{e^{-ikx}}{\sqrt{V}}, \tag{5}$$

so that

$$\langle \phi_{\mathbf{k}} | \phi_{\mathbf{k}} \rangle = \frac{1}{V} \int e^{ikx} e^{-ikx} d^3 x = 1\,, \tag{6}$$

or more generally,

$$\langle \phi_{\mathbf{k}} | \phi_{\mathbf{k}'} \rangle = \frac{1}{V} \int e^{ikx} e^{-ikx'} d^3 x = \delta_{\mathbf{k}\mathbf{k}'}\,. \tag{7}$$

2.1.1 Probability for Discrete Solutions

For a single particle state in RQM the probability density[1] is

$$\rho = i\left(\langle \phi | \phi_{,0} \rangle_{n.i.} - \langle \phi_{,0} | \phi \rangle_{n.i.} \right) = \left(2 \sum_{\mathbf{k}} \frac{A_{\mathbf{k}}^{\dagger}}{\sqrt{2\omega_{\mathbf{k}}}} \frac{e^{ikx}}{\sqrt{V}} \right)\left(\sum_{\mathbf{k}'} \frac{\omega_{\mathbf{k}'} A_{\mathbf{k}'}}{\sqrt{2\omega_{\mathbf{k}'}}} \frac{e^{-ik'x}}{\sqrt{V}} \right) \tag{8}$$

where the subscript "*n.i.*" implies we are not integrating over space inside the bracket. When we do integrate, using the Kronecker delta function relation of (7), we get

$$\int \rho d^3 x = \sum_{\mathbf{k}} | A_{\mathbf{k}} |^2 = 1\,, \tag{9}$$

where $|A_{\mathbf{k}}|^2$ is the probability of measuring the **k**th eigenstate.

Note that this is the reason for the normalization factors $1/\sqrt{2\omega_{\mathbf{k}} V}$ used in (2). Those factors result in a total probability of one for a single particle and $|A_{\mathbf{k}}|^2$ as the probability for measuring the **k**th state. That is, the form of the relativistic field equation gave us the form of the probability density in the middle of (8). (See footnote 1.) The time derivatives in (8) gave us a factor of $\omega_{\mathbf{k}}$, and the two terms a factor of 2. These cancel in (9) with the $2\omega_{\mathbf{k}}$ in the denominators of the terms in (2). The V term in the denominator cancels in the integration over volume in (9) and the result is a total probability of 1.

This probability value of unity is a relativistic invariant. If we change our frame, the energy spectrum (i.e., the $\omega_{\mathbf{k}}$ values) will change (K.E. looks different for a given energy-momentum eigenstate). But these factors cancel out in the probability calculation and always result in one for any frame. Further, the $A_{\mathbf{k}}$ here are constants that do not vary with frame, so the probability of finding any particular state is also independent of what frame the measurements are taken in.

As an aside, note that

$$\langle \phi | \phi \rangle = \sum_{\mathbf{k}} \frac{(A_{\mathbf{k}})^2}{2\omega_{\mathbf{k}}} \neq 1 \tag{10}$$

because (unlike in NRQM) the LHS of (10) does not represent the integral of the probability density over space in RQM.

2.1.2 Expectation Values for Discrete Solutions

An expectation value, for energy in this example, is found using the probability density (8) in parallel fashion to that of NRQM. That is, we "sandwich" the energy operator $i\frac{\partial}{\partial t}$ inside the probability density and integrate over the volume, i.e.,

$$\bar{E} = i\left(\langle \phi | i\tfrac{\partial}{\partial t} | \phi_{,0} \rangle - \langle \phi_{,0} | i\tfrac{\partial}{\partial t} | \phi \rangle \right) = \sum_{\mathbf{k}} \langle \phi_{\mathbf{k}} | (A_{\mathbf{k}})^2 i\tfrac{\partial}{\partial t} | \phi_{\mathbf{k}} \rangle = \sum_{\mathbf{k}} (A_{\mathbf{k}})^2 \omega_{\mathbf{k}}\,. \tag{11}$$

This is for a single particle state and equals the statistically weighted average of the single particle eigenstate energies, as it must.

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[1] Similar to non-relativistic quantum mechanics (NRQM), take the field equation (Klein-Gordon rather than Schroedinger) and post multiply by $|\phi\rangle$, then subtract from it the same equation pre-multiplied by $\langle\phi|$, and note the result has the form of the continuity equation (conservation of probability not mass or charge in this case.) The $\frac{\partial \rho}{\partial t}$ term in this equation has ρ of the form of the middle relation in (8).

For a multiparticle state $\left|\phi_p\phi_q\phi_r....\right\rangle$ where the particles are all general rather than eigenstates, the expectation value for the total energy of all states is found by

$$\bar{E} = i\left(\left\langle \phi_p\phi_q\phi_r....\right| i\tfrac{\partial}{\partial t}\left|\phi_p\phi_q\phi_r....\right\rangle_{,0} - \left\langle (\phi_p\phi_q\phi_r....)_{,0}\right| i\tfrac{\partial}{\partial t}\left|\phi_p\phi_q\phi_r....\right\rangle\right) \tag{12}$$

and turns out to be

$$\bar{E}_{total} = \bar{E}_p + \bar{E}_q + \bar{E}_r + \dots \tag{13}$$

i.e, the sum of expectation energies of all individual (general state) particles.

For a multiparticle state $\left|\phi_p\phi_q\phi_r....\right\rangle$ where the particles are all in energy eigenstates, the expectation value for the total energy of all states is found by

$$E = i\left(\left\langle \phi_p\phi_q\phi_r....\right| H\left|\phi_p\phi_q\phi_r....\right\rangle_{,0} - \left\langle (\phi_p\phi_q\phi_r....)_{,0}\right| H\left|\phi_p\phi_q\phi_r....\right\rangle\right) \tag{14}$$

and turns out to be

$$E_{total} = E_p + E_q + E_r + \dots \tag{15}$$

i.e, the sum of the energies of all individual (energy eigenstate) particles.

2.2 Continuous Solutions

The continuous solutions (3) in RQM are single particle wave packet states of form (where we substitute the Fourier amplitude $A(\mathbf{k})$ [a continuous numerical function of **k]** for operator $a(\mathbf{k})$, etc.)

$$\left|\phi(x)\right\rangle = \frac{1}{\sqrt{(2\pi)^3}}\int \frac{d\boldsymbol{k}}{\sqrt{2\omega_{\mathbf{k}}}} A(\mathbf{k})e^{-ikx} . \tag{16}$$

2.2.1 Probability for Continuous Solutions

For a single particle wave packet in RQM the probability density is

$$\begin{aligned}\rho &= i\left(\left\langle\phi\middle|\phi_{,0}\right\rangle_{n.i.} - \left\langle\phi_{,0}\middle|\phi\right\rangle_{n.i.}\right)\\ &= 2\left(\frac{1}{\sqrt{(2\pi)^3}}\int\frac{d\boldsymbol{k}}{\sqrt{2\omega_{\mathbf{k}}}}A(\mathbf{k})e^{-ikx}\right)\left(\frac{1}{\sqrt{(2\pi)^3}}\int\frac{d\boldsymbol{k}'}{\sqrt{2\omega_{\mathbf{k}'}}}\omega_{\mathbf{k}'}A(\mathbf{k}')e^{-ik'x}\right)^{\dagger}\end{aligned} \tag{17}$$

We integrate this over space, using the Dirac delta function relation (which is the continuous solution case analog of (7))

$$\delta^{(3)}(\mathbf{k}-\mathbf{k}') = \frac{1}{(2\pi)^3}\int e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}d^3x . \tag{18}$$

We thus find the total probability

$$\int \rho d^3x = \int |A(\mathbf{k})|^2\, d\mathbf{k} = 1 , \tag{19}$$

which is the correct result if $A(\mathbf{k})$ is the properly normalized Fourier amplitude[2].

2.2.2 Expectation Values for Continuous Solutions

The energy expectation value (with $H = i\frac{\partial}{\partial t}$) for the wave packet is

$$\bar{E} = i\left(\left\langle\phi\right|H\left|\phi_{,0}\right\rangle - \left\langle\phi_{,0}\right|H\left|\phi\right\rangle\right) = \int |A(\mathbf{k})|^2\,\omega_{\mathbf{k}}d\mathbf{k} , \tag{20}$$

which again equals the statistically weighted average.

For a multiparticle state $\left|\phi_p\phi_q\phi_r....\right\rangle$ where the particles are wave packets, the expectation value for the total energy of all states turns out to be

---

[2] We note as another aside, that for wave packets in RQM $\left\langle\phi\middle|\phi\right\rangle = \int \frac{|A(\mathbf{k})|^2}{2\omega_{\mathbf{k}}}d\mathbf{k} \neq 1$, unlike the corresponding result for NRQM wave packets.

$$\bar{E}_{total} = \bar{E}_p + \bar{E}_q + \bar{E}_r + \dots, \tag{21}$$

the sum of expectation energies of all individual wave packets.

3. Quantum Field Theory (QFT)

3.1 The Hamiltonian

3.1.1 Hamiltonian Density Operator

$$\mathcal{L} = \partial_\mu \phi^\dagger \partial^\mu \phi - \mu^2 \phi^\dagger \phi \tag{22}$$

$$\begin{aligned}\mathcal{H} &= \sum \pi_i \dot{\phi}^i - \mathcal{L} = \dot{\phi}^\dagger \dot{\phi} + \dot{\phi}\dot{\phi}^\dagger - \partial_\mu \phi^\dagger \partial^\mu \phi + \mu^2 \phi^\dagger \phi \\ &= \dot{\phi}\dot{\phi}^\dagger + \nabla \phi^\dagger \cdot \nabla \phi + \mu^2 \phi^\dagger \phi\end{aligned} \tag{23}$$

3.1.2 Hamiltonian Operator

<u>Discrete solutions</u>

$$\begin{aligned}H &= \int \mathcal{H} d^3x = \int \left(\dot{\phi}\dot{\phi}^\dagger + \nabla \phi^\dagger \cdot \nabla \phi + \mu^2 \phi^\dagger \phi \right) d^3x \\ &= \int \left(\sum_{\mathbf{k}} \frac{\partial}{\partial t} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} \left[a(\mathbf{k}) e^{-ikx} + b^\dagger(\mathbf{k}) e^{ikx} \right] \right) \left(\sum_{\mathbf{k}'} \frac{\partial}{\partial t} \frac{1}{\sqrt{2V\omega_{\mathbf{k}'}}} \left[b(\mathbf{k}') e^{-ik'x} + a^\dagger(\mathbf{k}') e^{ik'x} \right] \right) d^3x \\ &\qquad + \int \left(-\partial_i \phi^\dagger \partial^i \phi + \mu^2 \phi^\dagger \phi \right) d^3x\end{aligned} \tag{24}$$

The middle line of (24), i.e., the $\int \dot{\phi}\dot{\phi}^\dagger d^3x$ part, becomes

$$\int \left(\sum_{\mathbf{k}} \frac{i\omega_{\mathbf{k}}}{\sqrt{2V\omega_{\mathbf{k}}}} \left[-a(\mathbf{k}) e^{-ikx} + b^\dagger(\mathbf{k}) e^{ikx} \right] \right) \left(\sum_{\mathbf{k}'} \frac{i\omega_{\mathbf{k}'}}{\sqrt{2V\omega_{\mathbf{k}'}}} \left[-b(\mathbf{k}') e^{-ik'x} + a^\dagger(\mathbf{k}') e^{ik'x} \right] \right) d^3x \tag{25}$$

or

$$\sum_{\mathbf{k}} \sum_{\mathbf{k}'} \left(\frac{-\sqrt{\omega_{\mathbf{k}}}\sqrt{\omega_{\mathbf{k}'}}}{2V} \int \begin{bmatrix} a(\mathbf{k}) b(\mathbf{k}') e^{-ikx} e^{-ik'x} - a(\mathbf{k}) a^\dagger(\mathbf{k}') e^{-ikx} e^{ik'x} \\ -b^\dagger(\mathbf{k}) b(\mathbf{k}') e^{ikx} e^{-ik'x} + b^\dagger(\mathbf{k}) a^\dagger(\mathbf{k}') e^{ikx} e^{ik'x} \end{bmatrix} d^3x \right). \tag{26}$$

Note: One can shortcut the steps from here to (31) if the concern is only with finding expectation values for energy, i.e., $\bar{E} = \langle \phi | H | \phi \rangle$, and not considering eigenvalue determination, i.e., $H|\phi\rangle = E|\phi\rangle$. For the former case, all terms except those of form $\mathbf{a}^\dagger(\mathbf{k})\mathbf{a}(\mathbf{k}) + \mathbf{b}^\dagger(\mathbf{k})\mathbf{b}(\mathbf{k})$ will drop out as kets will not match bras in **k** otherwise. For the latter case, terms will survive in *H* that, for example, raise the ket by one particle, and hence there will be no eigenstate solution.

All terms in the integration in (26) result in zero except when $\mathbf{k}=\mathbf{k}'$ or $\mathbf{k}=-\mathbf{k}'$. (Note that the sum over $\mathbf{k}$ and $\mathbf{k}'$ is from negative infinity to positive infinity in the x, y, and z directions.) Since the volume of integration in (26) is finite and equal to *V*, we end up with

$$\int \dot{\phi}\dot{\phi}^\dagger d^3x = \sum_{\mathbf{k}} \frac{\omega_{\mathbf{k}}}{2} \left(-a(\mathbf{k}) b(-\mathbf{k}) e^{-i2\omega_{\mathbf{k}} t} + a(\mathbf{k}) a^\dagger(\mathbf{k}) + b^\dagger(\mathbf{k}) b(\mathbf{k}) - b^\dagger(\mathbf{k}) a^\dagger(-\mathbf{k}) e^{i2\omega_{\mathbf{k}} t} \right). \tag{27}$$

Following similar steps for the next term in (24) we get

$$\begin{aligned}&-\int \partial_i \phi^\dagger \partial^i \phi d^3x = \int \partial_i \phi^\dagger \partial_i \phi d^3x \\ &= \int \left(\sum_{\mathbf{k}} \frac{ik_i}{\sqrt{2V\omega_{\mathbf{k}}}} \left[b(\mathbf{k}) e^{-ikx} - a^\dagger(\mathbf{k}) e^{ikx} \right] \right) \left(\sum_{\mathbf{k}'} \frac{ik'_i}{\sqrt{2V\omega_{\mathbf{k}'}}} \left[a(\mathbf{k}') e^{-ik'x} - b^\dagger(\mathbf{k}') e^{ik'x} \right] \right) d^3x \\ &= \sum_{\mathbf{k}} \frac{\mathbf{k}^2}{2\omega_{\mathbf{k}}} \left(b(\mathbf{k}) a(-\mathbf{k}) e^{-i2\omega_{\mathbf{k}} t} + a^\dagger(\mathbf{k}) a(\mathbf{k}) + b(\mathbf{k}) b^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k}) b^\dagger(-\mathbf{k}) e^{i2\omega_{\mathbf{k}} t} \right)\end{aligned} \tag{28}$$

where we note that terms in the summation with both **k** and **- k** have a extra sign change since $k_i = -k'_i$ in the multiplication in the second line of (28).

Similarly, for the mass term in (24) we get

$$\int \mu^2 \phi^\dagger \phi d^3x =$$
$$\int \mu^2 \left(\sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} \left[b(\mathbf{k}) e^{-ikx} + a^\dagger(\mathbf{k}) e^{ikx} \right] \right) \left(\sum_{\mathbf{k}'} \frac{1}{\sqrt{2V\omega_{\mathbf{k}'}}} \left[a(\mathbf{k}') e^{-ik'x} + b^\dagger(\mathbf{k}') e^{ik'x} \right] \right) d^3x \qquad (29)$$
$$= \sum_{\mathbf{k}} \frac{\mu^2}{2\omega_{\mathbf{k}}} \left(b(\mathbf{k}) a(-\mathbf{k}) e^{-i2\omega_{\mathbf{k}} t} + b(\mathbf{k}) b^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k}) a(\mathbf{k}) + a^\dagger(\mathbf{k}) b^\dagger(-\mathbf{k}) e^{i2\omega_{\mathbf{k}} t} \right)$$

Adding the last lines of (27),(28), and (29), and using $\mathbf{k}^2 + \mu^2 = (\omega_{\mathbf{k}})^2$ along with the coefficient commutation relations,

$$\left[a(\mathbf{k}), a^\dagger(\mathbf{k}') \right] = \left[b(\mathbf{k}), b^\dagger(\mathbf{k}') \right] = \delta_{\mathbf{k}\mathbf{k}'} \text{ (discrete)}; \quad = \delta(\mathbf{k} - \mathbf{k}') \text{ (continuous)} \qquad (30)$$

we end up with

$$H = \sum_{\mathbf{k}} \frac{\omega_{\mathbf{k}}}{2} \left(a(\mathbf{k}) a^\dagger(\mathbf{k}) + a^\dagger(\mathbf{k}) a(\mathbf{k}) + b^\dagger(\mathbf{k}) b(\mathbf{k}) + b(\mathbf{k}) b^\dagger(\mathbf{k}) \right)$$
$$= \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(a^\dagger(\mathbf{k}) a(\mathbf{k}) + \tfrac{1}{2} + b^\dagger(\mathbf{k}) b(\mathbf{k}) + \tfrac{1}{2} \right) \qquad (31)(a)$$

or simply

$$H = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(N_a(\mathbf{k}) + \tfrac{1}{2} + N_b(\mathbf{k}) + \tfrac{1}{2} \right). \qquad (31)(b)$$

This is the Hamiltonian operator that acts on discrete solution states. If it is correct, to be consistent, its eigen value for a state must be the total energy of the state. For example, for a multiparticle state with 1 particle having energy eigenvalue ω_p, 2 particles having ω_q, 1 particle having ω_r, we have

$$E_{Tot} \left| \phi_p 2\phi_q \phi_r \right\rangle = \left(\omega_p + 2\omega_q + \omega_r \right) \left| \phi_p 2\phi_q \phi_r \right\rangle$$
$$= H \left| \phi_p 2\phi_q \phi_r \right\rangle = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left(N_a(\mathbf{k}) + \tfrac{1}{2} + N_b(\mathbf{k}) + \tfrac{1}{2} \right) \left| \phi_p 2\phi_q \phi_r \right\rangle \qquad (32)$$
$$= \left(n_p \omega_p + n_q \omega_q + n_r \omega_r + (\text{half integer energy states of vacuum}) \right) \left| \phi_p 2\phi_q \phi_r \right\rangle.$$

This leads us to conclude that the N_a and N_b operators must be number operators, which are unitless.

Note that if normal ordering (where one simply assumes non-commuting operators commute) were used in the first line of (31), then we would have no ½ factors in the above.

<u>Continuous solutions</u>

$$H = \int \mathcal{H} d^3x = \int \left(\dot{\phi}\dot{\phi}^\dagger + \nabla\phi^\dagger \nabla\phi + \mu^2 \phi^\dagger \phi \right) d^3x$$
$$= \int \left(\frac{1}{2(2\pi)^3} \int \frac{d\boldsymbol{k}}{\sqrt{\omega_{\mathbf{k}}}} i\omega_{\mathbf{k}} \left[-a(\mathbf{k}) e^{-ikx} + b^\dagger(\mathbf{k}) e^{ikx} \right] \right) \left(\int \frac{d\boldsymbol{k}'}{\sqrt{\omega_{\mathbf{k}'}}} i\omega_{\mathbf{k}'} \left[-b(\mathbf{k}') e^{-ik'x} + a^\dagger(\mathbf{k}') e^{ik'x} \right] \right) d^3x \quad (33)$$
$$+ \int \left(\nabla\phi^\dagger \nabla\phi + \mu^2 \phi^\dagger \phi \right) d^3x$$

The middle line of (33), i.e., the $\int \dot{\phi}\dot{\phi}^\dagger d^3x$ part, becomes

$$\int\left(\int\left(\frac{1}{2(2\pi)^3}\int\frac{(-\omega_{\mathbf{k}}\omega_{\mathbf{k}'})}{\sqrt{\omega_{\mathbf{k}}}\sqrt{\omega_{\mathbf{k}'}}}\left[-a(\mathbf{k})e^{-ikx}+b^\dagger(\mathbf{k})e^{ikx}\right]\left[-b(\mathbf{k}')e^{-ik'x}+a^\dagger(\mathbf{k}')e^{ik'x}\right]d\mathbf{k}'\right)d\mathbf{k}\right)d^3x \qquad (34)$$

or

$$\int\left(\int\left(\frac{1}{2(2\pi)^3}\frac{-\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}{\sqrt{\omega_{\mathbf{k}}}\sqrt{\omega_{\mathbf{k}'}}}\int\begin{bmatrix}a(\mathbf{k})b(\mathbf{k}')e^{-ikx}e^{-ik'x}-a(\mathbf{k})a^\dagger(\mathbf{k}')e^{-ikx}e^{ik'x}\\ -b^\dagger(\mathbf{k})b(\mathbf{k}')e^{ikx}e^{-ik'x}+b^\dagger(\mathbf{k})a^\dagger(\mathbf{k}')e^{ikx}e^{ik'x}\end{bmatrix}d^3x\right)d\mathbf{k}'\right)d\mathbf{k}\,. \qquad (35)$$

Using the Dirac delta function relation (18) for integration over all (infinite) space in the integral over $d\mathbf{k}'$ in (35) results in a relation parallel to (27), i.e.,

$$\int\dot{\phi}\dot{\phi}^\dagger d^3x=\int\frac{\omega_{\mathbf{k}}}{2}\left(-a(\mathbf{k})b(-\mathbf{k})e^{-i2\omega_{\mathbf{k}}t}+\underbrace{a(\mathbf{k})a^\dagger(\mathbf{k})}_{a^\dagger(\mathbf{k})a(\mathbf{k})+\delta(\mathbf{k}-\mathbf{k})}+b^\dagger(\mathbf{k})b(\mathbf{k})-b^\dagger(\mathbf{k})a^\dagger(-\mathbf{k})e^{i2\omega_{\mathbf{k}}t}\right)d\mathbf{k}\,. (36)$$

Using the commutation relations (30) for the continuous case, and evaluating the other two terms in (33) (last line) in similar fashion to that of (28) through (31), one ends up with the parallel relation to (31)(b), i.e.,

$$H=\int\omega_{\mathbf{k}}\left(N_a(\mathbf{k})+\tfrac{1}{2}\delta(0)+N_b(\mathbf{k})+\tfrac{1}{2}\delta(0)\right)d\mathbf{k}\,. \qquad (37)$$

This is the form of the Hamiltonian for continuous solution states, i.e., to be used with wave packets. Note the $\delta(0)$, representing the vacuum contribution, equals infinity and has the units of $1/k^3$ (inverse of momentum dimension to third power). Since $k = 2\pi/\lambda$, this is the same as volume units (length to third power) in physical space. So, the $\delta(0)$ represents the infinite volume of all space. Thus, the density per unit volume of space of the vacuum energy is

$$\mathcal{H}_{vac}=\frac{H_{vac}}{V}=\int\omega_{\mathbf{k}}\left(\tfrac{1}{2}+\tfrac{1}{2}\right)d\mathbf{k}=\int\omega_{\mathbf{k}}\left(\tfrac{1}{2}+\tfrac{1}{2}\right)d\mathbf{k} \qquad \begin{pmatrix}\text{vacuum energy density per}\\ \text{unit volume in physical space}\end{pmatrix}$$

(37)(a)

For a single particle state wave packet, there is no energy eigenstate of energy as the packet, by definition is a superposition of eigenstates (of infinite number and infinitesimal width in **k** space). We discuss energy expectation values for general (non-eigenstate) single and multi particle states in Section 5.

Note that the integral in **k** vector space of (37) is a 3D integral (in that space, not physical space), so it can also be expressed as a scalar integral

$$H=\int\omega_{\mathbf{k}}\left(N_a(\mathbf{k})+N_b(\mathbf{k})\right)d^3k \qquad (\text{observable Hamiltonian})\,, \qquad (38)$$

where d^3k here is an infinitesimal volume in **k** space. **k** has magnitude $2\pi/\lambda$ and thus units of 1/length, so d^3k has units of 1/volume. From (38), the units of $N_a(\mathbf{k})$ and $N_b(\mathbf{k})$ must be then be volume, or length^3. And thus, from $N_a(\mathbf{k}) = a^\dagger(\mathbf{k})a(\mathbf{k})$ and $N_b(\mathbf{k}) = b^\dagger(\mathbf{k})b(\mathbf{k})$, $a(\mathbf{k})$ and $b(\mathbf{k})$ must have units of $\sqrt{volume}$ = length$^{3/2}$. This differs from the discrete case where all these operators were unitless.

4. *Creating and Destroying General (non-eigenstate) States*

Questions arise in QFT as to what is created or destroyed by the general solution $\phi(x)$ (or $\phi^\dagger(x)$), which for discrete eigenstates, is a summation of terms, each containing a single particle eigenstate creation/destruction operator. Does operation of $\phi^\dagger(x)$ on the vacuum, for instance, create an infinite number of single particles, or a single particle comprising an infinite number of momentum eigenstates? If the latter, what amplitudes (whose squares are probabilities) are assigned to each such eigenstate?

Similar questions also arise regarding the general continuous eigenstate solution of (3). These are compounded by the continuous nature of $\phi(x)$. Does $\phi^\dagger(x)$ acting on the vacuum create a single particle wave packet state? If so, what (continuous) Fourier amplitude spectrum does the wave packet have? That is, how do we determine how "spread out" or how "tight" the created wave packet is?

Answer:

We do not use $\phi^\dagger(x)$ to create particles, so we should not be worried about the sum of terms in $\phi^\dagger(x)$ for creating states. We use $\mathbf{a}^\dagger(\mathbf{k})$ to create a unit normed state. Field operators like $\phi^\dagger(x)$ appear in bi-linear form (such as $\phi^\dagger\phi$) in all observable operators like H, and it is only these operators that have expectation values, e.g., $\overline{E} = \langle \phi | H | \phi \rangle$. In these cases all factors like $e^{-ikx}/\sqrt{2\omega_{\mathbf{k}} V}$ drop out and we are left with just number operators (and things like $\omega_{\mathbf{k}}$).

Confusion can arise here when one considers the heuristic treatment for finding the propagator in which the relation

$$\langle 0 | \left[\phi(x), \phi^\dagger(y) \right] | 0 \rangle = i\Delta(x-y) \tag{39}$$

was used to describe a particle created out of the vacuum at y and annihilated at x. This led to the Feynman propagator, i.e., the amplitude for a virtual particle traveling from y to x. One can then begin to think in terms of $\phi^\dagger$ as the operator to use to create and destroy states.

In reality, the propagator comes out of the mathematics in finding the S operator between initial and final states. In the Interaction Picture, the equation of motion for the states involved the Hamiltonian operator H. Integrating this equation involved the Dyson-Wicks expansion in which terms therein ended up containing factors of the form of (39). The bi-linear operator form of H led to such factors. These factors are the propagators for the virtual particles between y and x.

One can think of these factors (i.e., of (39)) roughly as $\phi^\dagger$ creating a state at y that ϕ destroys at x, but that is not completely accurate, and as noted, can lead to confusion. In reality the $\mathbf{a}^\dagger$ operator does the creating, and the other factors in a particular term in $\phi^\dagger$ lead to the correct form for the propagator in $e^{-ik(x-y)}$ etc.

4.1 Discrete Eigenstates

4.1.1 Creating a Single Particle State (Discrete Solutions Form)

Single Eigenstate for Single Particle (Discrete Solution Form)

We know that

$$a^\dagger(\mathbf{k}) | 0 \rangle = | \phi_{\mathbf{k}} \rangle = \left| \frac{e^{-ik\tilde{x}}}{\sqrt{V}} \right\rangle, \tag{40}$$

which has unit norm, and for which we employ "~" over x to distinguish it from the x dependence in field operators such as $\phi^\dagger$. The reason for this follows.

Aside

Suppose we wish to evaluate an expression similar to (39), such as (41) below. Using (2) on half of the commutator, we would have

$$\langle 0 | \phi\phi^\dagger | 0 \rangle = \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \left(\langle \phi_{\mathbf{k}'}(\tilde{y}) | \frac{e^{ik'y}}{\sqrt{2\omega_{\mathbf{k}'} V}} \frac{e^{-ikx}}{\sqrt{2\omega_{\mathbf{k}} V}} | \phi_{\mathbf{k}}(\tilde{x}) \rangle \right). \tag{41}$$

The point is that the integration implied by the inner product of the bracket is over the "~" coordinates, not the xy coordinates. The result of (41) is a function (without operators involved) of y-x.

The state created by $a^\dagger(\mathbf{k})$, i.e., $|\phi_{\mathbf{k}}(\tilde{x})\rangle$, is a function of $\tilde{x}$, which is a different position variable than x in the e^{-ikx} factor shown in (41). That is, the created state has its own particular function of position and time that is unrelated to that of the other position dependent term in $\phi^\dagger$.

In QFT the accustomed manner of treating states is simply to use the ket form $|\phi_{\mathbf{k}}\rangle$ without showing, or dealing with, the inherent spacetime dependence explicitly. We will gravitate towards this usage as well, but for some of the derivations that follow directly, it can help if that spacetime dependence is shown explicitly. The interested reader can verify for him/herself that if the created state depended on the same spacetime coordinates x as the e^{ikx} factor in $\phi^{\dagger}$, then incorrect results arise.

Each $|\phi_{\mathbf{k}}\rangle$ in (41)) has unit norm and is orthogonal to every other such eigenstate. That is,

$$|\phi_{\mathbf{k}}\rangle = \frac{e^{-ik\tilde{x}}}{\sqrt{V}}, \tag{42}$$

so that[3]

$$\langle \phi_{\mathbf{k}} | \phi_{\mathbf{k}} \rangle = \frac{1}{V}\int e^{ik\tilde{x}} e^{-ik\tilde{x}} d^3x' = 1 \tag{43}$$

or more generally,

$$\langle \phi_{\mathbf{k}} | \phi_{\mathbf{k}'} \rangle = \delta_{\mathbf{k}\mathbf{k}'} . \tag{44}$$

In QFT the middle part of (43) is rarely expressed and one simply uses (44).

General non-Eigen State for Single Particle (Discrete Solution Form)

To create a general particle state, which is a sum of eigenstates, we would need an operator of form

$$C = \sum_{\mathbf{k}} A_{\mathbf{k}} \mathbf{a}^{\dagger}_{\mathbf{k}} , \tag{45}$$

so that

$$\begin{aligned} C|0\rangle &= \sum_{\mathbf{k}} A_{\mathbf{k}} \mathbf{a}^{\dagger}_{\mathbf{k}} |0\rangle = A_1 \left| \frac{e^{-ik_1 x}}{\sqrt{V}} \right\rangle + A_2 \left| \frac{e^{-ik_2 x}}{\sqrt{V}} \right\rangle + A_3 \left| \frac{e^{-ik_3 x}}{\sqrt{V}} \right\rangle + ... \\ &= A_1 |\phi_1\rangle + A_2 |\phi_2\rangle + A_3 |\phi_3\rangle + ... = |\phi\rangle . \end{aligned} \tag{46}$$

In (45) and (46) $A_{\mathbf{k}}$ is a numerical coefficient, the square of which (for proper normalization) equals the probability of finding the **k** eigenstate. (See (4), (8), and (9).)

If only one term in C is used, then only one eigenstate with $|A_{\mathbf{k}}| = 1$ is created. If a more general state, comprising a sum of eigenstates, is created, then we are free to select the $A_{\mathbf{k}}$ as we please in order to create the particular general state we like, provided (for conservation of probability and correct normalization so total probability is unity)

$$\sum_{\mathbf{k}} | A_{\mathbf{k}} |^2 = 1 . \tag{47}$$

Important point: Note in QFT we have

$$\langle \phi | \phi \rangle = \sum_{\mathbf{k}} | A_{\mathbf{k}} |^2 = 1 \tag{48}$$

whereas in NRQM, we had (see (10), repeated below)

$$\langle \phi | \phi \rangle = \sum_{\mathbf{k}} \frac{(A_{\mathbf{k}})^2}{2\omega_{\mathbf{k}}} \neq 1 . \tag{49}$$

---

[3] Actually, though it is a subtle point at this stage, $|e^{-ikx'}\rangle$ here has no energy (time) dependence in the exponent as long as we are working in with the Heisenberg picture (which we do with free fields in the usual development of QFT.) In the Schroedinger picture, the state would have time dependence. When going to the interaction picture (for interacting fields in QFT) the time dependence for states will be on the interaction part of the Hamiltonian (but not the free part.)

This is because the kets created in QFT via $\mathbf{a}_{\mathbf{k}}^{\dagger}$ have unit norm, whereas the ket solutions to the field equations in NRQM do not.

4.1.2 Destroying a Single Particle State (Discrete)

Note that the operator

$$D = \sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}} \tag{50}$$

acting on any single particle general state will lower that state to the vacuum. If acting on the vacuum, each term in (50) will destroy it. That is,

$$\begin{aligned}\left(\sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}\right)\left|\phi\right\rangle &= \left(\sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}\right)\left| A_1\left|\phi_1\right\rangle + A_2\left|\phi_2\right\rangle + A_3\left|\phi_3\right\rangle + \ldots\right\rangle \\ &= \left(\left(\sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}\right)A_1\left|\phi_1\right\rangle + \left(\sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}\right)A_2\left|\phi_2\right\rangle + \left(\sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}\right)A_3\left|\phi_3\right\rangle + \ldots\right) \\ &= A_1\left|0\right\rangle + 0 + 0 + \ldots + 0 + A_2\left|0\right\rangle + 0 + \ldots = \left|0\right\rangle\end{aligned} \tag{51}$$

(We re-normalized the vacuum on the RHS above.)

4.1.3 Creating a Multi-particle State (Discrete Solution Form)

Applying operators similar in form to (45) (with typically different values for $A_{\mathbf{k}}$ in each operator) twice in succession creates a two particle state where each particle is a single particle general state (i.e., each is a summation of momentum eigenstates.) Any number of such operators may be applied to create a state of any number of particles, each in a general (not eigen) state.

Multiparticle states have unit norms, e.g.,

$$\left\langle \phi_p 2\phi_q \phi_r \middle|\middle| \phi_p 2\phi_q \phi_r \right\rangle = 1 \,. \tag{52}$$

4.1.4 Destroying a Multi-particle State (Discrete Solution Form)

Application of (50) repeatedly will destroy one general state single particle upon each application.

4.2 Continuous Eigenstates

4.2.1 Creating a Wave Packet (Single Particle State of Continuous Solution Form)

For continuous solution form states, we parallel our use in 4.1 above of the creation operators $\mathbf{a}_{\mathbf{k}}^{\dagger}$ in (2) to create a general creation operator. (Note there is no such thing as an eigenstate of continuous solution form.) We use the operators in (3) to create a single particle wave packet composed of an integral of continuous momenta eigenstates. That is, by analogy,

$$C = \int d\boldsymbol{k}\, A(\mathbf{k})\mathbf{a}^{\dagger}(\mathbf{k}) \,, \tag{53}$$

which can be seen with the aid of the table below.

	Discrete Solution Form	Continuous Solution Form
Eigenstate creation operator	$\mathbf{a}^{\dagger}{}_{\mathbf{k}}\lvert 0\rangle = \lvert\phi_{\mathbf{k}}\rangle = \left\lvert \frac{e^{-ikx}}{\sqrt{V}}\right\rangle$	$\mathbf{a}^{\dagger}(\mathbf{k})\lvert 0\rangle = \lvert\phi_{\mathbf{k}}\rangle = \left\lvert \frac{e^{-ikx}}{\sqrt{(2\pi)^3}}\right\rangle$
General state creation operator	$C = \sum_{\mathbf{k}} A_{\mathbf{k}}\mathbf{a}^{\dagger}_{\mathbf{k}}$	$C = \int d\boldsymbol{k}\, A(\mathbf{k})\mathbf{a}^{\dagger}(\mathbf{k})$
General state	$\lvert\phi\rangle = C\lvert 0\rangle = A_1\left\lvert\frac{e^{-ik_1x}}{\sqrt{V}}\right\rangle + A_2\left\lvert\frac{e^{-ik_2x}}{\sqrt{V}}\right\rangle + \ldots$ $= A_1\lvert\phi_1\rangle + A_2\lvert\phi_2\rangle + \ldots$ $= \sum_{\mathbf{k}} A_{\mathbf{k}}\left\lvert\frac{e^{-ikx}}{\sqrt{V}}\right\rangle$	$\lvert\phi\rangle = C\lvert 0\rangle$ $= \int d\boldsymbol{k}\, A(\mathbf{k})\left\lvert\frac{e^{-ikx}}{\sqrt{(2\pi)^3}}\right\rangle$

$A(\mathbf{k})$ is the Fourier amplitude, which is a numerical continuous function of $\mathbf{k}$, and which we can choose as we like to create the wave packet shape desired.

4.2.2 Destroying a Wave Packet (Single Particle State of Continuous Solution Form)

Once again, by analogy, we have a wave packet destruction operator

$$D = \int d\boldsymbol{k}\,\mathbf{a}(\mathbf{k}), \tag{54}$$

which can be seen with the aid of the table below.

	Discrete Solution Form	Continuous Solution Form
Eigenstate destruction operator	$\mathbf{a}_{\mathbf{k}}\lvert\phi_{\mathbf{k}}\rangle = \mathbf{a}_{\mathbf{k}}\left\lvert\frac{e^{-ikx}}{\sqrt{V}}\right\rangle = \lvert 0\rangle$	$\mathbf{a}(\mathbf{k})\lvert\phi_{\mathbf{k}}\rangle = \mathbf{a}_{\mathbf{k}}\left\lvert\frac{e^{-ikx}}{\sqrt{(2\pi)^3}}\right\rangle = \lvert 0\rangle$
General state destruction operator	$D = \sum_{\mathbf{k}} \mathbf{a}_{\mathbf{k}}$	$D = \int d\boldsymbol{k}\,\mathbf{a}(\mathbf{k})$

4.2.3 Creating a Multi-Wave Packet State (Multi-particle Continuous Solution Form)

Applying operators similar in form to C of (53) (with typically different Fourier spectra $A(\mathbf{k})$ in each operator) twice in succession creates a two particle state where each particle is a wave packet.

4.2.4 Destroying a Multi-Wave Packet State (Multi-particle Continuous Solution Form)

Application of (54) repeatedly will destroy one wave packet particle upon each application.

5. Probability and Expectation Values in QFT

As described in footnote 1 on page 5, we can determine a continuity (conservation) equation, i.e., a 4D current divergence equal to zero, in similar fashion to what was done in NRQM to find the probability conservation relation. Take the field equation (Klein-Gordon rather than Schroedinger) and pre multiply by $\phi^{\dagger}$, then subtract it from the complex conjugate Klein-Gordon equation post multiplied by ϕ, and note the result has the form of the continuity equation

$$\frac{\partial\rho'_{oper}}{\partial t} + \nabla\cdot\mathbf{j}'_{\mathbf{oper}} = j'_{oper}{}^{\mu}{}_{,\mu} = 0 \tag{55}$$

where

$$\rho'_{oper} = j'^{\,0}_{oper} = i\left(\phi^{\dagger}\phi_{,0} - \phi^{\dagger}{}_{,0}\,\phi\right) \qquad \mathbf{j}'_{oper} = j'^{\,i}_{oper} = -i\left(\phi^{\dagger}\phi_{,i} - \phi^{\dagger}{}_{,i}\phi\right). \tag{56}$$

We use the subscript "oper" to distinguish between the ρ of RQM, which represented the numerical particle density, and ρ'_{oper} of QFT, which is composed of operators and is therefore itself an operator. We also use a prime on ρ'_{oper} for reasons which will be seen. We derive below a single particle density *operator* ρ_{oper} that is closely related to ρ'_{oper}.

5.1 Probability Density for Discrete Solutions in QFT

Note that from (2) ρ'_{oper} has the form

$$\begin{aligned}\rho'_{oper} = &\left(2\sum_{\mathbf{k}}\frac{\mathbf{a}^{\dagger}_{\mathbf{k}}}{\sqrt{2\omega_{\mathbf{k}}}}\frac{e^{ikx}}{\sqrt{V}}\right)\left(\sum_{\mathbf{k}'}\frac{\omega_{\mathbf{k}'}\mathbf{a}_{\mathbf{k}'}}{\sqrt{2\omega_{\mathbf{k}'}}}\frac{e^{-ik'x}}{\sqrt{V}}\right) - \left(2\sum_{\mathbf{k}}\frac{\omega_{\mathbf{k}}\mathbf{b}^{\dagger}_{\mathbf{k}}}{\sqrt{2\omega_{\mathbf{k}}}}\frac{e^{ikx}}{\sqrt{V}}\right)\left(\sum_{\mathbf{k}'}\frac{\mathbf{b}_{\mathbf{k}'}}{\sqrt{2\omega_{\mathbf{k}'}}}\frac{e^{-ik'x}}{\sqrt{V}}\right) \\ &-\left(2\sum_{\mathbf{k}}\frac{\omega_{\mathbf{k}}}{\sqrt{2\omega_{\mathbf{k}}}}\frac{e^{ikx}}{\sqrt{V}}\right)\left(\sum_{\mathbf{k}'}\frac{1}{\sqrt{2\omega_{\mathbf{k}'}}}\frac{e^{-ik'x}}{\sqrt{V}}\right) + (\text{terms in } \mathbf{a}^{\dagger}{}_{\mathbf{k}}\mathbf{b}^{\dagger}{}_{\mathbf{k}'} \text{ and } \mathbf{b}_{\mathbf{k}}\mathbf{a}_{\mathbf{k}})\end{aligned}. \tag{57}$$

The third term in (57) will cause us problems later on. We can circumvent those problems by noting that ρ'_{oper} is not the only entity that satisfies the continuity equation (55).

Take the field equation (Klein-Gordon here) and *post* multiply it by $\phi^{\dagger}$, then subtract that from the complex conjugate field equation *pre* multiplied by ϕ. You obtain a ρ''_{oper} and $\mathbf{j}''_{oper}$ that satisfy the continuity equation (55), for which

$$\rho''_{oper} = i\left(\phi\phi^{\dagger}{}_{,0} - \phi_{,0}\,\phi^{\dagger}\right) \qquad j''^{\,i} = -i\left(\phi\phi^{\dagger}{}_{,i} - \phi_{,i}\phi^{\dagger}\right). \tag{58}$$

XXX Need to check signs here XXX The complete form for the probability density operator should then be a linear combination of ρ'_{oper} and ρ''_{oper}. We take this to be the average of the two, i.e.,

$$\rho_{oper} = \frac{\rho'_{oper} + \rho''_{oper}}{2}. \tag{59}$$

In (59), not only do terms like the third one in (57) cancel out, but the entire bottom row in (57) does as well. Thus, we find

$$\rho_{oper} = \left(2\sum_{\mathbf{k}}\frac{\mathbf{a}^{\dagger}_{\mathbf{k}}}{\sqrt{2\omega_{\mathbf{k}}}}\frac{e^{ikx}}{\sqrt{V}}\right)\left(\sum_{\mathbf{k}'}\frac{\omega_{\mathbf{k}'}\mathbf{a}_{\mathbf{k}'}}{\sqrt{2\omega_{\mathbf{k}'}}}\frac{e^{-ik'x}}{\sqrt{V}}\right) - \left(2\sum_{\mathbf{k}}\frac{\omega_{\mathbf{k}}\mathbf{b}^{\dagger}_{\mathbf{k}}}{\sqrt{2\omega_{\mathbf{k}}}}\frac{e^{ikx}}{\sqrt{V}}\right)\left(\sum_{\mathbf{k}'}\frac{\mathbf{b}_{\mathbf{k}'}}{\sqrt{2\omega_{\mathbf{k}'}}}\frac{e^{-ik'x}}{\sqrt{V}}\right). \tag{60}$$

5.1.1 Single Particle Probability Density (QFT, Discrete)

Single Particle Eigenstate

Hence, for a single particle in an eigenstate $|\phi_{\mathbf{k}''}\rangle$, the numerical probability density is the expectation value of the corresponding operator,

$$\rho = \langle\phi_{\mathbf{k}''}|\rho_{oper}|\phi_{\mathbf{k}''}\rangle = \langle\phi_{\mathbf{k}''}(\tilde{x})|\rho_{oper}(x)|\phi_{\mathbf{k}''}(\tilde{x})\rangle. \tag{61}$$

All terms in (60) with $\mathbf{k} \neq \mathbf{k}'$ will result in different particles (in orthogonal states) in the bra and ket, and drop out, leaving

$$\begin{aligned}\rho &= \langle\phi_{\mathbf{k}''}|\frac{\sum_{\mathbf{k}}(\mathbf{a}^{\dagger}{}_{\mathbf{k}}\mathbf{a}_{\mathbf{k}} - \mathbf{b}^{\dagger}{}_{\mathbf{k}}\mathbf{b}_{\mathbf{k}})}{V}|\phi_{\mathbf{k}''}\rangle = \langle\phi_{\mathbf{k}''}|\frac{\sum_{\mathbf{k}}(N_{\mathbf{a}}(\mathbf{k}) - N_{\mathbf{b}}(\mathbf{k}))}{V}|\phi_{\mathbf{k}''}\rangle, \\ &= \frac{1}{V}.\end{aligned} \tag{62}$$

Note that the bracket integration over $\tilde{x}$ causes only terms where $\mathbf{k} = \mathbf{k}'$ to survive. This also results in the cancellation of factors in the numerators and denominators, and the severing of dependence on *x*.

The final result in (62) is what we would expect. The total probability is the integral of ρ over the volume and equals unity. Note that an antiparticle state would have a negative probability density (from the $N_{\mathbf{b}}(\mathbf{k})$ operator) and a total probability of negative one. This led to the interpretation of ρ as charge density (probability of finding the given charge at any particular location) and its integral over volume as the particle/antiparticle charge.

Note further, that probability density in QFT for a unit norm ket is not invariant, due to the relativistic change in volume V for a different frame. But total probability is invariant (and always equals one), since in the integration over volume, the V factors cancel.

Single Particle General State

For a general single particle state, composed of a superposition of eigenstates, where

$$\left|\phi\right\rangle = A_1\left|\phi_1\right\rangle + A_2\left|\phi_2\right\rangle + A_3\left|\phi_3\right\rangle + \ldots, \tag{63}$$

we have, ignoring anti-particles for simplicity,

$$\begin{aligned}\rho &= \left\langle\phi\right|\rho_{oper}\left|\phi\right\rangle = \left\langle\phi(\tilde{x})\right|\rho_{oper}(x)\left|\phi(\tilde{x})\right\rangle = \\ &\left\langle\sum_{\mathbf{k}} A_{\mathbf{k}}^{\dagger}\frac{e^{ik\tilde{x}}}{\sqrt{V}}\right|\left(2\sum_{\mathbf{k}'}\frac{\mathbf{a}_{\mathbf{k}'}^{\dagger}}{\sqrt{2\omega_{\mathbf{k}'}}}\frac{e^{ik'x}}{\sqrt{V}}\right)\left(\sum_{\mathbf{k}''}\frac{\omega_{\mathbf{k}''}\mathbf{a}_{\mathbf{k}''}}{\sqrt{2\omega_{\mathbf{k}''}}}\frac{e^{-ik''x}}{\sqrt{V}}\right)\left|\sum_{\mathbf{k}'''} A_{\mathbf{k}'''}\frac{e^{ik'''\tilde{x}}}{\sqrt{V}}\right\rangle.\end{aligned} \tag{64}$$

To help in evaluating (64), look initially at only the first two terms in each of the ket and the right hand operator summations.

$$\begin{aligned}&\left(\sum_{\mathbf{k}''}\frac{\omega_{\mathbf{k}''}\mathbf{a}_{\mathbf{k}''}}{\sqrt{2\omega_{\mathbf{k}''}}}\frac{e^{-ik''x}}{\sqrt{V}}\right)\left|\sum_{\mathbf{k}'''} A_{\mathbf{k}'''}\frac{e^{-ik'''\tilde{x}}}{\sqrt{V}}\right\rangle \to \text{1st two terms} = \\ &\left(\frac{\omega_{\mathbf{k}_1}\mathbf{a}_{\mathbf{k}_1}}{\sqrt{2\omega_{\mathbf{k}_1}}}\frac{e^{-ik_1x}}{\sqrt{V}} + \frac{\omega_{\mathbf{k}_2}\mathbf{a}_{\mathbf{k}_2}}{\sqrt{2\omega_{\mathbf{k}_2}}}\frac{e^{-ik_2x}}{\sqrt{V}}\right)\left|A_{\mathbf{k}_1}\frac{e^{-ik_1\tilde{x}}}{\sqrt{V}} + A_{\mathbf{k}_2}\frac{e^{-ik_2\tilde{x}}}{\sqrt{V}}\right\rangle = \\ &\frac{\omega_{\mathbf{k}_1}}{\sqrt{2\omega_{\mathbf{k}_1}}}\frac{e^{-ik_1x}}{\sqrt{V}}A_{\mathbf{k}_1}\left|0\right\rangle + \frac{\omega_{\mathbf{k}_2}}{\sqrt{2\omega_{\mathbf{k}_2}}}\frac{e^{-ik_2x}}{\sqrt{V}}A_{\mathbf{k}_2}\left|\frac{e^{-ik_2\tilde{x}}}{\sqrt{V}}\right\rangle\end{aligned} \tag{65}$$

The two summations (in $\mathbf{k}$ and $\mathbf{k}'$) on the left side of (64) look like

$$2\left\langle 0\right|A_{\mathbf{k}_1}^{\dagger}\frac{1}{\sqrt{2\omega_{\mathbf{k}_1}}}\frac{e^{ik_1x}}{\sqrt{V}} + 2\left\langle\frac{e^{ik_1\tilde{x}}}{\sqrt{V}}\right|A_{\mathbf{k}_2}^{\dagger}\frac{1}{\sqrt{2\omega_{\mathbf{k}_2}}}\frac{e^{ik_2x}}{\sqrt{V}}. \tag{66}$$

If we take the bra-ket, i.e., the integral over $\tilde{\mathbf{x}}$, of (64), using (66) and the last line of (65), we get (including all terms, not just the first two)

$$\rho = \frac{1}{V}\sum_{\mathbf{k}} A_{\mathbf{k}}^{\dagger}\sum_{\mathbf{k}''} A_{\mathbf{k}}, \tag{67}$$

which is the probability density. If we integrate it over all space to get total probability, we find

$$\int\rho dV = \sum_{\mathbf{k}}\left|A_{\mathbf{k}}\right|^2 = 1, \tag{68}$$

which is what it should be, and also equals the total number of particles.

Parallel remarks to those made above with regard to single particle eigenstates for total probability, antiparticle charge/probability density, and invariance apply to general single particle states, as well.

5.1.2 Multiple Particle State Probability Density (QFT, Discrete)

All Particles in Eigenstates

For a multi particle state in which all particles are in eigenstates, such as

$$\left|\phi\right\rangle = \left|\phi_p 2\phi_q \phi_r\right\rangle \tag{69}$$

we have

$$\rho = \left\langle \phi_p 2\phi_q \phi_r \right| \rho_{oper} \left| \phi_p 2\phi_q \phi_r \right\rangle . \tag{70}$$

Any operator acts on a multi particle ket one particle at a time, much like a derivative on a product of fucntions. Hence, for a destruction operator $\mathbf{a}_{\mathbf{k}'}$, one would have

$$\begin{aligned}\sum_{\mathbf{k}'} \mathbf{a}_{\mathbf{k}'} \left|\phi_p 2\phi_q \phi_r\right\rangle &= \left|\left(\sum_{\mathbf{k}'} \mathbf{a}_{\mathbf{k}'} \phi_p\right) 2\phi_q \phi_r\right\rangle + \left|\phi_p \left(\sum_{\mathbf{k}'} \mathbf{a}_{\mathbf{k}'} \phi_q\right) \phi_q \phi_r\right\rangle \\ &+ \left|\phi_p \phi_q \left(\sum_{\mathbf{k}'} \mathbf{a}_{\mathbf{k}'} \phi_q\right) \phi_r\right\rangle + \left|\phi_p 2\phi_q \left(\sum_{\mathbf{k}'} \mathbf{a}_{\mathbf{k}'} \phi_r\right)\right\rangle\end{aligned} . \tag{71}$$

with a parallel relation for the action of $\mathbf{a}^\dagger_{\mathbf{k}}$ on the bra. When (71) is used with (60) in (70), all kets are destroyed (become equal to zero) except those for which $\mathbf{k}'$ equals the eigen momentum of one of the particles. This leaves only those eigen momentum terms inside (70), and thus we have a relationship similar to that for a single particle eigenstate (62), i.e.,

$$\begin{aligned}\rho &= \left\langle\phi\right| \frac{\sum_{\mathbf{k}} (\mathbf{a}^\dagger{}_{\mathbf{k}} \mathbf{a}_{\mathbf{k}} - \mathbf{b}^\dagger{}_{\mathbf{k}} \mathbf{b}_{\mathbf{k}})}{V} \left|\phi\right\rangle = \left\langle \phi_p 2\phi_q \phi_r \right| \frac{\sum_{\mathbf{k}} (N_{\mathbf{a}}(\mathbf{k}) - N_{\mathbf{b}}(\mathbf{k}))}{V} \left| \phi_p 2\phi_q \phi_r \right\rangle \\ &= \frac{1+2+1}{V} = \frac{4}{V} .\end{aligned} \tag{72}$$

The integral of this over the volume yields a total probability of 4, which for 4 particles, might make sense in some sort of way. Since this integral equals the number of particles, ρ can thus be more properly interpreted as particle number density (or charge density) where antiparticles have negative numbers.

In QFT, which invariably deals with multiparticle states it is more advantageous to focus on the number operators. In fact, we can think of the total number operator as the integral of ρ_{oper} over the volume.

$$N = \int \rho_{oper} dV = \sum_{\mathbf{k}} (N_{\mathbf{a}}(\mathbf{k}) - N_{\mathbf{b}}(\mathbf{k})) . \tag{73}$$

Particles in General States

Consider multi particle states where the particles are in general (non eigen) states, i.e., $\left|\phi_p 2\phi_q \phi_r\right\rangle$, where, for example,

$$\left|\phi_p\right\rangle = \left|\sum_{\mathbf{k}'''} A_{\mathbf{k}'''} \frac{e^{-ik'''x}}{\sqrt{V}}\right\rangle_p , \tag{74}$$

and similar relations hold for the other particles in the multi particle state.

When (71) and its parallel relation for the bra are used in (70), we get a term similar to (67) for each ket term on the right side of (71), i.e.,

$$\rho = \frac{1}{V}\left\{\begin{aligned}&\left(\sum_{\mathbf{k}'} A^\dagger_{\mathbf{k}'} \frac{e^{ik'x}}{\sqrt{2\omega_{\mathbf{k}'}}}\right)_{\phi_p} \left(\sum_{\mathbf{k}''} \omega_{\mathbf{k}''} \frac{e^{-ik''x}}{\sqrt{2\omega_{\mathbf{k}''}}} A_{\mathbf{k}''}\right)_{\phi_p} \\ &+ \left(\sum_{\mathbf{k}'} A^\dagger_{\mathbf{k}'} \frac{e^{ik'x}}{\sqrt{2\omega_{\mathbf{k}'}}}\right)_{\phi_q} \left(\sum_{\mathbf{k}''} \omega_{\mathbf{k}''} \frac{e^{-ik''x}}{\sqrt{2\omega_{\mathbf{k}''}}} A_{\mathbf{k}''}\right)_{\phi_q} + \ldots\end{aligned}\right\} \tag{75}$$

When we integrate (75) over all space we get

$$\int \rho dV = \begin{Bmatrix} \delta_{\mathbf{k}'\mathbf{k}''}\left(\sum_{\mathbf{k}'}\frac{A^{\dagger}_{\mathbf{k}'}}{\sqrt{2\omega_{\mathbf{k}'}}}\right)_{\phi_p}\left(\sum_{\mathbf{k}''}\omega_{\mathbf{k}''}\frac{A_{\mathbf{k}''}}{\sqrt{2\omega_{\mathbf{k}''}}}\right)_{\phi_p} \\ +2\delta_{\mathbf{k}'\mathbf{k}''}\left(\sum_{\mathbf{k}'}\frac{A^{\dagger}_{\mathbf{k}'}}{\sqrt{2\omega_{\mathbf{k}'}}}\right)_{\phi_q}\left(\sum_{\mathbf{k}''}\omega_{\mathbf{k}''}\frac{A_{\mathbf{k}''}}{\sqrt{2\omega_{\mathbf{k}''}}}\right)_{\phi_q} \\ +\delta_{\mathbf{k}'\mathbf{k}''}\left(\sum_{\mathbf{k}'}\frac{A^{\dagger}_{\mathbf{k}'}}{\sqrt{2\omega_{\mathbf{k}'}}}\right)_{\phi_r}\left(\sum_{\mathbf{k}''}\omega_{\mathbf{k}''}\frac{A_{\mathbf{k}''}}{\sqrt{2\omega_{\mathbf{k}''}}}\right)_{\phi_r} \end{Bmatrix} \tag{76}$$

or

$$\int \rho dV = \sum_{\mathbf{k}'}\left|{}_p A_{\mathbf{k}'}\right|^2 + 2\sum_{\mathbf{k}'}\left|{}_q A_{\mathbf{k}'}\right|^2 + \sum_{\mathbf{k}'}\left|{}_r A_{\mathbf{k}'}\right|^2 = 1+2+1 = 4\,. \tag{77}$$

Relation (75) is cumbersome to say the least, whereas (77) is quite simple and equals the total number of particles. In QFT, it turns out to be invariably simpler to focus on the number operators, for which

$$\begin{aligned} &\text{Number of particles} = \int \rho dV = \int \langle \phi | \rho_{oper}(x) | \phi \rangle d^3\mathbf{x} \\ &= \text{Expectation value of number operator} \\ &= \langle \phi | \sum_{\mathbf{k}} (\mathbf{a}^{\dagger}{}_{\mathbf{k}}\mathbf{a}_{\mathbf{k}} - \mathbf{b}^{\dagger}{}_{\mathbf{k}}\mathbf{b}_{\mathbf{k}}) | \phi \rangle = \langle \phi | \sum_{\mathbf{k}} (N_{\mathbf{a}}(\mathbf{k}) - N_{\mathbf{b}}(\mathbf{k})) | \phi \rangle \\ &= n_a - n_b\,. \end{aligned} \tag{78}$$

In our example,

$$\begin{aligned} &= \left\langle \phi_p 2\phi_q \phi_r \right| \frac{\sum_{\mathbf{k}} (N_{\mathbf{a}}(\mathbf{k}) - N_{\mathbf{b}}(\mathbf{k}))}{V} \left| \phi_p 2\phi_q \phi_r \right\rangle \\ &= \frac{1+2+1}{V} \end{aligned} \tag{79}$$

For a multi particle state $|\phi\rangle = \left|\left(A_{p1}\phi_{p1} + A_{p2}\phi_{p2} + ...\right), 2\left(A_{q1}\phi_{q1} + A_{q2}\phi_{q2} + ...\right), ...\right\rangle$ in which the particles are in general, not eigen, states, we have

$$\begin{aligned} \rho = \langle \phi | \rho_{oper} | \phi \rangle &= \langle \phi | \frac{\sum_{\mathbf{k}} (N_{\mathbf{a}}(\mathbf{k}) - N_{\mathbf{b}}(\mathbf{k}))}{V} | \phi \rangle \\ &= \frac{\left(A_{p1}^2 + A_{p2}^2 + A_{p3}^2 + ...\right) + 2\left(A_{q1}^2 + A_{q2}^2 + A_{q3}^2 + ...\right) + ...}{V} \\ &= \frac{1+2+...}{V} = \frac{\text{Total num of particles}}{V}\,. \end{aligned} \tag{80}$$

Again, we can consider the total particle number operator as having the form in (73).

5.2 Probability Density for Continuous Solutions in QFT

The continuous solution probability density and number operator relations are developed below in direct parallel with the discrete solutions development above. Note that, in analogy with (60)

$$\rho_{oper} = 2\left(\int \frac{\mathbf{a}^{\dagger}(\mathbf{k}')}{\sqrt{2\omega_{\mathbf{k}'}}}\frac{e^{ik'x}}{\sqrt{(2\pi)^3}}d\mathbf{k}'\right)\left(\int \frac{\omega_{\mathbf{k}''}\mathbf{a}(\mathbf{k}'')}{\sqrt{2\omega_{\mathbf{k}''}}}\frac{e^{-ik''x}}{\sqrt{(2\pi)^3}}d\mathbf{k}''\right) - 2\left(\int \frac{\mathbf{b}^{\dagger}(\mathbf{k}')}{\sqrt{2\omega_{\mathbf{k}'}}}\frac{e^{ik'x}}{\sqrt{(2\pi)^3}}d\mathbf{k}'\right)\left(\int \frac{\omega_{\mathbf{k}''}\mathbf{b}(\mathbf{k}'')}{\sqrt{2\omega_{\mathbf{k}''}}}\frac{e^{-ik''x}}{\sqrt{(2\pi)^3}}d\mathbf{k}''\right), \tag{81}$$

and as before, the numerical probability density is the expectation value of (81),

$$\rho = \langle \phi(\tilde{x}) | \rho_{oper}(x) | \phi(\tilde{x}) \rangle . \tag{82}$$

5.2.1 Single Particle Wave Packet Probability Density (QFT, Continuous)

Consider $|\phi\rangle$ as a single particle wave packet where, if for simplicity we ignore antiparticles,

$$|\phi(\tilde{x})\rangle = \left| \int A(\mathbf{k}''')\frac{e^{-ik'''\tilde{x}}}{\sqrt{(2\pi)^3}}d\mathbf{k}''' \right\rangle, \tag{83}$$

where proper normalization for $A(\mathbf{k}''')$ is assumed. As an aside, note that (need to have defined $\mathbf{a}$, $\mathbf{a}^+$, and $N_{\mathbf{a}}$ operator action on continuous ket before here)

$$\langle \phi(\tilde{x}) | \mathbf{a}^{\dagger}(\mathbf{k}')\mathbf{a}(\mathbf{k}'') | \phi(\tilde{x}) \rangle = A^{\dagger}(\mathbf{k}')A(\mathbf{k}'') \tag{84}$$

and this is only non-zero when $\mathbf{k}' = \mathbf{k}''$.

By analogy to (67), we have probability density

$$\rho = \frac{1}{\sqrt{(2\pi)^3}}\left(\int A^{\dagger}(\mathbf{k}')\frac{e^{ik'x}}{\sqrt{2\omega_{\mathbf{k}'}}}d\mathbf{k}'\right)\left(\int \omega_{\mathbf{k}''}\frac{e^{-ik''x}}{\sqrt{2\omega_{\mathbf{k}''}}}A(\mathbf{k}'')d\mathbf{k}''\right). \tag{85}$$

Integrating (85) over all space (and using the Dirac delta relation (18)) results in

$$\int \rho dV = \int |A(\mathbf{k}')|^2 d\mathbf{k}' = 1 . \tag{86}$$

This equals the total probability of finding a single wave packet somewhere over all space and looks familiar to what we have seen in non-relativistic quantum mechanics. It also equals the number of particles. Thus we may define a number operator as

$$N = \int \rho_{oper} dV = \int \left(N_a(\mathbf{k}) - N_b(\mathbf{k}) \right) d\mathbf{k} \tag{87}$$

in analogy with (73) for discrete solution states and consonant with (37).

5.2.2 Multiple Particle General State (QFT, Continuous)

Consider continuous solution multi particle states where the particles are in general (non eigen) states, i.e., $|\phi_p 2\phi_q \phi_r\rangle$, where, for example,

$$|\phi_p\rangle = \left| \int {}_pA(\mathbf{k}''')\frac{e^{-ik'''\tilde{x}}}{\sqrt{(2\pi)^3}}d\mathbf{k}''' \right\rangle, \tag{88}$$

and similar relations hold for the other particles in the multi particle state. By analogy to (75)

$$\rho = \frac{1}{(2\pi)^3}\left\{ \begin{aligned} &\left(\int {}_pA^{\dagger}(\mathbf{k}')\frac{e^{ik'x}}{\sqrt{2\omega_{\mathbf{k}'}}}d\mathbf{k}'\right)_{\phi_p}\left(\int \omega_{\mathbf{k}''}\frac{e^{-ik''x}}{\sqrt{2\omega_{\mathbf{k}''}}}\,{}_pA(\mathbf{k}'')d\mathbf{k}''\right)_{\phi_p} \\ &+\left(\int {}_qA^{\dagger}(\mathbf{k}')\frac{e^{ik'x}}{\sqrt{2\omega_{\mathbf{k}'}}}d\mathbf{k}'\right)_{\phi_q}\left(\int \omega_{\mathbf{k}''}\frac{e^{-ik''x}}{\sqrt{2\omega_{\mathbf{k}''}}}\,{}_qA(\mathbf{k}'')d\mathbf{k}''\right)_{\phi_q} + \ldots \end{aligned} \right\} \tag{89}$$

Thus,

$$\int \rho dV = \int \left| {}_pA_{\mathbf{k}'} \right|^2 d\mathbf{k}' + 2\int \left| {}_qA_{\mathbf{k}'} \right|^2 d\mathbf{k}' + \int \left| {}_rA_{\mathbf{k}'} \right|^2 d\mathbf{k}' = 1 + 2 + 1 = 4 . \tag{90}$$

This, again, equals the number of particles and hence

$$\begin{aligned}&\text{Number of particles} = \int \rho dV = \int \langle \phi | \rho_{oper}(x) | \phi \rangle d^3\mathbf{x} \\ &= \text{Expectation value of number operator} \\ &= \langle \phi | \int \left(\mathbf{a}^\dagger(\mathbf{k})\mathbf{a}(\mathbf{k}) - \mathbf{b}^\dagger(\mathbf{k})\mathbf{b}(\mathbf{k}) \right) d\mathbf{k} \,|\, \phi \rangle = \langle \phi | \int \left(N_\mathbf{a}(\mathbf{k}) - N_\mathbf{b}(\mathbf{k}) \right) d\mathbf{k} \,|\, \phi \rangle \\ &= n_a - n_b .\end{aligned} \tag{91}$$

6. *Action of Hamiltonian on States (QFT)*

6.1 Discrete Eigenstates (QFT)

We treat only the general state particle case, as the eigen state particle case is a special case where all $A_\mathbf{k}$ are zero except one, with that one having an absolute value (modulus) of 1.

6.1.1 General Single Particle State (QFT, Discrete)

For the Hamiltonian of **Error! Reference source not found.**, and again concentrating for simplicity only on particles (and not anti-particles) kets, the energy expectation value is

$$\begin{aligned}\bar{E} &= \langle \phi | H | \phi \rangle \\ &= \left\langle \sum_\mathbf{k} A_\mathbf{k}^\dagger \frac{e^{ik\tilde{x}}}{\sqrt{V}} \right| \sum_{\mathbf{k}'} \omega_{\mathbf{k}'} \left(N_a(\mathbf{k}') + \tfrac{1}{2} + N_b(\mathbf{k}') + \tfrac{1}{2} \right) \left| \sum_{\mathbf{k}'''} A_{\mathbf{k}'''} \frac{e^{ik'''\tilde{x}}}{\sqrt{V}} \right\rangle \\ &= \sum_\mathbf{k} A_\mathbf{k}^\dagger \sum_{\mathbf{k}'} \omega_{\mathbf{k}'} A_{\mathbf{k}'} \delta_{\mathbf{k}\mathbf{k}'} = \sum_\mathbf{k} \left| A_\mathbf{k} \right|^2 \omega_\mathbf{k} .\end{aligned} \tag{92}$$

In the last line we ignored the $\frac{1}{2}\omega_\mathbf{k}$ contributions from the vacuum.

For an eigenstate $|\phi\rangle = |\phi_\mathbf{k}\rangle$ all but one coefficient in (92) equals zero, and we have $E = \bar{E} = \omega_\mathbf{k}$.

6.1.2 General Multi Particle State (QFT, Discrete)

For multi particle states where at least some of the particles are in general states, we have

$$\bar{E} = \langle \phi | H | \phi \rangle = \left\langle \phi_p 2\phi_q \phi_r \right| \sum_{\mathbf{k}'} \omega_{\mathbf{k}'} \left(N_a(\mathbf{k}') + \tfrac{1}{2} + N_b(\mathbf{k}') + \tfrac{1}{2} \right) \left| \phi_p 2\phi_q \phi_r \right\rangle . \tag{93}$$

With the Hamiltonian operator acting on the ket as the $\mathbf{a}_\mathbf{k}$ operator did in (71), this results in

$$\bar{E} = \sum_\mathbf{k} \omega_\mathbf{k} \left(\left| {}_p A_\mathbf{k} \right|^2 + 2 \left| {}_q A_\mathbf{k} \right|^2 \left| {}_r A_\mathbf{k} \right|^2 \right) = \bar{E}_p + 2\bar{E}_q + \bar{E}_r , \tag{94}$$

wherein the total expected energy value equals the sum of the expectation energies for each particle in the state, and we have again ignored the vacuum contribution.

For all particles in eigenstates of energy, this reduces to $E = \omega_p + 2\omega_q + \omega_r$.

6.2 Continuous Eigenstates

6.2.1 Single Particle Wave Packet State (QFT, Continuous)

For a single particle wave packet, the ket has form

$$|\phi(\tilde{x})\rangle = \left| \int A(\mathbf{k}''') \frac{e^{-ik'''\tilde{x}}}{\sqrt{(2\pi)^3}} d\mathbf{k}''' \right\rangle , \tag{95}$$

and the energy expectation value is

$$\bar{E} = \langle \phi | H | \phi \rangle$$
$$= \left\langle \int A^{\dagger}(\mathbf{k}) \frac{e^{ik\tilde{x}}}{\sqrt{(2\pi)^3}} d\mathbf{k} \left| \int \omega_{\mathbf{k}'} \left(N_a(\mathbf{k}') + \tfrac{1}{2}\delta(0) + N_b(\mathbf{k}') + \tfrac{1}{2}\delta(0) \right) d\mathbf{k}' \right| \int A(\mathbf{k}''') \frac{e^{-ik'''\tilde{x}}}{\sqrt{(2\pi)^3}} d\mathbf{k}''' \right\rangle . \quad (96)$$

Noting that each $N_a(\mathbf{k}')$ operator acting on the ket leaves zero except when $\mathbf{k}' = \mathbf{k}'''$, we have

$$\bar{E} = \left\langle \int A^{\dagger}(\mathbf{k}) \frac{e^{ik\tilde{x}}}{\sqrt{(2\pi)^3}} d\mathbf{k} \middle\| \int \omega_{\mathbf{k}'} A(\mathbf{k}') \frac{e^{-ik'\tilde{x}}}{\sqrt{(2\pi)^3}} d\mathbf{k}' \right\rangle . \quad (97)$$

Integrating this over all space and using the Dirac delta function again, we end up with

$$\bar{E} = \int \omega_{\mathbf{k}} A^{\dagger}(\mathbf{k}) A(\mathbf{k}) d\mathbf{k} = \int \omega_{\mathbf{k}} |A(\mathbf{k})|^2 d\mathbf{k} \quad (98)$$

in complete analogy with (92).

6.2.2 Multi Particle Wave Packet States (QFT, Continuous)

For a multiparticle state where the particles are wave packets,

$$\begin{aligned} \bar{E} &= \langle \phi | H | \phi \rangle \\ &= \left\langle \phi_p 2\phi_q \phi_r \left| \int \omega_{\mathbf{k}'} \left(N_a(\mathbf{k}') + \tfrac{1}{2}\delta(0) + N_b(\mathbf{k}') + \tfrac{1}{2}\delta(0) \right) d\mathbf{k}' \right| \phi_p 2\phi_q \phi_r \right\rangle \end{aligned} \quad (99)$$

and once again we have the operator acting sequentially on each particle in the ket. Ignoring the vacuum contribution, this results in a series of terms like (98), i.e., XXX Think thru XXX

$$\bar{E} = \int \omega_{\mathbf{k}} \left(\left|{}_p A(\mathbf{k})\right|^2 + 2\left|{}_q A(\mathbf{k})\right|^2 + \left|{}_r A(\mathbf{k})\right|^2 \right) d\mathbf{k} = \bar{E}_p + 2\bar{E}_q + \bar{E}_r . \quad (100)$$

Thus, the expected energy is the sum of the expected energies for each wave packet particle.

7. Action of Hamiltonian on the Vacuum

Rough thoughts only as of March 13, 2010..