Fourier Transforms

Follows G.D.Mahan,"Many Particle Physics".

Discrete case:

$$f_l = \frac{1}{\sqrt{N}} \sum_k e^{i k a l} f_k$$

$$f_k = \frac{1}{\sqrt{N}} \sum_l e^{-i k a l} f_l$$

$$\sum_l e^{i (k-k') a l} = N \delta_{k k'}$$

$$\sum_l x_l x_{l+m} = \frac{1}{N} \sum_l \sum_{k,k'} e^{i k a l} x_k e^{i k' a (l+m)} x_{k'}$$

$$= \sum_{k,k'} \delta_{k,-k'} x_k e^{i k' a m} x_{k'}$$

$$= \sum_k e^{-i k a m} x_k x_{-k}$$

$$= \sum_k e^{i k a m} x_k x_{-k}$$

$$\sum_l x_l^2 = \sum_k x_k x_{-k}$$

Continuous case:

$$\boldsymbol{k} = \frac{2\pi}{V^{1/3}} (n_x, n_y, n_z) \quad \to \quad \sum_{\boldsymbol{k}} \approx \frac{V}{(2\pi)^3} \int d^3 k \qquad \text{for } V >> 1$$

$$\sum_{\boldsymbol{k}} \delta_{\boldsymbol{k} \boldsymbol{k}'} = 1 = \int d^3 k \, \delta(\boldsymbol{k} - \boldsymbol{k}')$$

$$\approx \frac{V}{(2\pi)^3} \int d^3 k \, \delta_{\boldsymbol{k} \boldsymbol{k}'}$$

$$\to \qquad \delta_{\boldsymbol{k} \boldsymbol{k}'} \approx \frac{(2\pi)^3}{V} \delta(\boldsymbol{k} - \boldsymbol{k}')$$

$$\int d^3 k \, e^{-i \boldsymbol{k} \cdot (\boldsymbol{r} - \boldsymbol{r}')} = (2\pi)^3 \delta(\boldsymbol{r} - \boldsymbol{r}')$$

$$\to \qquad \sum_{\boldsymbol{k}} e^{-i \boldsymbol{k} \cdot (\boldsymbol{r} - \boldsymbol{r}')} \approx \frac{V}{(2\pi)^3} \int d^3 k \, e^{-i \boldsymbol{k} \cdot (\boldsymbol{r} - \boldsymbol{r}')} = V \delta(\boldsymbol{r} - \boldsymbol{r}')$$

$$\int d^3 r \, e^{i (\boldsymbol{k} - \boldsymbol{k}') \cdot \boldsymbol{r}} = V \delta_{\boldsymbol{k},\boldsymbol{k}'} \qquad (\ \boldsymbol{k} \text{ discrete, } V \text{ finite}\ )$$

$$= (2\pi)^3 \delta(\boldsymbol{k} - \boldsymbol{k}') \qquad (\ \boldsymbol{k} \text{ continuous, } V \text{ infinite}\ )$$

Fourier transform:

$$f(\boldsymbol{k}) = \int d^3 r \, f(\boldsymbol{r}) \, e^{-i \boldsymbol{k} \cdot \boldsymbol{r}}$$

$$f(\boldsymbol{r}) = \frac{1}{V} \sum_{\boldsymbol{k}} e^{i \boldsymbol{k} \cdot \boldsymbol{r}} f(\boldsymbol{k}) = \frac{1}{V} \sum_{\boldsymbol{k}} e^{i \boldsymbol{k} \cdot \boldsymbol{r}} \int d^3 r' \, f(\boldsymbol{r}') \, e^{-i \boldsymbol{k} \cdot \boldsymbol{r}'} = f(\boldsymbol{r})$$

$$\approx \int \frac{d^3 k}{(2\pi)^3} f(\boldsymbol{k})\, e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}}$$

$$\frac{1}{V}\sum_{\boldsymbol{k}} e^{i\,\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} \approx \delta(\boldsymbol{r}-\boldsymbol{r}') = \int \frac{d^3 k}{(2\pi)^3} e^{i\,\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}$$

Field operator:

$$\psi(\boldsymbol{r}) = \sum_{\boldsymbol{k}} \phi_{\boldsymbol{k}}(\boldsymbol{r})\, a_{\boldsymbol{k}} = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}}\, a_{\boldsymbol{k}}$$

where $\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}}$

$$\int d^3 r\, \phi^*_{\boldsymbol{k}'}(\boldsymbol{r})\, \phi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{V}\int d^3 r\, e^{i\,(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} = \delta_{\boldsymbol{k}\,\boldsymbol{k}'}$$

(1 particle in V.)

Free particles:

$$\begin{aligned}
H &= -\int d^3 r\, \psi^+(\boldsymbol{r}) \frac{\hbar^2}{2m} \nabla^2\, \psi(\boldsymbol{r}) \\
&= \frac{1}{V}\sum_{\boldsymbol{k},\boldsymbol{k}'} \int d^3 r\; e^{i\,(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}\, \frac{\hbar^2 \boldsymbol{k}^2}{2m}\, a^+_{\boldsymbol{k}'}\, a_{\boldsymbol{k}} \\
&= \sum_{\boldsymbol{k}} \frac{\hbar^2 \boldsymbol{k}^2}{2m}\, a^+_{\boldsymbol{k}}\, a_{\boldsymbol{k}} \\
&= \sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}}\, a^+_{\boldsymbol{k}}\, a_{\boldsymbol{k}}
\end{aligned}$$

For $\boldsymbol{k}$ continuous:

$$\psi(\boldsymbol{r}) = \int d^3 k\, \varphi_{\boldsymbol{k}}(\boldsymbol{r})\, \tilde{a}_{\boldsymbol{k}} = \frac{1}{(2\pi)^{3/2}} \int d^3 k\, e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}}\, \tilde{a}_{\boldsymbol{k}}$$

where $\varphi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}}$

$$\int d^3 r\, \varphi^*_{\boldsymbol{k}'}(\boldsymbol{r})\, \varphi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int d^3 r\, e^{i\,(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} = \delta(\boldsymbol{k}-\boldsymbol{k}')$$

(1 particle in all space.)

$$\begin{aligned}
H &= -\int d^3 r\, \psi^+(\boldsymbol{r}) \frac{\hbar^2}{2m} \nabla^2\, \psi(\boldsymbol{r}) \\
&= \frac{1}{(2\pi)^3} \int d^3 k \int d^3 k' \int d^3 r\; e^{i\,(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}\, \frac{\hbar^2 \boldsymbol{k}^2}{2m}\, \tilde{a}^+_{\boldsymbol{k}'}\, \tilde{a}_{\boldsymbol{k}} \\
&= \int d^3 k\, \frac{\hbar^2 \boldsymbol{k}^2}{2m}\, \tilde{a}^+_{\boldsymbol{k}}\, \tilde{a}_{\boldsymbol{k}} \\
&= \int d^3 k\, \epsilon_{\boldsymbol{k}}\, \tilde{a}^+_{\boldsymbol{k}}\, \tilde{a}_{\boldsymbol{k}}
\end{aligned}$$

Hence, $a_{\boldsymbol{k}} = \sqrt{\frac{(2\pi)^3}{V}}\; \tilde{a}_{\boldsymbol{k}}$

Caution: It's common practice to use $a_{\boldsymbol{k}}$ to denote both $a_{\boldsymbol{k}}$ & $\tilde{a}_{\boldsymbol{k}}$, which results in the seemingly erroneous relation:

$$\sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}}\, a_{\boldsymbol{k}}^{+}\, a_{\boldsymbol{k}} \approx \int d^3 k\, \epsilon_{\boldsymbol{k}}\, a_{\boldsymbol{k}}^{+}\, a_{\boldsymbol{k}}$$