Dirac's Expansion Postulate and Completeness of an Eigenfon Set {4n}

Several times in the necent past, we have used Dirac's expansion postulate (#5) on p. Prop. 27 of these notes), i.e. the claim that if a QM system is characterized by a set of orthonormal eigenfens $\{\Psi_n(x)\}$, then an <u>arbitrary</u> state $\Psi(x)$ of the system (like the wavepackets we have been using) can be written as the superposition: $\Psi(x) = \sum_n C_n \Psi_n(x)$, and $|C_n|^2$ then measures the probability that the $n^{\frac{1}{2}}$ eigenstate will be found present in a measurement on state Ψ . When all this can be done, the set $\{\Psi_n(x)\}$ is said to be "Complete" -- i.e. it can completely specify any arbitrary $\Psi(x)$ relevant to the system.

Here we want to sharpen our notion of "completeness" for an eigenfen set $\{\frac{1}{4}, |x|\}$ and also to address the question of completeness and normalization for free particle eigenfons $\exp(+\frac{i}{\hbar}p \cdot r)$.

4) Start with the eigenfons { Ψ_n } generated by some Hermitian operator Q, via $Q\Psi_n(x) = q_n \Psi_n(x)$ } the { q_n } = {cnsts} are eigenvalues; (1) the { Ψ_n } are orthonormal! (Ψ_n) = θ_n .

Now try expanding an arbitrary state I of Q in terms of the {4, 7, i.e.

The expansion coefficients on in Eq. (2) are readily found ...

$$\rightarrow \langle \Psi_m | \Psi \rangle = \sum_n c_n \langle \Psi_m | \Psi_n \rangle = \sum_n c_n \delta_{mn} = c_m$$

Sol
$$C_n = \langle \psi_n | \Psi \rangle = \int \psi_n^*(x') \Psi(x') dx'$$

Now we demand self-consistency: we should be able to put Cn of Eq. (3) back into the RHS of Eq. (2) and thereby regenerate Y(x). We find...

(3)

$$\Psi(x) = \sum_{n} \left[\int \Psi_{n}^{*}(x') \Psi(x') dx' \right] \Psi_{n}(x) = \int \left[\sum_{n} \Psi_{n}^{*}(x') \Psi_{n}(x) \right] \Psi(x') dx'$$
This is an identity if the last [] behaves must act like $\delta(x'-x)$

like a Dirac delta fen. Then, indeed: \$[81x'-x]] \P(x') dx' = \P(x). Claim:

CLOSURE RELATION

The expansion $\Psi(x) = \sum_{n=1}^{\infty} C_n \Psi_n(x)$ is possible if and only if the $\{\Psi_n\} > (5)$ obey: $\sum_{n=1}^{\infty} \frac{\Psi_n^*(x') \Psi_n(x)}{\Psi_n(x)} = \frac{S(x'-x)}{N}$. The $\{\Psi_n\}$ are then a complete set.

The Closure Relation is the principal criterion for completeness of the {4,1.

2) Normalization of I proceeds apace...

$$\rightarrow \langle \Psi | \Psi \rangle = 1 \Rightarrow \langle \sum_{m} c_{m} \Psi_{m} | \sum_{n} c_{n} \Psi_{n} \rangle = \sum_{m,n} c_{m} c_{n} \langle \Psi_{m} | \Psi_{n} \rangle = \sum_{n} \frac{|c_{n}|^{2} = 1}{n}. \quad (6)$$

For discrete states, this is the analogue of Parseval's Theorem (see NOTES, b. Sch. 12). In fact we have parallel constructions...

(7A)

 $\frac{\Psi(x)}{\sqrt{2\pi}} = \frac{1}{\sqrt{2\pi}} \int \Phi(q) e^{iqx} dq; \qquad \text{Norm: } \int |\Psi(x)|^2 dx = 1 = \int |\Phi(q)|^2 dq.$ $\Rightarrow \text{Spectral for } \Phi(q) \text{ is:} \qquad \frac{\text{Interpretation: } |\Phi(q)|^2 dq = \text{probability of finding } \Psi \text{ with momentum in } dq \text{ at } q.$

GENERAL QM System (Meigenvalus qu discrete).

(7B)

Y(x) = Z Cn Yn(x); => Spectral Cn are: coefficients

cn= Synta) Y(x)dx.

Norm: $S|\Psi(x)|^2 dx = 1 = \sum_{n=1}^{\infty} |C_n|^2$.

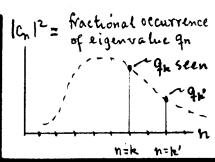
Interpretation: $|C_n|^2 = \text{probability of finding}$ I with eigenvalue q_n in state Ψ_n .

This analogy makes plansible Dirac's postulate #6 (p. Prop. 27), namely that the {1cn12} are a probability distribution for the eigenvalues In

The { 1 cn 12 } as a probability distribution. Completeness for SHO { 4,}. Complete

In fact, the expectation value of Q in the composite state I is...

A given single measurement of Q in the state I cornot yield anything other than some eigenvalue qx (because these are the only observables -- recall work on p. Prop. 19). The next measurement of (Q) may



yield $q_{k'}$, then $q_{k''}$, $q_{k'''}$ etc. The <u>probability</u> of any given q_n showing up--when working with $\Psi = \sum_{n} c_n \Psi_n - -is$ girst $|c_n|^2$. Then the value $\langle Q \rangle = \sum_{n} |c_n|^2 q_n$ in Eq.(8) has an obvious meaning as the average of all these measurements.

3) ASIDE Completeness for the SHO Rigenfons.

We shall show that the SHO eigenfons $\Psi_n(x)$ are complete, by demonstrating that the closure relation [Eq.(5) above] holds: $\sum \Psi_n^*(x) \Psi_n(x') = \delta(x-x')$.

$$\frac{1. E_{q.}(40)}{p. Soles 18} \left\{ \Psi_{n}(x) = \left(\frac{\alpha / \sqrt{\pi}}{2^{n} n!} \right)^{\frac{1}{2}} e^{-\frac{1}{2} \xi^{2}} H_{n}(\xi) , \quad \forall \xi = \alpha x \quad \forall \alpha = \sqrt{\frac{m \omega}{\hbar}} ; \quad (A1)$$

$$\frac{S_{\text{VM}}}{S_{\text{VM}}} = \sum_{n=0}^{\infty} \Psi_{n}^{*}(x) \Psi_{n}(x') = \frac{\alpha}{\sqrt{n}} e^{-\frac{1}{2}(\xi^{2} + \xi'^{2})} \sum_{n=0}^{\infty} \frac{1}{2^{n} n!} H_{n}(\xi) H_{n}(\xi'). \quad (A2)$$

2. We process the SUM in Eq. (Az) by using Rodrigues' formula...

$$\rightarrow H_n(\xi') = (-)^n e^{+\xi'^2} (d/d\xi')^n e^{-\xi'^2},$$
(A3)

... and the tabulated integral (from 500 e-au2 + bu du = 100 eb2/40) ...

$$\rightarrow \int_{-\infty}^{\infty} e^{-\frac{1}{4}\sigma^2 - i\xi'\sigma} d\sigma = 2\sqrt{\pi} e^{-\xi'^2}.$$
(A4)

Use the et 2 in (A4) on the RHS of (A3), i.e. form...

Completeness for the SHO eigenfens (cont'd)

$$\rightarrow H_n(\xi') = (-)^n e^{\xi'^2} \left(\frac{d}{d\xi'}\right)^n \cdot \frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{4}\sigma^2 - i\,\xi'\sigma} d\sigma \int_{\text{under the integral}}^{\text{differentiate}} d\sigma = \frac{i^n}{2\sqrt{\pi}} e^{\xi'^2} \int_{-\infty}^{\infty} \sigma^n e^{-\frac{1}{4}\sigma^2 - i\,\xi'\sigma} d\sigma. \tag{A5}$$

This is evidently an integral representation of the Hermite polynomials 3. Use (A5) in the SUM of (Az) to write...

$$\underline{SUM} = \frac{Q}{\sqrt{\pi}} e^{-\frac{1}{2}(\xi^2 + \xi'^2)} \sum_{n=0}^{\infty} \frac{H_n(\xi)}{2^n n!} \cdot \frac{i^n}{2\sqrt{\pi}} e^{\xi'^2} \int_{-\infty}^{\infty} \sigma^n e^{-\frac{1}{4}\sigma^2 - i\xi'\sigma} d\sigma. \quad (A6)$$

... Interchange order of \(\tilde{\Sigma}\) and \(\tilde{\Sigma}\), and rearrange factors ...

$$\underline{\underline{SUM}} = \frac{\alpha}{2\pi} e^{-\frac{1}{2}(\xi^2 - \xi'^2)} \int_{-\infty}^{\infty} \left[\sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i\sigma}{2} \right)^n H_n(\xi) \right] e^{-\frac{1}{4}\sigma^2 - i\xi'\sigma} d\sigma \qquad (A7)$$

generating fen for the Hn is: $g(s,\xi) = \sum_{n=0}^{\infty} \frac{s^n}{n!} H_n(\xi) = e^{-s^2 + 2\xi s} \int_{p. Solus 17}^{Eq. (30)} g(s,\xi) \Big|_{s=\frac{i\sigma}{2}} = e^{\frac{1}{4}\sigma^2 + i\xi\sigma}.$ (A8)

4. Use of this result in (A7) simplifies things considerably, viz.

$$\underline{\underline{SUM}} = \alpha e^{-\frac{1}{2}(\xi^2 - \xi'^2)} \cdot \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(\xi - \xi')\sigma} d\sigma \cdot \frac{1}{(\xi - \xi')}$$
(A9)

The remaining integral is just a rept of Dirac's delta for $\delta(\xi-\xi')$, $\frac{1}{2}$ $\xi=\alpha x$. So we can write (A9), using $\delta(\alpha u)=\frac{1}{\alpha}\delta(u)$, as...

$$\underline{SUM} = e^{-\frac{1}{2}\alpha^2(x^2-x'^2)} \cdot \delta(x-x') = \delta(x-x'), \qquad (A10)$$

The exponential factor is just $\equiv 1$ in effect, since the RHS is nonzero only when x = x'. Altogether then, we have Shown closure for the SHO 4.15:

$$\sum_{n} \Psi_{n}^{*}(x) \Psi_{n}(x') = \delta(x-x') \iff \text{the SHO} \{\Psi_{n}\} \text{ is complete.}$$
(A11)

Evidently, the analytic demonstration of closure for a set {\mathcal{Y}_n} is intricate. Other tests for completeness can be used (e.g. "convergence-in-the-mean" for \(\frac{\mathcal{Z}}{n} \, \mathcal{Y}_n \).

4) Not all eigenfons and eigenvalues work into our normalization-orthogonalitycompleteness scheme so neatly. For example, consider free-particle wavefons, which are eigenfons of momentum. The following catastrophe seems plausible...

PROOF THAT to = 0.

1: Let ϕ be an eigenfon of the (Hermitian) momentum operator, i.e.

2. Consider the commutator it = [x, p.]. Take expectation values on both sides

then it =
$$\langle \phi | x | p_{up} \phi \rangle - \langle p_{up} \phi | x | \phi \rangle \leftarrow \text{use } p_{up} \phi = p \phi \dots$$
 (9d)

in =
$$\beta\langle\phi|x|\phi\rangle - \beta^*\langle\phi|x|\phi\rangle \equiv 0$$
, since β is real. (9e)

3. (9e)
$$\Rightarrow$$
 h = 0. QED. Corollary: QM \rightarrow 0 ([x,p.,]=0, etc.). (9f)

Something must be wrong with this proof, even though we've done "orthodox" operations (provined, pop Hermitian, etc.).

There are two things wrong with this proof, namely the assumptions in (9b) & (9c) that $(\phi|\phi)=1$ & pop is Hermitian w.n.t. to the ϕ -fens. Both of these "orthodox" assumptions fail because free-particle wavefens have the (unique) peculiar feature that they do not vanish at ∞ . To see this, solve (9a)...

$$-i\hbar \frac{\partial}{\partial x} \phi = \phi \Rightarrow \frac{\phi = Ce \frac{i}{\hbar} \phi x = \phi_{\rho}(x)}{\text{eigenfen}; C = "morm" enst.}$$

$$\langle \phi_{\ell} | \phi_{\ell} \rangle = |C|^2 \int_{-\infty}^{\infty} e^{-(i/k)} p^{\chi} \cdot e^{+(i/k)} p^{\chi} d\chi = |C|^2 \int_{-\infty}^{\infty} d\chi \rightarrow \infty; \qquad (11)$$

and (next page)

$$\rightarrow \langle \phi | p_{+}(x\phi) \rangle = \langle p_{+}\phi | x\phi \rangle - i \hbar \underbrace{(x|\phi|^{2})|_{x=-\infty}^{x=+\infty}}_{\text{|C|}^{2}[(+)\infty-(-)\infty]} = \infty.$$

(12)

5 By the example of Eqs. (9)-121, it is clear that the procedures for normali-3 attorn, orthogonality, and completeness for (free-particle) momentum eigenfons must be treated as a special case. In 3D, these eigenfons are...

$$\begin{bmatrix}
-ik \nabla \phi = p \phi \implies \phi = C_p e^{|i/h|} p \cdot r = \phi_p | r \\
... put: \underline{p = h k} (de Broglie), so: \underline{\phi_k | r |} = C_k e^{ik \cdot r}; \\
... and: \phi_k(x, y, z) = C_k e^{ik_x x} e^{ik_y y} e^{ik_z z}, \text{ in rect}^{\perp} cds.$$
(13)

One way of normalizing the $\phi_k(t)$ is to imagine the space they are in to be a very large cubical box of side $L\to\infty$, and to impose periodic boundary conditions", i.e. with the L-box repeated indefinitely...

 $\oint \phi_{k}(x+L, y, z) = \phi_{k}(x, y, z), \text{ and similarly for } y \notin z;$ $\begin{cases}
SON & k = (k_{x}, k_{y}, k_{z}) = \frac{2\pi}{L}(n_{x}, n_{y}, n_{z}) \text{ integers: } 0, \pm 1, \dots
\end{cases}$

We did a similar procedure in our analysis off BB radiation $x \leftarrow L \rightarrow$ (See Notes, p. Intro. 2). It is now discrete, and so is the energy $E_k = h^2 k^2 / 2m$, but the spacing $\Delta k = 2\pi/L$ between adjacent k-values can be made as small as desired by letting $L \rightarrow \infty$; that is the way we recover the continuum of k-values (and E_k -values) that characterize a free particle.

The main reason why -- in Eq. (14) -- we require that $\phi_k(r)$ repeat itself on the walls, rather than requiring $\phi_k(r) \equiv 0$ there (as for the BB radiation case), is that we want to be able to recover the case of a truly free particle, where $|\phi_k|^2$ need not vanish at ∞ (i.e. $L \rightarrow \infty$). The requirement $\phi_k \equiv 0$ on the walls

Normalization, Orthogonality & Completeness for the OK(F).

would imply that the walls provided an actual physical containment -- they would act as though there were a potential V -> 00 at the boundaries.

6) With the so-called "box normalization" in Eq. (14), we can carry out the standard procedures for the free-particle eigenfens $\phi_k(\mathbf{r})$, viz...

NORMALIZATION

ORTHOGONALITY

This depends explicitly on the quasi-discrete nature of Ik, as follows ...

$$\rightarrow \langle \phi_{k} | \phi_{l} \rangle = \frac{1}{L^{3}} \int_{bax} e^{-i(k-1)\cdot r} d^{3}r$$

$$= \frac{1}{L^{3}} \int_{-L/2}^{+L/2} e^{-i(k_{x}-l_{x})} dx \times \left[\text{Similar integral} \right] \times \left[\text{Similar result} \right] \times \left[\text{Similar result} \right]$$

$$= \frac{1}{L^{3}} \left[\frac{2}{k_{x}-l_{x}} \text{Sim}(k_{x}-l_{x}) \frac{L}{2} \right] \times \left[\text{Similar result} \right] \times \left[\text{Similar result} \right]. \tag{16}$$

But: kx-1x = (2π/L) Δnx, where Δnx = some integer = 0, ±1, ±2, ... So...

$$\langle \phi_{k} | \phi_{1} \rangle = \left[\frac{\sin \pi \Delta n_{x}}{\pi \Delta n_{x}} \right] \times \left[\frac{\sin \pi \Delta n_{y}}{\pi \Delta n_{y}} \right] \times \left[\frac{\sin \pi \Delta n_{z}}{\pi \Delta n_{z}} \right] = \begin{cases} 0, & \text{if any } \Delta n_{i} \neq 0; \\ 1, & \text{only if all } \Delta n_{i} = 0. \end{cases}$$

So (\$k | \$p_) = 0, unless 1 = k. The shorthand for this orthogonality is ...

$$\langle \phi_k | \phi_1 \rangle = \delta_{kB}$$
 \int orthonormality for free-particle ligenfens (still in a cubical bix).

<u>Completeness</u>

This can be demonstrated by converting the closure sum to an integral, as ...

Completeness for free-particle $\phi_{k}(\mathbf{F})^{1/2}$. S-for normalization. Complete $\sum_{k} \phi_{k}^{*}(\mathbf{F}^{1}) \phi_{k}(\mathbf{F}) = \frac{1}{L^{3}} \sum_{n_{x}=-\infty}^{\infty} \sum_{n_{y}=-\infty}^{\infty} \sum_{n_{z}=-\infty}^{\infty} \frac{2\pi i}{L} [n_{x}(x-x')+n_{y}(y-y')+n_{z}(z-z')]$... as $L \to \infty$, $\frac{replace}{n_{x}=-\infty} \sum_{n_{x}=-\infty}^{\infty} b_{y} \int_{-\infty}^{\infty} dn_{x} = (L/2\pi) \int_{-\infty}^{\infty} dk_{x} \int_{-\infty}^{\infty} different way. Then...$ $\sum_{k} \frac{\phi_{k}^{*}(\mathbf{F}^{1}) \phi_{k}(\mathbf{F})}{k} = \frac{1}{(2\pi)^{3}} \cdot \int_{-\infty}^{\infty} dk_{x} \int_{-\infty}^{\infty} dk_{y} \int_{-\infty}^{\infty} dk_{z} e^{i \left[k_{x}(x-x')+k_{y}(y-y')+k_{z}(z-z')\right]} = S(x-x') S(y-y') S(z-z') = S(x-x').$ [20]

QED: Momentum eigenfons $\phi_k(R) = (1/L^{3/2})e^{i \cdot k \cdot r}$, subject to periodic boundary conditions in a cultical box of side L, are both orthonormal and complete. That means we can describe the most general free perticle motion by: $\Psi(R) = \sum_{k} a_k \phi_k(R) \rightarrow \int_{-\infty}^{\infty} d^3k A(k)e^{i \cdot k \cdot r}$. We took this Fourier-type wave packet as a given when we worked with free-particle motion.

An alternate approach to free-particle eigenfens is sometimes taken in a "box" which is already so in size. We put...

$$\frac{\langle \phi_{\mathbf{k}} | \phi_{\mathbf{l}} \rangle}{\langle \phi_{\mathbf{k}} | \phi_{\mathbf{l}} \rangle} = \int_{\infty}^{\infty} \phi_{\mathbf{k}}^{*} | \mathbf{k}^{*} \rangle \phi_{\mathbf{l}}(\mathbf{k}^{*}) d^{3}\tau = \frac{1}{(2\pi)^{3}} \int_{\infty}^{\infty} e^{-i(\mathbf{k} \cdot \mathbf{l}_{\mathbf{k}}) \cdot \mathbf{k}} d^{3}\tau$$

$$= \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i(\mathbf{k}_{\mathbf{k}} - \mathbf{l}_{\mathbf{k}}) \times d\mathbf{k}} \right] \times \begin{bmatrix} \text{similar} \\ \text{integral} \\ \text{in 2} \end{bmatrix} \times \begin{bmatrix} \text{Similar} \\ \text{in 2} \end{bmatrix} = \underbrace{S(\mathbf{k} - \mathbf{l}_{\mathbf{k}})}_{\infty}. \tag{21}$$

In this ease, we get a <u>Dirac</u> delta instead of the <u>Kronecker</u> S_{RR} in Eq. (18). The procedure here is called "delta-for normalization". The completeness condition is:

- $\int_{\infty} \Phi_{k}^{*}(r') \Phi_{k}(r') d^{3}k = (1/2\pi)^{3} \int_{\infty} e^{i k \cdot (r-r')} d^{3}k = S(r-r')$.

The closure sum & pklr') pklr) on the IHS has become an integral, a priori.

For the interested student: Stay in a box with the free-particle $\phi_k(x)^{is}$, and see What the "proof" in Eqs. (9a) - (9f) really does say.