QUANTUM MECHANICS II
A Second Course in Quantum Theory
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APPENDIX B

DIRAC NOTATION AND REPRESENTATIONS

This appendix is meant for reference. See elementary texts such as Merzbacher (1970) and Gottfried (1966) for a proper introduction, and Chapters 5–7 for applications.

B.1 Dirac Notation

A **state** is represented by the *ket* $|\psi\rangle$. This state is a ray in a linear vector space of infinite dimension, that is, an abstract vector in a Hilbert space.

A **dual or adjoint-space** state is represented by the *bra* $\langle\psi|$. The 1:1 correspondence between the spaces of kets and bras is shown by the adjoint operation:

$$\langle\psi| = |\psi\rangle^\dagger . \tag{B.1}$$

The **scalar or inner product** of states $|\phi\rangle$ and $|\psi\rangle$ is given by the juxtaposed "bra-ket" = *braket*,

$$\langle\phi\,|\psi\rangle \equiv (\phi, \psi) = \langle\psi\,|\phi\rangle^*. \tag{B.2}$$

General operators O or $\tilde{O}$ are objects which transform one state into another:

$$O\,|\psi\rangle = |\phi\rangle = |O\psi\rangle . \tag{B.3}$$

Accordingly, $O\,|\psi\rangle$ is *not* proportional to $|\psi\rangle$—although it may look that way.

An **operator** is formed by the juxtaposition $|\psi\rangle\,\langle\phi|$ of a ket and a bra. This is an operator and not a scalar product because it changes one ket into another.

A **complete set of states** is obtained as the eigenstates of any Hermitian operator H,

$$H\,|\phi_a\rangle = a\,|\phi_a\rangle , \quad a = 1, \infty. \tag{B.4}$$

A **basis** is formed by a complete set such as ϕ_a. Any state can be expanded as a sum of the ϕ_a's:

$$|\psi\rangle = \sum\!\!\!\!\!\!\int_a c_a\,|\phi_a\rangle , \quad c_a = \langle\phi_a\,|\psi\rangle . \tag{B.5}$$

Here the sum is for discrete states and the integral is for continuum states. When integrating, there is a phase space factor, $\int \rightarrow \int d^3k/(2\pi)^3$. The quantity c_a is the probability amplitude for $|\psi\rangle$ to "contain" $|\phi_a\rangle$ or to be "at" a.

The **orthogonality relation** is

$$\langle\phi_a|\phi_{a'}\rangle = \begin{cases} \delta_{aa'}, & \text{discrete states,} \\ \delta(a-a')/\rho_a, & \text{continuum states.} \end{cases} \tag{B.6}$$

In (B.6) the ρ_a is the *density-of-states factor*:

$$\rho_a \stackrel{\text{def}}{=} \frac{dN}{da} = \begin{cases} 1, & \text{for } \phi_a = \exp(i\mathbf{k}\cdot\mathbf{r})/(2\pi)^{3/2}, \quad \text{(our choice),} \\ (2\pi)^{-3}, & \text{for } \phi_a = \exp(i\mathbf{k}\cdot\mathbf{r}), \quad \text{(others).} \end{cases} \tag{B.7}$$

The a **representation** of a state is the expansion of that state:

$$|\psi\rangle = \sum\!\!\!\!\!\!\int_a c_a\,|\phi_a\rangle, \quad c_a = \langle\phi_a|\psi\rangle. \tag{B.8}$$

The **completeness relation** follows from the preceding expansion,

$$|\psi\rangle = \sum\!\!\!\!\!\!\int_a c_a\,|\phi_a\rangle = \sum\!\!\!\!\!\!\int_a |\phi_a\rangle\langle\phi_a|\psi\rangle \tag{B.9}$$

$$\Rightarrow \quad \tilde{1} = \sum\!\!\!\!\!\!\int_a |\phi_a\rangle\langle\phi_a|, \tag{B.10}$$

where $\tilde{1}$ is the *unit operator*.

The **matrix representation** of an operator O in the a representation is the bracket $\langle a'|O|a\rangle$. By changing basis we change the representation of an operator:

$$\langle b'|O|b\rangle = \sum\!\!\!\!\!\!\int_{a'a} \langle b'|a'\rangle\langle a'|O|a\rangle\langle a|b\rangle. \tag{B.11}$$

The **complex conjugate** of a bracket can take different forms:

$$\langle\phi|O|\psi\rangle = \langle O^\dagger\phi|\psi\rangle = \langle\psi|O^\dagger\phi\rangle^* = \langle\psi|O^\dagger|\phi\rangle^*. \tag{B.12}$$

The **wave function** in Dirac notation is

$$\psi(\mathbf{r}) \equiv \langle\mathbf{r}|\psi\rangle, \tag{B.13}$$

which is just the probability amplitude for finding the state ψ at $\mathbf{r}$, that is, its projection onto the $\mathbf{r}$ basis (see too next section).

B.2 Explicit Representations

Examples of *explicit representations* include $|\mathbf{r}\rangle$, $|\mathbf{k}\rangle$, and $|klm\rangle$; that is, coordinate, momentum, and energy plus angular momentum space. These are developed in Chapters 5–8.

Coordinate Space

$$\langle \mathbf{r} | \psi \rangle \equiv \psi(\mathbf{r}) = \langle \psi | \mathbf{r} \rangle^* = \text{probability amplitude to be at } \mathbf{r} \tag{B.14}$$

$$\langle \mathbf{r} | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}') \tag{B.15}$$

$$\int d^3r \, |\mathbf{r}\rangle \langle \mathbf{r}| = \tilde{1} \Rightarrow |\psi\rangle = \int d^3r \, |\mathbf{r}\rangle \langle \mathbf{r} | \psi \rangle = \int d^3r \, \psi(\mathbf{r}) \, |\mathbf{r}\rangle \tag{B.16}$$

Momentum Space

$$|\phi_{\mathbf{k}}\rangle \equiv |\mathbf{k}\rangle = \text{plane wave ray} \tag{B.17}$$

$$\langle \mathbf{r} | \phi_{\mathbf{k}} \rangle \equiv \langle \mathbf{r} | \mathbf{k} \rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}}, \quad \langle \mathbf{k} | \mathbf{r} \rangle = \frac{e^{-i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}} \tag{B.18}$$

$$\langle \mathbf{k} | \mathbf{k}' \rangle = \langle \mathbf{k} | \phi_{\mathbf{k}'} \rangle = \langle \phi_{\mathbf{k}} | \phi_{\mathbf{k}'} \rangle = \delta(\mathbf{k}' - \mathbf{k}) \tag{B.19}$$

$$\tilde{1} = \int d^3k \, |\mathbf{k}\rangle \langle \mathbf{k}| \tag{B.20}$$

$$\psi(\mathbf{k}) \equiv \langle \mathbf{k} | \psi \rangle = \text{probability amplitude to contain } \mathbf{k} \tag{B.21}$$

Change of representations occur via insertion of completeness relations:

$$\psi(\mathbf{r}) = \langle \mathbf{r} | \psi \rangle = \int d^3k \, \langle \mathbf{r} | \mathbf{k} \rangle \langle \mathbf{k} | \psi \rangle = \int d^3k \, \langle \mathbf{r} | \mathbf{k} \rangle \, \psi(\mathbf{k}) \tag{B.22}$$

$$= \int d^3k \, \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}} \psi(\mathbf{k}) \tag{B.23}$$

$$\psi(\mathbf{k}) = \langle \mathbf{k} | \psi \rangle = \int d^3r \, \langle \mathbf{k} | \mathbf{r} \rangle \langle \mathbf{r} | \psi \rangle = \int d^3r \, \frac{e^{-i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}} \psi(\mathbf{r}) \tag{B.24}$$

$$\langle \mathbf{r} | klm \rangle \equiv \langle \mathbf{r} | \phi_{klm} \rangle = i^l \frac{F_l(kr)}{kr} Y_{lm}(\Omega_r) \tag{B.25}$$

$$\langle \mathbf{r} | \psi_{klm} \rangle = i^l \frac{u_l(kr)}{kr} Y_{lm}(\Omega_r) \tag{B.26}$$

$$\langle k'lm | \psi_k \rangle = \frac{(\pi/2)^{1/2} Y^*_{l,m}(\Omega_k)}{kk'} u_l(k'; E_k) \tag{B.27}$$

K and G Operators (Nonrelativistic)

$$\langle \mathbf{r}' | K | \mathbf{r} \rangle = \delta(\mathbf{r} - \mathbf{r}') \frac{-\nabla_r^2}{2\mu} \quad \text{(kinetic energy)} \tag{B.28}$$

$$\langle \mathbf{k}' | K | \mathbf{k} \rangle = \frac{\delta(\mathbf{k}' - \mathbf{k})}{2\mu} k^2 \tag{B.29}$$

$$\langle \mathbf{r}' | G_E^{(+)} | \mathbf{r} \rangle = \frac{-m}{2\pi} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \quad \text{(Green's function)} \tag{B.30}$$

$$\langle \mathbf{k}' | G_E | \mathbf{k} \rangle = \langle \mathbf{k}' | \frac{1}{E - K} | \mathbf{k} \rangle = \frac{\delta(\mathbf{k} - \mathbf{k}')}{E - k^2/2\mu} \tag{B.31}$$

$$\langle plm| G_E^{(+)} |p'l'm'\rangle = \frac{\pi}{2}\frac{\delta(p-p')}{p^2}\frac{\delta_{ll'}\delta_{mm'}}{E-E_p+i\epsilon} \tag{B.32}$$

$$g_l^{(+)}(r,r';E) = \frac{-2\mu}{k}F_l(kr_<)H_l^{(+)}(kr_>) \tag{B.33}$$

Scattering Amplitude and T Matrix

$$T_E(\mathbf{k}',\mathbf{k}) = \langle\phi_{\mathbf{k}'}|T_E|\phi_{\mathbf{k}}\rangle = \langle\phi_{\mathbf{k}'}|V|\psi_{\mathbf{k}}^{(+)}\rangle \tag{B.34}$$

$$f_E(\theta,\phi) = -4\pi^2\mu T_E(\mathbf{k}',\mathbf{k})\big|_{k'=k} = -4\pi^2\mu\langle\phi_{\mathbf{k}'}|V|\psi_{\mathbf{k}}^{(+)}\rangle\Big|_{k'=k} \tag{B.35}$$

Energy and Angular Momentum Basis

Plane Wave

$$\langle\mathbf{r}|\mathbf{k}\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi)^{3/2}} = \sum_{l=0}^{\infty} i^l j_l(kr)\frac{(2l+1)P_l(\cos\theta)}{(2\pi)^{3/2}} \tag{B.36}$$

$$\sum_{l,m} Y_{lm}^*(\Omega_k)Y_{lm}(\Omega_r)4\pi = \sum_l (2l+1)P_l(\cos\theta_{kr}) \tag{B.37}$$

Distorted Wave

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = \langle\mathbf{r}|\psi(\mathbf{r})\rangle = \sum_{l,m} i^l\frac{u_l(kr)}{kr}\frac{Y_{lm}^*(\Omega_k)Y_{lm}(\Omega_r)4\pi}{(2\pi)^{3/2}} \tag{B.38}$$

Angular Momentum and Energy Eigenstate

$$\phi_{klm}(\mathbf{r}) \equiv \langle\mathbf{r}|klm\rangle = i^l\frac{F_l(kr)}{kr}Y_{lm}(\Omega_r) \tag{B.39}$$

Free Waves

$$F_l(kr) \equiv krj_l(kr) = \begin{cases}\frac{(kr)^{l+1}}{1\cdot3\cdot5\cdots(2l+1)}, & \text{when } r\to 0\\ \sin(kr-l\pi/2), & \text{when } r\sim\infty\end{cases} \tag{B.40}$$

$$G_l(kr) \equiv -krn_l(kr) = \begin{cases}\frac{1\cdot3\cdot5\cdots(2l-1)}{(kr)^l}, & \text{when } r\to 0\\ \cos(kr-l\pi/2), & \text{when } r\sim\infty\end{cases} \tag{B.41}$$

Momentum Ket Expansion

$$|\mathbf{k}\rangle = \sqrt{\frac{2}{\pi}}\sum_{l,m} Y_{lm}^*(\Omega_k)\,|klm\rangle \tag{B.42}$$

Completeness Relation, Identity Operator

$$\tilde{1} = \frac{2}{\pi}\mathop{\sum\!\!\!\!\!\!\int}_{l,m} dk\,k^2\,|klm\rangle\langle klm| = \frac{2\mu}{\pi}\mathop{\sum\!\!\!\!\!\!\int}_{l,m} dE_k\,k\,|klm\rangle\langle klm| \tag{B.43}$$

T and V Matrix Expansions, p Space

$$\langle \mathbf{k}'| \begin{pmatrix} V \\ T \end{pmatrix} |\mathbf{k}\rangle = \frac{2}{\pi}\sum_{l,m} \begin{pmatrix} V_l(k',k) \\ T_l(k',k) \end{pmatrix} Y^*_{lm}(\Omega_{k'})Y_{lm}(\Omega_k) \tag{B.44}$$

$$= \frac{1}{2\pi^2}\sum_{l,m}(2l+1) \begin{pmatrix} V_l(k',k) \\ T_l(k',k) \end{pmatrix} P_l(\cos\theta_{kk'}) \tag{B.45}$$

Rotational Invariance

$$\langle k'l'm'| \begin{pmatrix} V \\ T \end{pmatrix} |klm\rangle = \delta_{ll'}\delta_{mm'} \begin{pmatrix} V_l(k',k) \\ T_l(k',k) \end{pmatrix} \tag{B.46}$$

T and V Matrix Expansions, r Space

$$\langle \mathbf{r}'| \begin{pmatrix} V \\ T \end{pmatrix} |\mathbf{r}\rangle = \sum_{l,m} \begin{pmatrix} V_l(r',r) \\ T_l(r',r) \end{pmatrix} Y^*_{lm}(\Omega_{r'})Y_{lm}(\Omega_r) \tag{B.47}$$

Local Potential

$$V_l(r',r) = \frac{\delta(r-r')}{r^2}V(r) \quad \text{(all } l\text{'s)} \tag{B.48}$$

Wave function Transform, Non-Local Potential

$$V_l(k',k) = \frac{1}{k'k}\int_0^\infty dr \int_0^\infty dr'\, rr' F_l(k'r')V_l(r',r)F_l(kr) \tag{B.49}$$

Wave function Transform, Local Potential

$$V_l(k',k) = \frac{1}{k'k}\int_0^\infty dr\, F_l(k'r)V(r)F_l(kr) \tag{B.50}$$

T matrix

$$T_l(k',k;E_k) = \frac{1}{k'k}\int_0^\infty dr \int_0^\infty dr'\, rr' F_l(k'r')V_l(r',r)u_l(kr) \tag{B.51}$$

On-Energy-Shell Values

$$T_l(k,k;E_k) = -\frac{e^{2i\delta_l}-1}{2i\rho_T} = \frac{R_l}{1+i\rho_T R_l} \tag{B.52}$$

$$R_l(k,k;E_k) = -\frac{\tan\delta_l(k)}{\rho_T}, \quad \rho_T = 2\mu k \tag{B.53}$$

$$S_l(E[k]) = e^{2i\delta_l} \quad \text{(only defined on shell)} \tag{B.54}$$

Scattering Amplitude

$$f_E(\theta,\phi) = -4\pi^2\mu\,\langle \mathbf{k}'|\,T_E\,|\mathbf{k}\rangle\,|_{k'=k=k_0} \tag{B.55}$$

$$= \sum_l (2l+1)\frac{e^{2i\delta_l}-1}{2ik}P_l(\cos\theta_{kk'}) \tag{B.56}$$

One-Dimensional Integral Equations

$$u_l(kr) = F_l(kr) + 2\mu \int_0^\infty dr'\, F_l(kr_<) H_l^{(+)}(kr_>) V(r') u_l(kr') \quad \text{(B.57)}$$

$$u_l(k'; E_k) = \delta(k' - k) + \frac{2k' \int_0^\infty dp\, p V_l(k', p) u_l(p; E_k)}{\pi(E_k - E_{k'} + i\epsilon)} \quad \text{(B.58)}$$

$$T_l(k', k; E) = V_l(k', k) + \frac{2}{\pi} \int_0^\infty dp\, p^2 \frac{V_l(k', p) T_l(p, k)}{E + i\epsilon - E_p} \quad \text{(B.59)}$$

$$R_l(k', k) = V_l(k', k) + \frac{2}{\pi} \mathcal{P} \int_0^\infty dp\, p^2 \frac{V_l(k', p) R_l(p, k)}{E - E_p} \quad \text{(B.60)}$$