



TWO-STATE SYSTEMS

Introduction. Relative to some/any discretely indexed orthonormal basis $\{|n\rangle\}$ the abstract Schrödinger equation $\mathbf{H}|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle$ can be represented

$$\sum_n \langle m|\mathbf{H}|n\rangle\langle n|\psi\rangle = i\hbar\frac{\partial}{\partial t}\langle m|\psi\rangle$$

which can be notated
$$\sum_n H_{mn}\psi_n = i\hbar\frac{\partial}{\partial t}\psi_m$$

or again
$$\mathbb{H}|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle$$

We found it to be the fundamental commutation relation $[\mathbf{x}, \mathbf{p}] = i\hbar\mathbf{1}$ which forced the matrices/vectors thus encountered to be ∞ -dimensional. If we are willing

- to live without continuous spectra (therefore without \mathbf{x})
- to live without analogs/implications of the fundamental commutator

then it becomes possible to contemplate “toy quantum theories” in which all matrices/vectors are finite-dimensional. One loses some physics, it need hardly be said, but surprisingly much of genuine physical interest does survive. And one gains the advantage of sharpened analytical power: “finite-dimensional quantum mechanics” provides a methodological laboratory in which, not infrequently, the essentials of complicated computational procedures can be exposed with closed-form transparency. Finally, the toy theory serves to identify some unanticipated formal links—permitting ideas to flow back and forth—between quantum mechanics and other branches of physics.

Here we will carry the technique to the limit: we will look to “2-dimensional quantum mechanics.” The theory preserves the linearity that dominates the full-blown theory, and is of the least-possible size in which it is possible for the effects of non-commutivity to become manifest.

We have seen that quantum mechanics can be portrayed as a theory in which

- states are represented by self-adjoint linear operators ρ ;
- motion is generated by self-adjoint linear operators \mathbf{H} ;
- measurement devices are represented by self-adjoint linear operators \mathbf{A} .

In orthonormal representation those self-adjoint operators become Hermitian matrices

$$\mathbb{R} = \|(m|\rho|n)\|, \quad \mathbb{H} = \|(m|\mathbf{H}|n)\| \quad \text{and} \quad \mathbb{A} = \|(m|\mathbf{A}|n)\|$$

which in the toy theory become 2×2 . We begin, therefore, with review of the

Properties of 2x2 Hermitian matrices. The most general such matrix can be described¹

$$\mathbb{H} = \begin{pmatrix} h_0 + h_3 & h_1 - ih_2 \\ h_1 + ih_2 & h_0 - h_3 \end{pmatrix} \quad (1)$$

and contains a total of 4 adjustable real parameters. Evidently

$$\text{tr } \mathbb{H} = 2h_0 \quad \text{and} \quad \det \mathbb{H} = h_0^2 - h_1^2 - h_2^2 - h_3^2 \quad (2)$$

so we have

$$\begin{aligned} \det(\mathbb{H} - \lambda \mathbb{I}) &= \lambda^2 - 2h_0\lambda + (h_0^2 - h_1^2 - h_2^2 - h_3^2) \\ &= \lambda^2 - (\text{tr } \mathbb{H})\lambda + \det \mathbb{H} \end{aligned} \quad (3)$$

By the Cayley-Hamilton theorem

$$\mathbb{H}^2 - (\text{tr } \mathbb{H}) \cdot \mathbb{H} + (\det \mathbb{H}) \cdot \mathbb{I} = \mathbb{O} \quad (4)$$

from which it follows that

$$\begin{aligned} \mathbb{H}^{-1} &= (\det \mathbb{H})^{-1} [(\text{tr } \mathbb{H}) \cdot \mathbb{I} - \mathbb{H}] \\ &= (h_0^2 - h_1^2 - h_2^2 - h_3^2)^{-1} \begin{pmatrix} h_0 - h_3 & h_1 + ih_2 \\ h_1 - ih_2 & h_0 + h_3 \end{pmatrix} \end{aligned} \quad (5)$$

Returning to (1), we can write

$$\mathbb{H} = h_0\sigma_0 + h_1\sigma_1 + h_2\sigma_2 + h_3\sigma_3 \quad (6)$$

where $\sigma_0 \equiv \mathbb{I}$ and

$$\sigma_1 \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (7)$$

¹ Here \mathbb{H} is intended to evoke not Hamilton but Hermite . . . though, since we are developing what is in effect the theory of quaternions (the invention closest to Hamilton's heart), the former evocation would not be totally inappropriate.

are the familiar “Pauli matrices.” The linearly independent σ -matrices span the 4-dimensional real vector space of 2×2 Hermitian matrices \mathbb{H} , in which they comprise an algebraically convenient basis. Each of the three Pauli matrices is traceless, Hermitian and has $\det \sigma = -1$; their multiplicative properties can be summarized

$$\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = \mathbb{I} \quad (8.1)$$

$$\left. \begin{aligned} \sigma_1 \sigma_2 &= i \sigma_3 = -\sigma_2 \sigma_1 \\ \sigma_2 \sigma_3 &= i \sigma_1 = -\sigma_3 \sigma_2 \\ \sigma_3 \sigma_1 &= i \sigma_2 = -\sigma_1 \sigma_3 \end{aligned} \right\} \quad (8.2)$$

Equations (8) imply (and can be recovered from) the multiplication formula²

$$\begin{aligned} \mathbb{A}\mathbb{B} &= (a_0\sigma_0 + a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3)(b_0\sigma_0 + b_1\sigma_1 + b_2\sigma_2 + b_3\sigma_3) \\ &= (a_0b_0 + a_1b_1 + a_2b_2 + a_3b_3)\sigma_0 \\ &\quad + (a_0b_1 + a_1b_0 + ia_2b_3 - ia_3b_2)\sigma_1 \\ &\quad + (a_0b_2 + a_2b_0 + ia_3b_1 - ia_1b_3)\sigma_2 \\ &\quad + (a_0b_3 + a_3b_0 + ia_1b_2 - ia_2b_1)\sigma_3 \\ &= (a_0b_0 + \mathbf{a} \cdot \mathbf{b})\sigma_0 + (a_0\mathbf{b} + b_0\mathbf{a} + i\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma} \end{aligned} \quad (9)$$

If we agree to write

$$\left. \begin{aligned} \mathbb{A} &= a_0\sigma_0 + \mathbf{a} \cdot \boldsymbol{\sigma} \\ \bar{\mathbb{A}} &= a_0\sigma_0 - \mathbf{a} \cdot \boldsymbol{\sigma} \end{aligned} \right\} \quad (10)$$

then (9) supplies

$$\bar{\mathbb{A}}\mathbb{A} = (\det \mathbb{A})\mathbb{I} \quad (11)$$

Also

$$[\mathbb{A}, \mathbb{B}] = 2i(\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma} \quad (12)$$

which conforms to the general principle that

$$[\text{hermitian}, \text{hermitian}] = i(\text{hermitian}) = \text{antihermitian}$$

From (12) it becomes explicitly clear that/why

$$[\mathbb{X}, \mathbb{P}] = i\hbar\mathbb{I} \quad \text{is impossible}$$

and that \mathbb{A} and \mathbb{B} will commute if and only if $\mathbf{a} \sim \mathbf{b}$:

$$[\mathbb{A}, \mathbb{B}] = \mathbb{O} \quad \text{requires} \quad \mathbb{B} = \alpha\mathbb{A} + \beta\mathbb{I} \quad (13)$$

² This is the formula that had Hamilton so excited, and which inspired Gibbs to say “Let’s just define the \cdot and \times products, and be done with it!” Whence the 3-vector algebra of the elementary physics books.

Looking back again to (3), we see that

$$\text{if } \mathbb{H} \text{ is traceless } (h_0 = 0) \text{ then } \det \mathbb{H} = -\mathbf{h} \cdot \mathbf{h}$$

If, moreover, \mathbf{h} is a unit vector ($\mathbf{h} \cdot \mathbf{h} = 1$) then $\det(\mathbb{H} - \lambda \mathbb{I}) = \lambda^2 - 1 = 0$. The eigenvalues of such a matrix are ± 1 . In particular, the eigenvalues of each of the three Pauli matrices are ± 1 . The eigenvalues of \mathbb{H} in the *general* case (1) are

$$h_{\pm} = (h_0 \pm h) \quad (14)$$

$$h \equiv \sqrt{\mathbf{h} \cdot \mathbf{h}} = (h_1^2 + h_2^2 + h_3^2)^{\frac{1}{2}} \geq 0$$

Evidently *spectral degeneracy* requires $\mathbf{h} \cdot \mathbf{h} = 0$, so occurs only in the cases $\mathbb{H} \sim \mathbb{I}$.

To simplify discussion of the associated eigenvectors we write $\mathbb{H} = h_0 \mathbb{I} + \mathbf{h}$ with $\mathbf{h} \equiv \mathbf{h} \cdot \boldsymbol{\sigma}$ and on the supposition that $\mathbf{h}|h_{\pm}\rangle = \pm h|h_{\pm}\rangle$ obtain

$$\mathbb{H}|h_{\pm}\rangle = (h_0 \pm h)|h_{\pm}\rangle$$

In short, the spectrum of \mathbb{H} is displaced relative to that of \mathbf{h} , but they share the same eigenvectors: the eigenvectors of \mathbb{H} must therefore be h_0 -independent, and could more easily be computed from \mathbf{h} . And for the purposes of that computation one can without loss of generality assume \mathbf{h} to be a unit vector, which proves convenient. We look, therefore, to the solution of

$$\begin{pmatrix} h_3 & h_1 - ih_2 \\ h_1 + ih_2 & h_3 \end{pmatrix} |h_{\pm}\rangle = \pm |h_{\pm}\rangle$$

and, on the assumption that $\mathbf{h} \cdot \mathbf{h} = 1$ and $1 \pm h_3 \neq 0$, readily obtain normalized eigenvectors

$$|h_{\pm}\rangle = \begin{pmatrix} \sqrt{\frac{1 \pm h_3}{2}} \\ \pm \sqrt{\frac{1}{2(1 \pm h_3)}} (h_1 + ih_2) \end{pmatrix} \cdot e^{i\alpha} \quad : \quad \alpha \text{ arbitrary} \quad (15.1)$$

To mechanize compliance with the condition $h_1^2 + h_2^2 = 1 - h_3^2$ let us write

$$h_1 = \sqrt{1 - h_3^2} \cos \phi$$

$$h_2 = \sqrt{1 - h_3^2} \sin \phi$$

We then have

$$|h_{\pm}\rangle = \begin{pmatrix} \sqrt{\frac{1 \pm h_3}{2}} \\ \pm \sqrt{\frac{1 \mp h_3}{2}} e^{i\phi} \end{pmatrix} \quad (15.2)$$

Finally we set $h_3 = \cos \theta$ and obtain³

$$|h_+\rangle = \begin{pmatrix} \cos \frac{1}{2}\theta \\ + \sin \frac{1}{2}\theta \cdot e^{i\phi} \end{pmatrix}, \quad |h_-\rangle = \begin{pmatrix} \sin \frac{1}{2}\theta \\ - \cos \frac{1}{2}\theta \cdot e^{i\phi} \end{pmatrix} \quad (15.3)$$

Our objective in the manipulations which led to (15.2)/(15.3) was to escape the force of the circumstance that (15.1) becomes meaningless when $1 \pm h_3 = 0$. Working now most directly from (15.2),⁴ we find

$$\begin{aligned} \sigma_1|1\pm\rangle &= \pm 1 \cdot |1\pm\rangle & \text{with } |1+\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ +1 \end{pmatrix}, & |1-\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \\ \sigma_2|2\pm\rangle &= \pm 1 \cdot |2\pm\rangle & \text{with } |2+\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ +i \end{pmatrix}, & |2-\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \\ \sigma_3|3\pm\rangle &= \pm 1 \cdot |3\pm\rangle & \text{with } |3+\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}, & |3-\rangle &= \begin{pmatrix} 0 \\ -1 \end{pmatrix} \end{aligned}$$

Observables. Let the Hermitian matrix

$$\begin{aligned} a_0 \mathbb{I} + \mathbf{a} \cdot \boldsymbol{\sigma} &\equiv \mathbb{A} & \text{represent an } A \text{-meter} \\ \hat{\mathbf{a}} \cdot \boldsymbol{\sigma} &\equiv \mathbb{A}_0 & \text{represent an } A_0\text{-meter} \end{aligned}$$

where $\hat{\mathbf{a}}$ is a unit vector, and where $\mathbf{a} = k\hat{\mathbf{a}}$. As we've seen, \mathbb{A}_0 and \mathbb{A} have share the same population of eigenvectors, but the spectrum of the latter is got by dilating/shifting the spectrum of the other:

$$\mathbb{A}_0|a\rangle = a|a\rangle \iff \mathbb{A}|a\rangle = (a_0 + ka)|a\rangle$$

To say the same thing in more physical terms: the A_0 -meter and the A -meter function identically, but the former is calibrated to read $a = \pm 1$, the latter to read $a_0 \pm k$. Both are “two-state devices.” In the interest of simplicity we agree henceforth to use only A_0 -meters, but to drop the decorative hat and $_0$, writing

$$\mathbb{A} = a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3 \quad \text{with } \mathbf{a} \text{ a unit vector}$$

We find ourselves now in position to associate

$$\boxed{A\text{-meters}} \longleftrightarrow \boxed{\text{points on unit sphere } a_1^2 + a_2^2 + a_3^2 = 1}$$

and from the spherical coordinates of such a point, as introduced by

$$\left. \begin{aligned} a_1 &= \sin \theta \cos \phi \\ a_2 &= \sin \theta \sin \phi \\ a_3 &= \cos \theta \end{aligned} \right\} \quad (16)$$

³ Compare Griffiths, p. 160, whose conventions I have contrived to mimic.

⁴ Set $h_0 = 0$ and $\mathbf{h} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, else $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, else $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.

to be able to read off, by (15.3), explicit descriptions of the output states $|a_{\pm}\rangle$ characteristic of the device. And, in terms of those states—as an instance of $\mathbf{A} = \int |a\rangle da$ (a —to have

$$\mathbb{A} = |a_+\rangle\langle a_+| - |a_-\rangle\langle a_-| \quad (17)$$

It is interesting to notice what has happened to the concept of “physical dimension.” We recognize a physical parameter t with the dimensionality of “time,” which we read from the “clock on the wall,” not from the printed output of a “meter” as here construed: *time we are prepared to place in a class by itself*. Turning to the things we measure with meters, we might be inclined to say that we are

- “measuring a variable with the dimension $[a]$ ” as a way of announcing our intention to use an A -meter;
- “measuring a variable with the dimension $[b]$ ” as a way of announcing our intention to use a B -meter; etc.

To adopt such practice would be to assign distinct physical dimension to every point on the \mathbf{a} -sphere. Which would be fine and natural if we possessed only a limited collection of meters.

Made attractive by the circumstance that they are *addressable* (if not, at the moment, by us) are some of the questions which now arise:

- Under what conditions (i.e., equipped with what minimal collection of meters $P, Q, R \dots$) does it become feasible for us to “play scientist”—to expect to find *reproducible functional relationships* $f_i(\bar{p}, \bar{q}, \bar{r}, \dots) = 0$ among the numbers produced by our experiments?
- Under what conditions does a “dimensional analysis” become available as a guide to the construction of such relationships?
- How—and with what guarantee of uniqueness—would you work backwards from the “classical” relationships $f_i(p, q, r, \dots) = 0$ I hand you (or that you deduce from experiment) to the quantum theory from which I obtained them?

We gain the impression that two-state theory might profitably be pressed into service as a LABORATORY FOR THE PHILOSOPHY OF SCIENCE, and are not surprised to learn that the laboratory has in fact had occasional users . . . though most of them (with names like Einstein, Pololsky, Rosen, Bell, . . .) have not been card-carrying philosophers.

The expected result of presenting a quantum system in (pure) state $|\psi\rangle$ to an A -meter can be represented

$$|\psi\rangle \longrightarrow \boxed{A\text{-meter}} \longrightarrow \begin{cases} |a_+\rangle & \text{with probability } |(a_+|\psi)|^2 \\ |a_-\rangle & \text{with probability } |(a_-|\psi)|^2 \end{cases}$$

The meter registers + or – to report which projection has, in the particular instance, actually taken place.

Suppose—downstream from the A -meter—we have installed an “ $|a_+$)-gate” which passes $|a_+$) states, but excludes $|a_-)$ states. And—downstream from the

gate—a B -meter. Activity of the latter can be represented

$$|a_+\rangle \longrightarrow \boxed{B\text{-meter}} \longrightarrow \begin{cases} |b_+\rangle & \text{with probability } |(b_+|a_+\rangle|^2 \\ |b_-\rangle & \text{with probability } |(b_-|a_+\rangle|^2 \end{cases}$$

The B -meter will act *disruptively* upon the $|a_+\rangle$ -state (the output of the gated A -meter) unless $|a_+\rangle$ —an eigenstate of \mathbb{A} —is an eigenstate also of \mathbb{B} (i.e., unless $|a_+\rangle = |b_+\rangle$ else $|b_-\rangle$). In the former case $\mathbf{b} = +\mathbf{a}$: the B -meter is in reality a second A -meter and, even if the gate were removed, would *always* replicate the result yielded by the first A -meter: *it is on those grounds alone that we can assert that the first meter actually measured something!* In the alternative case $\mathbf{b} = -\mathbf{a}$: the B -meter acts like an A -meter in which the read-out device has been cross-wired, so that $+$ reads $-$ and *vice versa*. In the former case $\mathbb{B} = \mathbb{A}$; in the latter case $\mathbb{B} = \mathbb{A}^{-1}$... in which regard it must be emphasized that \mathbb{A}^{-1} *does not act like an A -meter run backwards* (does not “un-project”).

Recent remarks can be further clarified if one retreats for a moment to general quantum theory ... where one encounters the

\mathbf{B} acts non-disruptively upon the states
output by \mathbf{A} if and only if $[\mathbf{A}, \mathbf{B}] = \mathbf{0}$

(though \mathbf{B} may be non-disruptive of a *subset* of the \mathbf{A} -states under weaker conditions). Looking back in this light to (12) we see that

$$[\mathbb{A}, \mathbb{B}] = \mathbb{O} \quad \text{requires} \quad \mathbf{a} \sim \mathbf{b}$$

Which if \mathbf{a} and \mathbf{b} are both unit vectors requires $\mathbf{b} = \pm \mathbf{a}$.

We recently had occasion to draw casually upon the concept of a “gate.” How do we construct/represent such a device, a “filter transparent to some specified state $|\gamma\rangle$ ”? Two (ultimately equivalent) procedures recommend themselves. If $|\gamma\rangle$ is represented

$$|\gamma\rangle = \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix}$$

then we have only to construct the projection operator $\mathbb{G} \equiv |\gamma\rangle\langle\gamma|$ —represented

$$\mathbb{G} \equiv |\gamma\rangle\langle\gamma| = \begin{pmatrix} \gamma_1\gamma_1^* & \gamma_1\gamma_2^* \\ \gamma_2\gamma_1^* & \gamma_2\gamma_2^* \end{pmatrix} \tag{18.1}$$

—to achieve the desired result, for clearly $\mathbb{G}|\gamma\rangle = |\gamma\rangle$. In some circumstances it is, however, convenient—drawing upon (15.3)—to use

$$\begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix} = \begin{pmatrix} \cos \frac{1}{2}\theta \\ \sin \frac{1}{2}\theta \cdot e^{i\phi} \end{pmatrix} e^{i\alpha}$$

to ascribe “spherical coordinates” (and an overall phase) to $|\gamma\rangle$, and to use those coordinates in (16) to construct a unit 3-vector \mathbf{g} . This we do because we know $\mathbb{H} = h_0\mathbb{I} + h\mathbf{g}\cdot\boldsymbol{\sigma}$ to be the Hermitian matrix which

assigns eigenvalue $h_0 + h$ to eigenvector $|\gamma\rangle$
 assigns eigenvalue $h_0 - h$ to eigenvector $|\gamma\rangle_\perp$

and which *annihilates* $|\gamma\rangle_\perp$ if $h_0 - h = 0$. Setting $h_0 = h = \frac{1}{2}$ we are led to the representation

$$\mathbb{G} = \frac{1}{2}(\mathbb{I} + \mathbf{g}\cdot\boldsymbol{\sigma}) = \frac{1}{2} \begin{pmatrix} 1 + g_3 & g_1 - ig_2 \\ g_1 + ig_2 & 1 - g_3 \end{pmatrix} \quad (18.2)$$

which does not much resemble (18.1), but can be shown to be equivalent . . . to one another and to the “spectral representation”

$$\mathbb{G} = |\gamma\rangle \cdot 1 \cdot \langle\gamma| + |\gamma\rangle_\perp \cdot 0 \cdot \langle\gamma|_\perp$$

I end this discussion with a question, which I must, for the moment, be content to leave hanging in the air: How does one represent a measuring device of *imperfect resolution*?

Equivalent mixtures. To describe a statistical mixture of states $|u\rangle$, $|v\rangle$ and $|w\rangle$ ⁵ we write $\boldsymbol{\rho} = |u\rangle p_u \langle u| + |v\rangle p_v \langle v| + |w\rangle p_w \langle w|$, represented

$$\mathbb{R} = |u\rangle p_u \langle u| + |v\rangle p_v \langle v| + |w\rangle p_w \langle w| \quad (19.1)$$

with $p_u + p_v + p_w = 1$. The 2×2 matrix \mathbb{R} is Hermitian, therefore possesses real eigenvalues r_1, r_2 and orthonormal eigenvectors $|r_1\rangle, |r_2\rangle$ in terms of which it can be displayed

$$\mathbb{R} = |r_1\rangle r_1 \langle r_1| + |r_2\rangle r_2 \langle r_2| \quad (19.2)$$

with $\text{tr}\mathbb{R} = r_1 + r_2 = p_u + p_v + p_w = 1$. We may consider (19.2) to describe a mixture of states—and “eigenmixture” distinct from but equivalent to the original mixture. The right sides of (19) express a “distinction without a difference:” \mathbb{R} (rather: the $\boldsymbol{\rho}$ which it represents) is the object of physical significance, and its display as a “mixture” is, to a large degree, arbitrary.

From this fundamental fact arises a technical problem: *Describe the set of equivalent mixtures.* This is a problem which, in two-state theory, admits of illuminating geometrical solution, which I now describe.⁶

⁵ I mix *three* states to emphasize that no orthogonality assumption has been made. You may consider any number of arbitrarily selected additional states to be present in the mixture with (in this case) zero probability.

⁶ It was at 2:55 p.m. on 5 May 1998, as a senior oral on which we both sat was breaking up, that I posed the problem to Tom Wieting. He instantly outlined the argument I am about to present, and by 5:00 p.m., when we emerged from our next orals, he had ironed out all the wrinkles and written a sketch.

We have learned to associate unit complex 2-vectors $|a\rangle$ with unit real 2-vectors \mathbf{a} , and in terms of the latter to describe the matrix

$$|a\rangle\langle a| = \frac{1}{2}\{\mathbb{I} + \mathbf{a}\cdot\boldsymbol{\sigma}\} \quad (20)$$

which projects onto $|a\rangle$. We are in position, therefore, to associate the right side of (19.1) with a trio of weighted points

point \mathbf{u} with weight p_u
 point \mathbf{v} with weight p_v
 point \mathbf{w} with weight p_w

marked on the surface of the 3-ball. Bringing (20) to (19.1) we have

$$\begin{aligned} \mathbb{R} &= \frac{1}{2}\{(p_u + p_v + p_w)\mathbb{I} + (p_u\mathbf{u} + p_v\mathbf{v} + p_w\mathbf{w})\cdot\boldsymbol{\sigma}\} \\ &= \frac{1}{2}\{\mathbb{I} + \mathbf{r}\cdot\boldsymbol{\sigma}\} \\ \mathbf{r} &\equiv p_u\mathbf{u} + p_v\mathbf{v} + p_w\mathbf{w} = r\hat{\mathbf{r}} \end{aligned} \quad (21)$$

Introducing r_1 and r_2 by

$$\left. \begin{array}{l} r_1 + r_2 = 1 \\ r_1 - r_2 = r \end{array} \right\} \implies \left\{ \begin{array}{l} r_1 = \frac{1}{2}(1 + r) \\ r_2 = \frac{1}{2}(1 - r) \end{array} \right.$$

we have

$$\begin{aligned} \mathbb{R} &= r_1 \cdot \frac{1}{2}\{\mathbb{I} + \hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\} + r_2 \cdot \frac{1}{2}\{\mathbb{I} - \hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\} \\ &= \text{weighted sum of } \textit{orthogonal} \text{ projection matrices} \end{aligned} \quad (22)$$

If $\mathbb{P}_+ \equiv \frac{1}{2}\{\mathbb{I} + \hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\}$ projects onto $|r_1\rangle$ then \mathbb{P}_- projects onto $|r_2\rangle \equiv |r_1\rangle_{\perp}$, the orthogonal complement of $|r_1\rangle$: in (22) we have recovered precisely (19.2).

We are brought thus to the conclusion that density matrices $\mathbb{R}, \mathbb{R}', \mathbb{R}'', \dots$ describe physically indistinguishable equivalent mixtures if and only if, when written in the form (21), they share the same “center of mass” vector $\mathbf{r} = \sum p_i \hat{\mathbf{r}}_i$. And to help us comprehend the meaning of membership in the equivalence set $\{\mathbb{R}, \mathbb{R}', \mathbb{R}'', \dots\}$ we have now this geometrical imagery: take a string of unit length, attach one end to the origin, the other end to a point \mathbf{r} ($r \leq 1$) and think of the class of “string curves” $\mathbf{0} \rightarrow \mathbf{r}$. To each corresponds an \mathbb{R} . Obviously $\{\mathbb{R}, \mathbb{R}', \mathbb{R}'', \dots\}$ contains only a single element if $r = 1$, and—in some difficult-to-quantify sense contains increasing more elements as r becomes smaller.

Though some celebrated physicists have been known to assert (mistakenly) the uniqueness of quantum mixtures, modern authors—if they mention the point at all—tend to have it right,⁷ but to remain unaware of Wieting’s pretty

⁷ See L. E. Ballentine, *Quantum Mechanics* (1990), §2–3; K. Blum, *Density Matrix Theory and Applications* (2nd edition 1996), p. 16.

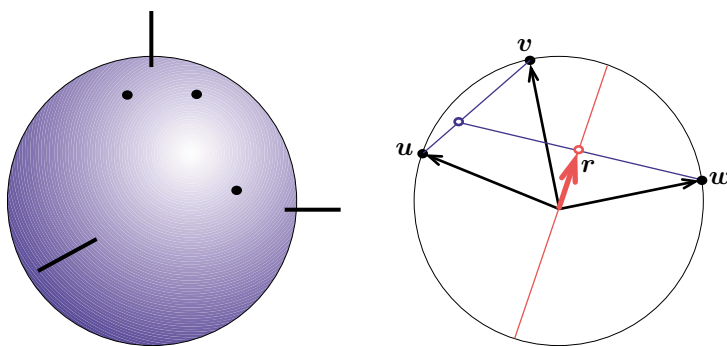


FIGURE 1: At left, three weighted points on the unit 3-ball represent a mixture of three quantum states. On the right a dimension has been discarded: the unit 3-ball has become the unit circle, on which weighted points $\{\mathbf{u}, \mathbf{v}, \mathbf{w}\}$ are deposited. Constructions indicate how one might compute the center of mass of $\{\mathbf{u}, \mathbf{v}\}$, then of $\{\mathbf{u}, \mathbf{v}, \mathbf{w}\}$ to determine finally the location of the \mathbf{r} which enters into the “eigenrepresentation” (21) of the mixture. The figure illustrates the procedure—due to Wieting—that takes one from (19.1) to (22).

demonstration of the point. Thus far, neither Weiting nor I have been able to discover, for ourselves or in the literature, a generalized construction that extends to N -state systems with $N > 2$.

It becomes fairly natural at this point to introduce a

$$\text{“degree of mixedness” } Q \equiv 1 - r = \begin{cases} 0 & \text{for pure states} \\ 1 & \text{for maximally mixed states} \end{cases}$$

This idea is (as will emerge) closely analogous to the “degree of polarization” introduced by George Stokes (and even more closely analogous to what might be called the “degree of depolarization”). But it proves to be often more useful to associate an “entropy” with quantum mixtures (as von Neumann was the first to do), writing

$$\text{“entropy” } S \equiv -r_1 \log r_1 - r_2 \log r_2 \quad (23.1)$$

Using $\lim_{x \downarrow 0} x \log x = \lim_{x \uparrow 1} x \log x = 0$ we have

$$S = \begin{cases} 0 & \text{for pure states} \\ \log 2 & \text{for maximally mixed states} \end{cases}$$

It is fairly easy to show, as a general proposition, that if \mathbb{P} is a projection matrix then

$$\log(\alpha \mathbb{I} + \beta \mathbb{P}) = (\log \alpha) \cdot \mathbb{I} + (1 + \beta/\alpha) \cdot \mathbb{P}$$

and, on this basis, that (working from (21)) it makes sense to write⁸

$$\begin{aligned} S &= -\text{tr}\{\mathbb{R} \log \mathbb{R}\} \\ &= -\text{tr}\{\boldsymbol{\rho} \log \boldsymbol{\rho}\} \text{ more abstractly/generally} \end{aligned} \quad (23.2)$$

Measurement on mixtures, with devices of imperfect resolution. When a mixture

$$\mathbb{R}_{\text{in}} = |r_1\rangle r_1 \langle r_1| + |r_2\rangle r_2 \langle r_2|$$

is presented to an *ideal* device

$$\mathbb{A} = |a_1\rangle a_1 \langle a_1| + |a_2\rangle a_2 \langle a_2|$$

the output (displayed as a density matrix) will be the

$$\begin{aligned} &\text{pure state } |a_1\rangle \langle a_1| \text{ with probability } \langle a_1 | \mathbb{R}_{\text{in}} | a_1 \rangle = \text{tr}\{|a_1\rangle \langle a_1 | \mathbb{R}_{\text{in}}\} \\ &\text{pure state } |a_2\rangle \langle a_2| \text{ with probability } \langle a_2 | \mathbb{R}_{\text{in}} | a_2 \rangle = \text{tr}\{|a_2\rangle \langle a_2 | \mathbb{R}_{\text{in}}\} \end{aligned}$$

but one will not know *which* was, in that event, the case until after the meter has been read.⁹ The entropy of the mixture representative of the system \mathfrak{S} has (unless the system was already in a pure state) decreased (the mixture has become “less disordered”), from

$$-r_1 \log r_1 - r_2 \log r_2 \quad \longrightarrow \quad 0$$

... which we interpret to mean that, by that individual act of measurement, we have

$$\text{gained “information”} = -r_1 \log r_1 - r_2 \log r_2$$

Let us, as at (21), again write

$$\mathbb{R}_{\text{in}} = \frac{1}{2} \{ \mathbb{I} + r_1 \boldsymbol{\sigma}_1 + r_2 \boldsymbol{\sigma}_2 + r_3 \boldsymbol{\sigma}_3 \}$$

to describe the pre-measurement state of \mathfrak{S} . By any of a variety of appropriately contrived *sequences* of measurements one can discover the values of r_1, r_2, r_3 . I describe what is certainly the simplest such procedure: the Hermitian matrices $\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3$ are, by quick implication of (7) and (8), *tracewise orthogonal* and individually traceless:

$$\text{tr } \boldsymbol{\sigma}_i \boldsymbol{\sigma}_j = 2 \delta_{ij} \quad \text{and} \quad \text{tr } \boldsymbol{\sigma}_i = 0 \quad (24)$$

⁸ See p. 57 in “Ellipsometry: Stokes’ parameters & related constructs in optics & classical/quantum mechanics” (1999).

⁹ The number $\langle \mathbf{A} \rangle = \text{tr } \mathbb{A} \mathbb{R}$ refers to the *average* of the meter readings obtained in a long experimental run.

Look upon the σ matrices as representatives of “Pauli meters” (which come in three different flavors), and observe that

$$s_i \equiv \langle \sigma_i \rangle = \text{tr}\{\sigma_i \mathbb{R}\} = r_i \quad (25)$$

We can, in particular, look to

$$s^2 \equiv s_1^2 + s_2^2 + s_3^2 \leq 1 \quad (26)$$

to discover whether or not \mathfrak{S} was in a pure state.

Suppose it were, and that had resurrected (from (15.3)) a former notation

$$|\psi\rangle = \begin{pmatrix} \cos \frac{1}{2}\theta \\ \sin \frac{1}{2}\theta \cdot e^{i\phi} \end{pmatrix} \quad (27)$$

to describe that state. We would then have

$$\left. \begin{aligned} s_1 &= \langle \psi | \sigma_1 | \psi \rangle = \sin \theta \cos \phi \\ s_2 &= \langle \psi | \sigma_2 | \psi \rangle = \sin \theta \sin \phi \\ s_3 &= \langle \psi | \sigma_3 | \psi \rangle = \cos \theta \end{aligned} \right\} \quad (28.1)$$

which are familiar from (16), and which in the impure case are replaced by

$$\left. \begin{aligned} s_1 &= s \sin \theta \cos \phi \\ s_2 &= s \sin \theta \sin \phi \\ s_3 &= s \cos \theta \end{aligned} \quad : \quad 0 \leq s \leq 1 \right\} \quad (28.2)$$

We are doing 2-state quantum mechanics, but have at this point reproduced the essentials of pretty mathematics introduced into the *theory of polarized light beams* by Stokes (1852), Poincaré (1892), Clark Jones (1941) and others.¹⁰

Consider now the action of an *imperfect* measurement device—a device with the property that its output remains to some degree uncertain. We may be tempted to say of the output that it is a “statistical distribution” of states (as might be described by positing some distribution function on the surface of the 3-ball), but the phrase conveys a more detailed meaning that we can justify (“misplaced concreteness” again): we can assert that the device delivers a mixed state, but not how that mixture has been concocted.

I propose—tentatively, in the absence (so far as I am aware) of any well established theory—to model imperfect *A*-meters as otherwise “perfect” meters speak with fuzzy imprecision: when

$$\mathbf{A} = \int |a\rangle da \langle a| \quad : \quad \text{imperfect}$$

¹⁰ See E. Hecht, *Optics* (2nd edition 1990), §8.12; C. Brosseau, *Fundamentals of Polarized Light: A Statistical Optics Approach* (1998) or ELECTRODYNAMICS (1980), pp. 344–370 for details.

looks at ρ_{in} and announces “ a_0 ” it signifies that it has constructed not the pure state $\rho_{\text{out}} = |a_0\rangle\langle a_0|$ characteristic of a perfect meter, but an a_0 -centered *mixed* state . . . something like

$$\rho_{\text{out}}(a_0) = \int |a\rangle p(a_0; a) da \quad |a\rangle \quad \text{with} \quad \langle a\rangle = \int p(a_0; a) a da = a_0 \quad (29)$$

Formally, by this account, the action of an imperfect device is nearly but not quite that of a projection operator, and \mathbf{A} by itself provides only a partial characterization of the device: full description of an imperfect A -meter requires presentation of the duplex data $\{\mathbf{A}; p(a_0, a)\}$.¹¹

The probability that an imperfect A -meter will, upon examination of ρ_{in} , announce “ a_0 ” is (we postulate) given by

$$P(a_0) = Z^{-1} \cdot \int (a|\rho_{\text{in}}|a) p(a_0; a) da = \text{tr}\{\rho_{\text{in}} \rho_{\text{out}}(a_0)\} \quad (30.1)$$

where

$$Z = Z(\rho_{\text{in}}) \equiv \int \text{tr}\{\rho_{\text{in}} \rho_{\text{out}}(a_0)\} da_0 \quad (30.2)$$

is a normalization factor, introduced to insure that $\int P(a_0) da_0 = 1$. For perfect meters the statements (30) assume the simpler form

$$\left. \begin{aligned} P(a_0) &= Z^{-1} \cdot (a_0|\rho_{\text{in}}|a_0) \\ Z &= Z(\rho_{\text{in}}) = 1 \quad : \quad (\text{all } \rho_{\text{in}}) \end{aligned} \right\} \quad (31)$$

If we use a perfect device then we find that prompt remeasurement after a measurement has yielded a_0 will again yield a_0 with certainty. Not so if we are less well equipped, for prompt remeasurement after our device has yielded a_0 will yield a_1 with conditional probability

$$\begin{aligned} P(a_0; a_1) &= Z^{-1} \cdot \int (a|\rho_{\text{out}}(a_0)|a) p(a_1; a) da = Z^{-1} \text{tr}\{\rho_{\text{out}}(a_0) \rho_{\text{out}}(a_1)\} \\ Z &= Z(\rho_{\text{out}}(a_0)) \end{aligned} \quad (32)$$

¹¹ It is perhaps most natural (but certainly not necessary) to assume

$$p(a_0; a) = \frac{1}{\epsilon\sqrt{2\pi}} \exp\left\{-\frac{1}{2}\left[\frac{a-a_0}{\epsilon}\right]^2\right\} \equiv g(a - a_0; \epsilon)$$

as was suggested on p. 51 of Chapter 0. In this instance $p(a; a_0)$ depends upon its arguments only through their difference, which we may expect to be a commonplace simplification. In any event, we expect to have

$$p(a_0; a) \longrightarrow \delta(a - a_0)$$

as instrumental precision is increased.

An imperfect instrument examines a mixture $\rho_{\text{in}} = \int |r\rangle p_r \langle r| dr$ with entropy

$$S_{\text{in}} \equiv S(\rho_{\text{in}}) = - \int p_r \log p_r dr \quad (33.1)$$

announces “ a_0 ,” and delivers the mixture (29), of which the entropy is

$$S_{\text{out}} \equiv S(\rho_{\text{out}}(a_0)) = - \int p(a_0; a) \log p(a_0; a) da \geq 0 \quad (33.2)$$

(with equality if and only if the instrument is in fact perfect). From

$$\text{information gained} = S_{\text{in}} - S_{\text{out}} \leq S_{\text{in}} \quad (34)$$

we see that the information gained by imperfect measurement is always less than would have been gained by perfect measurement. It is entirely possible for information to be *lost rather than gained*: in such cases we would have a “device” all right, but one hardly worthy of being called a “measuring device.”¹² If ρ_{in} referred in fact to a pure state (output of some prior perfect device), then measurement with an imperfect device *always serves to mess things up* (i.e., to produce mixtures of increased entropy, with negative information gain).

I suspect that one would be able to argue in quantitative detail to the effect that *all measurement devices are imperfect*. For example: one does not expect to be able to measure position with accuracy greater than $\Delta x \sim \hbar/mc$, where m is the mass of the least massive particle (electron?). Or angular momentum with accuracy much greater than $\Delta \ell \sim \hbar$. But I can cite no source in which such argument is undertaken with serious intent, and would be inclined to read with reservation any such paper not written by an experimentalist of the first rank.

Let’s look to see what the general theory sketched above has to say when applied to two-state systems. To describe ρ_{in} we have learned at (21/22) to write

$$\begin{aligned} \mathbb{R}_{\text{in}} &= \frac{1}{2} \{ \mathbb{I} + \mathbf{r} \cdot \boldsymbol{\sigma} \} \\ &= r_1 \cdot \frac{1}{2} \{ \mathbb{I} + \hat{\mathbf{r}} \cdot \boldsymbol{\sigma} \} + r_2 \cdot \frac{1}{2} \{ \mathbb{I} - \hat{\mathbf{r}} \cdot \boldsymbol{\sigma} \} \end{aligned} \quad (35)$$

A similar construction $\mathbb{A} = a_1 \cdot \frac{1}{2} \{ \mathbb{I} + \hat{\mathbf{a}} \cdot \boldsymbol{\sigma} \} + a_2 \cdot \frac{1}{2} \{ \mathbb{I} - \hat{\mathbf{a}} \cdot \boldsymbol{\sigma} \}$ is available to describe the Hermitian matrix representative of an ideal device, though in that context we can/will exercise the option to set $a_1 = +1$ and $a_2 = -1$, giving

$$\mathbb{A} = \hat{\mathbf{a}} \cdot \boldsymbol{\sigma} \quad (36)$$

¹² Optical depolarizers provide a case in point.

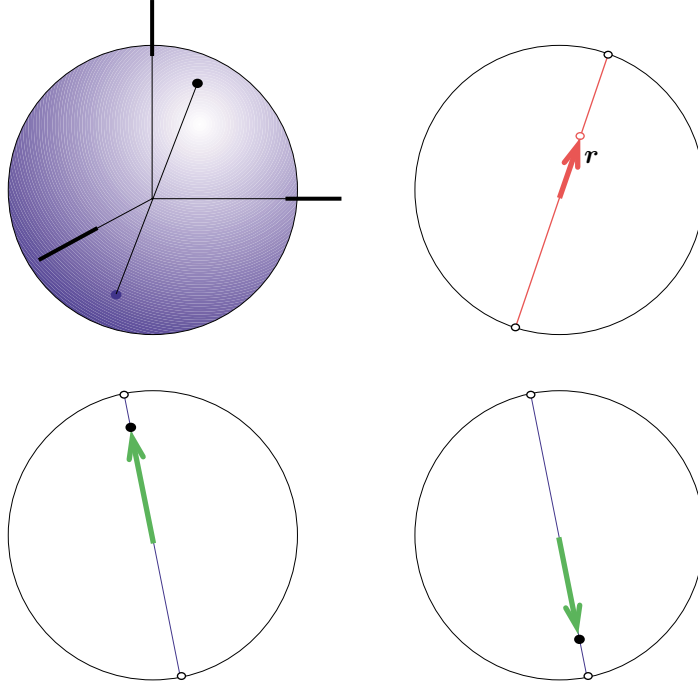


FIGURE 2: The figure at upper left stands as a reminder that the other figures refer to diametrically placed points on spheres, not circles. At upper right is a representation of the description (35) of the mixture \mathbb{R}_{in} to be examined by the imperfect device. When the device announces “ \pm ” it burps out the mixture (37) represented by the figure at lower left/right.

Those two ideas become fused when we undertake to describe $\rho_{\text{out}}(\pm)$:

$$\left. \begin{aligned} \mathbb{R}_{\text{out}}(+)&= p(+,+) \cdot \frac{1}{2}\{\mathbb{I} + \hat{\mathbf{a}} \cdot \boldsymbol{\sigma}\} + p(+,-) \cdot \frac{1}{2}\{\mathbb{I} - \hat{\mathbf{a}} \cdot \boldsymbol{\sigma}\} \\ &= \frac{1}{2}\{\mathbb{I} + \mathbf{a}_+ \cdot \boldsymbol{\sigma}\} \\ \mathbb{R}_{\text{out}}(-)&= p(-,+) \cdot \frac{1}{2}\{\mathbb{I} + \hat{\mathbf{a}} \cdot \boldsymbol{\sigma}\} + p(-,-) \cdot \frac{1}{2}\{\mathbb{I} - \hat{\mathbf{a}} \cdot \boldsymbol{\sigma}\} \\ &= \frac{1}{2}\{\mathbb{I} + \mathbf{a}_- \cdot \boldsymbol{\sigma}\} \end{aligned} \right\} \quad (37)$$

where $\mathbf{a}_+ \equiv [p(+,+) - p(+,-)]\hat{\mathbf{a}}$, and \mathbf{a}_- is defined similarly. If, in an effort to reduce notational clutter, we implement $p(\bullet,+) + p(\bullet,-) = 1$ by writing

$$\begin{aligned} p(+,+) &= 1 - \epsilon_+ & ; & & p(+,-) &= \epsilon_+ \\ p(-,+) &= \epsilon_- & ; & & p(-,-) &= 1 - \epsilon_- \end{aligned} \quad (38.1)$$

then (37) becomes

$$\begin{aligned} \mathbb{R}_{\text{out}}(+)&= \frac{1}{2}\{\mathbb{I} + (1 - 2\epsilon_+)\hat{\mathbf{a}} \cdot \boldsymbol{\sigma}\} \\ \mathbb{R}_{\text{out}}(-)&= \frac{1}{2}\{\mathbb{I} - (1 - 2\epsilon_-)\hat{\mathbf{a}} \cdot \boldsymbol{\sigma}\} \end{aligned} \quad (38.2)$$

The entropy of those mixtures is given by expressions of the form

$$\begin{aligned} S(\epsilon) &= -(1 - \epsilon) \log(1 - \epsilon) - \epsilon \log \epsilon \\ &= \epsilon(1 - \log \epsilon) - \frac{1}{2}\epsilon^2 + \dots \end{aligned}$$

and the mixtures become pure (operation of the instrument becomes perfect) as $\epsilon \downarrow 0$.

Presentation of \mathbb{R}_{in} to our imperfect device yields the response “ \pm ” with probabilities¹³

$$\begin{aligned} P(\pm) &= Z^{-1} \cdot \text{tr}\{\mathbb{R}_{\text{in}} \mathbb{R}_{\text{out}}(\pm)\} \\ &= Z^{-1} \cdot \frac{1}{2}(1 + \mathbf{r} \cdot \mathbf{a}_{\pm}) \end{aligned} \quad (39.1)$$

where $\mathbf{a}_+ \equiv +(1 - 2\epsilon_+)\hat{\mathbf{a}}$, $\mathbf{a}_- \equiv -(1 - 2\epsilon_-)\hat{\mathbf{a}}$ and

$$Z = 1 + \frac{1}{2}\mathbf{r} \cdot (\mathbf{a}_+ + \mathbf{a}_-) = 1 - (\epsilon_+ - \epsilon_-)\mathbf{r} \cdot \hat{\mathbf{a}} \quad (39.2)$$

Motivated again by a desire to reduce notational clutter, I restrict my attention henceforth to the case in which the device is of “symmetric design,” in the sense that $\epsilon_+ = \epsilon_- \equiv \epsilon$: then $\mathbf{a}_+ = -\mathbf{a}_- = \mathbf{a} \equiv (1 - 2\epsilon)\hat{\mathbf{a}}$ and $Z = 1$.

A “+” response is confirmed by prompt (but imperfect) remeasurement with probability

$$\begin{aligned} P(+, +) &= \text{tr}\{\mathbb{R}_{\text{out}}(+)\mathbb{R}_{\text{out}}(+)\} \\ &= \frac{1}{2}(1 + \mathbf{a} \cdot \mathbf{a}) \end{aligned} \quad (40.1)$$

and contradicted with probability

$$P(+, -) = \frac{1}{2}(1 - \mathbf{a} \cdot \mathbf{a}) \quad (40.2)$$

and the same can be said of $P(-, -)$ and $P(-, +)$. In ϵ -notation the preceding equations read

$$\left. \begin{aligned} P(+) &= \frac{1}{2}\{1 + (1 - 2\epsilon)\mathbf{r} \cdot \hat{\mathbf{a}}\} \\ P(+, +) &= \frac{1}{2}\{1 + (1 - 2\epsilon)^2\} \\ P(+, -) &= \frac{1}{2}\{1 - (1 - 2\epsilon)^2\} \\ \\ P(-) &= \frac{1}{2}\{1 - (1 - 2\epsilon)\mathbf{r} \cdot \hat{\mathbf{a}}\} \\ P(-, -) &= \frac{1}{2}\{1 + (1 - 2\epsilon)^2\} \\ P(-, +) &= \frac{1}{2}\{1 - (1 - 2\epsilon)^2\} \end{aligned} \right\} \quad (41)$$

¹³ See again (30). Essential use will be made here of the “traceless tracewise orthogonality” properties (24) of the σ -matrices.

In the special case $\epsilon = 0$ of an ideal instrument we on this basis have

$$\left. \begin{aligned} P(+) &= \frac{1}{2}\{1 + \mathbf{r} \cdot \hat{\mathbf{a}}\} \\ P(+, +) &= 1 \\ P(+, -) &= 0 \\ \\ P(-) &= \frac{1}{2}\{1 - \mathbf{r} \cdot \hat{\mathbf{a}}\} \\ P(-, -) &= 1 \\ P(-, +) &= 0 \end{aligned} \right\}$$

(confirmation is certain) while in the rather more interesting case of a “perfectly worthless instrument” ($\epsilon = \frac{1}{2}$) we have

$$\left. \begin{aligned} P(+) &= \frac{1}{2} \\ P(+, +) &= \frac{1}{2} \\ P(-, +) &= \frac{1}{2} \\ \\ P(-) &= \frac{1}{2} \\ P(-, -) &= \frac{1}{2} \\ P(+, -) &= \frac{1}{2} \end{aligned} \right\}$$

—irrespective of any/all properties of the state (mixture) being examined.

The discussion could be extended: one might inquire into the *moments* of imperfectly measure data, the *correlations* that arise when a second imperfect device B is brought into play ...but this is not the place. While the little “theory of imperfect measurement” sketched above might (in my view) be held to be intuitively/formally quite satisfying, I must stress that the question *Does it conform to the observed facts of the matter?* remains open. We have interest, therefore, in the results of experiments designed to expose its defects (if any). The main purpose of the discussion was to underscore the proposition that the proper formal repository for the concept of “quantum state” is (not $|\psi\rangle$) but ρ ...and that it is a meaningless frivolity to ask for the “identities of the states present in a mixture:” no specific answer to the latter question is objectively defensible, and none is needed to do practical computation.

Dynamics of two-state systems. I have recently had occasion to speak of *prompt* remeasurement, where “prompt” means “before the system has had an opportunity to move dynamically away from its measured state.” I turn now from the projective/irreversible state-adjustments we call “measurements” to the Hamiltonian-driven unitary (and therefore formally reversible) adjustments which we imagine to be taking place *between* observations.

Assume the Hamiltonian to be time-independent. We then have

$$|\psi\rangle_0 \longrightarrow |\psi\rangle_t = \mathbf{U}(t)|\psi\rangle_0 \quad \text{with} \quad \mathbf{U}(t) \equiv \exp\left\{-\frac{i}{\hbar}\mathbf{H}t\right\} \quad (42)$$

or again (and more generally)

$$\boldsymbol{\rho}_0 \longrightarrow \boldsymbol{\rho}_t = \mathbf{U}(t) \boldsymbol{\rho}_0 \mathbf{U}^{-1}(t) \quad (43)$$

In orthonormal representation the propagator $\mathbf{U}(t)$ becomes a unitary matrix

$$\mathbf{U}(t) = \exp \left\{ -\frac{i}{\hbar} \mathbb{H} t \right\} \quad (44)$$

which in two-state theory is 2×2 . The Hermitian Hamiltonian matrix can be described (see again (6))

$$\mathbb{H} = h_0 \boldsymbol{\sigma}_0 + h_1 \boldsymbol{\sigma}_1 + h_2 \boldsymbol{\sigma}_2 + h_3 \boldsymbol{\sigma}_3 = \hbar(\omega_0 \mathbb{I} + \boldsymbol{\omega} \hat{\mathbf{h}} \cdot \boldsymbol{\sigma}) \quad (45)$$

and (see again (14)) has eigenvalues

$$E_{\pm} = \hbar(\omega_0 \pm \omega) \quad (46)$$

Writing

$$\mathbf{U}(t) = e^{-i\omega_0 t} \cdot \mathbb{S}(t) \quad \text{with} \quad \mathbb{S}(t) \equiv \exp \left\{ -i\boldsymbol{\omega} \mathbf{h} t \right\} \quad (47)$$

$$\mathbf{h} \equiv \hat{\mathbf{h}} \cdot \boldsymbol{\sigma}$$

we observe¹⁴ that, because \mathbf{h} is traceless, $\mathbb{S}(t)$ is unimodular: $\det \mathbb{S}(t) = 1$. And because, by (2) and (4), $\det \mathbf{h} = -1$ we have $\mathbf{h}^2 = \mathbb{I}$. Therefore

$$\begin{aligned} \mathbb{S}(t) &= \cosh(-i\boldsymbol{\omega} t) \cdot \mathbb{I} + \sinh(-i\boldsymbol{\omega} t) \cdot \mathbf{h} \\ &= \cos \boldsymbol{\omega} t \cdot \mathbb{I} - i \sin \boldsymbol{\omega} t \cdot \mathbf{h} \end{aligned} \quad (48)$$

whence finally

$$\mathbf{U}(t) = e^{-i\omega_0 t} \left\{ \cos \boldsymbol{\omega} t \cdot \mathbb{I} - i \sin \boldsymbol{\omega} t \cdot \mathbf{h} \right\} \quad (49)$$

So the description of $|\psi\rangle_t = \mathbf{U}(t)|\psi\rangle_0$ has been reduced to a matter of simple matrix multiplication, and becomes even simpler if one works in terms of the energy eigenbasis, defined

$$\mathbb{H} |\pm\rangle = \hbar(\omega_0 \pm \omega) |\pm\rangle \quad (50)$$

For then

$$\begin{aligned} |\psi\rangle_0 &= |+\rangle \langle + | \psi \rangle_0 + |-\rangle \langle - | \psi \rangle_0 \\ &\downarrow \\ |\psi\rangle_t &= |+\rangle e^{-i(\omega_0 + \omega)t} \langle + | \psi \rangle_0 + |-\rangle e^{-i(\omega_0 - \omega)t} \langle - | \psi \rangle_0 \end{aligned} \quad (51)$$

The $|+\rangle$ and $|-\rangle$ components of $|\psi\rangle_0$ simply “buzz,” each with its own frequency.

¹⁴ Use $\det \mathbb{M} = e^{\text{tr} \log \mathbb{M}}$.

But it is perhaps more illuminating—certainly more comprehensive—to look to the motion of

$$\mathbb{R}_t = \frac{1}{2} \{ \mathbb{I} + \mathbf{r}(t) \cdot \boldsymbol{\sigma} \} \quad (52)$$

to which, we notice, ω_0 makes no contribution. The problem before us is to extract useful information from

$$\begin{aligned} \mathbb{R}_t &= \mathbb{S}(t) \mathbb{R}_0 \mathbb{S}^{-1}(t) \\ &= \{ \cos \omega t \cdot \mathbb{I} - i \sin \omega t \cdot \hat{\mathbf{h}} \} \frac{1}{2} \{ \mathbb{I} + \mathbf{r}(0) \cdot \boldsymbol{\sigma} \} \{ \cos \omega t \cdot \mathbb{I} + i \sin \omega t \cdot \hat{\mathbf{h}} \} \end{aligned} \quad (53)$$

There are many ways to proceed. We might proceed from the observation that when t is small the preceding equation reads (if we allow ourselves temporary liberty to write \mathbf{r} for $\mathbf{r}(0)$)

$$\mathbb{R}_\tau = \mathbb{R}_0 - \frac{1}{2} i \omega \tau [\hat{\mathbf{h}} \cdot \boldsymbol{\sigma}, \mathbf{r} \cdot \boldsymbol{\sigma}] + \dots$$

By (12) $[\hat{\mathbf{h}} \cdot \boldsymbol{\sigma}, \mathbf{r} \cdot \boldsymbol{\sigma}] = 2i(\hat{\mathbf{h}} \times \mathbf{r}) \cdot \boldsymbol{\sigma}$ so we have

$$\mathbb{R}_\tau = \mathbb{R}_0 + \omega \tau (\hat{\mathbf{h}} \times \mathbf{r}) \cdot \boldsymbol{\sigma} + \dots$$

which can be expressed

$$\mathbf{r}(\tau) = \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + 2\omega\tau \begin{pmatrix} 0 & -\hat{h}_3 & \hat{h}_2 \\ \hat{h}_3 & 0 & -\hat{h}_1 \\ -\hat{h}_2 & \hat{h}_1 & 0 \end{pmatrix} + \dots \right\} \mathbf{r}(0)$$

and clearly speaks of rotation about the $\hat{\mathbf{h}}$ -axis, through the doubled angle $2\omega\tau$. Iteration leads to

$$\begin{aligned} \mathbb{U}(t) &= e^{-i\omega_0 t} \cdot \exp \left\{ -i\omega t \begin{pmatrix} \hat{h}_3 & \hat{h}_1 - i\hat{h}_2 \\ \hat{h}_1 + i\hat{h}_2 & -\hat{h}_3 \end{pmatrix} \right\} \\ &\quad \downarrow \\ &\exp \left\{ 2\omega t \begin{pmatrix} 0 & -\hat{h}_3 & \hat{h}_2 \\ \hat{h}_3 & 0 & -\hat{h}_1 \\ -\hat{h}_2 & \hat{h}_1 & 0 \end{pmatrix} \right\} \end{aligned} \quad (54)$$

where the 2×2 top matrix either hits $|\psi\rangle$ (pure case) or wraps around \mathbb{R} , while the 3×3 bottom matrix hits \mathbf{r} (either case) to achieve the same effect. The top matrix is unitary ... the bottom matrix rotational. Alternatively, we might—having resolved \mathbf{r} into components parallel/perpendicular to $\hat{\mathbf{h}}$

$$\mathbf{r} = \mathbf{r}_\parallel + \mathbf{r}_\perp \quad \text{with} \quad \begin{cases} \mathbf{r}_\parallel = (\mathbf{r} \cdot \hat{\mathbf{h}}) \hat{\mathbf{h}} \\ \mathbf{r}_\perp = \mathbf{r} - \mathbf{r}_\parallel \end{cases}$$

—write

$$\mathbb{R} = \mathbb{R}_\parallel + \mathbb{R}_\perp \quad \text{with} \quad \begin{cases} \mathbb{R}_\parallel = \frac{1}{2} (\mathbb{I} + \mathbf{r}_\parallel \cdot \boldsymbol{\sigma}) \\ \mathbb{R}_\perp = \frac{1}{2} (\mathbb{I} + \mathbf{r}_\perp \cdot \boldsymbol{\sigma}) \end{cases}$$

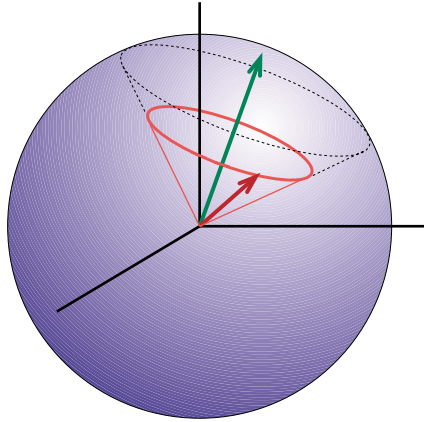


FIGURE 3: The long (green) arrow is set by the Hamiltonian, and points fore/aft to points representative of the energy eigenstates. The shorter (red) arrow describes the mixture (pure if the arrow is of unit length, otherwise an impure mixture of non-zero entropy), and twirls around the Hamiltonian axis with angular frequency 2ω .

and ask what $i\hbar\frac{d}{dt}\mathbb{R} = [\mathbb{H}, \mathbb{R}]$ says about the motion of \mathbb{R}_{\parallel} and \mathbb{R}_{\perp} . We are led promptly to the statements

$$\left. \begin{aligned} \frac{d}{dt}\mathbf{r}_{\parallel} &= \mathbf{0} \\ \frac{d}{dt}\mathbf{r}_{\perp} &= 2\omega\hat{\mathbf{h}} \times \mathbf{r}_{\perp} \end{aligned} \right\} \quad (55)$$

By either line of argument, we are led to the motion illustrated in the figure. Several points now merit comment:

The motion of $|\psi\rangle$ depends, according to (49), on ω_0 , but the motion of the density matrix—whether one works from (54) or from (55)—depends only on

$$\omega = \frac{1}{2\hbar}\{E_+ - E_-\} \sim \text{energy difference}$$

from which we infer that ω_0 is (at least in the absence of relativity/gravitation) not physically observable/meaningful. But this is hardly surprising, since in classical physics one can always assign any desired value to the energy reference level, and only energy differences matter. Let us agree henceforth to

$$\text{set } \omega_0 = 0$$

At time $t = \frac{1}{2}\tau = \pi/\omega$ the unitary matrix $\mathbb{U}(t)$ has, according to (49) (from which the unphysical $e^{i\omega_0 t}$ -factor has now been discarded), advanced through half a period, and we have $\mathbb{U}(\frac{1}{2}\tau) = -\mathbb{I}$: the original state vector has reappeared, but with reversed sign. The density matrix is, however, assembled quadratically from state vectors, and insensitive to sign flips: it has returned

to its original value $\mathbb{R}(\frac{1}{2}\tau) = +\mathbb{I}$ and the \mathbf{r} vector in Figure 3—which moves with doubled frequency—has made one *complete* tour of the cone. What we have encountered here once again is the celebrated double-valuedness of the spinor representations of the 3-dimensional rotation group $O(3)$. But here the encounter is peculiar in one particular: usually (as historically) one starts from a system which exhibits overt $O(3)$ symmetry, and is led to the spinors as a discovered resource. But here $O(3)$ has emerged as a “hidden symmetry” latent in the simplicity of the two-state model . . . pretty nearly the reverse of the more common progression.

The manifest dynamical constancy of the length of the \mathbf{r} vector—made obvious by the figure—can be read as an illustration of what we may take to be a general proposition:

$$\text{Quantum dynamical motion is isentropic: } \frac{d}{dt}S = 0 \quad (56)$$

Two-state theory as a theory of spin systems. From (8.2) we have

$$\begin{aligned} [\sigma_1, \sigma_2] &= 2i\sigma_3 \\ [\sigma_2, \sigma_3] &= 2i\sigma_1 \\ [\sigma_3, \sigma_1] &= 2i\sigma_2 \end{aligned}$$

which, if we introduce dimensioned Hermitian matrices $\mathbb{S}_k \equiv \frac{\hbar}{2}\sigma_k$, can be expressed

$$\left. \begin{aligned} [\mathbb{S}_1, \mathbb{S}_2] &= i\hbar \mathbb{S}_3 \\ [\mathbb{S}_2, \mathbb{S}_3] &= i\hbar \mathbb{S}_1 \\ [\mathbb{S}_3, \mathbb{S}_1] &= i\hbar \mathbb{S}_2 \end{aligned} \right\} \quad (57)$$

But these are precisely the commutation relations which at (1–50) were found to be characteristic of the *angular momentum* operators $\mathbf{L}_1, \mathbf{L}_2, \mathbf{L}_3$. The algebraic quantum theory of angular momentum¹⁵ derives much of its shape from the circumstance that the set $\{\mathbf{L}_1, \mathbf{L}_2, \mathbf{L}_3\}$ is—though closed with respect to commutation—*not multiplicatively closed*, in the sense that it is not possible to write $\mathbf{L}_i \mathbf{L}_j = \sum_k c_i^k{}^j \mathbf{L}_k$. In this important sense the \mathbb{S} matrices—for which one by (8.2) has equations of form $\mathbb{S}_1 \mathbb{S}_2 = i\frac{\hbar}{2} \mathbb{S}_3$ —are distinguished by the relative richness of their algebraic properties.

In the general theory one constructs

$$\mathbf{L}^2 \equiv \mathbf{L}_1^2 + \mathbf{L}_2^2 + \mathbf{L}_3^2 \quad (58.1)$$

and shows (*i*) that

$$[\mathbf{L}^2, \mathbf{L}_1^2] = [\mathbf{L}^2, \mathbf{L}_2^2] = [\mathbf{L}^2, \mathbf{L}_3^2] = \mathbf{0} \quad (58.2)$$

¹⁵ For a good brief account see Griffiths, pp. 146–149.

and (ii) that

$$\text{if } \mathbf{L}^2|\ell\rangle = \lambda|\ell\rangle \text{ then } \lambda = \hbar^2\ell(\ell+1) \quad : \quad \ell = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, \dots$$

On the other hand, in \mathbb{S} theory it follows from (8.1) that

$$\mathbb{S}^2 \equiv \mathbb{S}_1^2 + \mathbb{S}_2^2 + \mathbb{S}_3^2 = 3 \cdot \left(\frac{\hbar}{2}\right)^2 \mathbb{I} = \hbar^2 \frac{1}{2} \left(\frac{1}{2} + 1\right) \mathbb{I} \quad (59)$$

which enforces $\ell = \frac{1}{2}$ and informs us that in fact *every* 2-component $|\psi\rangle$ is an eigenvector of the “total spin” matrix \mathbb{S}^2 . We therefore expect \mathbb{S}^2 to play an insignificant role in the theory of spin $\frac{1}{2}$ systems; the operators of interest are $\{\mathbb{S}_1, \mathbb{S}_2, \mathbb{S}_3\}$, each of which has eigenvalues $\pm\frac{1}{2}\hbar$.

If we had had spin on our minds then the (most general) Hamiltonian introduced at (45) might have been notated $\mathbb{H} = \frac{1}{2}(\omega_0 \mathbb{I} + \omega \hat{\mathbf{h}} \cdot \mathbb{S})$ or again—if we exercise our option to set $\omega_0 = 0$, and adopt Griffiths’ physically motivated notation¹⁶—

$$\mathbb{H} = -\gamma \mathbf{B} \cdot \mathbb{S}$$

We would then interpret dynamical results obtained in the preceding section as having to do with the “precession of an electron in an impressed magnetic field.”¹⁷ Good physics, nothing wrong with that . . . and its gratifying to learn that “toy quantum mechanics” has something to say about the real world. The point I would emphasize, however, is that one is under no *obligation* to adopt spin language when thinking/talking about two-state systems: such language is always available, but sometimes it is liberating to put it out of mind.

Suppose one had *two* (or more) two-state systems, and wanted to assemble from them a *composite* system (a “molecule,” a “system of spins” or “spin system”); how would one proceed?

If a particle m were moving quantum mechanically in one dimension we might write $|\psi\rangle$ to indicate the state of the particle, and would find it natural to introduce an operator \mathbf{x} responsive to the question “Where is the particle?” Then $\psi(x) = \langle x|\psi\rangle$ becomes available as a descriptor of the particle’s location. If the system were comprised of *two* particles m_1 and m_2 then we would have need of a *pair* of operators, \mathbf{x}_1 and \mathbf{x}_2 , responsive to the questions “Where is m_1 ?” and “Where is m_2 ?” On the presumption that those are computable questions (formally, that $[\mathbf{x}_1, \mathbf{x}_2] = \mathbf{0}$) it becomes possible to introduce a doubly-indexed orthonormal basis $\{|x_1, x_2\rangle\}$ and obtain $\psi(x_1, x_2) = \langle x_1, x_2|\psi\rangle$. The operator \mathbf{x}_1 has a degenerate spectrum, and so does \mathbf{x}_2 :

$$\begin{aligned} \mathbf{x}_1|x_1, x_2\rangle &= x_1|x_1, x_2\rangle \\ \mathbf{x}_2|x_1, x_2\rangle &= x_2|x_1, x_2\rangle \end{aligned}$$

¹⁶ See Griffiths, p. 160.

¹⁷ For classical discussion of the same problem—presented as an exercise in Poisson bracket algebra, so as to look “maximally quantum mechanical”—see pp. 276–279 in CLASSICAL MECHANICS (1983).

But when announces its own individual eigenvalue they *collaboratively* identify a unique element $|x_1, x_2\rangle$ of the composite basis. In general, therefore, we expect to write

$$\psi(x_1, x_2), \text{ not (say) } \begin{pmatrix} \psi_1(x_1) \\ \psi_2(x_2) \end{pmatrix}$$

As a point of mathematical technique we may undertake to write something like

$$\psi(x_1, x_2) = \sum_{m,n} \varphi_m(x_1) \varphi_n(x_2) \quad (59.1)$$

and do not, in general, expect to see the sum reduce to a single term. If, however, m_1 and m_2 were on opposite sides of the room—were physically non-interactive, though *mentally* conjoined—then we *would* expect to have

$$\begin{aligned} &\downarrow \\ &= \psi_1(x_1) \cdot \psi_1(x_2) \end{aligned} \quad (59.2)$$

In the latter circumstance one has

$$\text{joint distribution} = (x_1\text{-distribution}) \cdot (x_1\text{-distribution}) \quad (60)$$

and says of x_1 and x_2 that they *independent* random variables—*uncorrelated*—that knowledge of the value of one conveys no information concerning the value of the other. It is with those general observations in mind that we return to consideration of how composite systems $\mathfrak{S} = \mathfrak{S}_1 \times \mathfrak{S}_2 \times \dots$ might be assembled from 2-state elements.

While the state of an individual 2-state element might (with respect to some arbitrarily selected orthonormal basis) be described

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \quad (61.1)$$

it could equally well (as we have seen) be described

$$\mathbb{R} = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} (\psi_1^* \quad \psi_2^*) = \begin{pmatrix} \psi_1 \psi_1^* & \psi_1 \psi_2^* \\ \psi_2 \psi_1^* & \psi_2 \psi_2^* \end{pmatrix} \quad : \quad \text{pure state} \quad (61.2)$$

$$\begin{aligned} &\downarrow \\ &= \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \quad : \quad \text{mixed state} \end{aligned} \quad (61.3)$$

The (latently more general) density matrix language is, as will emerge, uniquely well suited to the work before us, but its efficient management requires some familiarity with an elementary mathematical device which I now digress to describe.¹⁸

¹⁸ The following material has been excerpted from Chapter 3 of my *Classical Theory of Fields* (1999), where it appears on pp. 32–33.

The “Kronecker product” (sometimes called the “direct product”) of

- an $m \times n$ matrix \mathbb{A} onto
- a $p \times q$ matrix \mathbb{B}

is the $mp \times nq$ matrix defined¹⁹

$$\mathbb{A} \otimes \mathbb{B} \equiv \|a_{ij}\mathbb{B}\| \quad (62)$$

Manipulation of expressions involving Kronecker products is accomplished by appeal to general statements such as the following:

$$k(\mathbb{A} \otimes \mathbb{B}) = (k\mathbb{A}) \otimes \mathbb{B} = \mathbb{A} \otimes (k\mathbb{B}) \quad (63.1)$$

$$\left. \begin{aligned} (\mathbb{A} + \mathbb{B}) \otimes \mathbb{C} &= \mathbb{A} \otimes \mathbb{C} + \mathbb{B} \otimes \mathbb{C} \\ \mathbb{A} \otimes (\mathbb{B} + \mathbb{C}) &= \mathbb{A} \otimes \mathbb{B} + \mathbb{A} \otimes \mathbb{C} \end{aligned} \right\} \quad (63.2)$$

$$\mathbb{A} \otimes (\mathbb{B} \otimes \mathbb{C}) = (\mathbb{A} \otimes \mathbb{B}) \otimes \mathbb{C} \equiv \mathbb{A} \otimes \mathbb{B} \otimes \mathbb{C} \quad (63.3)$$

$$(\mathbb{A} \otimes \mathbb{B})^\top = \mathbb{A}^\top \otimes \mathbb{B}^\top \quad (63.4)$$

$$\text{tr}(\mathbb{A} \otimes \mathbb{B}) = \text{tr}\mathbb{A} \cdot \text{tr}\mathbb{B} \quad (63.5)$$

—all of which are valid except when meaningless.²⁰ Less obviously (but often very usefully)

$$(\mathbb{A} \otimes \mathbb{B})(\mathbb{C} \otimes \mathbb{D}) = \mathbb{A}\mathbb{C} \otimes \mathbb{B}\mathbb{D} \quad \text{if} \quad \left\{ \begin{array}{l} \mathbb{A} \text{ and } \mathbb{C} \text{ are } m \times m \\ \mathbb{B} \text{ and } \mathbb{D} \text{ are } n \times n \end{array} \right. \quad (63.6)$$

from which one can extract²¹

$$\mathbb{A} \otimes \mathbb{B} = (\mathbb{A} \otimes \mathbb{I}_n)(\mathbb{I}_m \otimes \mathbb{B}) \quad (63.7)$$

$$\det(\mathbb{A} \otimes \mathbb{B}) = (\det \mathbb{A})^n (\det \mathbb{B})^m \quad (63.8)$$

$$(\mathbb{A} \otimes \mathbb{B})^{-1} = \mathbb{A}^{-1} \otimes \mathbb{B}^{-1} \quad (63.9)$$

Here I have used \mathbb{I}_m to designate the $m \times m$ identity matrix; when the dimension is obvious from the context I will, in the future, allow myself to omit the subscript. The identities (63) are proven in each case by direct computation, and their great power will soon become evident.

I will write $\mathfrak{S} = \mathfrak{S}_1 \otimes \mathfrak{S}_2$ when I intend the non-interactive “mental” conjoin of two (or more) systems, and $\mathfrak{S}_1 \times \mathfrak{S}_2$ when elements of the composite

¹⁹ The alternative definition $\mathbb{A} \otimes \mathbb{B} \equiv \|a_{ij}b_{ij}\|$ gives rise to a “mirror image” of the standard theory. Good discussions can be found in E. P. Wigner, *Group Theory and its Application to the Quantum Theory of Atomic Spectra* (1959), Chapter 2; P. Lancaster, *Theory of Matrices* (1969), §8.2; Richard Bellman, *Introduction to Matrix Analysis* (2nd edition 1970), Chapter 12, §§5–13.

²⁰ Recall that one cannot add matrices unless they are co-dimensional, and does not speak of the trace of a matrix unless it is square.

²¹ See Lancaster³² for the detailed arguments.

system are permitted to interact physically. To describe the state of $\mathfrak{S}_1 \otimes \mathfrak{S}_2$ I propose to write

$$\mathbf{R} = \mathbb{R}_1 \otimes \mathbb{R}_2 \quad : \quad 4 \times 4 \quad (64)$$

in connection with which we notice that (by (63.5) and (61.2))

$$\text{tr } \mathbf{R} = \text{tr } \mathbb{R}_1 \cdot \text{tr } \mathbb{R}_2 = \begin{cases} (\psi_1 \psi_1^* + \psi_2 \psi_2^*)_1 \cdot (\psi_1 \psi_1^* + \psi_2 \psi_2^*)_2 = 1 & : \text{ pure case} \\ 1 \cdot 1 = 1 & \text{ even in the mixed case} \end{cases}$$

Drawing upon (63.6) we have

$$\begin{aligned} (\mathbb{A}_1 \otimes \mathbb{I}) \mathbf{R} (\mathbb{B}_1 \otimes \mathbb{I}) &= \mathbb{A}_1 \mathbb{R}_1 \mathbb{B}_1 \otimes \mathbb{R}_2 \\ (\mathbb{I} \otimes \mathbb{A}_2) \mathbf{R} (\mathbb{I} \otimes \mathbb{B}_2) &= \mathbb{R}_1 \otimes \mathbb{A}_2 \mathbb{R}_2 \mathbb{B}_2 \end{aligned}$$

which tells us in general terms how to construct

- operators which act upon \mathfrak{S}_1 but ignore \mathfrak{S}_2 ;
- operators which ignore \mathfrak{S}_1 but act upon \mathfrak{S}_2 .

We note also in this connection that if \mathbb{A} and \mathbb{B} are 2×2 Hermitian, then (by (63.4)) $\mathbb{A} \otimes \mathbb{B}$ is necessarily 4×4 Hermitian.

It becomes natural, in the light of preceding remarks, to introduce

$$\mathbf{S}_k \equiv (\mathbb{S}_k \otimes \mathbb{I}) + (\mathbb{I} \otimes \mathbb{S}_k) \quad : \quad k = 1, 2, 3 \quad (65.1)$$

as the operator which assigns “net k -component of spin” to the composite system, and to call

$$\mathbf{S}^2 \equiv \mathbf{S}_1^2 + \mathbf{S}_2^2 + \mathbf{S}_3^2 \quad (65.2)$$

the “total spin operator.” From (63.6) follows the useful identity

$$\begin{aligned} [(\mathbb{A} \otimes \mathbb{B}), (\mathbb{C} \otimes \mathbb{D})] &= (\mathbb{A}\mathbb{C} \otimes \mathbb{B}\mathbb{D}) + \{ -(\mathbb{C}\mathbb{A} \otimes \mathbb{B}\mathbb{D}) + (\mathbb{C}\mathbb{A} \otimes \mathbb{B}\mathbb{D}) \} - (\mathbb{C}\mathbb{A} \otimes \mathbb{D}\mathbb{B}) \\ &= ([\mathbb{A}, \mathbb{C}] \otimes \mathbb{B}\mathbb{D}) + (\mathbb{C}\mathbb{A} \otimes [\mathbb{B}, \mathbb{D}]) \end{aligned} \quad (66)$$

with the aid of which we quickly obtain

$$[\mathbf{S}_1, \mathbf{S}_2] = ([\mathbb{S}_1, \mathbb{S}_2] \otimes \mathbb{I}) + (\mathbb{I} \otimes [\mathbb{S}_1, \mathbb{S}_2]) = i\hbar \mathbf{S}_3, \text{ etc.} \quad (67)$$

Further computation

$$\begin{aligned} \mathbf{S}^2 &= \sum_k [(\mathbb{S}_k \otimes \mathbb{I}) + (\mathbb{I} \otimes \mathbb{S}_k)]^2 \\ &= \sum_k [(\mathbb{S}_k^2 \otimes \mathbb{I}) + 2(\mathbb{S}_k \otimes \mathbb{S}_k) + (\mathbb{I} \otimes \mathbb{S}_k^2)] \\ &= (\mathbb{S}^2 \otimes \mathbb{I}) + 2 \sum_k (\mathbb{S}_k \otimes \mathbb{S}_k) + (\mathbb{I} \otimes \mathbb{S}^2) \end{aligned}$$

gives (recall (59))

$$= \frac{3}{2} \hbar^2 (\mathbb{I} \otimes \mathbb{I}) + 2 \sum_k (\mathbb{S}_k \otimes \mathbb{S}_k) \quad (68)$$

and with this information, drawing again upon (66) and the commutation relations (57), we are led to

$$[\mathbf{S}^2, \mathbf{S}_1] = [\mathbf{S}^2, \mathbf{S}_2] = [\mathbf{S}^2, \mathbf{S}_3] = \mathbf{0} \quad (69)$$

Retreating again to generalities for a moment: in density matrix language the eigenvalue problem $\mathbb{A}|a\rangle = a|a\rangle$ becomes $\mathbb{A}\mathbb{R} = a\mathbb{R}$, and requires that the mixture contain only states that share the eigenvalue a (but puts no restriction on the relative weights assigned to those states, provided they sum to unity). If, in particular, the eigenvalue a is non-degenerate then necessarily $\mathbb{R} = |a\rangle\langle a|$ and $\mathbb{R}^2 = \mathbb{R}$. Building on this foundation, we find that

$$\begin{aligned} (\mathbb{A} \otimes \mathbb{B})(\mathbb{R}_1 \otimes \mathbb{R}_2) &= \lambda(\mathbb{R}_1 \otimes \mathbb{R}_2) \\ &\quad \updownarrow \\ \mathbb{A}\mathbb{R}_1 = a\mathbb{R}_1 \quad \text{and} \quad \mathbb{B}\mathbb{R}_2 &= b\mathbb{R}_2 \end{aligned} \quad (70.1)$$

and supplies $\lambda = ab$. And we find that

$$[(\mathbb{A} \otimes \mathbb{I}) + (\mathbb{I} \otimes \mathbb{B})](\mathbb{R}_1 \otimes \mathbb{R}_2) = \lambda(\mathbb{R}_1 \otimes \mathbb{R}_2) \quad (70.1)$$

imposes similar requirements upon \mathbb{R}_1 and \mathbb{R}_2 , while supplying $\lambda = a + b$.

Let us take \mathbf{S}^2 and (say) \mathbf{S}_3 to be simultaneous observables. Then

$$\mathbf{S}_3 \mathbf{R} = \mu \mathbf{R} \quad \text{entails} \quad \mathbb{S}_3 \mathbb{R}_1 = m_1 \mathbb{R}_1 \quad \text{and} \quad \mathbb{S}_3 \mathbb{R}_2 = m_2 \mathbb{R}_2$$

We know from previous work (see again (59)) that $m_1, m_2 = \pm \frac{1}{2}\hbar$, and will call the associated ‘‘eigendensities’’ \mathbb{R}_+ and \mathbb{R}_- . So the eigenvalues of \mathbf{S}_3 can be described

$$\mu = m_1 + m_2 \quad : \quad \text{ranges on} \quad \{-\hbar, 0, +\hbar\}$$

and the associated *eigendensities of the composite system* become

$$\mathbf{R}_{-1} = \mathbb{R}_- \otimes \mathbb{R}_- \quad : \quad \mathbf{R}_0 = \begin{cases} \mathbb{R}_+ \otimes \mathbb{R}_- \\ \mathbb{R}_- \otimes \mathbb{R}_+ \end{cases} \quad : \quad \mathbf{R}_{+1} = \mathbb{R}_+ \otimes \mathbb{R}_+$$

It is the degeneracy of \mathbf{R}_0 we ask \mathbf{S}^2 to resolve. In an effort to avoid confusing ‘‘formalism within formalism’’ I adopt an ‘‘experimentally computational’’ approach to the later problem:

We elect to work in the standard Pauli representation (7), and therefore have

$$\mathbb{S}_1 = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbb{S}_2 = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \mathbb{S}_3 = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (71)$$

The normalized eigenvectors of \mathbb{S}_3 are $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, with respective eigenvalues $\pm \frac{\hbar}{2}$, so we have

$$\mathbb{R}_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \mathbb{R}_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (72)$$

which, quite obviously, comprise a complete set of 2×2 orthogonal projection matrices. Building on this information, we obtain

$$\left. \begin{aligned} \mathbf{R}_{+1} &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, & \mathbf{R}_+ \otimes \mathbf{R}_- &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ \mathbf{R}_- \otimes \mathbf{R}_+ &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, & \mathbf{R}_{-1} &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{aligned} \right\} \quad (73)$$

(once again: a complete set of orthogonal projection matrices, but active now on 4-space). The names $\mathbf{R}_{\pm 1}$ will be motivated in a moment. Basic spin matrices for the composite system are

$$\mathbf{S}_1 = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, \quad \mathbf{S}_2 = \frac{\hbar}{2} \begin{pmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{pmatrix} \quad (74)$$

$$\mathbf{S}_3 = \hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

One verifies by direct matrix calculation that these possess the commutation properties alleged at (67), and that

$$\begin{aligned} \mathbf{S}_3 \mathbf{R}_{+1} &= +\hbar \mathbf{R}_{+1} \\ \mathbf{S}_3 \mathbf{R}_0 &= \mathbf{0} : \mathbf{R}_0 = \text{any linear combination of } \begin{cases} \mathbf{R}_+ \otimes \mathbf{R}_- \\ \mathbf{R}_- \otimes \mathbf{R}_+ \end{cases} \\ \mathbf{S}_3 \mathbf{R}_{-1} &= -\hbar \mathbf{R}_{-1} \end{aligned} \quad (75)$$

Finally we compute

$$\mathbf{S}^2 \equiv \mathbf{S}_1^2 + \mathbf{S}_2^2 + \mathbf{S}_3^2 = \hbar^2 \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \quad (76)$$

and observe that both \mathbf{R}_{+1} and \mathbf{R}_{-1} satisfy

$$\mathbf{S}^2 \mathbf{R} = \ell(\ell + 1)\hbar^2 \mathbf{R} \quad \text{with } \ell = 1 \quad (77)$$

To say the same thing another way: \mathbf{R}_{+1} and \mathbf{R}_{-1} project onto *simultaneous*

eigenvectors

$$|1, +1\rangle \equiv \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \equiv \uparrow\uparrow \quad \text{and} \quad |1, -1\rangle \equiv \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \equiv \downarrow\downarrow \quad (78.1)$$

of \mathbf{S}_3 and \mathbf{S}^2 . To obtain the final pair of such vectors we must diagonalize the central block $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ of the matrix described at (76); introducing

$$\mathbf{U} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} : \quad 45^\circ \text{ rotational unitary}$$

we obtain

$$\mathbf{U}^{-1} \mathbf{S}^2 \mathbf{U} = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & \mathbf{0} & 0 & 0 \\ 0 & 0 & \mathbf{2} & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$

and so, in $|\ell, m\rangle$ -notation and the frequently encountered²² “arrow notation,” we are led to write

$$|0, 0\rangle = \mathbf{U} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow), \quad |1, 0\rangle = \mathbf{U} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \quad (78.2)$$

The methods described above could (I presume) be extended to construct

- a theory of N -element composites of n -state systems;
- a general account of the addition of angular momentum.

We look now to results which arise when *measurements* are performed on composite systems. Continuing to work in the basis introduced at (73), we observe that the “spectral resolution” of (76) can be expressed

$$\mathbf{S}^2 = 2\hbar^2 \mathbf{P}_{\text{triplet}} + 0\hbar^2 \mathbf{P}_{\text{singlet}} \quad (79.1)$$

where

$$\mathbf{P}_{\text{triplet}} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{P}_{\text{singlet}} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (79.2)$$

comprise a complete orthogonal set of projection operators; the spectrum of $\mathbf{P}_{\text{triplet}}$ can be described $\{0, 1^3\}$ so that matrix projects onto a 3-space, while

²² Griffiths, §4.4.3.

$\mathbf{P}_{\text{singlet}}$, with spectrum $\{0^3, 1\}$, projects onto the orthogonal 1-space. When an (ideal) \mathbf{S}^2 -meter looks to a composite system in state

$$|\psi\rangle_{\text{in}} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

it announces “ $S^2 = 2\hbar^2$ ” and creates

$$|\psi\rangle_{\text{out}} = (\text{normalization factor}) \cdot \mathbf{P}_{\text{triplet}} |\psi\rangle_{\text{in}} \sim \begin{pmatrix} \psi_1 \\ (\psi_2 + \psi_3)/2 \\ (\psi_2 + \psi_3)/2 \\ \psi_4 \end{pmatrix} \quad (80.1)$$

with probability ${}_{\text{out}}\langle\psi|\psi\rangle_{\text{in}}|^2$. Else it announces “ $S^2 = 0\hbar^2$ ” and creates

$$|\psi\rangle_{\text{out}} = (\text{normalization factor}) \cdot \mathbf{P}_{\text{singlet}} |\psi\rangle_{\text{in}} \sim \begin{pmatrix} 0 \\ (\psi_2 - \psi_3)/2 \\ (\psi_3 - \psi_2)/2 \\ 0 \end{pmatrix} \quad (80.2)$$

with complementary probability. Similarly, the spectral resolution of \mathbf{S}_3 —which represents the action of a meter which looks to the S_3 of the entire composite system—can, by (74), be displayed

$$\mathbf{S}_3 = (+\hbar)\mathbf{P}_{+1} + (0\hbar)\mathbf{P}_0 + (-\hbar)\mathbf{P}_{-1} \quad (81)$$

with

$$\mathbf{P}_{+1} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{P}_0 \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{P}_{-1} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and supports an identical set of measurement-theoretic remarks. But if the meter looks only to the S_3 value of the #1 element then we must write

$$\mathbf{S}_3^{\#1} \equiv \mathbf{S}_3 \otimes \mathbb{I} = \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = (+\frac{1}{2}\hbar)\mathbf{P}_+^{\#1} + (-\frac{1}{2}\hbar)\mathbf{P}_-^{\#1} \quad (82.1)$$

with

$$\mathbf{P}_+^{\#1} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{P}_-^{\#1} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

while if the meter looks only to the #2 element we have

$$\mathbf{S}_3^{\#2} \equiv \mathbb{I}_3 \otimes \mathbb{S}_3 = \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = (+\frac{1}{2}\hbar)\mathbf{P}_+^{\#2} + (-\frac{1}{2}\hbar)\mathbf{P}_-^{\#2} \quad (82.2)$$

with

$$\mathbf{P}_+^{\#2} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{P}_-^{\#2} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Suppose, now, that an \mathbf{S}^2 -meter does respond “ $S^2 = 2\hbar^2$ ” when presented with some $|\psi\rangle_{\text{in}}$. The prepared state will, as we have seen, have then the form characteristic of triplet states:²³

$$|\psi\rangle_{\text{out}} = \begin{pmatrix} a \\ b \\ b \\ c \end{pmatrix} : \quad a^2 + 2b^2 + c^2 = 1 \quad (83)$$

Let that state be presented to a downstream $\mathbf{S}_3^{\#1}$ -meter, which will either

$$\text{respond “}S_3^{\#1} = +\frac{1}{2}\hbar\text{” and construct } |\psi\rangle_{\text{out/out}} = \frac{1}{\sqrt{a^2+b^2}} \begin{pmatrix} a \\ b \\ 0 \\ 0 \end{pmatrix}$$

or

$$\text{respond “}S_3^{\#1} = -\frac{1}{2}\hbar\text{” and construct } |\psi\rangle_{\text{out/out}} = \frac{1}{\sqrt{b^2+c^2}} \begin{pmatrix} 0 \\ 0 \\ b \\ c \end{pmatrix}$$

with

$$\text{probability given by } \begin{cases} \text{out}\langle\psi|\mathbf{P}_+^{\#1}|\psi\rangle_{\text{out}} = a^2 + b^2 \text{ in the former case} \\ \text{out}\langle\psi|\mathbf{P}_-^{\#1}|\psi\rangle_{\text{out}} = b^2 + c^2 \text{ in the latter case} \end{cases}$$

Now let a second S_3 -meter be placed downstream from the first. It it looks to subsystem #1 it will yield results which are simply confirmatory. But if it looks to subsystem #2 it will yield results which are *conditional upon the \pm recorded*

²³ In the following discussion—simply to reduce notational clutter—I will allow myself to write (for instance) a^2 when $|a|^2$ is intended. Maximal simplicity is achieved by setting $a = b = c = \frac{1}{2}$.

by the first meter. If the first meter were *disconnected* then the second meter would respond

$$\left. \begin{array}{l} \text{"+" with probability } \text{out}\langle\psi|\mathbf{P}_+^{\#2}|\psi\rangle_{\text{out}} = a^2 + b^2 \\ \text{"-" with probability } \text{out}\langle\psi|\mathbf{P}_-^{\#2}|\psi\rangle_{\text{out}} = b^2 + c^2 \end{array} \right\} \quad (84.1)$$

(which is to say: it would, owing to the special design (83) of triplet states, yield *data identical to that of the first meter*, though it would prepare a different population of states), but when the first meter is *reconnected* the expected responses of the second meter (which looks now to $|\psi\rangle_{\text{out/out}}$ states) might be described

$$\left. \begin{array}{l} \text{if "+" then } \left\{ \begin{array}{l} \text{"+" with probability } a^2/(a^2 + b^2) \\ \text{"-" with probability } b^2/(a^2 + b^2) \end{array} \right\} \\ \text{if "-" then } \left\{ \begin{array}{l} \text{"+" with probability } b^2/(b^2 + c^2) \\ \text{"-" with probability } c^2/(b^2 + c^2) \end{array} \right\} \end{array} \right\} \quad (84.2)$$

The point is that equations (84)—both of which describe activity of the second meter (under distinct experimental protocols)—differ from one another.

The situation becomes more starkly dramatic when the initial S^2 -meter announces that it has prepared a singlet state. The characteristic form of such a state was seen at (80.2) to be

$$|\psi\rangle_{\text{out}} = \begin{pmatrix} 0 \\ \frac{+1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \\ 0 \end{pmatrix} \quad (85)$$

Arguing as before, find that either downstream S_3 -meter, acting alone, (and though they prepare distinct populations of states) yields data which can be described

$$\left. \begin{array}{l} \text{"+" with probability } \frac{1}{2} \\ \text{"-" with probability } \frac{1}{2} \end{array} \right\} \quad (86.1)$$

but that when both meters are on-line the second meter gives

$$\left. \begin{array}{l} \text{if "+" then } \left\{ \begin{array}{l} \text{"+" with zero probability} \\ \text{"-" with certainty} \end{array} \right\} \\ \text{if "-" then } \left\{ \begin{array}{l} \text{"+" with certainty} \\ \text{"-" with zero probability} \end{array} \right\} \end{array} \right\} \quad (86.2)$$

The two meters are in this case *perfectly correlated*: the first meter-reading (whatever it may have turned out to be) caused—is that the right word?—the second meter-reading to be redundant/pre-determined.

We have come here upon a result which the many eminent physicists have found profoundly/disturbingly puzzling . . . which has caused a sea of ink to be spilled, and provoked occasionally strident controversy . . . and has stimulated

recent experimental work the results of which have been viewed with amazement by *all* participants in the dispute (if dispute there be). The points at issue continue to shake the foundations of quantum mechanics, and stem from the observation that ...

Elements \mathfrak{S}_1 and \mathfrak{S}_2 of the composite system may be *very far apart* at the moment we undertake to do measurement on \mathfrak{S}_1 . The idea that “news” of the outcome of that measurement should be transmitted instantaneously to \mathfrak{S}_2 (faster than allowed by relativity) struck Einstein and his collaborators²⁴ as absurd. One might

- argue that since we have worked non-relativistically we should not be surprised to find ourselves in conflict with relativity,²⁵ or
- attempt to construct a theory of the “delayed onset of correlation”

but such effort would be rendered pointless by observations which establish convincingly that *the onset of correlation is in fact instantaneous*.²⁶ One might on this evidence attempt to argue that the correlation was actually present from the outset, supported by “hidden variables” of which quantum theory takes no account, and that the theory is on this account “incomplete.” This

²⁴ A. Einstein, Boris Podolsky & Nathan Rosen, “Can quantum-mechanical description of physical reality be considered complete?” *Phys. Rev.* **47**, 777 (1935). This classic paper (only four pages long) is reprinted in J. A. Wheeler & W. H. Zurek, *Quantum Theory and Measurement* (1983), together with many of the papers (by Bohr, Schrödinger, others) which it stimulated. EPR spoke of composite systems in general terms, but the idea of looking to 2-state *spin* systems is due to David Bohm, §§15–19 in Chapter 22 of *Quantum Theory* (1951), reprinted as “The paradox of Einstein, Rosen & Podolsky” in Wheeler & Zurek.

²⁵ In fact our toy theory has so few moving parts that it is difficult to say whether it is or isn’t relativistic.

²⁶ A. Aspect, P. Grangier & G. Roger, “Experimental test of Bell’s inequalities using time-varying analyzers,” *Phys. Rev. Letters* **49**, 1804 (1982). The most recent results in that tradition are reported in W. Tittel, J. Brendel, H. Zbinden & N. Gisin, “Violation of Bell inequalities by photons more than 10km apart,” *Phys. Rev. Letters* **81**, 3563 (1998) and G. Wiehs, T. Jennewein, C. Simon, H. Weinfurter & A. Zeilinger, “Violation of Bell’s inequality under strict Einstein locality conditions,” *Phys. Rev. Letters* **81**, 5039 (1992). For a very nice brief review of the present status and significance of work in this field, see A. Aspect, “Bell’s inequality test: more ideal than ever,” *Nature* **398**, 189 (1999), which bears this subhead:

‘The experimental violation of Bell’s inequalities confirms that a pair of entangled photons separated by hundreds of metres must be considered a single non-separable object—it is impossible to assign local physical reality to each photon.’

Aspect remarks that the best available data lies 30 standard deviations away from the possibility that it might be in error.

hypothesis has added urgency to an already entrenched tradition in which the objective is to construct a deterministic “hidden variable theory” which would “explain” why the quantum mechanical world seems so profoundly random.²⁷ But this work, while it has taught us much of a formal nature, has thus far served only to sharpen the evidence on which we may hold orthodox quantum mechanics to be correct as it stands. “Instantaneous correlation” has come to be widely interpreted as an indication that quantum mechanics is, in some unsettling sense, *non-local* . . . that the states of the components of composite systems—even components so far removed from one another as to be physically non-interactive—remain (in Schrödinger’s phrase) “entangled.”

In the early/mid-1960’s John Bell—drawing inspiration jointly from a lecture presented at CERN (where he and I had recently served as colleagues in the Theory Division) by J. M. Jauch²⁸ and from his own prior exposure to EPR/Bohm and to Max Born’s account²⁹ of “von Neumann’s proof” that, subject to a few natural assumptions, hidden variable theories are impossible—looked again into the hidden variable question, as it relates to the EPR paradox. He was able to construct a hidden variable account of the quantum physics of simple spin systems, such as we have considered, and confronted then the question: Which of von Neumann’s “natural assumptions” did his toy theory violate? Bell argued that von Neumann’s “additivity postulate,” though it appears to have the status almost of a “law of thought,” is susceptible to physical challenge.³⁰ Bell’s work culminated in the development (while he was a visitor at Brandeis University) of “Bell’s inequality,” violation of which is interpreted to speak in favor of orthodox quantum mechanics, and against the existence of hidden variables. Einstein and Bohr had in the end to “agree to disagree” . . . as one must in all philosophical disputes. Bell’s inequality made it possible to resolve such issues by comparing one experimental number to another, and transformed the quality of the discussion.

Dynamics of composite spin systems. To describe (in the Schrödinger picture) the dynamics of a time-independent 2-state system we have only to write

$$\mathbb{H}|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle$$

²⁷ See F. J. Belinfante, *A Survey of Hidden-Variable Theories* (1973).

²⁸ J. M. Jauch & C. Piron, “Can hidden variables be excluded in quantum mechanics?” *Helvetica Physica Acta* 36, 827 (1963). Jauch was then at the University of Geneva.

²⁹ See p. 108 in *Natural Philosophy of Cause & Chance* (1949).

³⁰ For a readable account of “von Neumann’s impossibility proof” (including a list of his four postulates) see §7.4 in Max Jammer, *The Philosophy of Quantum Mechanics: The Interpretations of Quantum Mechanics in Historical Perspective* (1974). In §7.7 one finds a good account also of Bell’s contribution. Bell’s “On the Einstein-Podolsky-Rosen paradox” *Physics* 1, 195 (1964) and “On the problem of hidden variables in quantum mechanics” *Rev. Mod. Phys.* 38, 447 (1966) reproduced both in Wheeler & Zurek²⁴ and in his own collection of essays, *Speaking and unspeakable in quantum mechanics* (1987).

with

$$\begin{aligned}\mathbb{H} &= \hbar(\omega_0\boldsymbol{\sigma}_0 + \boldsymbol{\omega}\hat{\mathbf{h}}\cdot\boldsymbol{\sigma}) \\ &= \hbar\begin{pmatrix} \omega_0 + \omega\hat{h}_3 & \omega\hat{h}_2 - i\omega\hat{h}_2 \\ \omega\hat{h}_2 + i\omega\hat{h}_2 & \omega_0 - \omega\hat{h}_3 \end{pmatrix} \\ &= \sum_{\mu} h_{\mu}\boldsymbol{\sigma}_{\mu}\end{aligned}$$

with consequences which have already been described in the equations (45–55) which culminated in Figure 3. The motion of the associated density matrix is described

$$\mathbb{H}\mathbb{R} - \mathbb{R}\mathbb{H} = i\hbar\frac{\partial}{\partial t}\mathbb{R}$$

To describe the motion of elements of a non-interactive composite $\mathfrak{S}_1 \otimes \mathfrak{S}_2$ we might write

$$\left. \begin{aligned}\mathbb{H}_1\mathbb{R}_1 - \mathbb{R}_1\mathbb{H}_1 &= i\hbar\frac{\partial}{\partial t}\mathbb{R}_1 \\ \mathbb{H}_2\mathbb{R}_2 - \mathbb{R}_2\mathbb{H}_2 &= i\hbar\frac{\partial}{\partial t}\mathbb{R}_2\end{aligned}\right\} \quad (87)$$

But if we introduce

$$\left. \begin{aligned}\mathbf{R} &\equiv (\mathbb{R}_1 \otimes \mathbb{I}) + (\mathbb{I} \otimes \mathbb{R}_2) \\ \mathbf{H} &\equiv (\mathbb{H}_1 \otimes \mathbb{I}) + (\mathbb{I} \otimes \mathbb{H}_2)\end{aligned}\right\} \quad (88)$$

and notice that (after four of eight terms cancel)

$$[\mathbf{H}, \mathbf{R}] = ([\mathbb{H}_1, \mathbb{R}_1] \otimes \mathbb{I}) + (\mathbb{I} \otimes [\mathbb{H}_2, \mathbb{R}_2]) \quad (89)$$

t then equations (87) fuse, to become

$$\mathbf{H}\mathbf{R} - \mathbf{R}\mathbf{H} = i\hbar\frac{\partial}{\partial t}\mathbf{R} \quad : \quad \text{matrices now } 4 \times 4 \quad (90)$$

The problem now before us: How to describe motion of a composite system $\mathfrak{S}_1 \times \mathfrak{S}_2$ in which the elements are not just “mentally” conjoined, but physically —interactively?

The 2×2 Hermitian matrices \mathbb{H}_1 and \mathbb{H}_2 are 4-parameter objects, and when assembled yield a 4×4 Hermitian matrix of the specialized 7-parameter design³¹

$$\begin{aligned}\mathbf{H} &= \sum_{\mu} \{(a_{\mu}\boldsymbol{\sigma}_{\mu} \otimes \mathbb{I}) + (\mathbb{I} \otimes b_{\mu}\boldsymbol{\sigma}_{\mu})\} \\ &= \begin{pmatrix} a_0+a_3+b_0+b_3 & b_1-ib_2 & a_1-ia_2 & 0 \\ b_1+ib_2 & a_0+a_3+b_0-b_3 & 0 & a_1-ia_2 \\ a_1+ia_2 & 0 & a_0-a_3+b_0+b_3 & b_1-ib_2 \\ 0 & a_1+ia_2 & b_1-ib_2 & a_0-a_3+b_0-b_3 \end{pmatrix} \quad (91)\end{aligned}$$

The most general 4×4 Hermitian \mathbf{H} is, however, a 16-parameter object.

³¹ Seven (not eight) because a_0 and b_0 enter only in the fixed combination

$$a_0 + b_0 = \frac{1}{4} \text{tr } \mathbf{H}$$

We are led by this remark to construct the 16 matrices

$$\sigma_{\mu\nu} \equiv \sigma_{\mu} \otimes \sigma_{\nu} \quad (92)$$

The Pauli matrices themselves comprise a tracewise orthogonal basis in the 4-dimensional real vector space of 2×2 Hermitian matrices

$$\frac{1}{2} \operatorname{tr} \sigma_{\mu} \sigma_{\alpha} = \delta_{\mu\alpha}$$

and from this it follows that the $\sigma_{\mu\nu}$ -matrices are tracewise orthogonal

$$\begin{aligned} \frac{1}{4} \operatorname{tr} \sigma_{\mu\nu} \sigma_{\alpha\beta} &= \frac{1}{4} \operatorname{tr} \{ \sigma_{\mu} \sigma_{\alpha} \otimes \sigma_{\nu} \sigma_{\beta} \} \\ &= \frac{1}{4} (\operatorname{tr} \sigma_{\mu} \sigma_{\alpha}) (\operatorname{tr} \sigma_{\nu} \sigma_{\beta}) \\ &= \delta_{\mu\alpha} \delta_{\nu\beta} \end{aligned} \quad (93)$$

and therefore comprise a basis in the in the 16-dimensional real vector space of 4×4 Hermitian matrices. An arbitrary such matrix \mathbf{M} can be developed

$$\mathbf{M} = \sum_{\mu,\nu=0}^3 m_{\mu\nu} \sigma_{\mu\nu} \quad \text{with} \quad m_{\mu\nu} = \frac{1}{4} \operatorname{tr} \mathbf{M} \sigma_{\mu\nu}$$

For example: *Mathematica* (into which I have fed the $\sigma_{\mu\nu}$ -definitions³²) informs us (and we confirm by inspection) that

$$\begin{aligned} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} &= \frac{1}{4} \sigma_{00} + \frac{1}{4} \sigma_{03} + \frac{1}{4} \sigma_{30} + \frac{1}{4} \sigma_{33} \\ \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} &= \frac{1}{2} \sigma_{01} + \frac{1}{2} \sigma_{31} \\ \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} &= \frac{1}{2} \sigma_{02} + \frac{1}{2} \sigma_{32} \end{aligned}$$

We observe that

$$\frac{1}{4} \operatorname{tr} \sigma_{00} = 1 \quad : \quad \text{all other } \sigma_{\mu\nu}\text{-matrices traceless} \quad (94)$$

It follows that we can assign $\frac{1}{4} \operatorname{tr} \mathbf{H}$ any value we please by appropriate placement of the energy reference level; to set $\frac{1}{4} \operatorname{tr} \mathbf{H} = 0$ is to impose the spectral condition

$$E_1 + E_2 + E_3 + E_4 = 0 \quad (95)$$

³² I urge my reader to do the same. Take definitions of `Pauli0`, `Pauli1`, etc. from (7), then use `Outer[Times, Pauli0, Pauli0]//MatrixForm`, etc. to construct and examine the matrices σ_{00} , etc.

We are in position now to provide an answer to our motivating question: to achieve physical interaction between \mathfrak{S}_1 and \mathfrak{S}_2 we must introduce into the Hamiltonian terms which (while preserving Hermiticity) break the *symmetry with respect to the antidiagonal* which is so strikingly evident in (91); we must, in short, make an adjustment of the form

$$\mathbf{H} \longrightarrow \mathbf{H} + \lambda \mathbf{V} \quad (96)$$

with

$$\begin{aligned} \mathbf{H} &= (a_0 + b_0)\sigma_{00} + a_1\sigma_{10} + a_2\sigma_{20} + a_3\sigma_{30} + b_1\sigma_{01} + b_2\sigma_{02} + b_3\sigma_{03} \\ \mathbf{V} &= c_1\sigma_{13} + c_2\sigma_{23} + d_1\sigma_{31} + d_2\sigma_{32} + e_1\sigma_{22} + e_2\sigma_{21} + f_1\sigma_{11} + f_2\sigma_{12} + g\sigma_{33} \\ &= \begin{pmatrix} g & d_1 - id_2 & c_1 - ic_2 & -e_1 - ie_2 + f_1 - if_2 \\ d_1 + id_2 & -g & e_1 - ie_2 + f_1 + if_2 & -c_1 + ic_2 \\ c_1 + ic_2 & e_1 + ie_2 + f_1 - if_2 & -g & -d_1 + id_2 \\ -e_1 + ie_2 + f_1 - if_2 & -c_1 - ic_2 & -d_1 - id_2 & g \end{pmatrix} \end{aligned} \quad (97)$$

where the g -term has been included not for symmetry breaking reasons, but because otherwise σ_{33} would be excluded from both lists.

Our recent discussion of EPR spin correlation inspires interest in the conditions under which \mathbf{S}^2 commutes with \mathbf{H} and/or \mathbf{V} . While a fancy algebraic argument could be constructed (and would have the merit of being representation independent), I have found it simplest to work from the descriptions (76), (91) and (97) of the matrices in question; entrusting the matrix multiplication to *Mathematica*, we are led to the conclusions that

$$\left. \begin{aligned} [\mathbf{S}^2, \mathbf{H}] &= \mathbf{0} && \text{if and only if } a_1 = b_1, a_2 = b_2 \text{ \& } a_3 = b_3 \\ [\mathbf{S}^2, \mathbf{V}] &= \mathbf{0} && \text{if and only if } c_1 = d_1, c_2 = d_2 \text{ \& } e_2 = f_2 \end{aligned} \right\} \quad (98)$$

The former condition amounts to the requirement that

$$\mathbb{H}_2 = \mathbb{H}_1 + (\text{constant}) \cdot \mathbb{I}$$

and has this interesting implication: *every* 2×2 \mathbb{H} commutes with $\mathbb{S}^2 = \frac{3}{4}\hbar^2 \mathbb{I}$ (see again (59)), but the commutation of \mathbf{H} with \mathbf{S}^2 is strongly conditional. Preservation of the prepared singlet state—assumed in our discussion of the EPR phenomenon—therefore requires careful design of the over-all Hamiltonian (including the interactive \mathbf{V} component, which presumably is to be “turned off” as \mathfrak{S}_1 and \mathfrak{S}_2 become separated.)

The special design attributed to \mathbf{H} at (88) was attributed also to the joint density matrix \mathbf{R} , where it formalized the notion that $\mathfrak{S}_1 \otimes \mathfrak{S}_2$ is the “mental composite” of its elements. If the system were “physically composite” we would write $\mathfrak{S}_1 \times \mathfrak{S}_2$, and would expect the density matrix to contain additional terms:

$$\mathbf{R}_{\text{physical}} = \mathbf{R}_{\text{mental}} + \text{terms of the same design as } \mathbf{V}$$

The added terms are traceless, so their inclusion would not compromise the general requirement (imposed upon *all* density matrices) that $\text{tr } \rho = 1$.³³ It is in order to assess the significance of this result that I interpose here a reminder concerning how meter-operation is described in density matrix language:

When a perfect meter $\mathbf{A} = \sum |a\rangle a \langle a|$ looks at a system in the mixed state represented by the density matrix ρ_{in} and announces “ a_0 ” (which it will do with probability $\langle a_0 | \rho_{\text{in}} | a_0 \rangle$) it constructs

$$\rho_{\text{out}} = |a_0\rangle \langle a_0| = \frac{|a_0\rangle \langle a_0| \cdot \rho_{\text{in}} \cdot |a_0\rangle \langle a_0|}{\text{normalization factor}} \quad (99)$$

where the normalization factor is evidently just $\langle a_0 | \rho_{\text{in}} | a_0 \rangle = \text{tr} \{ \rho_{\text{in}} \cdot |a_0\rangle \langle a_0| \}$ and can (because of a property of the trace, together with the fact that $|a_0\rangle \langle a_0|$ is projective) be described

$$\text{normalization factor} = \text{tr} \left\{ |a_0\rangle \langle a_0| \cdot \rho_{\text{in}} \cdot |a_0\rangle \langle a_0| \right\}$$

Accordingly ... when at S^2 -meter looks at ρ_{in} and announces “singlet” it constructs

$$\rho_{\text{out}} = \frac{\mathbf{P}_{\text{singlet}} \rho_{\text{in}} \mathbf{P}_{\text{singlet}}}{\text{trace}} \quad (100)$$

We were supplied with a description of $\mathbf{P}_{\text{singlet}}$ at (79.2), and are in position now to write

$$\begin{aligned} \mathbf{P}_{\text{singlet}} &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ &= \frac{1}{4} \sigma_{00} - \frac{1}{4} \sigma_{11} - \frac{1}{4} \sigma_{22} - \frac{1}{4} \sigma_{33} \\ &= \frac{1}{4} \left\{ \mathbf{I} - (\sigma_1 \otimes \sigma_1) - (\sigma_2 \otimes \sigma_2) - (\sigma_3 \otimes \sigma_3) \right\} \end{aligned}$$

and to notice the the expression on the right displays “entangled terms”—terms not present in

$$\rho_{\text{mental}} = q_{00} \sigma_{00} + r_1 \sigma_{10} + r_2 \sigma_{20} + r_3 \sigma_{30} + s_1 \sigma_{01} + s_2 \sigma_{02} + s_3 \sigma_{03}$$

but present as honored citizens in

$$\begin{aligned} \rho_{\text{entangled}} &= r_1 \sigma_{13} + r_2 \sigma_{23} + s_1 \sigma_{31} + s_2 \sigma_{32} \\ &\quad + u_1 \sigma_{22} + u_2 \sigma_{21} + v_1 \sigma_{11} + v_2 \sigma_{12} + w_1 \sigma_{33} \end{aligned}$$

³³ Preservation of compliance with the requirement that all eigenvalues be non-negative seems, however, to be more difficult to insure.

Mathematica informs us that

$$\mathbb{P}_{\text{singlet}} \rho_{\text{mental}} \mathbb{P}_{\text{singlet}} = q_{00} \cdot \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

i.e., that when ρ_{mental} is presented to an S^2 -meter it constructs a singlet state with probability q_{00} . On the other hand,

$$\mathbb{P}_{\text{singlet}} \rho_{\text{entangled}} \mathbb{P}_{\text{singlet}} = -(v_1 + u_1 + w_1) \cdot \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The device then sees only the σ_{11} , σ_{22} and σ_{33} terms present in the entangled mixture. This is a satisfying result, not at all surprising ... but exposes—more clearly than before—this important point: S^2 -meters prepare (and some Hamiltonians preserve) entangled states, and it is upon this fact that the EPR phenomenon depends.

The preceding discussion exposes this deep (but, I suspect, attackable) problem: How does it come about that—in the classical limit; under what other circumstances?—the entangled component of the density matrix spontaneously and effectively *disappears* from the physics of composite systems?

Two-state theory as a perturbation laboratory. Perturbation theories come in many flavors. Some—some of those which assign a starring role to the wave function $\psi(x) = \langle x | \psi \rangle$, and are therefore representation-specific—are presented as exercises in the approximation theory of differential equations. Those have no analogs in 2-state theory (where no operators have continuous spectra). But many present exercises in matrix algebra, made complicated mainly by the circumstance that the matrices in question are ∞ -dimensional. Those can be modeled—sometimes advantageously, and variations of them explored—in the toy context provided by 2-state theory, where most matrix-theoretic questions can, after all, be settled by explicit/exact calculation.

Look in this light to the simplest version of time-independent perturbation theory.³⁴ We possess the solutions (eigenvalues and eigenvectors) of

$$\mathbb{H}^0 |n\rangle^0 = E_n^0 |n\rangle^0 \quad : \quad n = 1, 2$$

and seek solutions of

$$\mathbb{H} |n\rangle = E_n |n\rangle \quad : \quad \mathbb{H} = \mathbb{H}^0 + \lambda \mathbb{V}$$

Elect to work in the unperturbed eigenbasis, where

$$\mathbb{H}^0 = \begin{pmatrix} E_1^0 & 0 \\ 0 & E_2^0 \end{pmatrix}, \quad |1\rangle^0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |2\rangle^0 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

³⁴ The theory was first described by Schrödinger himself; See §6.1 in Griffiths.

and where to describe the Hermitian perturbation term we will agree to write

$$\mathbb{V} = \begin{pmatrix} \langle 1|\mathbb{V}|1\rangle^0 & \langle 1|\mathbb{V}|2\rangle^0 \\ \langle 2|\mathbb{V}|1\rangle^0 & \langle 2|\mathbb{V}|2\rangle^0 \end{pmatrix} = \begin{pmatrix} V_1 & U^* \\ U & V_2 \end{pmatrix}$$

The exact perturbed energy eigenvalues are easy enough to compute: from

$$\begin{aligned} & \det \begin{pmatrix} E_1^0 + \lambda V_1 - x & \lambda U^* \\ \lambda U & E_2^0 + \lambda V_2 - x \end{pmatrix} \\ &= x^2 - x[(E_1^0 + \lambda V_1) + (E_2^0 + \lambda V_2)] + [(E_1^0 + \lambda V_1) \cdot (E_2^0 + \lambda V_2) - \lambda^2 U^* U] \end{aligned}$$

we have

$$x = \frac{1}{2} \left\{ [(E_1^0 + \lambda V_1) + (E_2^0 + \lambda V_2)] \pm \sqrt{[(E_1^0 + \lambda V_1) - (E_2^0 + \lambda V_2)]^2 + 4\lambda^2 U^* U} \right\}$$

which upon expansion in powers of λ gives

$$\left. \begin{aligned} E_1 &= E_1^0 + \lambda E_1^1 + \lambda^2 E_1^2 + \dots \\ &= E_1^0 + \lambda V_1 - \lambda^2 \frac{U^* U}{E_2^0 - E_1^0} + \dots \\ E_2 &= E_2^0 + \lambda E_2^1 + \lambda^2 E_2^2 + \dots \\ &= E_2^0 + \lambda V_2 + \lambda^2 \frac{U^* U}{E_2^0 - E_1^0} + \dots \end{aligned} \right\} \quad (101.1)$$

when $E_1^0 < E_2^0$, and

$$\left. \begin{aligned} E_1 &= E^0 + \frac{1}{2}\lambda \left\{ (V_1 + V_2) - \sqrt{(V_1 - V_2)^2 + U^* U} \right\} \\ &\quad + \text{no } \lambda^2 \text{ term} + \dots \\ E_2 &= E^0 + \frac{1}{2}\lambda \left\{ (V_1 + V_2) + \sqrt{(V_1 - V_2)^2 + U^* U} \right\} \\ &\quad + \text{no } \lambda^2 \text{ term} + \dots \end{aligned} \right\} \quad (101.2)$$

when the unperturbed spectrum is degenerate: $E_1^0 = E_2^0 \equiv E^0$. Standard perturbation theory leads to (101) by a hierarchical method

$$\{ \dots \{ \{ \{ 0^{\text{th}} \rightarrow 1^{\text{st}} \} \rightarrow 2^{\text{nd}} \} \rightarrow 3^{\text{rd}} \} \rightarrow \dots \}$$

which—while it does not require one to develop/solve

$$\det (\mathbb{H}^0 + \lambda \mathbb{V} - E \mathbb{I}) = 0$$

—does require one to serially construct

- all lower-order spectral corrections $\{E_i^1, E_i^2, \dots, E_i^{p-1}\}$ (all i) and
- all lower-order corrections $\{|i\rangle^1, |i\rangle^2, \dots, |i\rangle^{p-1}\}$ (all i) to the eigenfunctions before one undertakes to describe

$$E_n^p \quad : \quad p^{\text{th}} \text{ correction to } n^{\text{th}} \text{ spectral value}$$

Our visit to the “toy quantum lab” has on this occasion rewarded us with the vision of an alternative—and potentially more efficient—3-step procedure:

STEP ONE Expand $\det(\mathbb{H}^0 + \lambda\mathbb{V} - E\mathbb{I})$ in powers of λ .

STEP TWO Replace E with $E_n^0 + \lambda E_n^1 + E_n^2 + \dots$ and collect terms:

$$\det = \lambda D(E_n^0, E_n^1) + \lambda^2 D(E_n^0, E_n^1, E_n^2) + \lambda^3 D(E_n^0, E_n^1, E_n^2, E_n^3) + \dots$$

STEP THREE Solve serially.

The first step is accomplished by writing

$$\det(\mathbb{H}^0 + \lambda\mathbb{V} - E\mathbb{I}) = \det(\mathbb{H}^0 - E\mathbb{I}) \cdot \det(\mathbb{I} + \lambda\mathbb{M})$$

$$\mathbb{M} = (\mathbb{H}^0 - E\mathbb{I})^{-1}\mathbb{V}$$

and using

$$\det(\mathbb{H}^0 - E\mathbb{I}) = \prod_i (E_i^0 - E)$$

and a remarkable identity³⁵ which deserves to be more widely known:

$$\det(\mathbb{I} + \lambda\mathbb{M}) = 1 + \lambda \operatorname{tr}\mathbb{M} + \frac{1}{2!}\lambda^2 \begin{vmatrix} \operatorname{tr}\mathbb{M} & \operatorname{tr}\mathbb{M}^2 \\ 1 & \operatorname{tr}\mathbb{M} \end{vmatrix} \quad (102)$$

$$+ \frac{1}{3!}\lambda^3 \begin{vmatrix} \operatorname{tr}\mathbb{M} & \operatorname{tr}\mathbb{M}^2 & \operatorname{tr}\mathbb{M}^3 \\ 1 & \operatorname{tr}\mathbb{M} & \operatorname{tr}\mathbb{M}^2 \\ 0 & 2 & \operatorname{tr}\mathbb{M} \end{vmatrix} + \dots$$

I regret that I must, on this occasion, leave further details to the delight of the curious reader.

Not to belabor the nearly obvious: in 2-state theory much can be done exactly that is usually done only approximately, and by comparing those exact procedures with various perturbation strategies³⁶ one has an opportunity to learn things ...and perhaps to come upon new strategies that may offer advantages in some situations.

It is in that spirit that we turn now to *time-dependent perturbation theory*, and to discussion of some the insight which in that important context can be gained from play with our toy quantum theory. Standardly, one elects to work in the Schrödinger picture, and writes

$$\mathbf{H}_0|n\rangle = E_n|n\rangle \quad (103)$$

³⁵ See CLASSICAL DYNAMICS (1964), Chapter 1, pp. 60–69 or “Applications of an elegant formula due to V. F. Ivanoff” in COLLECTED SEMINARS 1963–1970.

³⁶ Of which a fairly long and diverse (but by no means exhaustive) list can be found in QUANTUM PERTURBATION THEORY & CLASSICAL RADIATIVE PROCESSES (1969/74), pp. 1–50.

(note the altered/simplified notation) to describe the information that is assumed to be already in hand. The general solution of $\mathbf{H}_0|\psi\rangle_t = i\hbar\frac{\partial}{\partial t}|\psi\rangle_t$ can in this notation be developed

$$\begin{aligned} |\psi\rangle_t &= \sum_n |n\rangle e^{-i\omega_n t} \langle n|\psi\rangle_0 \quad : \quad \omega_n \equiv E_n/\hbar \\ &= \sum_n c_n \cdot e^{-i\omega_n t} |n\rangle \end{aligned} \quad (104)$$

as a c_n -weighted superposition of “harmonically buzzing eigenfunctions.” We now tickle the Hamiltonian

$$\mathbf{H}_0 \longrightarrow \mathbf{H} = \mathbf{H}_0 + \lambda\mathbf{V}(t) \quad : \quad t\text{-dependent perturbation}$$

and ask how the tickle alters the motion of $|\psi\rangle_t$. The question is standardly approached by launching the coefficients c_n into motion; one discovers by simple argument that

$$|\psi\rangle_t^{\text{perturbed}} \equiv \sum_n c_n(t) \cdot e^{-i\omega_n t} |n\rangle \quad (105)$$

will (exactly!) satisfy

$$\{\mathbf{H}_0 + \lambda\mathbf{V}(t)\}|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle$$

if and only if

$$i\hbar\frac{d}{dt}c_m(t) = \lambda \sum_n \langle m|\mathbf{V}(t)|n\rangle e^{i(\omega_m - \omega_n)t} c_n(t) \quad (106.1)$$

which we may express

$$i\hbar\frac{d}{dt}\mathbf{c} = \lambda\mathbb{W}(t)\mathbf{c} \quad \text{with} \quad \mathbf{c} \equiv \begin{pmatrix} c_1(t) \\ c_2(t) \\ \vdots \\ c_n(t) \\ \vdots \end{pmatrix} \quad (106.2)$$

Equivalently, we have the integral equation

$$\mathbf{c}(t) = \mathbf{c}_0 - \lambda\frac{i}{\hbar} \int_0^t \mathbb{W}(\tau)\mathbf{c}(\tau) d\tau \quad : \quad \mathbf{c}_0 \equiv \mathbf{c}(0) \quad (107)$$

which upon iteration gives

$$\begin{aligned} \mathbf{c}(t) = \left\{ \mathbb{I} - \lambda\frac{i}{\hbar} \int_0^t \mathbb{W}(\tau) d\tau + \left(\lambda\frac{i}{\hbar}\right)^2 \int_0^t \int_0^\tau \mathbb{W}(\tau)\mathbb{W}(\sigma) d\sigma d\tau \right. \\ \left. - \left(\lambda\frac{i}{\hbar}\right)^3 \int_0^t \int_0^\tau \int_0^\sigma \mathbb{W}(\tau)\mathbb{W}(\sigma)\mathbb{W}(\rho) d\rho d\sigma d\tau + \dots \right\} \mathbf{c}_0 \end{aligned} \quad (108.1)$$

This exact result can be rendered more compactly (and, at the same time, be made to fall more gracefully upon the eye: no staggered integrals) if we introduce the “chronological product operator” \mathcal{P} , which acts on products of non-commuting objects $\mathbb{A}(t_1)\mathbb{B}(t_2)\cdots\mathbb{Z}(t_n)$ by placing them in the order

(factor with latest argument) \cdot (factor with next latest) \cdots (earliest)

Thus

$$\mathcal{P}\{\mathbb{A}(\tau)\mathbb{B}(\sigma)\} \equiv \begin{cases} \mathbb{A}(\tau)\mathbb{B}(\sigma) & \text{if } \tau > \sigma \\ \mathbb{B}(\sigma)\mathbb{A}(\tau) & \text{if } \tau < \sigma \end{cases}$$

and we are enabled to write (note what’s happened to the upper limits)

$$\begin{aligned} \mathbf{c}(t) &= \left\{ \mathbb{I} - \lambda \frac{i}{\hbar} \int_0^t \mathbb{W}(\tau) d\tau + \left(\lambda \frac{i}{\hbar}\right)^2 \frac{1}{2!} \int_0^t \int_0^t \mathcal{P}\{\mathbb{W}(\tau)\mathbb{W}(\sigma)\} d\sigma d\tau \right. \\ &\quad \left. - \left(\lambda \frac{i}{\hbar}\right)^3 \frac{1}{3!} \int_0^t \int_0^t \int_0^t \mathcal{P}\{\mathbb{W}(\tau)\mathbb{W}(\sigma)\mathbb{W}(\rho)\} d\rho d\sigma d\tau + \cdots \right\} \mathbf{c}_0 \\ &\equiv \mathcal{P} \exp \left\{ -\lambda \frac{i}{\hbar} \int_0^t \mathbb{W}(\tau) d\tau \right\} \mathbf{c}_0 \end{aligned} \quad (108.2)$$

These last manipulations are merely cosmetic, but widely encountered.

The results achieved thus far are exact, but not terribly useful as they stand except in favorable special cases.³⁷ The theory becomes an *approximation scheme* when, in service of enhanced tractability, one *truncates the series* ... which means that in place of (108.1) we write

$$\mathbf{c}(t) = \left\{ \mathbb{I} - \lambda \frac{i}{\hbar} \int_0^t \mathbb{V}(\tau) d\tau \right\} \mathbf{c}_0 + \cdots \quad (109)$$

In the exact theory we had $\sum_n |c_n(t)|^2 = 1$, which is sacrificed when we truncate. But the damage done is readily seen to be always of higher order than the order in which we are working, so can be ignored.

In 2-dimensional quantum mechanics (104) becomes

$$|\psi\rangle_t = c_1 e^{-i\omega_1 t} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_2 e^{-i\omega_2 t} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

³⁷ Suppose, for example, that $\mathbb{V}(t)$ is in fact *constant*. Then (108.2) gives

$$\mathbf{c}(t) = \exp \left\{ -\lambda \frac{i}{\hbar} \mathbb{V} t \right\} \mathbf{c}_0$$

and we find ourselves doing what amounts to an odd kind of time-*independent* perturbation theory. Ambitious readers will find that tracing the details which lead “from here to there” is a rewarding challenge.

with $|c_1|^2 + |c_2|^2 = 1$, the perturbed Hamiltonian acquires (in the unperturbed eigenbasis) the representation

$$\mathbb{H} = \hbar \begin{pmatrix} \omega_1 & 0 \\ 0 & \omega_2 \end{pmatrix} + \lambda \begin{pmatrix} V_{11}(t) & V_{12}(t) \\ V_{21}(t) & V_{22}(t) \end{pmatrix}$$

and (106) reads

$$i\hbar \frac{d}{dt} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \lambda \begin{pmatrix} V_{11}(t) & V_{12}(t)e^{-i\omega t} \\ V_{21}(t)e^{+i\omega t} & V_{22}(t) \end{pmatrix} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}$$

with $\omega \equiv \omega_2 - \omega_1$. So in leading approximation we (according to (109)) have

$$\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \lambda \frac{i}{\hbar} \int_0^t \begin{pmatrix} V_{11}(\tau) & V_{12}(\tau)e^{-i\omega\tau} \\ V_{21}(\tau)e^{+i\omega\tau} & V_{22}(\tau) \end{pmatrix} d\tau \right\} \begin{pmatrix} c_1(0) \\ c_2(0) \end{pmatrix}$$

which in the textbooks³⁸ is, in a variety of special cases, used to illuminate a remarkable variety of fundamental physical processes.

Textbook accounts of time-dependent perturbation theory tend to mask its simple essence, which I would like to try here to expose. Let the Schrödinger equation $\{\mathbf{H}_0 + \lambda\mathbf{V}(t)\}|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle$ be written

$$\{i\hbar\frac{\partial}{\partial t} - \mathbf{H}_0\}|\psi\rangle = \lambda\mathbf{V}(t)|\psi\rangle$$

Use the shift rule $\{i\hbar\frac{\partial}{\partial t} - \mathbf{H}_0\} = e^{-\frac{i}{\hbar}\mathbf{H}_0 t} \cdot i\hbar\frac{\partial}{\partial t} \cdot e^{+\frac{i}{\hbar}\mathbf{H}_0 t}$ to obtain

$$i\hbar\frac{\partial}{\partial t}|c\rangle = \lambda\mathbf{W}(t)|c\rangle \quad (110.1)$$

with $|c\rangle \equiv e^{+\frac{i}{\hbar}\mathbf{H}_0 t}|\psi\rangle$ and $\mathbf{W}(t) \equiv e^{+\frac{i}{\hbar}\mathbf{H}_0 t} \cdot \mathbf{V}(t) \cdot e^{-\frac{i}{\hbar}\mathbf{H}_0 t}$. From the latter definition it follows that

$$i\hbar\frac{\partial}{\partial t}\mathbf{W} = -[\mathbf{H}_0, \mathbf{W}] \quad (110.2)$$

By unitary transformation we have moved from the Schrödinger picture to an instance of the “interaction picture:”³⁹ the unperturbed Hamiltonian moves observables around, while the perturbation \mathbf{V} (which by the adjustment just mentioned has become \mathbf{W}) moves the state vector. Our toy theory has (because of the diagrammatic possibilities made thus available; see again Figure 3) emphasized the importance of the density operator as a state-representation device, and in that connection we notice that

$$\mathbf{C} \equiv |c\rangle\langle c| = e^{+\frac{i}{\hbar}\mathbf{H}_0 t} \cdot |\psi\rangle\langle\psi| \cdot e^{-\frac{i}{\hbar}\mathbf{H}_0 t}$$

³⁸ See, for example (and especially), Griffiths’ Chapter 9, or L. E. Ballentine, *Quantum Mechanics* (1990); L. I. Schiff, *Quantum Mechanics* (3rd edition 1968), pp. 279–289.

³⁹ See Chapter 0, p. 19, footnote 12.

moves by the law

$$i\hbar \frac{\partial}{\partial t} \mathbf{C} = \lambda[\mathbf{W}(t), \mathbf{C}]$$

which in 2×2 representation becomes

$$i\hbar \frac{\partial}{\partial t} \mathbb{C} = \lambda[\mathbb{W}(t), \mathbb{C}]$$

with

$$\mathbb{C} = \frac{1}{2}(\mathbb{I} + \hat{\mathbf{c}} \cdot \boldsymbol{\sigma})$$

This result places us in position to comprehend and depict the perturbed motion of $|\psi\rangle$ by watching the motion of the real unit 3-vector $\hat{\mathbf{c}}$.

Abrupt/slow system adjustments. Dynamical systems—whether classical or quantum mechanical—with time-dependent Hamiltonians are systems with non-conserved energy

$$\partial H / \partial t \neq 0 \implies \text{energy non-conservation}$$

and it is that circumstance (loss of an “integral of the motion”) that makes their theory relatively difficult to discuss, except in favorable special cases. We have discussed a perturbation theory designed to handle cases of the form

$$\text{Hamiltonian} = \text{constant term} + \text{small excursion term}$$

We turn now to discussion of a pair of “favorable cases” which acquire their tractability not from a presumption that the excursion is “small” (in typical applications it won’t be) but from the presumption that

$$H_{\text{initial}} \longrightarrow H_{\text{final}} \quad \text{is either} \quad \begin{cases} \text{abrupt, or} \\ \text{very slow} \end{cases}$$

The former is much easier to discuss. Look, for example, to the classical oscillator

$$H(x, p; t) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2(t)x^2 \quad \text{with} \quad \omega^2(t) = \begin{cases} \omega_1^2 & : t < 0 \\ \omega_2^2 & : t > 0 \end{cases}$$

If the motion can be described $x(t) = A \cos \omega_1 t$ when $t < 0$ then necessarily $x(t) = A \cos \omega_2 t$ when $t > 0$, the “splice condition” being $x(0) = A$, $p(0) = 0$. The oscillator moves with conserved energy $E_1 = \frac{1}{2}m\omega_1^2 A^2$ at times prior to $t = 0$, and with different conserved energy

$$E_2 = E_1 + \frac{1}{2}m(\omega_2^2 - \omega_1^2)A^2$$

at subsequent times.

Or, within the 2-dimensional toy theory, suppose it to be the case that

$$\mathbb{H}(t) = \begin{cases} \hbar\{\omega_{01}\mathbb{I} + \omega_1 \hat{\mathbf{h}}_1 \cdot \boldsymbol{\sigma}\} & : t < 0 \\ \hbar\{\omega_{02}\mathbb{I} + \omega_2 \hat{\mathbf{h}}_2 \cdot \boldsymbol{\sigma}\} & : t > 0 \end{cases}$$

Then $\hat{\boldsymbol{\psi}}$ —which comes to us from the density matrix $|\psi\rangle\langle\psi| = \frac{1}{2}\{\mathbb{I} + \hat{\boldsymbol{\psi}}\cdot\boldsymbol{\sigma}\}$ —

twirls conically about $\begin{cases} \hat{\boldsymbol{h}}_1 \text{ with angular frequency } 2\omega_1 \text{ when } t < 0 \\ \hat{\boldsymbol{h}}_2 \text{ with angular frequency } 2\omega_2 \text{ when } t > 0 \end{cases}$

as illustrated in Figure 3. At negative times the density matrix has at every instant the form $|\psi\rangle\langle\psi| = \frac{1}{2}\{\mathbb{I} + (\hat{\boldsymbol{h}}_1 \cos \alpha + \hat{\boldsymbol{g}} \sin \alpha)\cdot\boldsymbol{\sigma}\}$ with $\hat{\boldsymbol{g}} \perp \hat{\boldsymbol{h}}_1$, so the expected energy, as computed from $\text{tr}\{|\psi\rangle\langle\psi| \mathbb{H}_1\}$, is given therefore by

$$E_1 = \hbar(\omega_{01} + \cos \alpha \cdot \omega_1) = \begin{cases} \hbar(\omega_{01} + \omega_1) & : \quad \alpha = 0 \\ \hbar(\omega_{01} - \omega_1) & : \quad \alpha = \frac{\pi}{2} \end{cases}$$

At positive times we have

$$E_2 = \hbar(\omega_{02} + \cos \beta \cdot \omega_2) = \begin{cases} \hbar(\omega_{02} + \omega_2) & : \quad \beta = 0 \\ \hbar(\omega_{02} - \omega_2) & : \quad \beta = \frac{\pi}{2} \end{cases}$$

where β is the angle which $\boldsymbol{\psi}$ (twirling about $\hat{\boldsymbol{h}}_1$) and $\hat{\boldsymbol{h}}_2$ happen to subtend at $t = 0$. The simple geometry of the situation is illustrated in Figures 4 & 5.⁴⁰

More interesting in many respects is the physics that results when $\mathbf{H}(t)$ changes not suddenly, but very slowly. Look again to the classical system

$$H(x, p; t) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2(t)x^2$$

or perhaps to the “gently transported oscillator”

$$H(x, p; t) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2[x - a(t)]^2$$

If the t-dependence were suppressed then the dynamical phase point $\{x(t), p(t)\}$ would trace an ellipse, with intercepts $\{\pm\sqrt{eE/m\omega^2}, \pm\sqrt{2mE}\}$ and area given therefore by

$$\text{area} = \oint p dx = 2\pi E/\omega \quad (111)$$

One can show by simple argument (but more informatively by an argument that proceeds with the aid of “action and angle variables” from Hamilton-Jacobi theory)⁴¹ that

$$E(t)/\omega(t) = \text{constant in the “adiabatic approximation”} \quad (112)$$

But Planck gave us

$$\text{area} = nh \quad : \quad n = 1, 2, 3, \dots$$

which historically supplied $E_n = n\hbar\omega$ but might now be used to support an expectation that

$$n = E(t)/\hbar\omega(t) \text{ is an adiabatic invariant} \quad (113)$$

⁴⁰ For more elaborate discussion, and reference to some pioneering work by Pauli, see pp. 292–295 in Schiff.³⁸

⁴¹ See CLASSICAL MECHANICS (1983), pp. 412–421 for details, references and historical remarks.

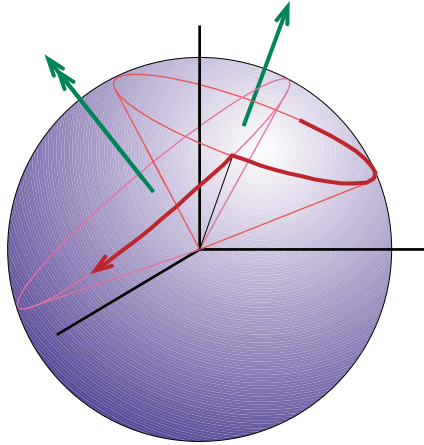


FIGURE 4: The 3-vector ψ twirls about the axis defined by \mathbb{H}_1 , but at $t = 0$ the old Hamiltonian is abruptly replaced by \mathbb{H}_2 (\rightarrow is replaced by $\rightarrow\rightarrow$).

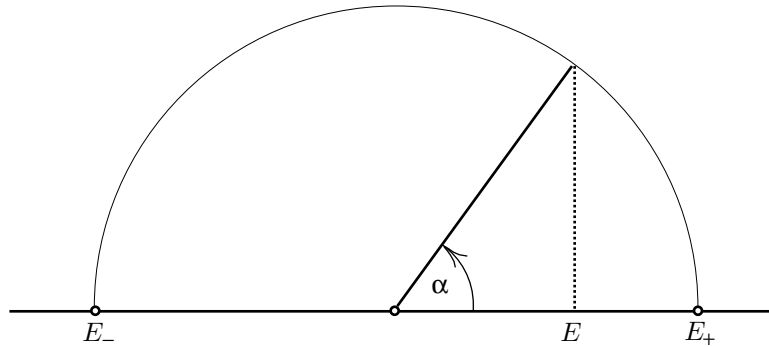


FIGURE 5: Illustration of the simple relationship

$$E = \hbar(\omega_0 + \omega \cos \alpha)$$

between the expected energy of a system in state ψ and the apex angle of the cone traced by ψ . The system is in energy eigenstate $|+\rangle$ when ψ is parallel to \mathbf{h} (i.e., when $\alpha = 0$), and in state $|-\rangle$ when antiparallel.

The “old quantum mechanics” leads, in other words, to the expectation that a system (here an oscillator) which begins in the n^{th} quantum state will, under adiabatic deformation, *remain* in the n^{th} quantum state. The classical basis for this expectation is illustrated in Figure 6. See §3.1 in Max Jammer’s *Conceptual Development of Quantum Mechanics* (1966) for a fascinating account of the important role played by the “Adiabatic Principle” in the transition from old quantum theory to the modern quantum mechanics of 1926. The placement of

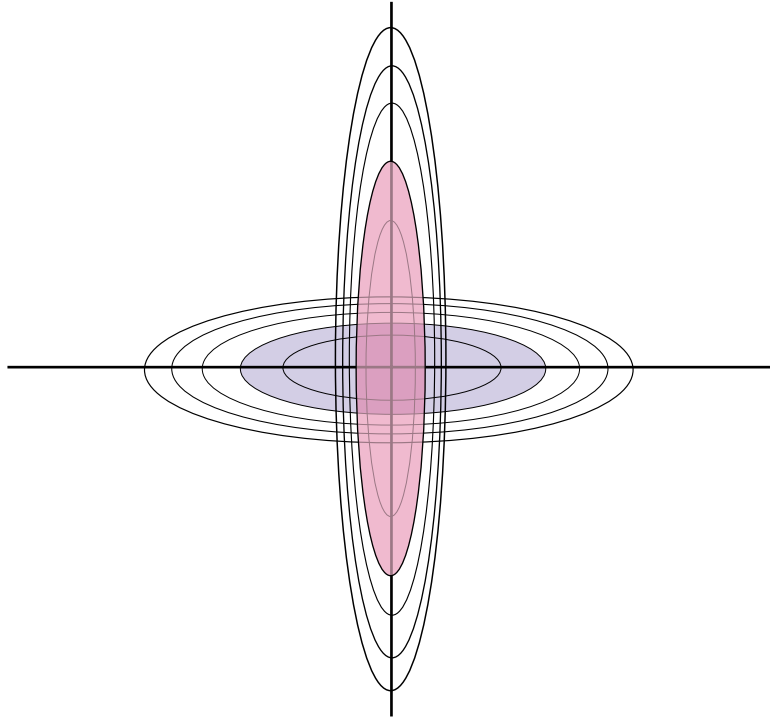


FIGURE 6: *The classical harmonic oscillator Hamiltonian inscribes isoenergetic ellipses on phase space. Temporal modification of the Hamiltonian (such as might be achieved by lending t -dependence to the spring constant) causes deformation of the associated elliptical orbits. An oscillator moves initially on the undeformed E -ellipse. In adiabatic approximation the modified system will be found to be tracing an ellipse of the same area, from which it follows that*

$$\begin{aligned} \text{work done on oscillator} &= E_{\text{final}} - E_{\text{initial}} \\ &= \frac{\omega_{\text{final}} - \omega_{\text{initial}}}{\omega_{\text{initial}}} \cdot E_{\text{initial}} \end{aligned}$$

that old idea *within* the modern theory was worked out by Fermi & Persico,⁴² and in greater detail by Born & Fock.⁴³ Griffiths devotes his §10.1 to the

⁴² E. Fermi & F. Persico, “Il principio della adiabatiche e la nozione de forza vivo nella nuova meccanica ondulatoria,” *Lincei Rend.* **4**, 452 (1926).

⁴³ M. Born & V. Fock, “Beweis des Adiabatenatzes,” *Z. Physik* **51**, 165 (1928). Appended to this paper is a valuable bibliography listing the principal contributions to adiabatic theory in language of the old quantum theory, from Ehrenfest (1916) through Dirac (1925).

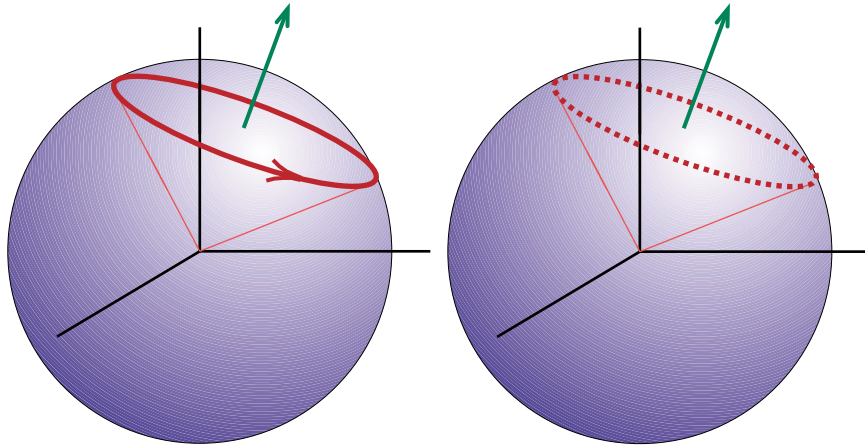


FIGURE 7: The figure on the left refers once again to the dynamical motion of the unit 3-vector ψ representative of a pure state $|\psi\rangle$, on the presumption that the Hamiltonian \mathbf{H}_0 is time-independent. The figure on the right refers to a population of pure states such as would be produced if $\psi(t)$ were sampled at times $t = n(\text{period})/N$ ($n = 1, 2, \dots, N$). Individual elements of the population circulate, but the population as a whole is time-independent. The “ergodic hypothesis” speaks to the equivalence of the two modes of averaging.

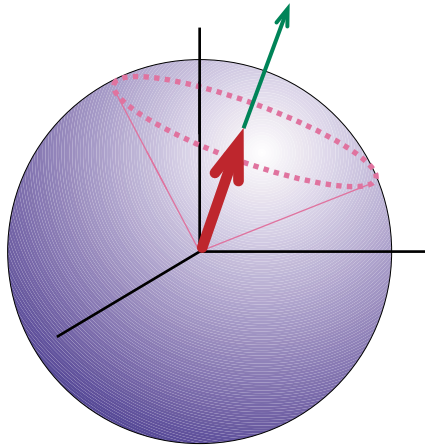


FIGURE 8: Representation of the mixed state which might have been constructed by time-averaging, but might equally well have resulted from averaging over the steady population shown at right in the preceding figure. Note that the steady red arrow representative of the mixture is parallel to the green arrow representative of the time-independent Hamiltonian.

subject, and an especially valuable discussion can be found in Schiff.³⁸ My own approach to the points at issue has been designed to exploit diagrammatic resources special to the two-state theory.

Figures 7–10 describe the plan of attack. The Hamiltonian

$$\mathbb{H}(t) = \hbar\{\omega_0(t)\mathbb{I} + \omega(t)\hat{\mathbf{h}}(t)\cdot\boldsymbol{\sigma}\} \quad (114)$$

interpolates between $\mathbb{H}_0 \equiv \mathbb{H}(t_0)$ and $\mathbb{H}_1 \equiv \mathbb{H}(t_1)$. The unit 3-vector $\boldsymbol{\psi}(t)$ serves by $\frac{1}{2}\{\mathbb{I} + \boldsymbol{\psi}(t)\cdot\boldsymbol{\sigma}\}$ to describe the projector onto the dynamical pure state $|\psi_t\rangle$. At times prior to t_0 the vector $\boldsymbol{\psi}(t)$ has been tracing a cone with apex angle α and spin-axis $\hat{\mathbf{h}}$. Time-averaging over a period (or equivalently: averaging over the ring-ensemble shown on the right in Figure 7) yields the mixed state described by the time-independent density matrix

$$\rho \equiv \frac{1}{\tau} \int_0^\tau |\psi_t\rangle dt \langle\psi_t| = \frac{1}{2}\{\mathbb{I} + \boldsymbol{\rho}\cdot\boldsymbol{\sigma}\} \quad (115)$$

where $\boldsymbol{\rho} = \boldsymbol{\psi}_\parallel = \cos\alpha \cdot \hat{\mathbf{h}}$. It is the time-independence of ρ that makes it, in comparison to $|\psi_t\rangle\langle\psi_t|$, such an attractive thing to watch. What we want to show is that

$$\boldsymbol{\rho}(t) = \cos\alpha \cdot \hat{\mathbf{h}}(t) \quad (116)$$

persists even when \mathbb{H} is subjected to slow adjustment, and that the value of $\cos\alpha$ remains constant. Such a result (see Figures 9 & 10) would entail that

$$\hbar \cos\alpha = \frac{\langle E - E_0 \rangle(t)}{\omega(t)} \quad \text{is adiabatically invariant} \quad (117)$$

and so would be neatly consistent with our classical experience. To expose most simply the mathematical essence of the issue before us, and to minimize the width of the chasm which might separate formalism from physical intuition, I will, in fact, revert to the language of classical mechanics, looking now in closer detail to a system to which passing reference has already been made.¹⁷

SYMMETRIC CHARGED TOP IN A SLOWLY WANDERING MAGNETIC FIELD

A rigid body—in effect, a “top”—spins with angular momentum \mathbf{S} about its center of mass. The top is assumed to be “symmetric” in the sense that its principal moments of inertia (relative to the center of mass) are equal. The top is assumed, moreover, to be made of some non-conductive material, and to be uniformly charged. It has, therefore, a magnetic moment $\boldsymbol{\mu} = g\mathbf{S}$, which in the presence of an impressed magnetic field \mathbf{B} contributes a term $\boldsymbol{\mu}\cdot\mathbf{B}$ to the energy of the system, so the Hamiltonian becomes

$$H = \frac{1}{2(\text{moment of inertia})} \mathbf{S}\cdot\mathbf{S} + \boldsymbol{\mu}\cdot\mathbf{B} = aS^2 + \omega \mathbf{a}\cdot\mathbf{S}$$

where a is a dimensioned constant, $\omega = gB$ bears the dimensions of a frequency, and \mathbf{a} is a dimensionless unit vector. From the Poisson bracket theory upon

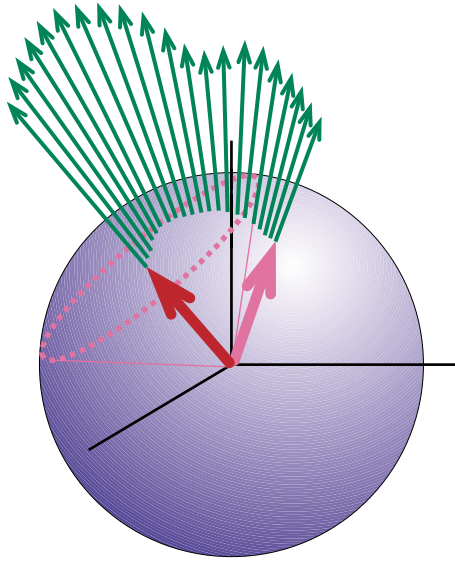


FIGURE 9: *An external agent slowly modifies the Hamiltonian:*

$$\mathbf{H}_0 \xrightarrow{\mathbf{H}(t)} \mathbf{H}_1$$

as represented by the sequenced green arrows (of which not only the direction but also the length is variable). It is claimed that in adiabatic approximation the arrow representative of the mixture remains parallel to the Hamiltonian arrow, and is of constant length. The mixed state is, in effect, “transported rigidly, without internal deformation or sloshing.”

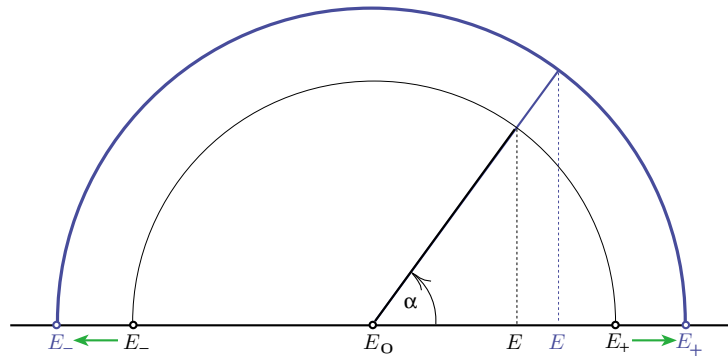


FIGURE 10: *Adiabatic adjustment of the Hamiltonian generally alters both the natural frequency $\omega = (E_+ - E_-)/\hbar$ and the expected energy $\langle E \rangle$, but in such a way that the angle α (which is to say: the entropy of the mixture) remains constant.*

which we based (0–50) we know that

$$\begin{aligned} [S_1, S_2] &= S_3, & [S_2, S_3] &= S_1, & [S_3, S_1] &= S_2 \\ [S_1, S^2] &= [S_2, S^2] = [S_3, S^2] &= 0 \end{aligned}$$

from which it follows that

$$\frac{d}{dt} S^2 = -[H, S^2] = 0 \quad : \quad S^2 \equiv \mathbf{S} \cdot \mathbf{S} \text{ is a constant of the motion}$$

and

$$\begin{aligned} \frac{d}{dt} \mathbf{S} &= -[H, \mathbf{S}] \\ &= \boldsymbol{\omega} \mathbf{a} \times \mathbf{S} = \boldsymbol{\omega} \mathbb{A} \mathbf{S} \quad \text{with} \quad \mathbb{A} \equiv \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix} \end{aligned}$$

Immediately

$$\mathbf{S}(t) = e^{\boldsymbol{\omega} \mathbb{A} t} \mathbf{S}(0)$$

where $\mathbb{R}(t) \equiv e^{\boldsymbol{\omega} \mathbb{A} t}$ is the rotation matrix that describes “twirling about the \mathbf{a} -axis with angular velocity $\boldsymbol{\omega}$.” The motion of the spin vector \mathbf{S} is therefore precessional, as illustrated on the left in Figure 7. Introducing

$$\mathbf{S}_{\parallel} = (\mathbf{S} \cdot \mathbf{a}) \mathbf{a} \quad : \quad \text{component of } \mathbf{S} \text{ parallel to } \mathbf{a} \quad (118)$$

we see that

$$\frac{d}{dt} \mathbf{S}_{\parallel} = \boldsymbol{\omega} (\mathbf{S} \cdot \mathbf{a}) \mathbf{a} \times \mathbf{a} = \mathbf{0}$$

\mathbf{S}_{\parallel} is a constant of the motion, and so in particular is its length $S_{\parallel} = (\mathbf{S} \cdot \mathbf{a})$.

If we assign arbitrary time-dependence to the *strength* of the magnetic field $\boldsymbol{\omega} \mapsto \boldsymbol{\omega}(t)$ then the preceding line of argument gives

$$\frac{d}{dt} \mathbf{S} = \boldsymbol{\omega}(t) \mathbb{A} \mathbf{S} \implies \mathbf{S}(t) = e^{\mathbb{A} \int_0^t \boldsymbol{\omega}(s) ds} \mathbf{S}(0) \quad (119)$$

The conservation of S^2 , \mathbf{S}_{\parallel} and S_{\parallel} is unaffected by such an adjustment.

Now assign arbitrary time-dependence also to the *direction* of the magnetic field; i.e., let $\mathbf{a} \mapsto \mathbf{a}(t)$ wander in some prescribed way on the surface of the unit sphere. Our time-dependent Hamilton has become

$$H(t) = a S^2 + \boldsymbol{\omega}(t) \mathbf{a}(t) \cdot \mathbf{S} \quad (120)$$

\uparrow would be pointless to deposit time-dependence here,
 since this term is dynamically inconsequential

Borrowing an idea from (108.2) we might in place of (119) write

$$\frac{d}{dt} \mathbf{S} = \boldsymbol{\omega}(t) \mathbb{A}(t) \mathbf{S} \implies \mathbf{S}(t) = \mathcal{P} \left\{ e^{\int_0^t \boldsymbol{\omega}(s) \mathbb{A}(s) ds} \right\} \mathbf{S}(0) \quad (121)$$

but the expression on the right is hardly more than a fancy name for a heavy computational program; it is, except in favorable special cases, uninformative as it stands. It is, however, evident that $[H(t), S^2] = 0$; however complicated the motion of $\mathbf{S}(t)$ may have become, the constancy of $S^2 = \mathbf{S}(t) \cdot \mathbf{S}(t)$ has been preserved.

Look now to the motion of \mathbf{S}_{\parallel} , which has become an observable with a *time-dependent definition*

$$\mathbf{S}_{\parallel} \equiv (\mathbf{S} \cdot \mathbf{a}(t)) \mathbf{a}(t) : \text{component of } \mathbf{S} \text{ instantaneously parallel to } \mathbf{a}(t)$$

so to describe the dynamical motion of \mathbf{S}_{\parallel} we must write

$$\frac{d}{dt} \mathbf{S}_{\parallel} = -[H(t), \mathbf{S}_{\parallel}] + \frac{\partial}{\partial t} \mathbf{S}_{\parallel} \quad (122)$$

The first term on the right vanishes as before, but if we write $\mathbf{b} \equiv \frac{d}{dt} \mathbf{a}$ then we have

$$\frac{d}{dt} \mathbf{S}_{\parallel} = \mathbf{0} + (\mathbf{S} \cdot \mathbf{b}) \mathbf{a} + (\mathbf{S} \cdot \mathbf{a}) \mathbf{b}$$

Similarly (or arguing from the result just obtained, with the aid of $\mathbf{a} \cdot \mathbf{b} = 0$, which follows upon differentiation of $\mathbf{a} \cdot \mathbf{a} = 1$)

$$\frac{d}{dt} S_{\parallel} = (\mathbf{S} \cdot \mathbf{b}) = (\mathbf{b} \cdot \mathbf{S}_{\perp}) \quad (123)$$

and it is upon implications of the latter equation that we will concentrate. From (123) and the established fact that S^2 is conserved it follows immediately that

$$S_{\parallel}(t) = S_{\parallel}(0) + \underbrace{\int_0^t b(u) \sqrt{S^2 - S_{\parallel}^2(u)} \cos \vartheta(u) du}_{\text{bounded by } \pm S \int_0^t b(u) \cos \vartheta(u) du}$$

where $\vartheta(t)$ refers to the angle instantaneously subtended by $\mathbf{S}_{\perp}(t)$ and $\mathbf{b}(t)$:

$$\vartheta(t) = \int_0^t \omega(s) ds + \left\{ \begin{array}{l} \text{relatively small correction term arising from} \\ \text{the geometry of the curve traced by } \mathbf{a}(t) \end{array} \right.$$

Our objective is to establish that under weak hypotheses

$$S_{\parallel}(t) = S_{\parallel}(0) \text{ for all } t \text{ in the adiabatic limit} \quad (124)$$

To expose most simply the meaning of the preceding assertion, and the mechanism at work, I look first to a simplified model:

Suppose $a(t)$ ramps linearly from a_0 to a_1 in time T :

$$a(t) = \begin{cases} a_0 & : t \leq 0 \\ a_0 + (a_1 - a_0)t/T & : 0 \leq t \leq T \\ a_1 & : T \leq t \end{cases}$$

Then

$$b(t) \equiv \dot{a}(t) = \begin{cases} 0 & : t \leq 0 \\ (a_1 - a_0)/T \equiv b & : 0 \leq t \leq T \\ 0 & : T \leq t \end{cases}$$

The constant $b \downarrow 0$ as $T \uparrow \infty$, but in such a way that $\int_0^T b(u) du$ remains dilationally invariant. Suppose additionally that $\omega(t)$ ramps linearly from ω_0 to ω_1 in time T :

$$\omega(t) = \begin{cases} \omega_0 & : t \leq 0 \\ \omega_0 + (\omega_1 - \omega_0)t/T & : 0 \leq t \leq T \\ \omega_1 & : T \leq t \end{cases}$$

Then

$$\vartheta(t) = \int_0^t \omega(s) ds = \omega_0 t + \frac{1}{2}(\omega_1 - \omega_0)t^2/T \quad : \quad 0 \leq t \leq T$$

and (ask *Mathematica* for the details) $\int \cos \vartheta(u) du$ can be described in terms of the so-called ‘‘Fresnel integrals’’⁴⁴

$$C(t) \equiv \int_0^t \cos \frac{1}{2}\pi u^2 du \quad \text{and} \quad S(t) \equiv \int_0^t \sin \frac{1}{2}\pi u^2 du$$

Look to a concrete case: let b assume unit value in the case $T = 10$ (therefore $b = \frac{1}{2}$ in the case $T = 20$, $b = \frac{1}{4}$ in the case $T = 40$, etc.), and let $\omega_1 = 2\omega_0$ with $\omega_0 = 2\pi$, giving $\vartheta(t) = 2\pi t + \pi t^2/T$. Then

$$\int_0^t b(u) \cos \vartheta(u) du = \begin{cases} \int_0^t \cos(2\pi u + \frac{1}{10}\pi u^2) du = \sqrt{\frac{5}{1}} \left\{ C\left(\frac{t+10}{\sqrt{5}}\right) - C\left(\frac{10}{\sqrt{5}}\right) \right\} \\ \frac{1}{2} \int_0^t \cos(2\pi u + \frac{1}{20}\pi u^2) du = \sqrt{\frac{5}{2}} \left\{ C\left(\frac{t+20}{\sqrt{10}}\right) - C\left(\frac{20}{\sqrt{10}}\right) \right\} \\ \frac{1}{4} \int_0^t \cos(2\pi u + \frac{1}{40}\pi u^2) du = \sqrt{\frac{5}{4}} \left\{ C\left(\frac{t+40}{\sqrt{20}}\right) - C\left(\frac{40}{\sqrt{20}}\right) \right\} \\ \downarrow \\ 0 \text{ asymptotically} \end{cases}$$

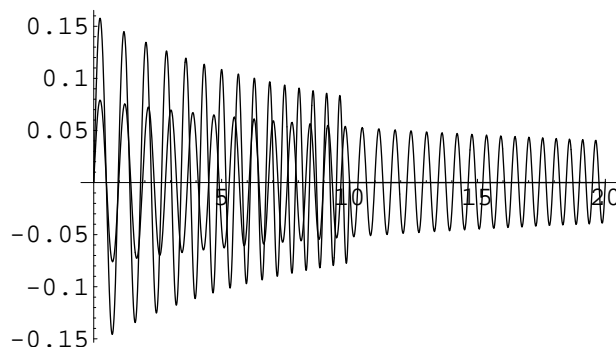
with consequences which are illustrated in Figure 11.

The preceding discussion is not so restrictively special as it might appear. For we might use the values assumed by $a(t)$ and $\omega(t)$ at times

$$t_n \equiv t_0 + n(T - t_0) \quad : \quad n = 1, 2, \dots, N$$

to construct *spline approximants* to those functions; since between consecutive nodal times t_n and t_{n+1} the approximants are in fact ramped, the preceding

⁴⁴ Good discussion of these important functions can be found in Spanier & Oldham, *An Atlas of Functions* (1987), Chapter 39; Gradshteyn & Ryzhik, §8.25; or Abramowitz & Stegun, §7.3.

FIGURE 11: *Superimposed graphs of*

$$\int_0^t \cos(2\pi u + \frac{1}{10}\pi u^2) du \quad : \quad 0 \leq t \leq 10$$

$$\int_0^t \frac{1}{2} \cos(2\pi u + \frac{1}{20}\pi u^2) du \quad : \quad 0 \leq t \leq 20$$

remarks pertain—internodal sector by internodal sector.

The essential point is that the dilation which sends $a(t) \rightarrow A(t) \equiv a(t/k)$ sends $a'(t) \rightarrow A'(t) \equiv \frac{1}{k}a'(t/k)$: we have the previously remarked dilational invariance statement

$$\int_0^{kT} A'(u) du = \int_0^{kT} \frac{1}{k} a'(u/k) du = \int_0^T a'(t) dt = a(T) - a(0)$$

But the introduction of an oscillatory factor which *does not participate* in the dilation serves to *break dilational invariance*

$$\int_0^{kT} A'(u) \cos \omega u du = \int_0^T a'(t) \cos k\omega t dt \neq \int_0^T a'(t) \cos \omega t dt$$

Moreover

$$\lim_{k \rightarrow \infty} \int_0^T a'(t) \cos k\omega t dt = 0 \quad (125)$$

under weak hypotheses which I will not attempt to spell out, but which permit ω also to be endowed with some t -dependence.

So (124) is established: S_{\parallel} is adiabatically invariant, and (since S is unrestrictedly invariant) so also is S_{\perp} . Slow reorientation of the magnetic field “leads the top by its nose” in Griffiths’ phrase. Slow adjustment of the strength of the field has no effect upon the rate of spin, but does affect the rate of precession.

The mathematics pertains with only interpretive change to the quantum theory of two-state systems: adiabatic adjustment of the Hamiltonian (see again Figure 9) leaves unchanged the length of the $\boldsymbol{\psi}_{\parallel}$ vector (and therefore also of the $\boldsymbol{\psi}_{\perp}$ vector). The 3-vector $\boldsymbol{\psi} = \boldsymbol{\psi}_{\parallel} + \boldsymbol{\psi}_{\perp}$ precesses about the momentary $\boldsymbol{\psi}_{\parallel}$ -axis at a rate determined by the momentary “strength” of $\mathbb{H}(t)$. The flying vector $\boldsymbol{\psi}(t)$ “points” (in the sense that $\frac{1}{2}\{\mathbb{I} + \boldsymbol{\psi}(t) \cdot \boldsymbol{\sigma}\}$ projects onto) a flying sequence $|\psi\rangle_t$ of complex 2-vectors which describe the dynamical quantum state of the system. One could (with Griffiths; see his §10.1.3) phrase the argument directly in terms of those state vectors, but then one must live with (and contrive to see the simplicity which lies beyond) the fussy complexity of those $|\psi\rangle$ -vectors (see again (15.3)). In the parallel theory of N -state systems ($N > 2$) there appears to be, in fact, no other way to go,⁴⁵ but it is my experience that even in that enlarged setting our toy theory does serve to *illuminate* what’s going on.

I have previously remarked (see again Figures 7 & 8) that the “flying” component of $\boldsymbol{\psi}(t)$ can be expunged by an averaging process, leaving $\boldsymbol{\psi}_{\parallel}$ as the descriptor of a *mixture*, with density matrix given by

$$\rho = \frac{1}{2}\{\mathbb{I} + \boldsymbol{\psi}_{\parallel} \cdot \boldsymbol{\sigma}\}$$

One might be tempted to interpret what we now know about the adiabatic motion of ρ to mean that “slow transport of a mixture preserves the relative placement of its constituents”—in a word: “generates no internal sloshing”—but to adopt such language entails risk of imputing an objective reality to the notion of “constituent” which we have found to be classically meaningful but quantum mechanically disallowed.

Possibly more useful therefore—or at least more sharply curious—is the observation that the adiabatic invariance of the

$$\text{length of } \boldsymbol{\psi}_{\parallel} = \sqrt{2\text{tr}\rho^2 - 1}$$

can be interpreted⁴⁶ to signify the

$$\text{adiabatic invariance of the entropy of } \rho \tag{126}$$

In thermodynamics one has, by the first law,

$$dU = dQ + dW$$

where dQ (differential “heat injected”) refers to the energy increase which results when a dynamical trajectory is flicked from an isoenergetic surface to one of higher energy (same Hamiltonian), while dW (differential “work done on”) refers to *slow adjustment of the parameters which control the design of the Hamiltonian*. And by the second law

$$dQ = TdS$$

⁴⁵ See Schiff, *Quantum Mechanics* (3rd edition 1968), pp. 289–292.

⁴⁶ See again (22) and (23).

in which sense “adiabatic” ($dQ = 0$) *means* “isentropic” ($dS = 0$). So the quantum mechanical statement (126) conforms very nicely to thermodynamic usage. I find it impossible to think that this confluence of ideas is *merely* verbal, yet must emphasize that on the thermodynamic side of the street essential reference is made to the famously elusive concept of a “thermized state,” while no such notion appears to inhabit the quantum mechanics.

It is interesting in this light to notice that *abrupt* adjustment of the Hamiltonian *followed by re-thermalization of the mixture* (quantum analog of Joule free expansion) in *non-isentropic*, and in fact entails

$$S_{\text{after}} > S_{\text{before}}$$

since (see again Figure 4) $\psi_{\parallel\text{after}}$ is necessarily shorter than $\psi_{\parallel\text{before}}$. It must, however, be emphasized that quantum mechanics—unenriched by any further principle—provides no mechanism by which “re-thermalization” might come about, no indication of how a mixture *acquires* the features of its time-average.

Geometric phase. Let the design of the Hamiltonian $\mathbb{H}(t)$ be adiabatically adjusted (Figure 9) in such a way that at time T it has returned to its *original* design (Figure 12):

$$\mathbb{H}(0) \xrightarrow{\text{adiabatic tour of a loop in parameter space}} \mathbb{H}(T) = \mathbb{H}(0)$$

Then $\hat{\mathbf{h}}(t)$ will trace a closed curve on the unit sphere, which $\psi_{\parallel}(t)$ will track. Initially (i.e., at times $t < 0$) $\psi(t)$ was tracing a circle, and upon completion of the tour (i.e., at times $t > T$) finds itself retracing that same circle, but it will in general be *out of phase with the comparison system which remained at home the whole time*.

Let $\mathbb{H}_{\text{tour}} = \hbar\omega(t)\hat{\mathbf{h}}(t)\cdot\sigma$ describe the system that takes the leisurely tour, and $\mathbb{H}_{\text{home}} = \hbar\omega(t)\hat{\mathbf{h}}\cdot\sigma$ the system that stays home and twiddles its thumb $\omega(t)$. Take it to be understood that $\hat{\mathbf{h}}(0) = \hat{\mathbf{h}}(T) = \hat{\mathbf{h}}$. By the time the tourist returns to its point of departure the stay-at-home system, according to (54), will have experienced a net precession given by

$$\theta_{\text{home}} = 2 \int_0^T \omega(t) dt$$

The tourist, on the other hand, will be relatively phase-advanced

$$\theta_{\text{tour}} = \theta_{\text{home}} + (\text{spherical area } \Omega \text{ enveloped by the tour}) \quad (127.1)$$

for the non-dynamical, purely geometrical reason described in the caption to Figure 13. Retreating from ψ -language to $|\psi\rangle$ -language, we find (see again (54)) that

$$\text{phase of } |\psi\rangle_{\text{tour}} = \text{phase of } |\psi\rangle_{\text{home}} + \frac{1}{2}\Omega \quad (127.2)$$

where the $\frac{1}{2}$ can be considered to reflect (not a minor mystery, as is sometimes alleged, but simply) the double-valuedness of the $SU(2)$ representation of $O(3)$.

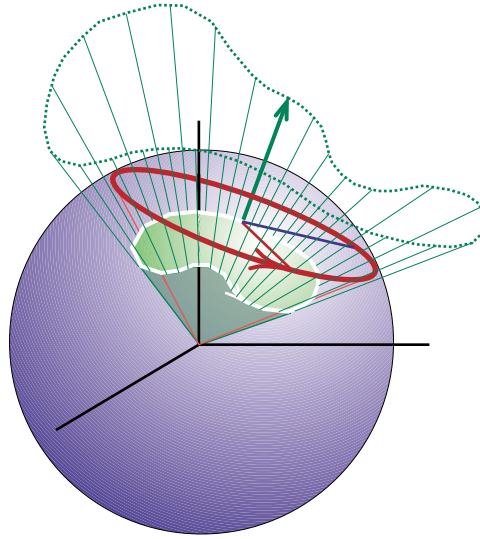


FIGURE 12: Representation the tour taken by $\mathbb{H}_{\text{tour}} = \hbar\omega(t)\hat{\mathbf{h}}(t)\cdot\boldsymbol{\sigma}$, who finally returns home at time $t = T$.

Equations (127) illustrate a point first noted, in a more general quantum mechanical setting, by Michael Berry in 1984.⁴⁷ J. H. Hannay, a colleague of Berry's at the University of Bristol, immediately demonstrated that the "geometrical phase" phenomenon is not intrinsically quantum mechanical, but is present also in classical mechanics (note in this connection that (127.1) could be taken to refer to the adiabatic mechanics of our toy top). It was noticed belatedly that an optical instance of the same phenomenon had been described already by S. Pancharatnam in 1956,⁴⁸ and within a few years the idea had been recognized to have significant applications to topics ranging from gauge field theory to the locomotion of robots and other creatures.⁴⁹

I digress to argue that "geometric phase" had been implicit in the work of mathematicians/physicists/engineers for more than a century by the time Pancharatnam published his paper—since 1854, to be precise, when

- "Stokes' theorem" (known to W^m Thomson (Lord Kelvin) already in 1850) made its first public appearance (as a problem to be solved by Cambridge undergraduates), and
- the "polar planimeter" was invented by Jakob Amsler.

⁴⁷ "Quantal phase factors accompanying adiabatic changes," Proc. Roy. Soc. (London) **A392**, 45 (1984).

⁴⁸ "Generalized theory of interference and its applications," Proceedings of the Indian Academy of Sciences **44**, 247 (1956).

⁴⁹ We move by semi-cyclic manipulation of our shape; i.e., by touring closed curves in high-dimensional "shape-space." For a collection of the classic papers in this young field, see A. Shapere & F. Wilczek, *Geometric Phases in Physics* (1989).

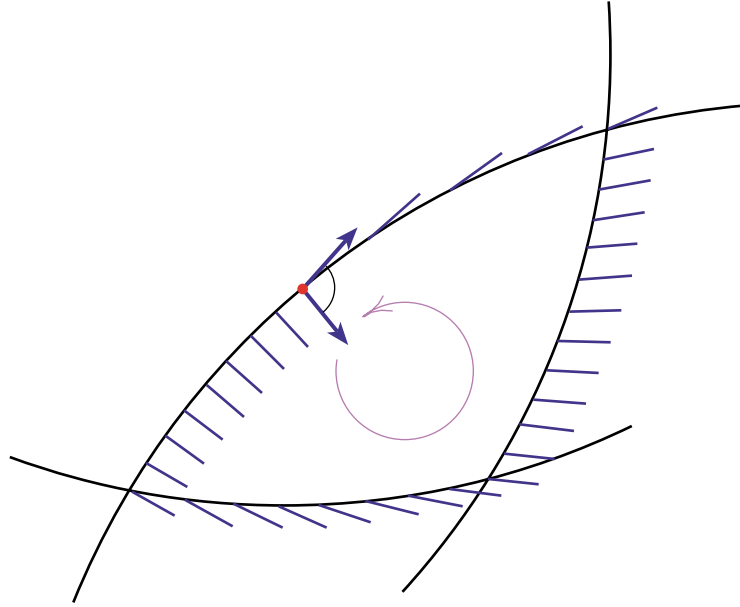


FIGURE 13: A spherical triangle (triangle bounded by geodesic arcs) is inscribed on the surface of a sphere of unit radius R . It has been known since antiquity that

$$\text{area} = R^2 \cdot \underbrace{\{(\text{sum of interior angles}) - \pi\}}_{\text{“spherical excess”}}$$

Of more recent vintage is the discovery that parallel transport of a vector around such curve results in an “angular misalignment” given by that same factor:

$$\begin{aligned} \text{misalignment} &= \text{spherical excess} \\ &= \frac{\text{area}}{R^2} \end{aligned}$$

The latter formula pertains, in fact, to the curves which bound arbitrary regions, by an easy argument based on the observation that such regions can be approximated to any degree of precision by fitting together spherical triangular tiles. Several more sophisticated modes of argument are also available.

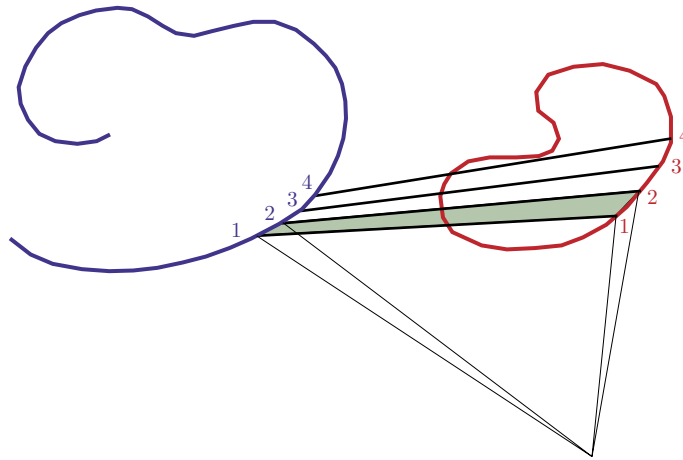


FIGURE 14: What is the area swept out by a rod of length ℓ that moves so that one end lies always on the blue curve \mathcal{C}_0 and the other tours once around the closed loop \mathcal{C} ? What, in other words, is the sum of the areas of the green quadrilaterals? The question presumes that all points of \mathcal{C} lie not greater than ℓ from the nearest point (and not less than ℓ from the most distant point) of \mathcal{C}_0 .

I discuss those developments in reverse order.

Amsler's planimeter⁵⁰ springs from the solution of the problem posed in the preceding figure. A detail is reproduced as Figure 15, for the purpose establishing an elegant mathematical principle, as profound as it is simple. Returning with that principle to the situation illustrated above, we find that

⁵⁰ Jakob Amsler (1823–1912), the son of a Swiss farmer, went to Königsberg to study theology, but was diverted into mathematical physics by influence of Franz Neumann (who figured prominently in the pre-Maxwellian history of electrodynamics, a subject to which Amsler himself also made youthful contributions). In 1851 he accepted a position as teacher in the Gymnasium of Schaffhausen, Switzerland, in order to secure his financial position and to gain time in which to do research. The success of his “polar planimeter” led him to found a firm devoted to the manufacture and sale of precision scientific instruments. Amsler's planimeter was for years used widely by shipbuilders and engineers, and was applied also to the computation of moments of inertia and Fourier coefficients. By the time of his death he had sold 50,000 of the things. Today one can buy digital planimeters which operate on the same principle. Further information concerning Amsler—whom Felix Klein (in the geometry volume of *Elementary Mathematics from an Advanced Standpoint* (1908)) describes somewhat condescendingly as a “mechanic,” though he has only good things to say about Amsler's invention (“highly ingenious and very useful”)—can be found in the *Dictionary of Scientific Biography* (1970).

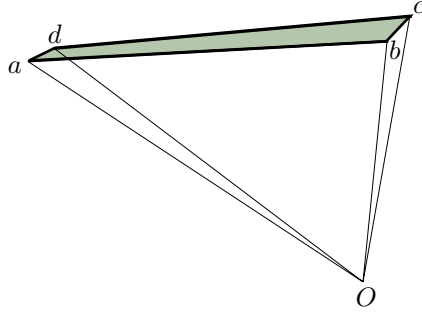


FIGURE 15: Let $(abcd)$ signify the area of the \curvearrowright -oriented green quadrilateral. Introducing an arbitrary reference point O we see that

$$(abcd) = (Oab) + (Obc) + (Ocd) + (Oca)$$

The triangles acquire their orientation from the quadrilateral:

- $\triangle Oab$ is \curvearrowright -oriented, so (Oab) is negative;
- $\triangle Obc$ is \curvearrowright -oriented, so (Obc) is negative;
- $\triangle Ocd$ is \curvearrowright -oriented, so (Ocd) is positive;
- $\triangle Oda$ is \curvearrowright -oriented, so (Oda) is positive.

we are at once able to proceed from

$$\text{swept area} = (1221) + (2332) + (3443) + \dots$$

to

$$\begin{aligned} \text{swept area} = & (O12) + (O22) + (O21) + (O11) \\ & + (O23) + (O33) + (O32) + (O22) \\ & + (O34) + (O44) + (O43) + (O33) \end{aligned}$$

But the terms of mixed color cancel pairwise ($\triangle O22$ and $\triangle O22$ have opposite orientation, so $(O22) + (O22) = 0$, and so on down the line), leaving

$$\begin{aligned} \text{swept area} = & \{(O12) + (O23) + (O34) + \dots\} \\ & - \{(O12) + (O23) + (O34) + \dots\} \\ = & \text{area of region bounded by } \mathcal{C} \\ & - \text{area of region bounded by } \mathcal{C}_0 \end{aligned}$$

But \mathcal{C}_0 bounds *no* area, so we have

$$\text{swept area} = \text{area of the region } \mathcal{R} \text{ bounded by } \mathcal{C}$$

which will be fairly obvious to anyone who has (like me) spent childhood hours contemplating the piston rods of steam locomotives.

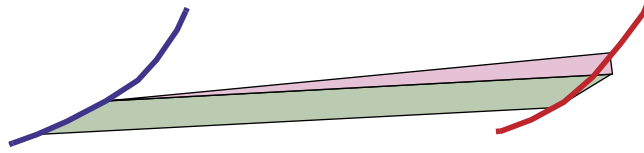


FIGURE 16: A different way to conceptualize the differential area shown in the preceding figure. The green parallelogram has length l and a differential width we will call dw . The area of the wedge is $\frac{1}{2}l^2 d\vartheta$, so the area of the entire shaded region can, in leading order, be described

$$dA = l dw + \frac{1}{2}l^2 d\vartheta$$

Alternatively, we might argue from the preceding figure to the conclusion that

$$\text{swept area} = l \oint dw + \frac{1}{2}l^2 \oint d\vartheta$$

But it is evident that $\oint d\vartheta = 0$, so we have at last the equation which lies at the heart of Amsel’s inspired contrivance:

$$\text{area of the region } \mathcal{R} \text{ bounded by } \mathcal{C} = l \oint dw \quad (128)$$

Given this pretty fact—which Klein holds up as an example of the kind of mathematics that should be presented to school kids—the planimeter almost invents itself; Amsel’s device is shown in Figure 17. The wheel serves as a mechanical integrator.

The point to notice is that the planimeter, upon completion of a circuit, returns home *in an altered state*: the wheel has experienced a phase advance which reflects a geometrical property of the excursion. This I present as a non-dynamical instance of “geometrical phase.”

What has this to do with Stokes’ theorem? Look to the (3-dimensional Cartesian) instance of Stokes theorem which reads

$$\iint_{\mathcal{R}} (\nabla \times \mathbf{A}) \cdot d\mathbf{S} = \oint_{\partial\mathcal{R}} \mathbf{A} \cdot d\mathbf{s}$$

Set

$$\mathbf{A} = \begin{pmatrix} -\frac{1}{2}y \\ +\frac{1}{2}x \\ 0 \end{pmatrix} \implies \nabla \times \mathbf{A} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

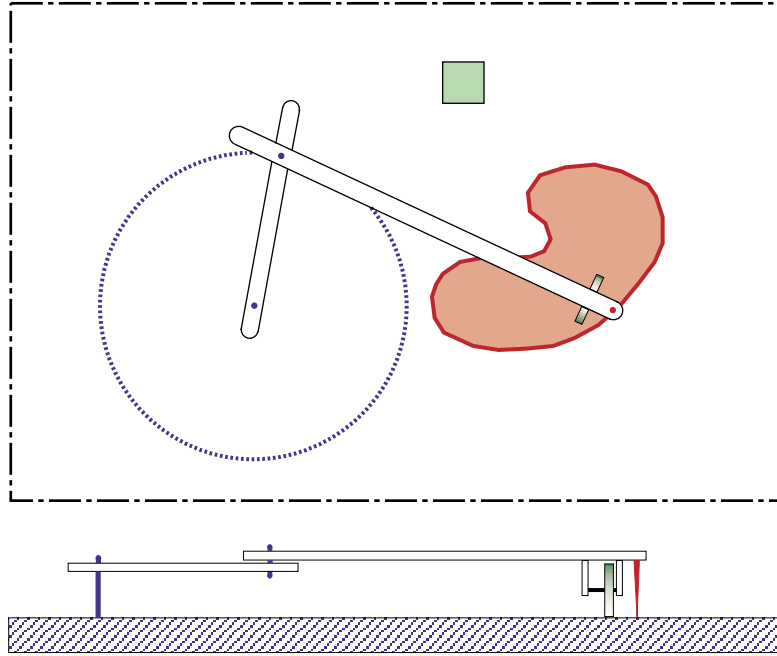


FIGURE 17: Amsel's "polar planimeter." It has been mechanically expedient to take the reference curve \mathcal{C}_0 to be circular. The wheel turns on a threaded axel, so rotation can be read as translation along a vernier. The green square is a "unit area," used to calibrate the device.

and with the aid of

$$d\mathbf{S} = \begin{pmatrix} dydz \\ dzdx \\ dxdy \end{pmatrix} \quad \text{and} \quad d\mathbf{s} = \begin{pmatrix} dx \\ dy \\ dz \end{pmatrix}$$

obtain

$$\iint_{\mathcal{R}} dxdy \equiv \text{area of } \mathcal{R} = \frac{1}{2} \oint (xdy - ydx) \quad (129)$$

Some other ways to say the same thing, each instructive in its own way:

$$\text{area} = \frac{1}{2} \oint \begin{vmatrix} 1 & 0 & 0 \\ 1 & x & y \\ 1 & x+dx & y+dy \end{vmatrix} = \frac{1}{2} \oint r^2 d\theta$$

The essence of the situation is exposed by the elementary observation that the differential form encountered at (129) is "inexact," in the sense that

$$\text{there exists no } f(x, y) \text{ such that } df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy = xdy - ydx$$

In some fields (thermodynamics, most notably) it has become standard to use \bar{d} -notation to register the distinction: one writes

$$\bar{d}f = f_x dx + f_y dy \quad \text{if} \quad \frac{\partial}{\partial x} f_y - \frac{\partial}{\partial y} f_x \neq 0$$

and in the contrary (or “exact”) case writes df . One has

$$\oint df = 0 \quad \text{invariably, but}$$

$$\oint \bar{d}f \neq 0 \quad \text{typically}$$

and observes that $\oint \bar{d}f$ is invariant under “gauge transformations” $\bar{d}f \rightarrow \bar{d}f + dg$.

The terms “inexact” and “anholonomic” refer to the same mathematical circumstance, and *geometrical phase is—in every instance, whatever the context—a manifestation of anholonomy*. One is therefore not surprised to find that the latter term is ubiquitous in the Berry phase literature.⁴⁹

Look back again in this light to Figure 16, were we encounter the equation $dA = \ell dw + \frac{1}{2}\ell^2 d\vartheta$. Given \mathcal{C}_0 and \mathcal{C} , one could in principle work out descriptions of the $dw = w_x dx + w_y dy$ and $d\vartheta = \vartheta_x dx + \vartheta_y dy$ that result from differential advance $(x, y) \rightarrow (x + dx, y + dy)$ along \mathcal{C} . Amsel’s construction hinges of the circumstance that $d\vartheta$ is exact (exploited when we wrote $\oint d\vartheta = 0$), while dw (more properly $\bar{d}w$) is inexact.

It is amusing to note that if you carried a gyro and a pair of accelerometers (integration of their output would yield $x(t)$ and $y(t)$) while walking around a fenced field, you could, upon completion of your hike, use (129) to compute the area of the field . . . without ever venturing onto it. Or more physically: let $x(t)$ and $y(t)$ refer to the periodic motion of a mass m around a closed track. Then

$$2m(\text{area enclosed by track}) = \int_0^{\text{period}} m(xy\dot{y} - y\dot{x}) dt$$

from which a number of interesting conclusions could be drawn. It was Kepler who (in effect) first noticed the implied relation between orbital area and angular momentum.

Return now to the sphere which launched this entire discussion. Tinkering leads me (in the notation of Figure 18) to introduce the vector field

$$\mathbf{A} = \begin{pmatrix} A_r(r, \theta, \phi) \\ A_\theta(r, \theta, \phi) \\ A_\phi(r, \theta, \phi) \end{pmatrix} = \begin{pmatrix} 0 \\ -\phi \frac{1}{2} r \sin \theta \\ -\frac{1}{2} r \cot \theta \end{pmatrix} \quad (130.1)$$

on grounds that, by calculation,

$$\nabla \times \mathbf{A} = \begin{pmatrix} 1 \\ \cot \theta \\ -\phi \sin \theta \end{pmatrix} \quad (130.2)$$

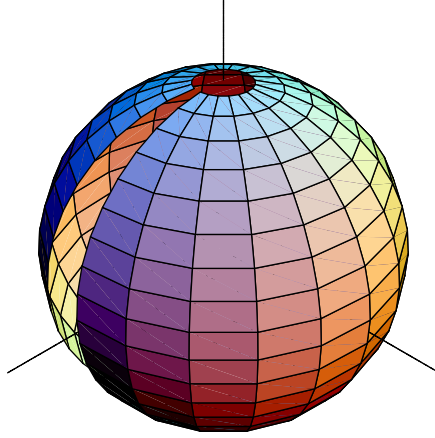


FIGURE 18: We employ spherical coordinates introduced in such a way

$$\begin{aligned} x &= r \sin \theta \cos \phi \\ y &= r \sin \theta \sin \phi \\ z &= r \cos \theta \end{aligned} \quad : \quad \begin{aligned} 0 &< \theta < \pi \\ 0 &\leq \phi < 2\pi \end{aligned}$$

as to render $\{\mathbf{dr}, \mathbf{d\theta}, \mathbf{d\phi}\}$ a righthanded frame. The convention is in agreement with that employed by Griffiths and by Mathematica, whose `<<Calculus\VectorAnalysis\` package can be used to remove the tedium from calculation involving the spherical identities which Griffiths reproduces on the front endboards of his *Introduction to Electrodynamics* (1981/89/99). Notice that θ here signifies not latitude but “co-latitude.” The figure is intended to emphasize that, for purposes of the present discussion, the poles must be carefully avoided, and that also one must be careful not to trip on the multivaluedness of ϕ . We agree to write $\hat{\mathbf{r}}, \hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ —directed as indicated by $\{dr, d\theta, d\phi\}$ —to denote orthonormal unit vectors in that particular element of the “frame field” which is associated with the point $\{r, \theta, \phi\}$.

Surface elements on the sphere can be described

$$\mathbf{dS} = r^2 \sin \theta \, d\theta d\phi \cdot \hat{\mathbf{r}} = \begin{pmatrix} r^2 \sin \theta \, d\theta d\phi \\ 0 \\ 0 \end{pmatrix} \quad (130.3)$$

so if \mathcal{R} does not violate restrictions imposed in the figure, then

$$\text{area of spherical region} = \iint_{\mathcal{R}} (\nabla \times \mathbf{A}) \cdot \mathbf{dS} = \iint_{\mathcal{R}} r^2 \sin \theta \, d\theta d\phi \quad (130.4)$$

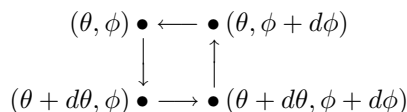
But by Stokes' theorem we expect to have

$$\begin{aligned} \text{area of spherical region} &= \oint_{\partial\mathcal{R}} \mathbf{A} \cdot d\mathbf{s} \quad \text{with} \quad d\mathbf{s} = \begin{pmatrix} 0 \\ r d\theta \\ r \sin \theta d\phi \end{pmatrix} \\ &= -\frac{1}{2} r^2 \oint_{\partial\mathcal{R}} (\phi \sin \theta d\theta + \cos \theta d\phi) \end{aligned} \quad (130.5)$$

which (as I will in a moment demonstrate) is readily established on independent grounds; the effort will supply evidence (if evidence were needed) that *Stokes' theorem works even in non-Euclidean settings*. It is, by the familiar



argument, sufficient to establish that (130.5) pertains accurately to the curves that bound infinitesimal patches:



We find in leading order that

$$\begin{aligned} &-\frac{1}{2} r^2 \oint_{\text{little patch boundary}} (\phi \sin \theta d\theta + \cos \theta d\phi) \\ &= -\frac{1}{2} r^2 \left\{ \phi \sin \theta d\theta + \cos(\theta + d\theta) d\phi - (\phi + d\phi) \sin \theta d\theta - \cos \theta d\phi \right\} \\ &= (\text{first-order terms cancel}) + \frac{1}{2} r^2 \sin \theta d\theta d\phi + \dots \end{aligned}$$

which is precisely the result we sought.⁵¹ We will soon have need of (130).

I turn finally to a discussion motivated by the question: *How might Berry phase be observed?*

Interference effects in quantum mechanics. Generally, we expect to have to use interferometric techniques to detect phase relationships ... at least when they occur in physical contexts that involve superimposable waves (optics, acoustics, wave mechanics). The generic idea is quite simple: one constructs

$$z(\delta) = z_1 + z_2 e^{i\delta} \quad : \quad \text{superimposed complex signals}$$

⁵¹ If, at (130.5), we in place of the co-latitude θ introduce the geographer's latitude $\vartheta \equiv \frac{\pi}{2} - \theta$ then we have

$$-\frac{1}{2} r^2 \oint_{\partial\mathcal{R}} (\phi \sin \theta d\theta + \cos \theta d\phi) = +\frac{1}{2} r^2 \oint_{\partial\mathcal{R}} (\phi \cos \vartheta d\vartheta - \sin \vartheta d\phi)$$

which is encountered in the discussion of Pancharatnam's phase⁴⁸ that can be found in "Ellipsometry" (1999).

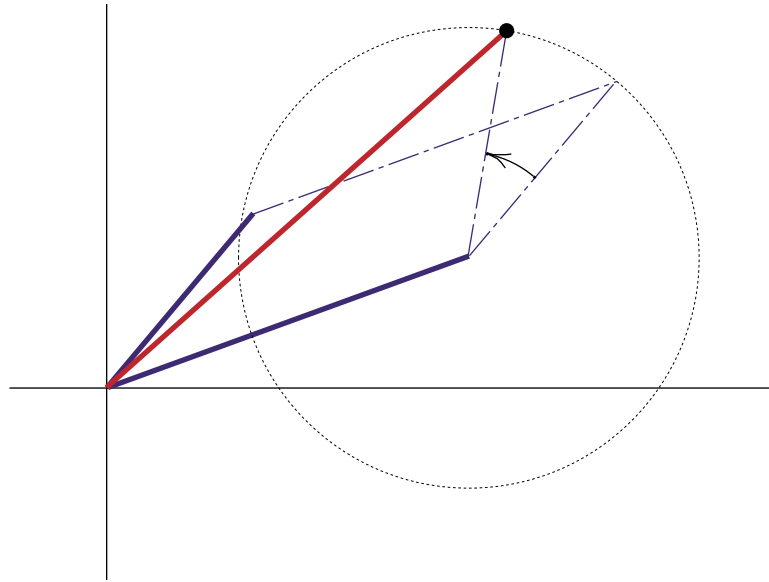


FIGURE 19: Representation of the superposition process

$$z = z_1 + z_2 e^{i\delta}$$

as it is encountered in (say) optics or acoustics. One has interest in the squared modulus of z as the relative phase δ ranges through all values; i.e., as \bullet ranges on the circle. The δ -values which serve to maximize/minimize $|z|^2$ are evident.

and looks to the δ -dependence of $|z(\delta)|^2$, which in optics/acoustics carries an “intensity-like” interpretation. The preceding figure illustrates the simple essence of the matter.

The quantum mechanical situation differs in one simple but characteristic and profoundly important respect (which—unaccountably—the texts typically neglect to mention): a ket vector is not admissible as a state-descriptor unless it has unit norm, so state superposition *must be followed by renormalization*

$$|\psi\rangle = \frac{|\psi_1\rangle + |\psi_2\rangle e^{i\delta}}{\text{normalization factor}} \quad : \quad \text{superimposed quantum states} \quad (131)$$

and it would therefore be senseless to inquire after the δ -dependence of $\langle\psi|\psi\rangle = 1$. To expose the phase-dependence hidden within the design of the superimposed state one must *make a measurement*: one must look (Figure 20) to the δ -dependence of some experimentally convenient *component* of $|\psi\rangle$... which is to say: one must look to how some selected *expectation value* depends upon the relative phase. Recall in this light the design of the two-slit experiment, where one looks to the squared modulus of $\psi(x) \equiv \langle x|\psi\rangle$.

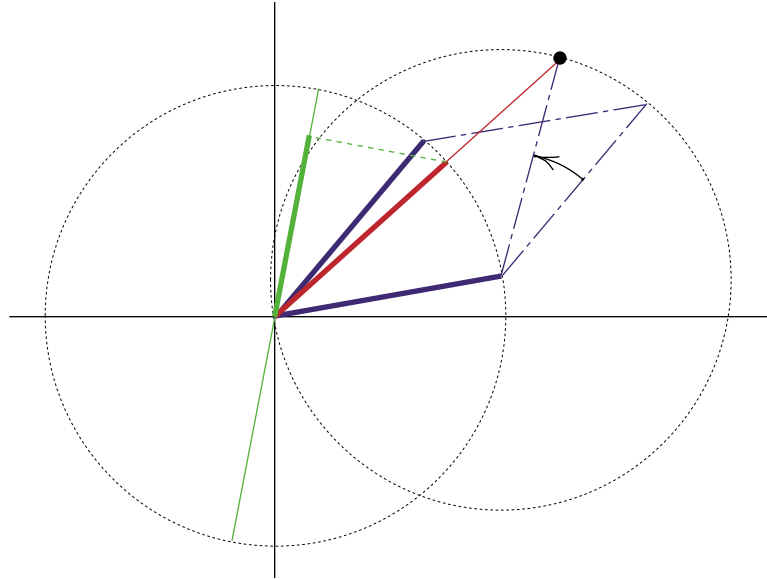


FIGURE 20: Representation of the superposition process

$$|\psi\rangle = \frac{|\psi_1\rangle + |\psi_2\rangle e^{i\delta}}{\text{normalization factor}}$$

as it is encountered in quantum mechanics. The unit value of $\langle\psi|\psi\rangle$ is enforced by fundamental postulate. The phase-dependence of the superimposed state becomes evident only when does a measurement; i.e., when one projects out some arbitrarily selected component of $|\psi\rangle$ —a process to which the green details refer.

Our “toy quantum mechanics” is too impoverished to support a two-slit experiment, but does permit one to inquire after the phase-dependence of expressions of the form $\langle\psi|\mathbf{a}\cdot\boldsymbol{\sigma}|\psi\rangle$ —in spin language: the expected spin in some specified direction. The normalization factor encountered at (131) can be described $\sqrt{\text{norm}}$ with

$$\text{norm} = 2[1 + m \cos(\mu + \delta)]$$

where I have written $\langle\psi_1|\psi_2\rangle \equiv m e^{i\mu}$, with m -notation intended to suggest “mixing.” In this notation we have

$$\langle\psi|\mathbb{A}|\psi\rangle = \frac{\langle\psi_1|\mathbb{A}|\psi_1\rangle + \langle\psi_2|\mathbb{A}|\psi_2\rangle + \langle\psi_1|\mathbb{A}|\psi_2\rangle e^{i\delta} + \langle\psi_2|\mathbb{A}|\psi_1\rangle e^{-i\delta}}{\text{norm}} \quad (132)$$

Berry, however, has contrived a situation in which $|\psi_1\rangle = |\psi_2\rangle$, at least to within the precision of the adiabatic approximation. In that special circumstance⁵²

⁵² Let the shared value of $|\psi_1\rangle$ and $|\psi_2\rangle$ be called $|\Psi\rangle$.

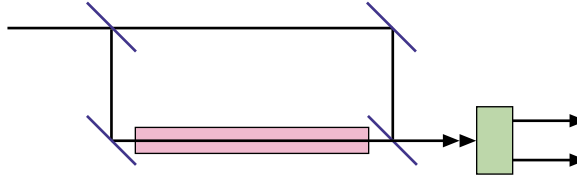


FIGURE 21: Schematic of an interferometer designed to observe Berry's phase. In that application, a prepared state $|\psi_0\rangle$ is resolved into two fractions, of which one proceeds under control of a fixed Hamiltonian to a detector (green), while the other is subjected to an adiabatic adventure (red), such as might be achieved by slow passage through a spatially variable impressed field. The reassembled state presented to the detector (which in two-state theory will register either plus or minus) is the renormalized superposition of $|\psi_1\rangle$ and $|\psi_2\rangle$.

we have

$$|\psi\rangle = \frac{1 + e^{i\delta}}{\sqrt{2(1 + \cos\delta)}} |\Psi\rangle = e^{\frac{1}{2}i\delta} \cdot |\Psi\rangle$$

Relative phase survives here only as an *unphysical phase factor which, in point of principle, no measurement can expose*: we have

$$(\psi|\mathbb{A}|\psi) = (\Psi|\mathbb{A}|\Psi) \quad \text{for all values of } \delta$$

which could, alternatively, have been extracted directly from (132). The surprising conclusion is that, while the interferometer shown above works fine as a detector of *optical* Berry phase,⁵³ it fails quantum mechanically.

Suppose, however, that adiabatic transport carries $|\psi_0\rangle$ to a state $|\psi_2\rangle$ distinct from $|\psi_1\rangle$; i.e., that progress around the loop *remains incomplete* by the time the reassembled state is presented to the detector. Prior to Berry's publication (1984) we might have expected to find

$$|\psi\rangle = \frac{|\psi_1\rangle e^{-i\omega t} + |\psi_2\rangle e^{-i\omega t}}{\sqrt{\text{norm}}} \quad \text{presented to the detector}$$

giving

$$(\psi|\mathbb{A}|\psi) = \frac{(\psi_1|\mathbb{A}|\psi_1) + (\psi_2|\mathbb{A}|\psi_2) + (\psi_1|\mathbb{A}|\psi_2) + (\psi_2|\mathbb{A}|\psi_1)}{\text{norm}}$$

Berry argues that we should in fact expect to have

⁵³ In optics no renormalization factor intrudes to mess things up.

$$|\psi\rangle = \frac{|\psi_1\rangle e^{-i\omega t} + |\psi_2\rangle e^{-i(\omega t + \gamma)}}{\sqrt{\text{norm}}} \quad : \quad \text{Berry phase now included}$$

giving

$$\langle\psi|\mathbb{A}|\psi\rangle = \frac{\langle\psi_1|\mathbb{A}|\psi_1\rangle + \langle\psi_2|\mathbb{A}|\psi_2\rangle + \langle\psi_1|\mathbb{A}|\psi_2\rangle e^{-i\gamma} + \langle\psi_2|\mathbb{A}|\psi_1\rangle e^{+i\gamma}}{\text{norm}}$$

He argues, moreover, that—within the context provided by two-state theory⁵⁴—for loops (*closed arcs*)

$$\begin{aligned} \gamma(\text{loop}) &= \frac{1}{2}(\text{area enclosed by loop}) = -\frac{1}{4} \oint_{\text{loop}} (\phi \sin \theta d\theta + \cos \theta d\phi) \\ &= \oint_{\text{loop}} \mathbf{A} \cdot d\mathbf{s} \end{aligned}$$

We are tempted to assert that for *open arcs*

$$\gamma(\text{open arc}) = \int_{\text{arc}} \mathbf{A} \cdot d\mathbf{s}$$

but confront the circumstance that \mathbf{A} is determined *only to within a gauge transformation*. In my account⁵¹ of the very closely related problem studied by Pancharatnam it emerges that a physical consideration (intensity maximization) permits one to discover the “right gauge.” In the present context a geometrical principle (parallel transport) might plausibly be pressed into similiar service . . . but to pursue that remark all the way to a theory of the “observable Berry phase for open arc transport” would take me too far afield. I have a bear by the tail, but must for now release my hold and run for protective cover, with this final remark:

It is interesting that the Berry phase presented by our toy top poses *no* observational difficulty, while observation of the formally identical “transported 2-state quantum system” is proscribed for at the most fundamental of quantum mechanical reasons.

⁵⁴ See again Figure 12 and (130.5).