Chapter 1

Basics of Kinematics and Dynamics

1.1 Brief review of basic kinematics

In quantum mechanics, the physical quantities are symbolized by linear operators A, B, ... that act on vectors — elements of a vector space, that is, not physical vectors in the three-dimensional space of our experience. We often speak of *observables* when referring to these linear operators, which is a sloppy use of terminology because, more precisely, the operators are the mathematical symbols that represent the physical "observable" properties, or simply "observables". The vectors they act on come in two kinds: ket vectors $\bigl|\ldots\bigr\rangle$ and bra vectors $\bigl\langle\ldots\bigr|$ (or right vectors and left vectors). The mathematical operation of hermitian conjugation, or as the physicists say: "taking the adjoint", relates them to each other,

$$\bigl\langle\ldots\bigr|^\dagger = \bigl|\ldots\bigr\rangle\,, \quad \bigl|\ldots\bigr\rangle^\dagger = \bigl\langle\ldots\bigr|\,, \tag{1.1.1}$$

where it is understood that the ellipses indicate identical sets of quantum numbers, which serve as the labels that identify the kets and bras.

A measurement of an observable A yields one of the possible measurement results $a_1, a_2, a_3, \ldots$, which are complex numbers in general. If it is known that a measurement of A will surely return the value a_j, then we say that the quantum mechanical system is in the state $\bigl|a_j\bigr\rangle$,

$$\bigl|a_j\bigr\rangle : \quad A\bigl|a_j\bigr\rangle = \bigl|a_j\bigr\rangle a_j\,, \tag{1.1.2}$$

which — mathematically speaking — is an eigenvector equation, here: an eigenket equation. There is also the corresponding eigenbra equation,

$$\bigl\langle a_j\bigr|A = a_j\bigl\langle a_j\bigr|\,. \tag{1.1.3}$$

The measurement results a_j is the eigenvalue of A in both the eigenket equation (1.1.2) and the eigenbra equation (1.1.3).

Under these circumstances, namely: the system is in state $|a_j\rangle$, the probability of finding the value b_k upon measuring observable B is given by

$$\mathrm{prob}(a_j \to b_k) = \left|\langle b_k|a_j\rangle\right|^2 . \tag{1.1.4}$$

The complex number $\langle b_k|a_j\rangle$ is the *probability amplitude* to measurement result b_k in state $|a_j\rangle$; its absolute square is the associated probability. This amplitude has all properties that are required of an inner product, in particular

$$\begin{aligned} |a\rangle = |a'\rangle + |a''\rangle : &\quad \langle b|a\rangle = \langle b|a'\rangle + \langle b|a''\rangle , \\ |a\rangle = |\alpha\rangle\lambda : &\quad \langle b|a\rangle = \langle b|\alpha\rangle\lambda , \end{aligned} \tag{1.1.5}$$

where λ is any complex number, and

$$\begin{aligned} &\langle a|b\rangle = \langle b|a\rangle^* , \\ &\langle a|a\rangle \geq 0 \quad \text{with “=” only if } |a\rangle = 0 . \end{aligned} \tag{1.1.6}$$

In mathematical terms, these properties characterize the kets as elements of an inner-product space or *Hilbert space* (David Hilbert). There is a Hilbert space for the bras as well, related to that of the kets by hermitian conjugation.

The mathematical property $\langle a|b\rangle = \langle b|a\rangle^*$ has a very important physical implication, namely the statement that the two probabilities $\mathrm{prob}(a \to b)$ and $\mathrm{prob}(b \to a)$ are equal,

$$\mathrm{prob}(a_j \to b_k) = \mathrm{prob}(b_k \to a_j) . \tag{1.1.7}$$

The probabilities for these related, yet different physical processes,

$$\begin{aligned} \text{on the left: } &\text{ probability of finding } b_k \text{ if } a_j \text{ is the case,} \\ \text{on the right: } &\text{ probability of finding } a_j \text{ if } b_k \text{ is the case,} \end{aligned}$$

are therefore always equal. There is, of course, a lot of circumstantial evidence for the validity of this fundamental symmetry, but — elementary situations aside — there does not seem to be a systematic direct experimental test.

Different measurement results for the same quantity A exclude each other. This physical fact is expressed by the mathematical statement of orthogonality,

$$\langle a_j | a_k \rangle = 0 \quad \text{if} \quad a_j \neq a_k\,, \quad \text{or} \quad j \neq k\,. \tag{1.1.8}$$

Inasmuch as $\mathrm{prob}(a_j \to a_j)$ is the probability that a control measurement confirms what is known, we must have

$$\mathrm{prob}(a_j \to a_j) = 1\,, \tag{1.1.9}$$

so that $\langle a_j | a_j \rangle = 1$ must hold. Thus

$$\langle a_j | a_k \rangle = \begin{Bmatrix} 0 & \text{if} & j \neq k \\ 1 & \text{if} & j = k \end{Bmatrix} = \delta_{jk}\,, \tag{1.1.10}$$

where we employ Leopold Kronecker's δ symbol for a compact presentation of this statement of orthonormality.

Each measurement has a result. This physical fact has a mathematical analog as well, namely the completeness relation

$$\sum_j |a_j\rangle\langle a_j| = 1 \quad (= \text{identity operator}). \tag{1.1.11}$$

As an immediate consequence we note that the eigenket equation

$$A|a_j\rangle = |a_j\rangle a_j\,, \tag{1.1.12}$$

multiplied by $\langle a_j|$ on the right, and then summed over j, yields

$$A = \sum_j |a_j\rangle a_j \langle a_j|\,, \tag{1.1.13}$$

the so-called spectral decomposition of A. We get the spectral decomposition of $A^\dagger$,

$$A^\dagger = \sum_j |a_j\rangle a_j^* \langle a_j|\,, \tag{1.1.14}$$

by making use of the familiar product rule for the adjoint,

$$\Big(|1\rangle\lambda\langle 2|\Big)^\dagger = |2\rangle\lambda^*\langle 1| \tag{1.1.15}$$

for any ket $|1\rangle$, complex number λ, and bra $\langle 2|$.

An apparatus that measures the physical property A, in fact measures all functions of A,

$$f(A)|a_j\rangle = |a_j\rangle f(a_j)\,, \tag{1.1.16}$$

because you just evaluate the function $f(a_j)$ after finding the value a_j. Put differently, it is our free choice whether we want to call the result a_j or $f(a_j)$ when the jth outcome is found. It follows that the spectral decomposition of $f(A)$ is given by

$$f(A) = \sum_j |a_j\rangle f(a_j)\langle a_j| \,. \tag{1.1.17}$$

It makes consistent sense to regard $f(A)$ thus defined as an operator-valued function of operator A. For example, consider the simple function A^2,

$$\begin{aligned} f(A) = A^2 &= \Bigl(\sum_j |a_j\rangle a_j \langle a_j|\Bigr)^2 \\ &= \sum_{j,k} (a_j) a_j \underbrace{\langle a_j|a_k\rangle}_{=\delta_{jk}} a_k \langle a_k| \\ &= \sum_j |a_j\rangle a_j^2 \langle a_j| = \sum_j |a_j\rangle f(a_j)\langle a_j| \,, \end{aligned} \tag{1.1.18}$$

indeed. Similarly, you easily show that it works for other powers of A, then for all polynomials, then for all functions that can be approximated by, or related to, polynomials, and so forth. But what is really needed to ensure that $f(A)$ is well defined, is that the numerical function $f(a_j)$ is well defined for all eigenvalues a_j. As a consequence, two functions of A are the same if they agree for all a_j:

$$f(A) = g(A) \quad \text{if} \quad f(a_j) = g(a_j) \quad \text{for all } j \,. \tag{1.1.19}$$

As an example consider the following exercise.

1-1 Operator A has eigenvalues 0, +1, and −1. Write

$$f(A) = \mathrm{e}^{\mathrm{i}\frac{2\pi}{3}A}$$

as a polynomial in A,

$$f(A) = c_0 + c_1 A + c_2 A^2 \,,$$

with numerical coefficients c_0, c_1, c_2, after first showing that such a polynomial is the most general function of A.

We recall that operators of two particular kinds play special roles in quantum mechanics. These are the *hermitian* operators, named in honor of Charles Hermite, which are equal to their adjoints,

$$\text{hermitian:} \quad H = H^\dagger\,, \tag{1.1.20}$$

and the *unitary* operators,

$$\text{unitary:} \quad U = \left(U^\dagger\right)^{-1}, \quad UU^\dagger = 1 = U^\dagger U\,, \tag{1.1.21}$$

for which the inverse equals the adjoint.

1-2 Consider the spectral decomposition (1.1.17) and show that $f(a_j)$ is real if $f(A)$ is hermitian, and that $|f(a_j)| = 1$ if $f(A)$ is unitary. That is: all eigenvalues of a hermitian operator are real; all eigenvalues of a unitary operator are phase factors.

Several observables A, B, C, ... have their state kets $|a_j\rangle$, $|b_k\rangle$, $|c_l\rangle$, ... with probability amplitudes $\langle a_j|b_k\rangle$, $\langle b_k|c_l\rangle$, $\langle c_l|a_j\rangle$, ... These amplitudes are not independent, however, but must obey the composition law

$$\langle a_j|b_k\rangle = \sum_l \langle a_j|c_l\rangle\langle c_l|b_k\rangle\,, \tag{1.1.22}$$

which we recognize to be a consequence of the completeness of the $|c_l\rangle$ kets. The self-suggesting interpretation

> "First there is $|b_k\rangle$, eventually $|a_j\rangle$, and in between $|c_l\rangle$,
> but we do not know which C value was actually the case
> and so we must sum over all c_l."

is *wrong*. The assumption of an actual C value at an intermediate stage leads to logical contradictions.

There are two main reasons for this. First, the l sum is not a sum of probabilities but of probability amplitudes. The resulting statement about probabilities reads

$$\begin{aligned}\mathrm{prob}(b_k \to a_j) &= \sum_l \mathrm{prob}(b_k \to c_l)\,\mathrm{prob}(c_l \to a_j) \\ &\quad + \sum_{l\neq l'} \langle c_l|b_k\rangle\langle b_k|c_{l'}\rangle\langle c_{l'}|a_j\rangle\langle a_j|c_l\rangle \end{aligned} \tag{1.1.23}$$

where the appearance of the $l \neq l'$ terms signifies the possible occurrence of quantum mechanical interferences. Only if the $l \neq l'$ sum happens to vanish, the interpretation above is justified.

Second, there is the fundamental aspect that some observables exclude each other mutually. This feature of quantum mechanics has no true analog in classical physics. In particular, there are pairs of complementary observables. The pair A, B is complementary if the probabilities

$$\operatorname{prob}(a_j \to b_k) = \left|\langle b_k | a_j \rangle\right|^2 \tag{1.1.24}$$

do not depend on the quantum numbers a_j and b_k. Physically speaking: If the system is prepared in a state in which the value of A is known, that is: we can predict with certainty the outcome of a measurement of property A, then all measurement results are equally probable in a measurement of B, and vice versa.

Now, if D were the complementary partner of C, we would have

$$\begin{aligned}\langle a_j | b_k \rangle &= \sum_l \langle a_j | c_l \rangle \langle c_l | b_k \rangle \\ &= \sum_m \langle a_j | d_m \rangle \langle d_m | b_k \rangle \,. \end{aligned} \tag{1.1.25}$$

The wrong interpretation after (1.1.22) would then imply that both C and D have definite, though unknown, values at the intermediate stage, because the two sums are on equal footing. But this is utterly impossible.

Given operator A with its (nondegenerate) eigenvalues a_j and the kets $|a_j\rangle$, can we always find another observable, B, such that A, B are a pair of complementary observables? Yes, we can by an explicit construction, for which

$$|b_k\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} |a_j\rangle \, \mathrm{e}^{\mathrm{i}\frac{2\pi}{N} jk} \tag{1.1.26}$$

is the basic example. (More about this shortly.) It is here assumed that we deal with a quantum degree of freedom for which there can be at most N different values for any measurement.

We need to verify that the B states of this construction are orthonormal,

$$\begin{aligned}\langle b_k | b_l \rangle &= \frac{1}{N} \sum_{j,m} \mathrm{e}^{-\mathrm{i}\frac{2\pi}{N} jk} \underbrace{\langle a_j | a_m \rangle}_{=\delta_{jm}} \mathrm{e}^{\mathrm{i}\frac{2\pi}{N} lm} \\ &= \frac{1}{N} \sum_{j=1}^{N} \mathrm{e}^{-\mathrm{i}\frac{2\pi}{N} j(k-l)} \\ &= \delta_{kl} \,, \quad \text{indeed.}\end{aligned} \tag{1.1.27}$$

Then

$$B = \sum_k \big|b_k\big\rangle b_k \big\langle b_k\big| \tag{1.1.28}$$

with any convenient choice for the nondegenerate B values b_k will do. By construction, we have

$$\left|\big\langle a_j\big|b_k\big\rangle\right|^2 = \left|\frac{1}{\sqrt{N}}\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}jk}\right|^2 = \frac{1}{N} \tag{1.1.29}$$

so that A, B are a complementary pair, indeed. We note that this property is actually primarily a property of the two bases of kets (and bras) associated with the pair of observables. A common terminology is to call such pairs of bases "mutually unbiased".

In passing, it is worth mentioning that there are quite basic questions about such mutually unbiased basis pairs that do not have a known answer. Quantum kinematics is not a closed subject but still the object of research despite the profound understanding that has resulted from eight decades of intense studies.

1.2 Bohr's principle of complementarity

1.2.1 *Complementary observables*

We consider the situation where we can have at most N different outcomes of a measurement, that is there are no more than N mutually orthogonal states available. One such set is composed of all the eigenstates of some observable A, with the respective kets denoted by $\big|a_1\big\rangle$, $\big|a_2\big\rangle$, $\ldots$, $\big|a_N\big\rangle$. Another set is obtained immediately by a cyclic permutation, effected by the unitary operator U,

$$\begin{aligned}
\big|a_1\big\rangle &\longrightarrow \big|a_2\big\rangle = U\big|a_1\big\rangle\,,\\
\big|a_2\big\rangle &\longrightarrow \big|a_3\big\rangle = U\big|a_2\big\rangle\,,\\
&\ \vdots\\
\big|a_N\big\rangle &\longrightarrow \big|a_1\big\rangle = U\big|a_N\big\rangle\,,
\end{aligned} \tag{1.2.1}$$

generally

$$U\big|a_j\big\rangle = \big|a_{j+1}\big\rangle\,, \tag{1.2.2}$$

where the index is to be understood modulo N, so that $|a_{N+1}\rangle = |a_1\rangle$, for example. Applying U twice shifts the index by 2,

$$U^2|a_j\rangle = |a_{j+2}\rangle\,, \tag{1.2.3}$$

and N such shifts amount to doing nothing,

$$U^N|a_j\rangle = |a_{j+N}\rangle = |a_j\rangle\,. \tag{1.2.4}$$

Accordingly, we have

$$U^N = 1 \tag{1.2.5}$$

so that U is a unitary operator of period N.

The eigenvalues of U must obey the same equation

$$u^N = 1 \quad \text{if} \quad U|u\rangle = |u\rangle u \tag{1.2.6}$$

for which

$$u_k = \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}k}\,, \quad k = 1, 2, \ldots, N \tag{1.2.7}$$

are the possible solutions, all of which occur. We can, therefore, write the equation for U also in the factorized form

$$\begin{aligned} U^N - 1 &= (U - u_1)(U - u_2)\cdots(U - u_N) \\ &= \prod_{k=1}^{N}(U - u_k)\,. \end{aligned} \tag{1.2.8}$$

Let us isolate one factor,

$$U^N - 1 = (U - u_k)\prod_{l(\neq k)}(U - u_l)\,, \tag{1.2.9}$$

and note the following

$$\prod_{l(\neq k)}(U - u_l)|u_m\rangle = \begin{cases} 0 & \text{if} \quad m \neq k\,, \\ |u_k\rangle\alpha & \text{if} \quad m = k\,, \end{cases} \tag{1.2.10}$$

with some complex number $\alpha \neq 0$, because one of the factors $U - u_l \to u_m - u_l$ vanishes if $m \neq k$ but all are nonzero if $m = k$. We conclude that the operator acting on $|u_m\rangle$ in (1.2.10) is a numerical multiple of $|u_k\rangle\langle u_k|$, the projector on the kth eigenstate. This product of $N-1$ factors is a polynomial in U of degree $N-1$, for which we can also give another construction. We apply the familiar identity

$$\begin{aligned} X^N - 1 &= (X-1)\big(1 + X + X^2 + \cdots + X^{N-1}\big) \\ &= (X-1)\sum_{l=0}^{N-1} X^l \end{aligned} \tag{1.2.11}$$

to $X = U/u_k$:

$$\begin{aligned} U^N - 1 = (U/u_k)^N - 1 &= (U/u_k - 1)\sum_{l=0}^{N-1} (U/u_k)^l \\ &= (U/u_k - 1)\sum_{l=1}^{N} (U/u_k)^l \end{aligned} \tag{1.2.12}$$

where the first step exploits $u_k^N = 1$ and the last step makes use of $(U/u_k)^0 = 1 = (U/u_k)^N$. Now, for $U \to u_k$ the sum equals N, and so we arrive at

$$|u_k\rangle\langle u_k| = \frac{1}{N}\sum_{l=1}^{N} (U/u_k)^l\,. \tag{1.2.13}$$

1-3 Verify explicitly that

$$\frac{1}{N}\sum_{l=1}^{N} (U/u_k)^l |u_m\rangle = |u_k\rangle\delta_{km}\,.$$

1-4 Verify directly that $\sum_{l=1}^{N} (U/u_k)^l$ is hermitian.

So we know the eigenvalues of U and have an explicit construction for the projectors on those eigenvalues as a function of U itself, and now we find out how the eigenkets of U are related to the original set of kets $|a_j\rangle$. We begin with

$$|u_k\rangle\langle u_k|a_N\rangle = \frac{1}{N}\sum_{l=1}^{N} u_k^{-l}\,\underbrace{U^l|a_N\rangle}_{=|a_l\rangle} \tag{1.2.14}$$

and then apply $\langle a_N |$ from the left,

$$\langle a_N | u_k \rangle \langle u_k | a_N \rangle = \left| \langle u_k | a_N \rangle \right|^2 = \frac{1}{N} u_k^{-N} = \frac{1}{N} \,. \tag{1.2.15}$$

We make use of the freedom to choose the overall complex phase of $|u_k\rangle$ and agree on

$$\langle u_k | a_N \rangle = \frac{1}{\sqrt{N}} \,, \tag{1.2.16}$$

with the consequence

$$\begin{aligned} |u_k\rangle &= \frac{1}{\sqrt{N}} \sum_{l=1}^{N} |a_l\rangle u_k^{-l} \\ &= \frac{1}{\sqrt{N}} \sum_{l=1}^{N} |a_l\rangle \, \mathrm{e}^{-\mathrm{i}\frac{2\pi}{N}kl} \end{aligned} \tag{1.2.17}$$

and, after taking the adjoint,

$$\langle u_k | = \frac{1}{\sqrt{N}} \sum_{l=1}^{N} \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}kl} \langle a_l | \,. \tag{1.2.18}$$

We read off that

$$\langle u_k | a_l \rangle = \frac{1}{\sqrt{N}} \, \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}kl} \,, \tag{1.2.19}$$

of which the $l = N$ case is (1.2.16).

We have now a second set of bras and kets, for which we can repeat the story of cyclic permutations, effected by the unitary operator V,

$$\begin{aligned} \langle u_k | V &= \langle u_{k+1} | \,, \\ \langle u_k | V^2 &= \langle u_{k+2} | \,, \\ &\;\;\vdots \\ \langle u_k | V^N &= \langle u_k | \,. \end{aligned} \tag{1.2.20}$$

In full analogy with what we did above for U, we conclude here that

$$V^N = 1 : \quad V \text{ is unitary with period } N \,, \tag{1.2.21}$$

that the eigenvalues of V are $v_l = \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}l}$, that the projector on the lth eigenvalue is

$$\big|v_l\big\rangle\big\langle v_l\big| = \frac{1}{N}\sum_{k=1}^{N}\left(V/v_l\right)^k, \tag{1.2.22}$$

and are led to

$$\big\langle u_N\big|v_l\big\rangle\big\langle v_l\big| = \frac{1}{N}\sum_{k=1}^{N} v_l^{-k}\big\langle u_k\big| \tag{1.2.23}$$

and then

$$\big\langle u_N\big|v_l\big\rangle\big\langle v_l\big|u_N\big\rangle = \left|\big\langle u_N\big|v_l\big\rangle\right|^2 = \frac{1}{N}\,. \tag{1.2.24}$$

Here, too, we choose $\big\langle u_N\big|v_l\big\rangle = \dfrac{1}{\sqrt{N}}$ and establish

$$\big\langle v_l\big| = \frac{1}{\sqrt{N}}\sum_{k=1}^{N}\mathrm{e}^{-\mathrm{i}\frac{2\pi}{N}kl}\big\langle u_k\big| \tag{1.2.25}$$

as well as

$$\big|v_l\big\rangle = \frac{1}{\sqrt{N}}\sum_{k=1}^{N}\big|u_k\big\rangle\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}kl}\,. \tag{1.2.26}$$

Can we continue like this and get more and more sets of kets? No! Because the kets $\big|v_l\big\rangle$ are identical with the kets $\big|a_l\big\rangle$, see

$$\begin{aligned}\big|v_l\big\rangle &= \sum_{k=1}^{N}\big|u_k\big\rangle\underbrace{\frac{1}{\sqrt{N}}\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}kl}}_{=\langle u_k|a_l\rangle} \\ &= \underbrace{\left(\sum_k\big|u_k\big\rangle\big\langle u_k\big|\right)}_{=1}\big|a_l\big\rangle = \big|a_l\big\rangle\,. \end{aligned} \tag{1.2.27}$$

We have been led back to the initial set of kets.

In summary, we have a pair of reciprocally defined unitary operators,

$$U\big|v_l\big\rangle = \big|v_{l+1}\big\rangle\,,\quad \big\langle u_k\big|V = \big\langle u_{k+1}\big|\,, \tag{1.2.28}$$

which are of period N,

$$U^N = 1\,, \quad V^N = 1\,. \tag{1.2.29}$$

Their eigenstates are related to each other by the probability amplitudes

$$\langle u_k | v_l \rangle = \frac{1}{\sqrt{N}}\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}kl}\,, \tag{1.2.30}$$

so that the probabilities

$$\bigl|\langle u_k | v_l \rangle\bigr|^2 = \frac{1}{N} \tag{1.2.31}$$

do not depend on k and l, which tells us that U and V are a pair of complementary observables.

Being complementary partners of each other, U and V should have a simple commutation relation. We find it by considering the effect of UV and VU upon $\langle u_k|$,

$$\begin{aligned} \langle u_k|UV &= u_k\langle u_k|V = u_k\langle u_{k+1}|\,,\\ \langle u_k|VU &= \langle u_{k+1}|U = u_{k+1}\langle u_{k+1}|\,, \end{aligned} \tag{1.2.32}$$

so that

$$\langle u_k|VU = \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}}u_k\langle u_{k+1}| = \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}}\langle u_k|UV \tag{1.2.33}$$

since

$$u_{k+1} = u_k\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}}\,. \tag{1.2.34}$$

The completeness of the bras $\langle u_k|$ now implies

$$\begin{aligned} UV &= \mathrm{e}^{-\mathrm{i}\frac{2\pi}{N}}VU\,,\\ VU &= \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}}UV\,, \end{aligned} \tag{1.2.35}$$

and their generalization to

$$\begin{aligned} U^kV^l &= \mathrm{e}^{-\mathrm{i}\frac{2\pi}{N}kl}V^lU^k\,,\\ V^lU^k &= \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}kl}U^kV^l \end{aligned} \tag{1.2.36}$$

is immediate. These are the *Weyl commutation relations* for the complementary pair U, V, named in honor of Hermann K. H. Weyl.

1.2.2 *Algebraic completeness*

Now, all functions of U are polynomials of degree $N-1$, and all functions of V are also such polynomials. Therefore, a general function of both U and V is always of the form

$$f(U,V) = \sum_{k,l=0}^{N-1} f_{kl} U^k V^l = \sum_{k,l=1}^{N} f_{kl} U^k V^l \tag{1.2.37}$$

or can be brought into this form. It is written here such that all Us are to the left of all Vs in the products, but this is no restriction because the relations (1.2.36) state that other products can always be brought into this U,V-ordered form.

In fact, all such functions of U and V make up all operators for this degree of freedom, which is to say that the complementary pair U,V is *algebraically complete*. To make this point, we consider an arbitrary operator F, and note that then the numbers $\langle u_k|F|v_l\rangle$ are known. We normalize these mixed matrix elements by dividing by $\langle u_k|v_l\rangle$, thus defining the set of N^2 numbers

$$f(u_k, v_l) = \frac{\langle u_k|F|v_l\rangle}{\langle u_k|v_l\rangle}\,. \tag{1.2.38}$$

Multiply by $|u_k\rangle\langle u_k|$ from the left, by $|v_l\rangle\langle v_l|$ from the right, and sum over k and l,

$$\begin{aligned}
\sum_{k,l} |u_k\rangle\langle u_k| f(u_k,v_l) |v_l\rangle\langle v_l| &= \sum_{k,l} |u_k\rangle \underbrace{\langle u_k|v_l\rangle f(u_k,v_l)}_{=\langle u_k|F|v_l\rangle} \langle v_l| \\
&= \underbrace{\sum_k |u_k\rangle\langle u_k|}_{=1}\, F \underbrace{\sum_l |v_l\rangle\langle v_l|}_{=1} \\
&= F\,.
\end{aligned} \tag{1.2.39}$$

Indeed, we have succeeded in writing F as a function of U and V, with all

Us to the left of all Vs,

$$\begin{aligned} F &= \sum_{k,l} \big|u_k\big\rangle\big\langle u_k\big| f(u_k, v_l) \big|v_l\big\rangle\big\langle v_l\big| \\ &= \frac{1}{N^2} \sum_{k,l,m,n} (U/u_k)^m f(u_k, v_l)(V/v_l)^n \\ &= \sum_{k,l} f_{kl} U^k V^l \end{aligned} \tag{1.2.40}$$

with

$$f_{kl} = \frac{1}{N^2} \sum_{m,n} u_m^{-k} f(u_m, v_n) v_n^{-l} \tag{1.2.41}$$

after interchanging $k \leftrightarrow m$, $l \leftrightarrow n$ in the summation.

1-5 Show that

$$\mathrm{tr}\big\{U^k V^l\big\} = 0 \quad \text{unless} \quad k = l = 0 \quad (\mathrm{mod}\ N)$$

and then relate f_{kl} to $\mathrm{tr}\big\{U^{-k} F V^{-l}\big\}$.

1-6 For $F = \sum_{k,l} f_{kl} U^k V^l$ and $G = \sum_{k,l} g_{kl} U^k V^l$, express $\mathrm{tr}\big\{F^\dagger G\big\}$ in terms of the coefficients f_{kl} and g_{kl}.

With the general version of the Kronecker δ symbol,

$$\delta(x, y) = \begin{cases} 1 & \text{if} \quad x = y\,, \\ 0 & \text{if} \quad x \neq y\,, \end{cases} \tag{1.2.42}$$

we can write

$$\begin{aligned} \big|u_k\big\rangle\big\langle u_k\big| &= \sum_j \big|u_j\big\rangle \delta(u_j, u_k) \big\langle u_j\big| \\ &= \delta(U, u_k) \end{aligned} \tag{1.2.43}$$

where the last step is an application of the general form of an operator function $f(A)$, the spectral decomposition in (1.1.17). Likewise we have

$$\big|v_l\big\rangle\big\langle v_l\big| = \delta(V, v_l)\,, \tag{1.2.44}$$

and then

$$F = \sum_{k,l} \delta(U, u_k)\, f(u_k, v_l)\, \delta(V, v_l)\,. \tag{1.2.45}$$

In view of the δ symbols, we can evaluate the sums over k and l and so arrive at

$$F = f(U;V) \tag{1.2.46}$$

where the semicolon is a reminder that all Us stand to the left of all Vs in this expression.

We return to (1.2.38) and reveal the following:

$$\begin{aligned} f(u_k, v_l) &= \frac{\langle u_k|F|v_l\rangle\langle v_l|u_k\rangle}{\langle u_k|v_l\rangle\langle v_l|u_k\rangle} \\ &= N\langle u_k|F|v_l\rangle\langle v_l|u_k\rangle \\ &= N\,\mathrm{tr}\{|u_k\rangle\langle u_k|F|v_l\rangle\langle v_l|\} \\ &= N\,\mathrm{tr}\{\delta(U,u_k)\,F\,\delta(V,v_l)\}\ , \end{aligned} \tag{1.2.47}$$

where we recall the defining property of the *trace*, that is

$$\mathrm{tr}\{|1\rangle\langle 2|\} = \langle 2|1\rangle \tag{1.2.48}$$

for any ket $|1\rangle$ and any bra $\langle 2|$. Relation (1.2.47) is the reciprocal to (1.2.45) inasmuch as we go from $F(U,V)$ to $f(u,v)$ in (1.2.47), and from $f(u,v)$ to $F(U,V)$ in (1.2.45).

We thus have a simple procedure for finding the U,V-ordered version of a given operator F:

First evaluate $f(u_k, v_l) = \dfrac{\langle u_k|F|v_l\rangle}{\langle u_k|v_l\rangle}$; then replace $u_k \to U$, $v_l \to V$ with due attention to the ordering in products, all U operators must stand to the left of all V operators. (1.2.49)

Here is an elementary example. For $F = VU$ we have

$$\begin{aligned} f(u_k, v_l) &= \frac{\langle u_k|VU|v_l\rangle}{\langle u_k|v_l\rangle} = \frac{\langle u_{k+1}|v_{l+1}\rangle}{\langle u_k|v_l\rangle} \\ &= \frac{\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}(k+1)(l+1)}/\sqrt{N}}{\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}kl}/\sqrt{N}} = \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}(k+l+1)} \end{aligned} \tag{1.2.50}$$

or

$$f(u_k, v_l) = u_k v_l\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}} \tag{1.2.51}$$

so that

$$VU = F = UV\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}}\,, \tag{1.2.52}$$

which we know already.

1-7 What is the U,V-ordered version of $|u_j\rangle\langle u_k|$, of $|v_j\rangle\langle v_k|$?

1-8 We have

$$|u_k\rangle\langle u_k| = \delta(U,u_k) = \frac{1}{N}\sum_l (U/u_k)^l\,.$$

Therefore,

$$\sum_k \frac{1}{N}\sum_l (U/u_k)^l = 1\,.$$

Verify this by a direct evaluation of this sum, that is: first sum over k, then over l.

1-9 We have

$$F = \sum_{k,l} f_{kl} U^k V^l = f(U;V)\,.$$

Express the trace of F in terms of the N^2 coefficients f_{kl}, and also in terms of the N^2 numbers $f(u_k,v_l)$.

1-10 Show that

(1) if F commutes with U, that is $FU = UF$, then F is a function of U only, $F = f(U)$;
(2) if F commutes with V, that is $FV = VF$, then F is a function of V only, $F = f(V)$.

What is implied for an operator F that commutes with both U and V? The answer to this question is *Schur's lemma*, named after Issai Schur.

1-11 Consider an arbitrary operator X and define F by

$$F = \sum_{k,l=1}^{N} V^{-l}U^{-k}XU^kV^l\,,$$

that is: F is the sum of all N^2 operators obtained from X by the basic unitary transformations that result from repeated applications of U and V. Show that F commutes with U and with V. Then conclude that

$$F = N\,\mathrm{tr}\{X\}\,.$$

1-12 For odd N, that is $N = 2M+1$ with $M = 1, 2, 3, \ldots$, we define N^2 operators in accordance with

$$W_{00} = \frac{1}{N}\sum_{j=-M}^{M}\sum_{k=-M}^{M} U^j V^k \,\mathrm{e}^{\mathrm{i}\pi jk/N} \quad \text{and} \quad W_{lm} = V^m U^{-l} W_{00} U^l V^{-m}$$

for $-M \le l, m \le M$. Show that all W_{lm}s are hermitian, and evaluate $\mathrm{tr}\{W_{lm}\}$ and $\mathrm{tr}\{W_{lm}W_{l'm'}\}$.

1-13 Establish that an arbitrary operator F can be written as a weighted sum of the W_{lm}s,

$$F = \frac{1}{N}\sum_{l,m} f_{lm} W_{lm} \quad \text{with} \quad f_{lm} = \mathrm{tr}\{F W_{lm}\}\ ,$$

and express $\mathrm{tr}\{F\}$ in terms of the coefficients f_{lm}.

1.2.3 *Bohr's principle. Technical formulation*

In summary, we have established a clear technical formulation of Niels H. D. Bohr's *principle of complementarity*:

(1) for each quantum degree of freedom there is a pair of complementary observables
and (2) all observables are functions of this pair.

This wording of the principle is a minor extension of the insights gained by Hermann K. H. Weyl and Julian Schwinger in their seminal work on quantum kinematics. We comment on the phenomenological implication of the complementarity principle in Section 1.2.7 below.

1.2.4 *Composite degrees of freedom*

In the above reasoning, the dimension N of the degree of freedom can be any integer number, prime or composite. In the case of composite numbers, we can regard the quantum degree of freedom as being composite as well, namely composed of simpler systems. It is sufficient to illustrate this in the example of $N = 6 = 2 \times 3$.

Here we have the periodic unitary operators

$$U^6 = 1 \quad \text{and} \quad V^6 = 1 \tag{1.2.53}$$

of period 6, but as

$$\left(U^3\right)^2 = 1\,, \quad \left(U^2\right)^3 = 1 \tag{1.2.54}$$

show, there are also operators with periods 2 and 3. This suggests that we can regard the $N = 6$ degree of freedom as composed of a $N = 2$ one and a $N = 3$ one.

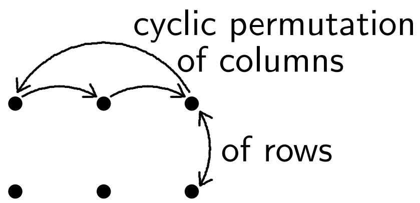
To make this point more explicitly, let us arrange the six basis states $|a_1\rangle, \ldots, |a_6\rangle\left(\equiv |v_1\rangle, \ldots, |v_6\rangle\right)$ in a two-dimensional array

$$\begin{array}{ccc} 1 & 2 & 3 \\ \bullet & \bullet & \bullet \\ \\ \bullet & \bullet & \bullet \\ 4 & 5 & 6 \end{array}$$

and then relabel them accordingly,

$$\begin{array}{ccc} 11 & 12 & 13 \\ \bullet & \bullet & \bullet \\ \\ \bullet & \bullet & \bullet \\ 21 & 22 & 23 \end{array}$$

Rather than the original cyclic permutation $1 \to 2 \to 3 \to 4 \to 5 \to 6 \to 1$, we now have cyclic permutations of the rows $11 \leftrightarrow 21$ & $12 \leftrightarrow 22$ & $13 \leftrightarrow 23$, and of the columns $11 \to 12 \to 13 \to 11$ & $21 \to 22 \to 23 \to 21$:



So, there are two operators effecting cyclic permutations, one with period 2 and the other with period 3,

$$U_1^2 = 1\,, \quad U_2^3 = 1\,, \tag{1.2.55}$$

which act on the respective indices,

$$\begin{aligned} U_1|v_{jk}\rangle &= |v_{j+1k}\rangle\,, \\ U_2|v_{jk}\rangle &= |v_{jk+1}\rangle\,, \end{aligned} \tag{1.2.56}$$

where the first index j is modulo 2, the second index k is modulo 3. Clearly, U_1 commutes with U_2

$$U_1 U_2 = U_2 U_1 \,, \tag{1.2.57}$$

and it is easy to show (do this yourself) that this is also true for their complementary partners V_1 and V_2. That is,

$$V_1 V_2 = V_2 V_1 \,, \quad U_1 V_2 = V_2 U_1 \,, \quad V_1 U_2 = U_2 V_1 \,. \tag{1.2.58}$$

But the pairs U_1, V_1 and U_2, V_2 are pairs of complementary observables of the $N = 2$ and $N = 3$ types, respectively,

$$U_1 V_1 = \mathrm{e}^{-\mathrm{i}\frac{2\pi}{2}} V_1 U_1 \,, \quad U_2 V_2 = \mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}} V_2 U_2 \,. \tag{1.2.59}$$

In short: U_1, V_1 and U_2, V_2 refer to independent degrees of freedom, the prime degrees of freedom that are the constituents of the composite degree of freedom with $N = 6$.

1-14 Show that $U = U_1 U_2$ has period 6. Begin with $\bigl|a_1\bigr\rangle \equiv \bigl|v_{11}\bigr\rangle$ and find $\bigl|a_2\bigr\rangle, \ldots, \bigl|a_6\bigr\rangle$ in accordance with (1.2.2).

In the general situation of a composite value of N other than 6, this process of factorization can be repeated until the given $N = N_1 N_2 \cdots N_n$ is broken up into the prime degrees of freedom of which it is composed, or can be thought of as being composed. As a consequence, the elementary quantum degrees of freedom have N values that are prime and cannot be decomposed further.

1.2.5 *The limit $N \to \infty$. Symmetric case*

The primes $N = 2, 3, 5, 7, 11, 13, \ldots$ are all odd, except for $N = 2$, so that we can restrict ourselves to odd N values in the limit $N \to \infty$. It is then possible to change from the numbering

$$k = 1, 2, \ldots, N \tag{1.2.60}$$

to a new numbering

$$k = 0, \pm 1, \pm 2, \ldots, \pm \frac{N-1}{2} \,. \tag{1.2.61}$$

Further, as N grows, the basic unit of complex phase $2\pi/N$ gets arbitrarily small. We introduce a small quantity, ϵ, to deal with this,

$$\frac{2\pi}{N} = \epsilon^2 . \tag{1.2.62}$$

Aiming at a continuous degree of freedom in the limit $N \to \infty$, we also relabel the states in the sense that

$$\begin{aligned} k &\longrightarrow k\epsilon = x = 0, \pm\epsilon, \pm 2\epsilon, \ldots, \pm\left(\frac{\pi}{\epsilon} - \frac{\epsilon}{2}\right), \\ l &\longrightarrow l\epsilon = p = 0, \pm\epsilon, \pm 2\epsilon, \ldots, \pm\left(\frac{\pi}{\epsilon} - \frac{\epsilon}{2}\right). \end{aligned} \tag{1.2.63}$$

Then the numbers x and p will cover the real axis, $-\infty < x, p < \infty$, when $N \to \infty$, $\epsilon \to 0$.

The unitary operator U acting on $\bigl|v_l\bigr\rangle$ increases l by 1, so that it effects $p \to p + \epsilon$. Likewise V applied to $\bigl\langle u_k\bigr|$ results in $x \to x + \epsilon$. This suggests the identification of hermitian operators X and P such that

$$\begin{aligned} U &= \mathrm{e}^{\mathrm{i}\epsilon X} \quad \text{with} \quad X = X^\dagger , \\ V &= \mathrm{e}^{\mathrm{i}\epsilon P} \quad \text{with} \quad P = P^\dagger . \end{aligned} \tag{1.2.64}$$

The Weyl commutator (1.2.36),

$$U^l V^k = \mathrm{e}^{-\mathrm{i}\frac{2\pi}{N}kl} V^k U^l , \tag{1.2.65}$$

then appears as

$$\mathrm{e}^{\mathrm{i}l\epsilon X}\,\mathrm{e}^{\mathrm{i}k\epsilon P} = \mathrm{e}^{-\mathrm{i}k\epsilon l\epsilon}\,\mathrm{e}^{\mathrm{i}k\epsilon P}\,\mathrm{e}^{\mathrm{i}l\epsilon X} , \tag{1.2.66}$$

that is

$$\mathrm{e}^{\mathrm{i}pX}\,\mathrm{e}^{\mathrm{i}xP} = \mathrm{e}^{-\mathrm{i}xp}\,\mathrm{e}^{\mathrm{i}xP}\,\mathrm{e}^{\mathrm{i}pX} . \tag{1.2.67}$$

The two equivalent versions

$$\begin{aligned} \mathrm{e}^{-\mathrm{i}xP}\,\mathrm{e}^{\mathrm{i}pX}\,\mathrm{e}^{\mathrm{i}xP} &= \mathrm{e}^{\mathrm{i}p(X-x)} , \\ \mathrm{e}^{\mathrm{i}pX}\,\mathrm{e}^{\mathrm{i}xP}\,\mathrm{e}^{-\mathrm{i}pX} &= \mathrm{e}^{\mathrm{i}x(P-p)} \end{aligned} \tag{1.2.68}$$

look much more conspicuous after we use the identity

$$U^{-1} f(A) U = f(U^{-1} A U) , \tag{1.2.69}$$

which — as we recall — is valid for any operator function $f(A)$ and any unitary operator U, twice to establish

$$\begin{aligned} \mathrm{e}^{\mathrm{i}p\left(\mathrm{e}^{-\mathrm{i}xP} X \,\mathrm{e}^{\mathrm{i}xP}\right)} &= \mathrm{e}^{\mathrm{i}p(X-x)}\,, \\ \mathrm{e}^{\mathrm{i}x\left(\mathrm{e}^{\mathrm{i}pX} P \,\mathrm{e}^{-\mathrm{i}pX}\right)} &= \mathrm{e}^{\mathrm{i}x(P-p)}\,. \end{aligned} \tag{1.2.70}$$

It is tempting to conclude that

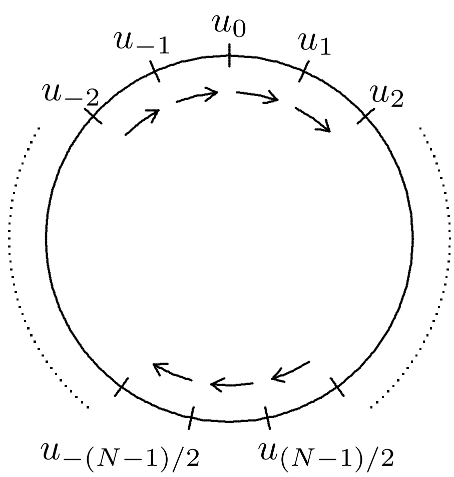
$$\begin{aligned} \mathrm{e}^{-\mathrm{i}xP} X \,\mathrm{e}^{\mathrm{i}xP} &= X - x\,, \\ \mathrm{e}^{\mathrm{i}pX} P \,\mathrm{e}^{-\mathrm{i}pX} &= P - p\,, \end{aligned} \tag{1.2.71}$$

but this does not follow without imposing a restricting condition, just as

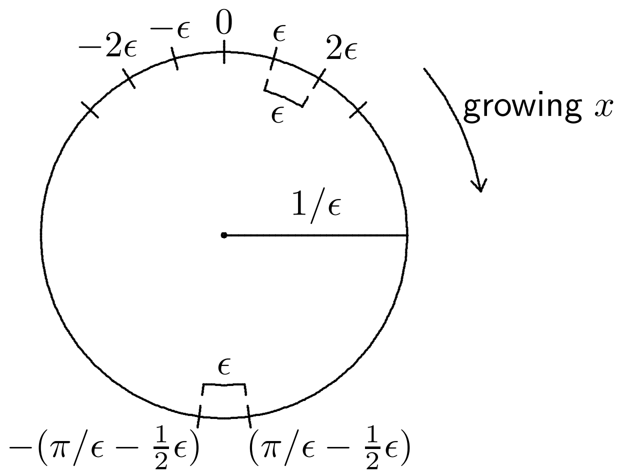
$$\mathrm{e}^{\mathrm{i}\alpha} = \mathrm{e}^{\mathrm{i}\beta} \quad (\alpha, \beta\text{: two real numbers}) \tag{1.2.72}$$

does not imply $\alpha = \beta$, but only that $\alpha - \beta$ is an integer multiple of 2π.

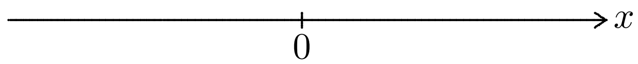
To understand the restricting condition, we visualize the cyclic permutation by a circle:



where an application of V turns the wheel of u_k states by one notch. For large N, small ϵ, the picture is this



The circumference of the circle is $N\epsilon = 2\pi/\epsilon$, so that the radius is $1/\epsilon$ and becomes infinitely large as $N \to \infty$, $\epsilon \to 0$. In this limit then, any *finite* portion of the circle is indistinguishable from a straight line,



If we thus restrict ourselves to situations in which only a finite range of x values matters, thereby explicitly giving up the periodicity that would force us to identify $x = +\infty$ with $x = -\infty$, the statements in (1.2.71) become correct.

By comparing terms that are of first order in x or p in (1.2.71) we get

$$XP - PX = \mathrm{i} \quad \text{or} \quad [X, P] = \mathrm{i}\,, \tag{1.2.73}$$

which is, of course, Werner Heisenberg's commutation relation for position X and momentum P, here for dimensionless operators, rather than the normal ones with metrical dimensions of length and mass $\times$ velocity. As a consequence, Planck's constant $\hbar$ (Max K. E. L. Planck) does not appear on the right-hand side.

With this commutator established by the 1st-order terms, all higher-order terms take care of themselves, which is seen most easily by differentiation. Consider, say, the first statement in (1.2.71), where we get

$$\begin{aligned}\frac{\partial}{\partial x}\left(\mathrm{e}^{-\mathrm{i}xP}X\,\mathrm{e}^{\mathrm{i}xP}\right) &= \mathrm{e}^{-\mathrm{i}xP}\underbrace{(-\mathrm{i}PX + X\mathrm{i}P)}_{=\,\mathrm{i}[X,P]\,=\,-1}\mathrm{e}^{\mathrm{i}xP}\\ &= -1 \end{aligned}\tag{1.2.74}$$

on the left and

$$\frac{\partial}{\partial x}(X - x) = -1 \tag{1.2.75}$$

on the right. Thus, these are two functions of x, which have the same derivative everywhere and agree in the vicinity of $x = 0$. It follows that the functions are the same for all values of x.

These $N \to \infty$ considerations for U and V have a counterpart in their respective kets and bras. It should be reasonably clear, given what we know about the X, P pair from *Basic Matters* and *Simple Systems*, or any other introductory text, that

$$\langle u_k | v_l \rangle = \frac{1}{\sqrt{N}}\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}kl} \tag{1.2.76}$$

turns into

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{\mathrm{i}xp}\,, \tag{1.2.77}$$

and the orthonormality and completeness relations

$$\langle u_k | u_{k'} \rangle = \delta_{kk'}\,, \quad \sum_k |u_k\rangle\langle u_k| = 1 \tag{1.2.78}$$

become

$$\langle x | x' \rangle = \delta(x - x')\,, \quad \int \mathrm{d}x\,|x\rangle\langle x| = 1\,, \tag{1.2.79}$$

and likewise for the momentum states, with consistent replacements of Kronecker δ symbols by Dirac δ functions (Paul A. M. Dirac), and summations by integrations.

More specifically, we need to identify

$$\langle x| = \frac{1}{\sqrt{\epsilon}}\langle u_k|\bigg|_{\epsilon \to 0} \quad \text{with} \quad k\epsilon = x \tag{1.2.80}$$

and

$$\big|p\big\rangle = \big|v_l\big\rangle \frac{1}{\sqrt{\epsilon}}\bigg|_{\epsilon\,\to\,0} \qquad \text{with} \quad l\epsilon = p\,, \tag{1.2.81}$$

and then we have

$$\frac{1}{\epsilon}\big\langle u_k\big|v_l\big\rangle \xrightarrow[\epsilon\,\to\,0]{} \big\langle x\big|p\big\rangle\,. \tag{1.2.82}$$

As one example of many that could be used for illustration equally well, let us take a look at the transition from

$$\delta(U, u_k) = \frac{1}{N}\sum_{l(\neq k)} \big(U/u_k\big)^l = \big|u_k\big\rangle\big\langle u_k\big| \tag{1.2.83}$$

to

$$\delta(X - x) = \int \frac{\mathrm{d}p}{2\pi}\, \mathrm{e}^{\mathrm{i}p(X\,-\,x)} = \big|x\big\rangle\big\langle x\big|\,. \tag{1.2.84}$$

We proceed from

$$\begin{aligned}\frac{1}{\epsilon}\delta(U, u_k) &= \frac{1}{N\epsilon}\sum_{l(\neq k)} \Big(\mathrm{e}^{\mathrm{i}\epsilon X}\,\mathrm{e}^{-\mathrm{i}\epsilon x}\Big)^l \\ &= \underbrace{\frac{1}{N\epsilon^2}}_{=\,1/(2\pi)}\sum_{l(\neq k)} \Delta p\ \mathrm{e}^{\mathrm{i}p(X\,-\,x)}\end{aligned} \tag{1.2.85}$$

with $p = l\epsilon$ and $\Delta p = \epsilon$ for the difference between successive p values. Upon recognizing that the l summation is the Riemann sum (G. F. Bernhard Riemann) for the integral in

$$\frac{1}{\epsilon}\delta(U, u_k) = \frac{1}{2\pi}\int_{\epsilon/2\,-\,\pi/\epsilon}^{\pi/\epsilon\,-\,\epsilon/2} \mathrm{d}p\ \mathrm{e}^{\mathrm{i}p(X\,-\,x)}\,, \tag{1.2.86}$$

the limit $\epsilon \to 0$ is immediate,

$$\frac{1}{\epsilon}\delta(U, u_k) \xrightarrow[\epsilon\,\to\,0]{} \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}p\ \mathrm{e}^{\mathrm{i}p(X\,-\,x)} = \delta(X - x)\,. \tag{1.2.87}$$

The familiar Fourier representation (Jean B. J. Fourier) of the Dirac δ function establishes the last identity. The other limit offered by (1.2.83) in conjunction with (1.2.80),

$$\frac{1}{\epsilon}\delta(U,u_k) = \left(\big|u_k\big\rangle\frac{1}{\sqrt{\epsilon}}\right)\left(\frac{1}{\sqrt{\epsilon}}\big\langle u_k\big|\right) \xrightarrow[\epsilon\to 0]{} \big|x\big\rangle\big\langle x\big|\,, \tag{1.2.88}$$

is consistent with what we get from the spectral decomposition of $\delta(X-x)$,

$$\delta(X-x) = \int \mathrm{d}x'\,\big|x'\big\rangle\delta(x'-x)\big\langle x'\big| = \big|x\big\rangle\big\langle x\big|\,, \tag{1.2.89}$$

as it should be.

It is natural and convenient to use dimensionless operators X and P for this study of the limit $N\to\infty$, but eventually we want to have the correct metrical dimensions of length for position X and mass $\times$ velocity for momentum P. All that is needed is the introduction of Planck's constant $\hbar$ in the right places, such as

$$\big[X,P\big] = \mathrm{i}\hbar \tag{1.2.90}$$

for the Heisenberg commutator rather than (1.2.73), and

$$\big\langle x\big|p\big\rangle = \frac{\mathrm{e}^{\mathrm{i}xp/\hbar}}{\sqrt{2\pi\hbar}} \tag{1.2.91}$$

for the xp transformation function rather than (1.2.77). The orthonormality and completeness relations for the position states in (1.2.79) continue to hold without change, but we should take note of the metrical dimension $(\text{length})^{-\frac{1}{2}}$ of $\big|x\big\rangle$ and $\big\langle x\big|$. Corresponding remarks apply to the momentum states.

For the record and future reference it is worth recalling the basic relations between commutators and differentiations,

$$\begin{aligned}\big[X,f(X,P)\big] &= \mathrm{i}\hbar\frac{\partial f(X,P)}{\partial P}\,,\\ \big[f(X,P),P\big] &= \mathrm{i}\hbar\frac{\partial f(X,P)}{\partial X}\,,\end{aligned} \tag{1.2.92}$$

where $f(X,P)$ is any well defined function of X and P. These generalizations of the Heisenberg commutator are in fact implications of (1.2.90), and in turn contain (1.2.90) as special cases.

1-15 Combine (1.2.71) with (1.2.69) to first establish that

$$\begin{aligned} &\mathrm{e}^{-\mathrm{i}xP/\hbar} f(X,P)\,\mathrm{e}^{\mathrm{i}xP/\hbar} = f(X-x,P) \\ \text{and}\quad &\mathrm{e}^{\mathrm{i}pX/\hbar} f(X,P)\,\mathrm{e}^{-\mathrm{i}pX/\hbar} = f(X,P-p)\,, \end{aligned}$$

and then use this in

$$\frac{\partial f(X,P)}{\partial X} = \frac{1}{x}\big[f(X,P) - f(X-x,P)\big]\bigg|_{x\,\to\,0}\,,$$

for example, to derive (1.2.92).

1.2.6 *The limit $N \to \infty$. Asymmetric case*

The limit $N \to \infty$ discussed in Section 1.2.5 is *symmetric* inasmuch as U and V are treated on completely equal footing. This symmetric procedure is, however, not the only way of performing the limit $N \to \infty$. There are, in fact, three important *asymmetric* limits, of which we shall consider one.

This time we start with the relation

$$\delta_{kl} = \sum_m \langle u_k|v_m\rangle\langle v_m|u_l\rangle \tag{1.2.93}$$

which states the completeness of the V states and the orthonormality of the U states. In

$$\langle u_k|v_m\rangle = \frac{1}{\sqrt{N}}\,\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}km} = \frac{1}{\sqrt{N}}\Big(\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}k}\Big)^m \tag{1.2.94}$$

we encounter a phase factor

$$\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}k} = \mathrm{e}^{\mathrm{i}\phi} \quad\text{with}\quad \phi = \frac{2\pi}{N}k \quad\text{and}\quad k = 0,\dots,N-1\,. \tag{1.2.95}$$

The phases $\phi = \frac{2\pi}{N}k$ and $\phi' = \frac{2\pi}{N}l$ will cover the whole range

$$0 \le \phi, \phi' < 2\pi \tag{1.2.96}$$

densely in the limit $N \to \infty$. We note immediately that the relation

$$\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}k} = \mathrm{e}^{\mathrm{i}\phi} \tag{1.2.97}$$

identifies ϕ only up to an arbitrary multiple of 2π, so that there is no point in distinguishing between ϕ and $\phi + 2\pi$.

For the m summation we choose $m = 0, \pm 1, \dots, \pm\frac{1}{2}(N-1)$, so that

$$\begin{aligned} N\delta_{kl} = \sum_{m=-\frac{1}{2}(N-1)}^{\frac{1}{2}(N-1)} \mathrm{e}^{im(\phi\,-\,\phi')} &= \left\{\begin{matrix} N & \text{if} & \phi = \phi' \pmod{2\pi} \\ 0 & \text{if} & \phi \neq \phi' \pmod{2\pi} \end{matrix}\right\} \\ &= N\delta(\phi, \phi') \quad \pmod{2\pi} \\ &= N \sum_{n=-\infty}^{\infty} \delta(\phi, \phi' + 2\pi n)\,. \end{aligned} \tag{1.2.98}$$

In the limit $N \to \infty$, the sum is

$$\sum_{m=-\infty}^{\infty} \mathrm{e}^{im(\phi\,-\,\phi')} = 2\pi \sum_{n=-\infty}^{\infty} \delta(\phi - \phi' - 2\pi n)\,. \tag{1.2.99}$$

This so-called *Poisson identity*, which is named after Siméon-Denis Poisson, can be verified by comparing the Fourier coefficients of these two periodic functions of ϕ. On the left we get

$$\int_0^{2\pi} \frac{\mathrm{d}\phi}{2\pi}\, \mathrm{e}^{-\mathrm{i}j\phi} \sum_{m=-\infty}^{\infty} \mathrm{e}^{im(\phi\,-\,\phi')} = \mathrm{e}^{-\mathrm{i}j\phi'}\,, \tag{1.2.100}$$

and on the right

$$\int_0^{2\pi} \frac{\mathrm{d}\phi}{2\pi}\, \mathrm{e}^{-\mathrm{i}j\phi} 2\pi \sum_{n=-\infty}^{\infty} \delta(\phi - \phi' - 2\pi n) = \mathrm{e}^{-\mathrm{i}j\phi'}\,. \tag{1.2.101}$$

Indeed, all Fourier coefficients are identical and, therefore, the functions are the same.

We are thus invited to introduce bras $\langle\phi|$ and kets $|m\rangle$ in accordance with

$$\langle\phi| = \langle\phi + 2\pi| \quad \text{(periodic)} \tag{1.2.102}$$

and

$$\langle\phi|m\rangle = \frac{1}{\sqrt{2\pi}}\, \mathrm{e}^{im\phi}\,. \tag{1.2.103}$$

These are such that

$$\begin{aligned} \langle\phi|\phi'\rangle &= \sum_{m=-\infty}^{\infty} \langle\phi|m\rangle\langle m|\phi'\rangle \\ &= \frac{1}{2\pi} \sum_m \mathrm{e}^{im(\phi\,-\,\phi')} = \sum_n \delta(\phi - \phi' - 2\pi n) \end{aligned} \tag{1.2.104}$$

and

$$\begin{aligned}\langle m|m'\rangle &= \int_{(2\pi)} \mathrm{d}\phi\, \langle m|\phi\rangle\langle\phi|m'\rangle \\ &= \int_{(2\pi)} \frac{\mathrm{d}\phi}{2\pi}\, \mathrm{e}^{-\mathrm{i}(m-m')\phi} = \delta_{mm'} \end{aligned} \tag{1.2.105}$$

state the orthonormality and completeness of both sets of vectors. The ϕ integration in (1.2.105) covers any interval of 2π, such as $0\cdots 2\pi$ or $-\pi\cdots\pi$.

In the unitary operator

$$\sum_{m=-\infty}^{\infty} |m\rangle\, \mathrm{e}^{\mathrm{i}m\varphi} \langle m| = \mathrm{e}^{\mathrm{i}\varphi L/\hbar} \tag{1.2.106}$$

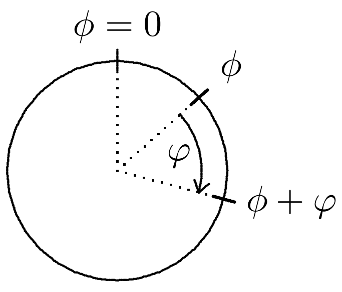
we recognize the hermitian operator

$$L = \sum_{m=-\infty}^{\infty} |m\rangle \hbar m \langle m| \tag{1.2.107}$$

that generates shifts of ϕ,

$$\begin{aligned}\langle\phi| \longrightarrow \langle\phi|\, \mathrm{e}^{\mathrm{i}\varphi L/\hbar} &= \sum_m \langle\phi|m\rangle\, \mathrm{e}^{\mathrm{i}m\varphi}\langle m| \\ &= \sum_m \underbrace{\frac{1}{\sqrt{2\pi}}\, \mathrm{e}^{\mathrm{i}m\phi}\, \mathrm{e}^{\mathrm{i}m\varphi}}_{=\,\mathrm{e}^{\mathrm{i}m(\phi+\varphi)}/\sqrt{2\pi} \,=\, \langle\phi+\varphi|m\rangle} \langle m| \\ &= \sum_m \langle\phi+\varphi|m\rangle\langle m| = \langle\phi+\varphi|\,, \end{aligned} \tag{1.2.108}$$

which are, geometrically speaking, rotations around a fixed axis:



As it should be, this picture is consistent with the periodic nature of the bras $\langle\phi|$. We conclude that L is the angular momentum operator associated with the rotation around this axis.

1-16 Consider the unitary operators

$$U^n = \int_{(2\pi)} \mathrm{d}\phi\, |\phi\rangle\, \mathrm{e}^{\mathrm{i}n\phi} \langle\phi| = \left(\int_{(2\pi)} \mathrm{d}\phi\, |\phi\rangle\, \mathrm{e}^{\mathrm{i}\phi} \langle\phi|\right)^n$$

where, as in (1.2.105), the integration is over any 2π interval and n is any integer, positive or negative. What is $U^n|m\rangle$?

1-17 Compare $U^n\, \mathrm{e}^{\mathrm{i}\varphi L/\hbar}$ with $\mathrm{e}^{\mathrm{i}\varphi L/\hbar} U^n$. Do you get what you anticipate?

The differential statement corresponding to

$$\langle\phi + \varphi| = \langle\phi|\, \mathrm{e}^{\mathrm{i}\varphi L/\hbar} \tag{1.2.109}$$

is

$$\frac{\partial}{\partial\varphi}\langle\phi + \varphi|\Big|_{\varphi=0} = \langle\phi|\frac{\mathrm{i}}{\hbar}L \tag{1.2.110}$$

or

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial\phi}\langle\phi| = \langle\phi|L\,. \tag{1.2.111}$$

This differential-operator representation of the angular momentum operator acting on an azimuth bra is the analog of

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}\langle x| = \langle x|P\,, \tag{1.2.112}$$

Erwin Schrödinger's relation for position bras and the operator of linear momentum. Indeed, in the context of orbital angular momentum the correspondence $L \to \dfrac{\hbar}{\mathrm{i}}\dfrac{\partial}{\partial\phi}$ appears in Section 4.3 of *Simple Systems*.

1-18 Get (1.2.112) as an implication of (1.2.91).

In closing this subject, let us note that, in addition to the X, P-type of continuous degree of freedom and the ϕ, L-type, there is also one for radial motion (position limited to positive values, corresponding momentum takes on all real values), and one for the polar angle or confinement to a finite range (position limited to a finite range, but without periodic values as for the ϕ variable, and momentum takes on all real values). All of them can be obtained as suitable limits $N \to \infty$.

1.2.7 *Bohr's principle. Quantum indeterminism*

Pairs of complementary observables are such that if the value of one observable is known, all outcomes are equally probable in a measurement of the second observable. Put differently, if one observable is sharp, the other is completely undetermined. The situation is clearly an extreme case of *quantum indeterminism*. But, as extreme as it may seem, it is not at all untypical. In fact, it is the generic situation, because there are always undetermined observables, irrespective of the preparation of the system.

Consider, therefore, the most general case, that is a quantum system prepared in a state described by a statistical operator ρ; see Section 2.15 in *Basic Matters* and Section 1.6 in *Simple Systems*. We write ρ in its diagonal form,

$$\rho = \sum_{j=1}^{N} |r_j\rangle r_j \langle r_j|$$
$$\text{with} \quad r_j \geq 0\,, \quad \sum_j r_j = 1\,, \quad \langle r_j|r_k\rangle = \delta_{jk}\,. \tag{1.2.113}$$

Then define

$$|a_k\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} |r_j\rangle\, \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}jk} \tag{1.2.114}$$

so that

$$\langle a_k|a_l\rangle = \delta_{kl} \tag{1.2.115}$$

as we know from (1.1.27). The observable introduced by

$$A = \sum_{k=1}^{N} |a_k\rangle k \langle a_k| \tag{1.2.116}$$

has values $k = 1, 2, \ldots, N$, and all of them have probability $1/N$, because

$$\langle a_k|\rho|a_k\rangle = \sum_{j=1}^{N} r_j \underbrace{\left|\langle a_k|r_j\rangle\right|^2}_{=1/N} = \frac{1}{N}\sum_{j=1}^{N} r_j = \frac{1}{N}\,. \tag{1.2.117}$$

Since ρ was quite arbitrary, and this construction for A is always possible, the above assertion is correct indeed, that is:

> Irrespective of the preparation of the quantum system, there are always observables that are completely undetermined.

One can regard this statement as another way of phrasing Bohr's principle of complementarity, a phrasing that emphasizes the phenomenology.

1-19 Guided by the φ, L example of Section 1.2.6, construct an undetermined observable for the case of $N = \infty$.

1.3 Brief review of basic dynamics

1.3.1 *Equations of motion*

Up to here, we have been reviewing quantum kinematics, that is the description of quantum systems. Now we turn to quantum dynamics, that is the evolution in time of quantum systems. One basic equation is Erwin Schrödinger's equation of motion, the *Schrödinger equation*, which we state both for bras and for kets,

$$\begin{aligned} \mathrm{i}\hbar\frac{\partial}{\partial t}\langle\ldots,t| &= \langle\ldots,t|H\bigl(A(t),t\bigr)\,, \\ -\mathrm{i}\hbar\frac{\partial}{\partial t}|\ldots,t\rangle &= H\bigl(A(t),t\bigr)|\ldots,t\rangle\,. \end{aligned} \tag{1.3.1}$$

The ellipses indicate fixed quantum numbers that identify the kets and bras, and $H\bigl(A(t),t\bigr)$ is the hermitian Hamilton operator at time t, regarded as a function of the dynamical variables $A(t)$, pairs of complementary observables for the various degrees of freedom under consideration, and perhaps of t itself.

All other operators are of the same general form, $F = F\bigl(A(t),t\bigr)$, and obey Werner Heisenberg's equation of motion, the *Heisenberg equation*,

$$\frac{\mathrm{d}}{\mathrm{d}t}F = \frac{\partial F}{\partial t} + \frac{1}{\mathrm{i}\hbar}[F,H] \tag{1.3.2}$$

where $\frac{\mathrm{d}}{\mathrm{d}t}$ differentiates t globally

$$\frac{\mathrm{d}}{\mathrm{d}t}F\bigl(A(t),t\bigr)\,, \tag{1.3.3}$$

whereas $\dfrac{\partial}{\partial t}$ means the *parametric* time derivative only,

$$\frac{\partial}{\partial t}F\bigl(A(t),t\bigr)\,. \tag{1.3.4}$$

only

Their difference

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}-\frac{\partial}{\partial t}\right)F\bigl(A(t),t\bigr)=\frac{1}{\mathrm{i}\hbar}\bigl[F\bigl(A(t),t\bigr),H\bigl(A(t),t\bigr)\bigr] \tag{1.3.5}$$

is the *dynamical* time derivative that originates in the dynamics of the system, that is the physical interactions of the constituents. Perhaps consult Chapter 3 of *Basic Matters* and Chapter 2 of *Simple Systems*, if you are uncertain about these matters.

We recall that there are some special cases. First, the Hamilton operator itself has no dynamical time dependence,

$$\frac{\mathrm{d}}{\mathrm{d}t}H=\frac{\partial}{\partial t}H\,, \tag{1.3.6}$$

so that it is constant in time if there is no parametric time dependence,

$$H\bigl(A(t)\bigr)=H\bigl(A(t_0)\bigr)\quad\text{if}\quad\frac{\partial H}{\partial t}=0\,. \tag{1.3.7}$$

Second, the dynamical variables themselves have only a dynamical time dependence,

$$\frac{\partial}{\partial t}A=0\,,\quad\frac{\mathrm{d}}{\mathrm{d}t}A=\frac{1}{\mathrm{i}\hbar}[A,H]\,. \tag{1.3.8}$$

In particular, for position X and momentum P as the dynamical variables, we have, by virtue of (1.2.92),

$$\frac{\mathrm{d}}{\mathrm{d}t}X=\frac{\partial H}{\partial P}\quad\text{and}\quad\frac{\mathrm{d}}{\mathrm{d}t}P=-\frac{\partial H}{\partial X}\,, \tag{1.3.9}$$

which have the same form as William R. Hamilton's equations of motion in classical mechanics.

Third, the statistical operator $\rho(A(t),t)$ has no total time dependence,

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho=0\,,\quad\rho\bigl(A(t),t\bigr)=\rho\bigl(A(t_0),t_0\bigr)\,. \tag{1.3.10}$$

This is to say that the parametric t dependence of ρ compensates fully for the dynamical t dependence. Therefore, the statistical operator obeys

$$\frac{\partial}{\partial t}\rho = -\frac{1}{\mathrm{i}\hbar}\bigl[\rho, H\bigr]\,; \tag{1.3.11}$$

this special case of the Heisenberg equation (1.3.2) is the so-called *von Neumann equation*, named after John von Neumann. It is the quantum analog of Joseph Liouville's equation of motion in classical statistical physics.

1.3.2 *Time transformation functions*

The descriptions at different times are related to each other by the time transformation functions, such as $\bigl\langle a, t_1\big|b, t_2\bigr\rangle$ for kets $\big|b\bigr\rangle$ at the early time t_2 and bras $\bigl\langle a\big|$ at the late time t_1. For example, if the state of the system is specified by the probability amplitudes $\bigl\langle b, t_2\big|\ \bigr\rangle$ at the early time t_2,

$$\big|\ \bigr\rangle = \sum_b \big|b, t_2\bigr\rangle\bigl\langle b, t_2\big|\ \bigr\rangle\,, \tag{1.3.12}$$

we find the amplitudes $\bigl\langle a, t_1\big|\ \bigr\rangle$ by means of

$$\bigl\langle a, t_1\big|\ \bigr\rangle = \sum_b \bigl\langle a, t_1\big|b, t_2\bigr\rangle\bigl\langle b, t_2\big|\ \bigr\rangle\,, \tag{1.3.13}$$

which follows from applying both sides of (1.3.12) to $\bigl\langle a, t_1\big|$. We can examine the evolution of any given state as soon as we know the time transformation functions.

Being conscious of the fact that all fundamental evolution equations in physics are differential equations, let us ask the following question:

> How does $\bigl\langle a, t_1\big|b, t_2\bigr\rangle$ change if there is a small change in the Hamilton operator at the intermediate time t?

The primary effect of such a change in H at time t is on $\bigl\langle a', t+\mathrm{d}t\big|b', t\bigr\rangle$, namely

$$\begin{aligned}\delta\bigl\langle a', t+\mathrm{d}t\big|b', t\bigr\rangle &= \delta\Bigl[\bigl\langle a', t\big|\Bigl(1-\frac{\mathrm{i}}{\hbar}H(t)\mathrm{d}t\Bigr)\big|b', t\bigr\rangle\Bigr]\\ &= \bigl\langle a', t\big|\Bigl(-\frac{\mathrm{i}}{\hbar}\delta H(t)\mathrm{d}t\Bigr)\big|b', t\bigr\rangle\\ &= \bigl\langle a', t+\mathrm{d}t\big|\Bigl(-\frac{\mathrm{i}}{\hbar}\delta H(t)\mathrm{d}t\Bigr)\big|b', t\bigr\rangle \end{aligned}\tag{1.3.14}$$

where $H(t) \equiv H\bigl(A(t),t\bigr)$ for brevity and the last step recognizes that we are only dealing with terms that are of first order in the time increment $\mathrm{d}t$. Thus, the effect on

$$\bigl\langle a,t_1\big|b,t_2\bigr\rangle = \sum_{a',b'}\bigl\langle a,t_1\big|a',t+\mathrm{d}t\bigr\rangle\bigl\langle a',t+\mathrm{d}t\big|b',t\bigr\rangle\bigl\langle b',t\big|b,t_2\bigr\rangle \tag{1.3.15}$$

is

$$\begin{aligned}
&\delta\bigl\langle a,t_1\big|b,t_2\bigr\rangle \\
&\quad= \sum_{a',b'}\bigl\langle a,t_1\big|a',t+\mathrm{d}t\bigr\rangle\bigl\langle a',t+\mathrm{d}t\big|\Bigl(-\frac{\mathrm{i}}{\hbar}\delta H(t)\mathrm{d}t\Bigr)\big|b',t\bigr\rangle\bigl\langle b',t\big|b,t_2\bigr\rangle \\
&\quad= \bigl\langle a,t_1\big|\Bigl(-\frac{\mathrm{i}}{\hbar}\delta H(t)\mathrm{d}t\Bigr)\big|b,t_2\bigr\rangle\,.
\end{aligned} \tag{1.3.16}$$

This is the contribution of an infinitesimal change of H, an infinitesimal change of the dynamics, at the particular intermediate time t, and we get the accumulated effect of small changes at all intermediate times by integration,

$$\delta\bigl\langle a,t_1\big|b,t_2\bigr\rangle = \bigl\langle a,t_1\big|\int_{t_2}^{t_1}\Bigl(-\frac{\mathrm{i}}{\hbar}\delta H(t)\mathrm{d}t\Bigr)\big|b,t_2\bigr\rangle\,. \tag{1.3.17}$$

As an elementary example, let us consider the mass dependence of the time transformation function

$$\bigl\langle x,t_1\big|x',t_2\bigr\rangle = \sqrt{\frac{M}{\mathrm{i}2\pi\hbar T}}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\frac{M}{2T}(x-x')^2}\,, \tag{1.3.18}$$

where $T = t_1 - t_2$ is the total duration and the underlying Hamilton operator

$$H = \frac{1}{2M}P^2 \tag{1.3.19}$$

is that of force-free motion in one dimension. We have

$$\delta_M H(t) = -\frac{\delta M}{2M^2}P(t)^2 \tag{1.3.20}$$

where

$$P(t) = \frac{M}{T}\Bigl(X(t_1) - X(t_2)\Bigr) = P(t_1) = P(t_2) \tag{1.3.21}$$

is constant in time (no force — no change of the momentum).

We wish to write

$$\delta_M H = -\frac{\delta M}{2M^2}\left(\frac{M}{T}\right)^2\Big(X(t_1) - X(t_2)\Big)^2 \tag{1.3.22}$$
$$= -\frac{\delta M}{2T^2}\Big(X(t_1)^2 + X(t_2)^2 - X(t_1)X(t_2) - X(t_2)X(t_1)\Big)$$

with the position operators $X(t_1), X(t_2)$ in their natural order: $X(t_1)$ to the left, $X(t_2)$ to the right, so that they will stand next to their respective eigenstates, namely bra $\langle x, t_1|$ for $X(t_1)$ and ket $|x', t_2\rangle$ for $X(t_2)$. We thus need the commutator

$$\big[X(t_1), X(t_2)\big] = \left[X(t_2) + \frac{T}{M}P(t_2), X(t_2)\right]$$
$$= -\mathrm{i}\hbar\frac{T}{M} \tag{1.3.23}$$

in

$$X(t_2)X(t_1) = X(t_1)X(t_2) - \big[X(t_1), X(t_2)\big]$$
$$= X(t_1)X(t_2) + \mathrm{i}\hbar\frac{T}{M}\,. \tag{1.3.24}$$

Accordingly,

$$\delta_M H = -\frac{\delta M}{2T^2}\left(X(t_1)^2 + X(t_2)^2 - 2X(t_1)X(t_2) - \mathrm{i}\hbar\frac{T}{M}\right) \tag{1.3.25}$$

and

$$\delta_M\langle x, t_1|x', t_2\rangle = \langle x, t_1|x', t_2\rangle \int_{t_2}^{t_1} \mathrm{d}t \left(-\frac{\mathrm{i}}{\hbar}\right)\left(-\frac{\delta M}{2T^2}\right)\left[(x-x')^2 - \mathrm{i}\hbar\frac{T}{M}\right]$$
$$= \langle x, t_1|x', t_2\rangle\left[\frac{\mathrm{i}}{\hbar}\frac{\delta M}{2T}(x-x')^2 + \frac{\delta M}{2M}\right], \tag{1.3.26}$$

implying first

$$\delta_M \log\langle x, t_1|x', t_2\rangle = \frac{\delta_M\langle x, t_1|x', t_2\rangle}{\langle x, t_1|x', t_2\rangle}$$
$$= \frac{\mathrm{i}}{\hbar}\frac{\delta M}{2T}(x-x')^2 + \frac{\delta M}{2M}$$
$$= \delta_M\left(\frac{\mathrm{i}}{\hbar}\frac{M}{2T}(x-x')^2 + \log\sqrt{M}\right) \tag{1.3.27}$$

and then

$$\langle x, t_1 | x', t_2 \rangle \propto \sqrt{M}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} \frac{M}{2T} (x - x')^2} \tag{1.3.28}$$

where the proportionality factor does not depend on M. We compare this with the known form of $\langle x, t_1 | x', t_2 \rangle$ in (1.3.18) and confirm that the M dependence thus found is correct.

1.4 Schwinger's quantum action principle

In view of (1.2.92) and (1.3.1), we also know how to deal with changes of the initial and final values of x and t,

$$\begin{aligned} \delta \langle x, t_1 | &= \langle x, t_1 | \frac{\mathrm{i}}{\hbar} \Big(P(t_1)\delta x - H(t_1)\delta t_1 \Big) , \\ \delta | x', t_2 \rangle &= -\frac{\mathrm{i}}{\hbar} \Big(P(t_2)\delta x' - H(t_2)\delta t_2 \Big) | x', t_2 \rangle , \end{aligned} \tag{1.4.1}$$

which we abbreviate as

$$\delta \langle x, t_1 | = \langle x, t_1 | \frac{\mathrm{i}}{\hbar} G_1 \tag{1.4.2}$$

and

$$\delta | x', t_2 \rangle = -\frac{\mathrm{i}}{\hbar} G_2 | x', t_2 \rangle \tag{1.4.3}$$

where G_1, G_2 are the appropriate *generators* for infinitesimal changes of the bras and kets. Their specifc form depends on the quantum numbers that characterize the initial and final states. For example, in the case of an initial momentum ket, we have

$$\begin{aligned} \delta | p, t_2 \rangle &= \left(\frac{\mathrm{i}}{\hbar} X(t_2)\delta p + \frac{\mathrm{i}}{\hbar} H(t_2)\delta t_2 \right) | p, t_2 \rangle \\ &= -\frac{\mathrm{i}}{\hbar} G_2 | p, t_2 \rangle \end{aligned} \tag{1.4.4}$$

with

$$G_2 = -X(t_2)\delta p - H(t_2)\delta t_2 \,. \tag{1.4.5}$$

Quite generally, then, the response of a time transformation function to variations of both the initial and final states and the dynamics at intermediate times is

$$\delta\bigl\langle a,t_1\big|b,t_2\bigr\rangle = \frac{\mathrm{i}}{\hbar}\bigl\langle a,t_1\big|\left(G_1 - G_2 - \int_{t_2}^{t_1} \mathrm{d}t\,\delta H(t)\right)\big|b,t_2\bigr\rangle\,. \tag{1.4.6}$$

Upon recognizing that we can derive the infinitesimal operators as variations of an *action* W_{12},

$$G_1 - G_2 - \int_{t_2}^{t_1} \mathrm{d}t\,\delta H(t) = \delta W_{12}\,, \tag{1.4.7}$$

this becomes Julian Schwinger's *quantum action principle*

$$\delta\bigl\langle a,t_1\big|b,t_2\bigr\rangle = \frac{\mathrm{i}}{\hbar}\bigl\langle a,t_1\big|\delta W_{12}\big|b,t_2\bigr\rangle\,. \tag{1.4.8}$$

The particular form of W_{12} depends thereby on the form of the generators G_1 and G_2 that are needed for the specified bras and kets. In particular, we have

$$W_{12} = \int_{t_2}^{t_1} \mathrm{d}t\,\left(P(t)\frac{\mathrm{d}X}{\mathrm{d}t} - H(t)\right) \tag{1.4.9}$$

for

$$\delta\bigl\langle x,t_1\big|x',t_2\bigr\rangle = \frac{\mathrm{i}}{\hbar}\bigl\langle x,t_1\big|\delta W_{12}\big|x',t_2\bigr\rangle\,. \tag{1.4.10}$$

We verify this by a more convenient reparameterization of the t integral, essentially identical with the parameterization in Section 4.10 of *Basic Matters*, for which purpose we introduce an integration parameter τ that ranges from $\tau = 0$ to $\tau = 1$, and regard $t, X(t), P(t)$ as functions of τ,

$$\begin{aligned} \tau = 0:\quad t(\tau) &= t_2\,,\\ \tau = 1:\quad t(\tau) &= t_1\,, \end{aligned} \tag{1.4.11}$$

where

$$\mathrm{d}t = \frac{\mathrm{d}t}{\mathrm{d}\tau}\mathrm{d}\tau \equiv \dot{t}\,\mathrm{d}\tau \tag{1.4.12}$$

and

$$\frac{\mathrm{d}X}{\mathrm{d}t} = \frac{\mathrm{d}X}{\mathrm{d}\tau}\frac{\mathrm{d}\tau}{\mathrm{d}t} \equiv \dot{X}/\dot{t} \tag{1.4.13}$$

with dots denoting τ derivatives. Then

$$W_{12} = \int_0^1 \mathrm{d}\tau\,\bigl(P\dot{X} - \dot{t}H\bigr)\,, \tag{1.4.14}$$

and variations of the "paths" $X(t), P(t)$ give

$$\delta W_{12} = \int_0^1 \mathrm{d}\tau \, \big(\delta P \, \dot{X} + P \, \delta\dot{X} - \delta\dot{t} \, H - \dot{t} \, \delta H\big) \tag{1.4.15}$$

where

$$\delta H = \delta H(X, P, t) = \frac{\partial H}{\partial X}\delta X + \delta P \frac{\partial H}{\partial P} + \delta t \frac{\partial H}{\partial t} \tag{1.4.16}$$

or, after recalling the equations of motion (1.3.9),

$$\delta H = -\frac{\mathrm{d}P}{\mathrm{d}t}\delta X + \delta P \frac{\mathrm{d}X}{\mathrm{d}t} + \delta t \frac{\partial H}{\partial t} \, . \tag{1.4.17}$$

Thus,

$$\begin{aligned}\delta W_{12} = \int_0^1 \mathrm{d}\tau \, \Bigg(\delta P \left(\dot{X} - \dot{t}\frac{\mathrm{d}X}{\mathrm{d}t}\right) + \left(P \, \delta\dot{X} + \dot{t} \, \frac{\mathrm{d}P}{\mathrm{d}t} \, \delta X\right) \\ - \left(\delta\dot{t} \, H + \dot{t} \, \delta t \, \frac{\partial H}{\partial t}\right)\Bigg) \, .\end{aligned} \tag{1.4.18}$$

Here, the first term vanishes because $\dot{t} \, \frac{\mathrm{d}X}{\mathrm{d}t} = \dot{X}$, and we have

$$\begin{aligned} P \, \delta\dot{X} + \dot{t} \, \frac{\mathrm{d}P}{\mathrm{d}t} \, \delta X &= P \, \delta\dot{X} + \dot{P} \, \delta X \\ &= \frac{\mathrm{d}}{\mathrm{d}\tau}(P \, \delta X) \end{aligned} \tag{1.4.19}$$

for the second term, and

$$\begin{aligned} \delta\dot{t} \, H + \dot{t} \, \delta t \, \frac{\partial H}{\partial t} &= \delta\dot{t} \, H + \delta t \, \dot{t} \, \frac{\mathrm{d}H}{\mathrm{d}t} \\ &= \delta\dot{t} \, H + \delta t \, \frac{\mathrm{d}H}{\mathrm{d}\tau} \\ &= \frac{\mathrm{d}}{\mathrm{d}\tau}(\delta t \, H) \end{aligned} \tag{1.4.20}$$

for the third term. Taken together they give

$$\begin{aligned} \delta W_{12} &= (P \, \delta X - H \, \delta t)\Big|_{\tau=0}^{\tau=1} \\ &= (P \, \delta X - H \, \delta t)\Big|_{t=t_2}^{t=t_1} = G_1 - G_2 \end{aligned} \tag{1.4.21}$$

with

$$G = P\,\delta X - H\,\delta t\,, \tag{1.4.22}$$

the generator of (1.4.1)–(1.4.5), indeed.

In arriving at this result, we paid little attention to the order of P and $\mathrm{d}X$ or P and δX. This is justified because eventually $\delta X \to \delta x$ or $\delta x'$, so that we only need to consider variations of $X(t)$ that are multiples of the identity, and then the order of multiplication is irrelevant. One can extend the treatment to slightly more general variations, but this is not so important for the sequel, as we shall mainly use the explicit differential statement (1.4.6).

In Sections 3.3 and 3.4 of *Simple Systems*, we have applications of the endpoint variations supplied by $G_1 - G_2$ in (1.4.6). We now supplement them by a simple example for the $\delta H(t)$ contribution.

1.4.1 *An example: Constant force*

As an illustrative example, we consider the motion under a constant force of strength F, for which

$$H = \frac{1}{2M}P^2 - FX \tag{1.4.23}$$

is the Hamilton operator. We already know the time transformation function $\langle x, t_1 | x', t_2 \rangle$ for $F = 0$, see (1.3.18), so we can get its $F \neq 0$ form by considering small changes of F. Now

$$\delta_F H = -\delta F\, X(t) \tag{1.4.24}$$

so that

$$\delta_F \langle x, t_1 | x', t_2 \rangle = \frac{\mathrm{i}}{\hbar}\delta F \langle x, t_1 | \int_{t_2}^{t_1} \mathrm{d}t\, X(t) | x', t_2 \rangle\,, \tag{1.4.25}$$

where we need $X(t)$ in terms of $X(t_1)$ and $X(t_2)$. The Heisenberg equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}X(t) = \frac{1}{M}P(t)\,, \quad \frac{\mathrm{d}}{\mathrm{d}t}P(t) = F \tag{1.4.26}$$

imply

$$X(t) = X(t_1)\frac{t - t_2}{T} + X(t_2)\frac{t_1 - t}{T} - \frac{F}{2M}(t_1 - t)(t - t_2) \tag{1.4.27}$$

as one verifies by inspection. Accordingly,

$$\delta_F\bigl\langle x,t_1\big|x',t_2\bigr\rangle = \frac{\mathrm{i}}{\hbar}\delta F\,\bigl\langle x,t_1\big|x',t_2\bigr\rangle \times \int_{t_2}^{t_1}\mathrm{d}t\left[x\frac{t-t_2}{T}+x'\frac{t_1-t}{T}-\frac{F}{2M}(t_1-t)(t-t_2)\right] \tag{1.4.28}$$

or

$$\begin{aligned}\delta_F\log\bigl\langle x,t_1\big|x',t_2\bigr\rangle &= \frac{\delta_F\bigl\langle x,t_1\big|x',t_2\bigr\rangle}{\bigl\langle x,t_1\big|x',t_2\bigr\rangle}\\ &= \frac{\mathrm{i}}{\hbar}\delta F\left(\frac{x+x'}{2}T-\frac{FT^3}{12M}\right)\end{aligned} \tag{1.4.29}$$

after making use of

$$\int_{t_2}^{t_1}\mathrm{d}t\,\frac{t-t_2}{T}=\frac{1}{2}T=\int_{t_2}^{t_1}\mathrm{d}t\,\frac{t_1-t}{T} \tag{1.4.30}$$

and

$$\int_{t_2}^{t_1}\mathrm{d}t\,(t_1-t)(t-t_2)=\frac{1}{6}T^3\,. \tag{1.4.31}$$

We recognize immediately that the right-hand side of (1.4.29) is a total variation in F,

$$\delta_F\log\bigl\langle x,t_1\big|x',t_2\bigr\rangle = \delta_F\left(\frac{\mathrm{i}}{\hbar}\frac{x+x'}{2}FT-\frac{\mathrm{i}}{\hbar}\frac{F^2T^3}{24M}\right), \tag{1.4.32}$$

which implies

$$\bigl\langle x,t_1\big|x',t_2\bigr\rangle = \bigl\langle x,t_1\big|x',t_2\bigr\rangle\Big|_{F=0}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\frac{x+x'}{2}FT-\frac{\mathrm{i}}{\hbar}\frac{F^2T^3}{24M}} \tag{1.4.33}$$

and we arrive at the time transformation function

$$\bigl\langle x,t_1\big|x',t_2\bigr\rangle = \sqrt{\frac{M}{\mathrm{i}2\pi\hbar T}}\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\frac{M}{2T}(x-x')^2+\frac{\mathrm{i}}{\hbar}\frac{x+x'}{2}FT-\frac{\mathrm{i}}{\hbar}\frac{F^2T^3}{24M}}\,, \tag{1.4.34}$$

in agreement with the result of Exercise 3-8 on page 67 in *Simple Systems*.

1-20 Repeat this for $\bigl\langle x,t_1\big|p,t_2\bigr\rangle$.

1-21 Consider the Hamilton operator

$$H = \frac{1}{2M}\left(P - \frac{\partial\lambda(X,t)}{\partial X}\right)^2 - \frac{\partial\lambda(X,t)}{\partial t}\,,$$

where $\lambda(X,t)$ is an arbitrary "gauge function" that depends on position operator X and parametrically on time t. Does the force $M\frac{\mathrm{d}^2}{\mathrm{d}t^2}X$ depend on λ? Find the λ dependence of $\langle x,t_1|x',t_2\rangle$.

1-22 Consider the Hamilton operator

$$H = \frac{1}{2M}P^2 + \frac{1}{2}\gamma(XP+PX)$$

with rate constant γ. Show that $\frac{\mathrm{d}}{\mathrm{d}t}(XP+PX) = \frac{2}{M}P^2$ and use this to find $X(t)P(t)+P(t)X(t)$ in terms of $X(t_1)$ and $P(t_2)$. Then employ the quantum action principle to determine first $\delta_\gamma\langle x,t_1|p,t_2\rangle$ and then $\langle x,t_1|p,t_2\rangle$.

1.4.2 *Insertion: Varying an exponential function*

As a preparation for the sequel, we derive an important mathematical formula for the response of e^A to infinitesimal variations of operator A. Begin with

$$\begin{aligned}\delta\,\mathrm{e}^A &= \delta\sum_{k=0}^{\infty}\frac{1}{k!}A^k = \delta\sum_{k=1}^{\infty}\frac{1}{k!}A^k \\ &= \delta\sum_{k=0}^{\infty}\frac{1}{(k+1)!}A^{k+1} \\ &= \sum_{k=0}^{\infty}\frac{1}{(k+1)!}\delta A^{k+1}\end{aligned} \tag{1.4.35}$$

where

$$\begin{aligned}\delta A^{k+1} &= \delta A\,A^k + A\,\delta A\,A^{k-1} + A^2\,\delta A\,A^{k-2} + \cdots + A^k\,\delta A \\ &= \sum_{j=0}^{k} A^j\,\delta A\,A^{k-j}\,.\end{aligned} \tag{1.4.36}$$

Therefore

$$\delta\, \mathrm{e}^{A} = \sum_{k=0}^{\infty} \frac{1}{(k+1)!} \sum_{j=0}^{k} A^j\, \delta A\, A^{k-j}\,, \tag{1.4.37}$$

or after rearranging the double sum

$$\delta\, \mathrm{e}^{A} = \sum_{j,k=0}^{\infty} \frac{1}{(j+k+1)!} A^j\, \delta A\, A^{k}\,. \tag{1.4.38}$$

With Leonhard Euler's so-called *beta function integral* ,

$$\begin{aligned} \frac{j!\,k!}{(j+k+1)!} &= \int_0^1 \mathrm{d}x\, x^j (1-x)^k \\ &= \int_0^1 \mathrm{d}x\, (1-x)^j x^k\,, \end{aligned} \tag{1.4.39}$$

this becomes

$$\begin{aligned} \delta\, \mathrm{e}^{A} &= \sum_{j,k=0}^{\infty} \int_0^1 \mathrm{d}x\, x^j (1-x)^k \frac{A^j}{j!}\, \delta A\, \frac{A^k}{k!} \\ &= \int_0^1 \mathrm{d}x \sum_{j=0}^{\infty} \frac{(xA)^j}{j!}\, \delta A \sum_{k=0}^{\infty} \frac{\bigl((1-x)A\bigr)^k}{k!} \end{aligned} \tag{1.4.40}$$

or

$$\begin{aligned} \delta\, \mathrm{e}^{A} &= \int_0^1 \mathrm{d}x\ \mathrm{e}^{xA}\, \delta A\ \mathrm{e}^{(1-x)A} \\ &= \int_0^1 \mathrm{d}x\ \mathrm{e}^{(1-x)A}\, \delta A\ \mathrm{e}^{xA}\,. \end{aligned} \tag{1.4.41}$$

This formula for the variation of an exponential operator function is worth memorizing. It contains all of perturbation theory *in nuce*.

1-23 Show that (1.4.41) implies

$$\delta\, \mathrm{e}^{\alpha A} = \int_0^{\infty} \mathrm{d}\alpha_1 \int_0^{\infty} \mathrm{d}\alpha_2\, \delta(\alpha_1+\alpha_2-\alpha)\, \mathrm{e}^{\alpha_1 A}\, \delta A\ \mathrm{e}^{\alpha_2 A}\,, \tag{1.4.42}$$

where α is a real parameter that is not varied along with A.

1-24 Now use this and the identity

$$(\beta - A)^{-1} = \frac{1}{\beta - A} = \int_0^\infty \mathrm{d}\alpha \; \mathrm{e}^{-\alpha\beta}\, \mathrm{e}^{\alpha A}$$

to establish

$$\delta \frac{1}{\beta - A} = \frac{1}{\beta - A}\delta A \frac{1}{\beta - A}\,.$$

Which restrictions apply to β to ensure the convergence of the integral?

1-25 Justify the statement

$$\delta X^{-1} = -X^{-1}\,\delta X\, X^{-1}\,,$$

and then use it to derive the result of the preceding exercise directly, that is without invoking the integral expression for $(\beta - A)^{-1}$.

1-26 First show that

$$\mathrm{e}^{-\epsilon B}\,\mathrm{e}^{A}\,\mathrm{e}^{\epsilon B} = \mathrm{e}^{\mathrm{e}^{-\epsilon B} A\, \mathrm{e}^{\epsilon B}}\,,$$

where A and B are operators and ϵ is a complex number, and then use this to demonstrate that

$$\Bigl[\mathrm{e}^{A}, B\Bigr] = \int_0^1 \mathrm{d}x \; \mathrm{e}^{(1-x)A}\bigl[A, B\bigr]\,\mathrm{e}^{xA}\,.$$

1-27 All eigenvalues of the hermitian operator A are positive. Verify that

$$\log A = \int_0^\infty \mathrm{d}\alpha \left(\frac{1}{\alpha + 1} - \frac{1}{\alpha + A}\right) = \int_0^\infty \mathrm{d}\beta \; \frac{\mathrm{e}^{-\beta} - \mathrm{e}^{-\beta A}}{\beta}$$

are two valid integral representations of $\log A$. Then consider an infinitesimal variation δA and establish

$$\delta \log A = \int_0^\infty \mathrm{d}\alpha \, \frac{1}{\alpha + A}\,\delta A\,\frac{1}{\alpha + A}\,.$$

1.4.3 *Time-independent Hamilton operator*

As an application of (1.4.41), which shows the connection with the quantum action principle, we consider the situation of a time-independent Hamilton operator, that is

$$\frac{\mathrm{d}}{\mathrm{d}t} H\bigl(A(t), t\bigr) = 0 \quad \text{implying} \quad H = H\bigl(A(t)\bigr) \equiv H(t) \tag{1.4.43}$$

so that $\dfrac{\partial H}{\partial t} = 0$ and $H(t) = H(t_1) = H(t_2)$. Then

$$\langle a, t_1| = \langle a, t_2|\, \mathrm{e}^{-\mathrm{i}H(t_2)(t_1 - t_2)/\hbar} \tag{1.4.44}$$

and, for variations of the Hamilton operator only,

$$\delta\langle a, t_1|b, t_2\rangle = \langle a, t_2|\Bigl(\delta\,\mathrm{e}^{-\mathrm{i}H(t_2)T/\hbar}\Bigr)|b, t_2\rangle \tag{1.4.45}$$

with $T = t_1 - t_2$ as always. Here we meet

$$\begin{aligned}\delta\,\mathrm{e}^{-\mathrm{i}H(t_2)T/\hbar} = \int_0^1 \mathrm{d}x\ \mathrm{e}^{(1-x)(-\mathrm{i}H(t_2)T/\hbar)}\Bigl(-\frac{\mathrm{i}}{\hbar}\delta H(t_2)T\Bigr)&\\ \times\ \mathrm{e}^{x(-\mathrm{i}H(t_2)T/\hbar)}&\end{aligned} \tag{1.4.46}$$

or with $xT = t - t_2$, $(1-x)T = t_1 - t$, $\mathrm{d}x\,T = \mathrm{d}t$,

$$\delta\,\mathrm{e}^{-\mathrm{i}H(t_2)T/\hbar} = \int_{t_2}^{t_1} \mathrm{d}t\ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t_2)(t_1-t)}\Bigl(-\frac{\mathrm{i}}{\hbar}\delta H(t_2)\Bigr)\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t_2)(t-t_2)}\,. \tag{1.4.47}$$

The unitary operator on the far right, $\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t_2)(t-t_2)}$, advances states and operators from time t_2 to time t, so that

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar}H(t_2)(t-t_2)}\delta H(t_2)\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(t_2)(t-t_2)} = \delta H(t) \tag{1.4.48}$$

and, therefore,

$$\begin{aligned}\delta\,\mathrm{e}^{-\mathrm{i}H(t_2)T/\hbar} &= \int_{t_2}^{t_1} \mathrm{d}t\ \mathrm{e}^{-\mathrm{i}H(t_2)(t_1-t_2)/\hbar}\Bigl(-\frac{\mathrm{i}}{\hbar}\delta H(t)\Bigr)\\ &= \mathrm{e}^{-\mathrm{i}H(t_2)T/\hbar}\int_{t_2}^{t_1} \mathrm{d}t\,\Bigl(-\frac{\mathrm{i}}{\hbar}\delta H(t)\Bigr)\,.\end{aligned} \tag{1.4.49}$$

It follows that

$$\begin{aligned}\delta\langle a, t_1|b, t_2\rangle &= \langle a, t_2|\,\mathrm{e}^{-\mathrm{i}H(t_2)T}\int_{t_2}^{t_1}\mathrm{d}t\,\Bigl(-\frac{\mathrm{i}}{\hbar}\delta H(t)\Bigr)|b, t_2\rangle\\ &= \langle a, t_1|\int_{t_2}^{t_1}\mathrm{d}t\,\Bigl(-\frac{\mathrm{i}}{\hbar}\delta H(t)\Bigr)|b, t_2\rangle\,,\end{aligned} \tag{1.4.50}$$

which is exactly what the quantum action principle tells us about variations of the dynamics at intermediate times.