

# Unitary Time Development and Born Rule

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## Reference:

CQT = R. B. Griffiths, *Consistent Quantum Theory* (Cambridge, 2002)

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## 1 Schrödinger Equation and Time Development Operators

- Reference: CQT Ch. 7

### 1.1 Schrödinger's equation

- ★ Schrödinger's (time-dependent) equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \quad (1)$$

applies to a *closed* or *isolated* quantum system, one that is not interacting with an external environment.

- However, the notion of “closed” is often extended to include cases in which one can for the purposes one is interested in replace the actual interaction with the environment with an “effective” Hamiltonian, which is often (but not always) time dependent, in such a way that (1) is a good approximation.

- ★ Quantum mechanics can also be applied to an “open system” which is some system of interest plus an environment with which it interacts. In principle what one needs to do is to work out the quantum

development of the combined system-plus-environment. But this is very difficult to do, so one makes various approximations for the environment and the effects of the environment on the system of interest. Consideration of open systems lies outside the scope of this set of notes.

- We call the time evolution resulting from Schrödinger's equation *unitary* time evolution (the name will be justified below) in contrast to the *probabilistic* time evolution of quantum systems taken up, for which see Sec. 2.

## 1.2 Time-dependent kets and operators

★ What does it mean to take the time derivative of a ket  $|\psi(t)\rangle$ ? What is meant by a time-dependent operator, and its time derivative? This section relates these concepts to derivatives of ordinary (complex-valued) functions. It can be skipped by readers who are already familiar with these ideas.

- In the technical sense all we mean when writing  $|\psi(t)\rangle$  is that we have a *collection* of kets, one for every possible value of  $t$ . Similarly,  $A(t)$  is a *collection* of operators, one for every possible value of  $t$ . The choice could be completely arbitrary. E.g.,  $A(t) = 0$  if  $t$  is a rational number,  $A(t) = I$  if  $t$  is irrational. But physicists are typically interested in cases where there is a continuous, differentiable, dependence on  $t$ .

★ A helpful perspective is to note the one-to-one correspondence between kets and column vectors, and between operators and matrices, when an orthonormal basis has been specified. We assume the  $\{|j\rangle\}$  basis,  $1 \leq j \leq d$  is *time independent*, i.e., we will be using the same basis for every time  $t$ . Then every element of a column vector and every matrix element

$$\psi_j(t) = \langle j|\psi(t)\rangle, \quad A_{jk}(t) = \langle j|A(t)|k\rangle \quad (2)$$

is an ordinary (complex-valued) function of  $t$ . Conversely, given a collection of  $d$  complex functions of time  $\psi_j(t)$ , or of  $d^2$  functions  $A_{jk}(t)$ , we can use them to construct the corresponding ket or time-dependent operator

$$|\psi(t)\rangle = \sum_j \psi_j(t) |j\rangle, \quad A(t) = \sum_{jk} A_{jk}(t) |j\rangle\langle k|. \quad (3)$$

◦ Why insist that the basis be time-independent? Who would ever use a time-dependent basis? Sometimes a time-dependent basis provides a very convenient way of thinking about the physics. See the example in Sec. 3.3 below. But for present purposes a time-independent basis is the simplest and shortest route to understanding.

★ Time derivative. If every function  $\psi_j(t)$  in the column vector that corresponds to  $|\psi(t)\rangle$ , (2), is differentiable, we can define  $d|\psi(t)\rangle/dt$  as the ket such that the  $j$ 'th component of the corresponding column vector is  $d\psi_j(t)/dt$ , or

$$\frac{d}{dt}|\psi(t)\rangle = \sum_j \frac{d\psi_j(t)}{dt} |j\rangle. \quad (4)$$

In the same way, if every  $A_{jk}(t)$  is differentiable we can define

$$A'(t) = dA/dt = \partial A/\partial t \quad (5)$$

as the operator whose matrix elements in our time-independent basis are given by:

$$\langle j|A'(t)|k\rangle = d\langle j|A(t)|k\rangle/dt = dA_{jk}/dt = A'_{jk}(t). \quad (6)$$

That is, the matrix of the time derivative is obtained by taking time derivatives of the original matrix elements. One can also write the result using dyads:

$$A'(t) = dA/dt = \sum_{jk} A'_{jk}(t) \cdot |j\rangle\langle k|. \quad (7)$$

◦ Some authors prefer to write  $\partial|\psi(t)\rangle/\partial t$  in place of  $d|\psi(t)\rangle/dt$ , or  $\partial A/\partial t$  in place of  $A'(t)$  or  $dA/dt$ . There is no particular reason to use partial derivative notation when there are no other continuous variables (e.g, positions in space) under consideration, but it also does no harm.

★ While the above discussion was carried out using a particular orthonormal basis  $\{|j\rangle\}$ , the relationship between  $|\psi(t)\rangle$  and  $d|\psi\rangle/dt$ , or between  $A(t)$  and  $dA/dt$  does not depend upon the choice of basis. The reason is that any other (time-independent, of course) orthonormal basis is related to the one we used by means of a time-independent unitary transformation, and one can check that, for example, (7) is still correct if both the dyads and the matrix elements in the final sum refer to this alternate basis.

□ Exercise. Make this argument explicit using an alternate basis  $\{|\bar{j}\rangle\}$

★ If kets or operators can be differentiated they can also be integrated. Again, it helps to use a basis, because while

$$B(t) = \int_0^t A(t') dt' \quad (8)$$

looks rather abstract,

$$B_{jk}(t) = \langle j|B(t)|k\rangle = \int_0^t \langle j|A(t')|k\rangle dt' = \int_0^t A_{jk}(t') dt' \quad (9)$$

simply tells us to integrate each of the matrix elements separately in order to get the matrix elements of the integral. From this it follows by the standard rules of calculus that

$$A(t) = dB(t)/dt. \quad (10)$$

- Similar expressions apply to integrals of kets.

### 1.3 Solutions to Schrödinger's equation

★ In (1) the Hamiltonian  $H$  may depend on time, but we shall assume that at every time it is a Hermitian operator:  $H(t) = H(t)^\dagger$ .

- Using a time-independent basis  $\{|j\rangle\}$  allows us to write (1) as a matrix equation

$$\frac{d\langle j|\psi(t)\rangle}{dt} = \sum_k \langle j|H(t)|k\rangle \langle k|\psi(t)\rangle, \quad (11)$$

which is to say

$$d\psi_j/dt = \sum_K H_{jk}(t)\psi_k(t), \quad (12)$$

that is to say, a collection of coupled first-order linear differential equations with, in general, time-dependent coefficients on the right side.

★ A standard result from the theory of differential equations is that (11), or equivalently (12) has a *unique* solution provided  $\psi(t_0)$ , i.e., all the  $\psi_j(t_0)$  are given at some reference time  $t_0$ .

◦ There are technical requirements that  $H(t)$ , equivalently the  $H_{jk}(t)$ , is not too badly behaved; they will be satisfied in the usual physics applications. Discontinuities in  $H(t)$  as a function of  $t$  are allowed if they are not too wild or too frequent.

◦ We are also assuming the Hilbert space is of finite dimension in order to avoid additional technical complications.

★ It is useful to think of a solution  $|\psi_t\rangle$  of Schrödinger's equation (1) as the quantum analog of a *trajectory* in classical phase space: the set of points traced out as a function of time by a solution to Hamilton's equations.

◦ The point a trajectory passes through at a particular time  $t_0$  determines the entire trajectory at all times, provided the classical Hamiltonian  $H(t)$  (which can be a function of time) is known.

- ★ Let  $|\phi(t)\rangle, |\psi(t)\rangle$  be any two solutions of Schrödinger's equation. Then

$$\frac{d}{dt} \langle \phi(t)|\psi(t)\rangle = 0 \quad (13)$$

follows from (1) and  $H = H^\dagger$ .

□ Exercise. Show it. Where did you use  $H = H^\dagger$ ?

• Consequence of (13): the linear Schrödinger equation (1) *preserves the norm* (“length of the vector”):  $\|\psi(t)\| = \sqrt{\langle \psi(t) | \psi(t) \rangle}$  is independent of time  $t$ . In quantum theory one refers to this as *unitarity*—more below.

◦ The classical analog of unitarity is *Liouville’s theorem* on the preservation of phase space “volume” in classical mechanics.

#### 1.4 Time development operator

★ Because (1) is a linear differential equation, one can show that if  $t$  and  $t'$  are any two times there is a linear operator  $T(t, t')$ , the *time development* operator, such that when  $|\psi(t')\rangle$  is a solution to Schrödinger’s equation

$$|\psi(t)\rangle = T(t, t')|\psi(t')\rangle. \quad (14)$$

• For a *given*  $t$  and  $t'$  there is a *single* operator  $T(t, t')$  such that for *every* solution to Schrödinger’s equation with the *given* Hamiltonian (and a given time dependence if  $H(t)$  depends on time), thus for *every* (quantum) trajectory, (14) is satisfied.

◦ Classical analogy: Given  $t$  and  $t'$ , there is a map  $T(t, t')$  of the phase space  $\Gamma$  to itself which carries a point  $\gamma'$  to  $\gamma$  by treating  $\gamma'$  at  $t'$  as an initial condition and integrating Hamilton’s equations from  $t'$  to  $t$  to get the point  $\gamma$ .

• Note that in writing  $T(t, t')$  we really have in mind a *family* of operators labeled by two real parameters,  $t$  and  $t'$ .

★ For each  $t$  and  $t'$ ,  $T(t, t')$  is a *unitary* operator. This is a consequence of the fact, see (13) and the following discussion, that

$$\langle \psi(t) | \psi(t) \rangle = \langle \psi_{t'} | T(t, t')^\dagger T(t, t') | \psi_{t'} \rangle = \langle \psi(t') | \psi(t') \rangle \quad (15)$$

holds whatever choice one makes for  $|\psi(t')\rangle$ , i.e., whatever trajectory one considers.

◦ See Sec. 1.5 below for some properties of unitary operators. We are, as usual, employing the rules for finite-dimensional Hilbert spaces, relying on the experts to assure us that they will (usually, anyway) work for the infinite-dimensional cases we may be interested in.

★ As well as unitarity, the time-development operators satisfy the following important relations:

$$T(t, t) = I, \quad (16)$$

$$T(t, t')T(t', t'') = T(t, t''), \quad (17)$$

$$T(t', t) = T(t, t')^\dagger = T(t, t')^{-1} \quad (18)$$

□ Exercise. Give brief arguments (not a proof) for the validity of each of these.

★ In place of  $T(t, t')$  with two arguments one can use

$$U(t) := T(t, 0), \quad (19)$$

where now the family of unitary operators depends on only a single argument rather than two, and

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle \quad (20)$$

◦ In (19) the time  $t = 0$  plays a special role. One could just as well use some other *fixed reference time*  $t_r$  and replace (19) with

$$U(t) := T(t + t_r, t_r), \quad (21)$$

In the following discussion we shall assume that  $t_r = 0$ , i.e., use the definition (19)

- In place of (16) to (18) we have the relations:

$$U(0) = I, \tag{22}$$

$$U(-t) = U(t)^\dagger = U(t)^{-1}. \tag{23}$$

- Exercise. Use the definition (19) to derive (23) from (18).
- Exercise. Show that (17) is a consequence of (23).
- If  $U(t)$  is known one can use it to define  $T(t, t')$ :

$$T(t, t') := U(t)U(t')^\dagger. \tag{24}$$

- The use of  $T(t, t')$  or  $U(t)$  is somewhat a matter of taste. For some purposes the former and for some purposes the latter gives simpler formulas.
- Schrödinger's equation for time-development operators:

$$i\hbar \frac{d}{dt}U(t) = H(t)U(t), \quad i\hbar \frac{\partial}{\partial t}T(t, t') = H(t)T(t, t'), \quad -i\hbar \frac{\partial}{\partial t'}T(t, t') = T(t, t')H(t') \tag{25}$$

where in the equations for  $T(t, t')$  we use a partial derivative because there are two arguments, and  $t'$  should be held fixed while carrying out  $\partial/\partial t$ . One could also write  $\partial U(t)/\partial t$ .

- Exercise. Derive these starting with (1), and (14) or (20).

## 1.5 Properties of unitary operators

- ★ An operator  $J$  that preserves the norm,

$$\|J|\psi\rangle\|^2 = \langle\psi|J^\dagger J|\psi\rangle = \langle\psi|\psi\rangle \tag{26}$$

for every  $|\psi\rangle$  in the Hilbert space is called an *isometry*. (It “preserves the metric”, which in this case is given by the norm.)

- An isometry  $J$  that maps the Hilbert space into itself is a *unitary* operator and satisfies the conditions

$$JJ^\dagger = J^\dagger J = I \tag{27}$$

- Exercise. Which of these equalities expresses the fact that  $J$  is an isometry?

• If the Hilbert space  $\mathcal{H}$  is *finite* and  $J$  maps  $\mathcal{H}$  into  $\mathcal{H}$  (rather than, for example, into some larger Hilbert space  $\mathcal{H}'$ ) then each equality in (27) implies the other, so only one of them needs to be checked to verify that the operator  $J$  is unitary.

- ★ Important properties of unitary operators

• The product  $UV$  of two unitary operators  $U$  and  $V$  is a unitary operator, and therefore also the product of any number of unitary operators is a unitary operator.

• The eigenvalues of a unitary operator are complex numbers of magnitude 1. (Real numbers  $\pm 1$  are also allowed.)

- The matrix of a unitary operator in an *orthonormal* basis  $\{|b_j\rangle\}$  is a unitary matrix.

$$U_{jk} = \langle b_j|U|b_k\rangle. \tag{28}$$

Conversely, if  $U_{jk}$  is a unitary matrix,  $\sum_{jk} U_{jk}|b_j\rangle\langle b_k|$  is a unitary operator.

◦ A unitary matrix is one in which the columns are mutually orthogonal and normalized column vectors. Equivalently, the rows are mutually orthogonal and normalized row vectors. As long as the matrix is finite these two characterizations are equivalent; one implies the other.

- Exercise. Explain why one of these characterizations corresponds to  $U \cdot U^\dagger = I$ , understanding this as matrix multiplication and  $I$  as the identity matrix, and the other to  $U^\dagger \cdot U = I$ .

- If  $K$  is a Hermitian operator,  $e^{iK}$  is a unitary operator, and if  $U$  is a unitary operator, then there is an operator  $K$  such that  $U = e^{iK}$ , and this  $K$  is Hermitian.

□ Exercise. Prove it. [Hint: spectral representation.]

□ Exercise. Show that any  $2 \times 2$  unitary matrix is of the form

$$e^{i\phi} \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}, \quad (29)$$

where  $\phi$  is a (real) phase, and  $\alpha$  and  $\beta$  are complex numbers that satisfy a certain condition (which you should work out).

## 1.6 Time-independent Hamiltonian

★ Important case: Hamiltonian  $H$  independent of time. Then  $T(t, t')$  depends only on  $t - t'$  and is equal to  $U(t - t')$ :

$$T(t, t') = U(t - t') = \exp[-i(t - t')H/\hbar]. \quad (30)$$

- In particular, if

$$H = \sum_n E_n |e_n\rangle\langle e_n| = \sum_j E'_j P_j \quad (31)$$

is the spectral representation of the time-independent Hamiltonian, where in the second form we assume that  $j \neq k$  means  $E'_j \neq E'_k$ , then

$$U(t) = \sum_n e^{-itE_n/\hbar} |e_n\rangle\langle e_n| = \sum_j e^{-itE'_j/\hbar} P_j, \quad (32)$$

which is often a very convenient way to write  $U(t) = T(t - t')$ .

★ The most general solution to the Schrödinger equation can be written in the form

$$|\psi(t)\rangle = \sum_n c_n e^{-iE_n t/\hbar} |e_n\rangle, \quad (33)$$

where the  $c_n$  are time-independent complex numbers.

□ Exercise. Show that  $|\psi(t)\rangle$  in (33) is indeed a solution of the Schrödinger equation (1) with  $H$  in (31) independent of the time.

□ Exercise. Discuss why (33) is the most general solution of the Schrödinger equation. [What can you say about  $t = 0$ ?]

★ A special case is that of a *stationary state* in which only one of the coefficients  $c_n$  in (33) is nonzero, i.e.,  $|\psi(t)\rangle$  is an energy eigenstate with a phase that varies with time. In this case the corresponding physical property, the projector  $|\psi(t)\rangle\langle\psi(t)|$ , is independent of time, and if  $|\psi(t)\rangle$  is thought of as a pre-probability, see Sec. 2, the probabilities it assigns to the properties in any time-independent decomposition of the identity  $\{P^k\}$  are independent of time.

- Hence any quantum state with a well-defined energy (which is to say an energy eigenstate) has no time dependence whatsoever. Contrast this with a classical system of fixed energy, e.g., a harmonic oscillator, which can have a quite nontrivial time dependence.

- Interesting time dependence in the case of a time-independent Hamiltonian is only possible when  $|\psi(t=0)\rangle$  is a *superposition* of states with different energies.

## 2 The Born Rule

### 2.1 Probabilities of properties

★ Starting with an initial state  $|\psi_0\rangle$  at time  $t_0$  Schrödinger's equation can be integrated to yield  $|\psi_1\rangle$  at a time  $t_1$ . What is the *physical significance* of  $|\psi_1\rangle$ ? How should one think about it? One way to think about it is in terms of the *probabilities it generates* via what is known as the *Born rule*.

- One can think of  $|\psi_1\rangle$  as a *pre-probability*, a mathematical tool for calculating probabilities of certain physical properties at the time  $t_1$ .

★ To be specific, suppose we are interested in the properties of the system at  $t_1$  corresponding to a decomposition of the identity  $\{P^k\}$ ,  $I = \sum_k P^k$ . Here we are using the superscript  $k$  as a label, not as a power, in order to reserve the subscript position to indicate the time.

- One possibility would be an orthonormal basis  $\{|\phi_1^k\rangle\}$ ;  $P^k = |\phi_1^k\rangle\langle\phi_1^k|$ .
- The *Born rule* states that these probabilities are given by

$$\Pr(P^k) = \langle\psi_1|P^k|\psi_1\rangle = \text{Tr}\{|\psi_1\rangle\langle\psi_1|P^k\}, \quad (34)$$

where we are assuming a normalized initial state, so that  $\|\psi_0\| = \|\psi_1\| = 1$ . Otherwise, divide the right side by  $\langle\psi_0|\psi_0\rangle = \langle\psi_1|\psi_1\rangle$ .

- In the case where the  $\{P^k\}$  are associated with an orthonormal basis  $\{|\phi_1^k\rangle\}$ ,  $P^k = |\phi_1^k\rangle\langle\phi_1^k|$ , one can also write

$$\Pr(\phi_1^k) = |\langle\phi_1^k|\psi_1\rangle|^2, \quad (35)$$

where the inner product  $\langle\phi_1^k|\psi_1\rangle$  is sometimes referred to as a *probability amplitude*.

□ Exercise. Show that the different expressions in (34) and (35) give the same result.

- These probabilities depend, of course, on the assumed state or property  $|\psi_0\rangle$  at  $t_0$ , and sometimes it is useful to include that fact in the notation by writing  $\Pr(P^k)$  as a *conditional probability*  $\Pr(P^k | \psi_0)$ , where the expression to the right of the vertical bar  $|$  is the condition; read this as “the probability of  $P^k$  at time  $t_1$  given  $[\psi_0]$  (or  $|\psi_0\rangle$ ) at  $t_0$ .”

★ As is obvious, these probabilities also depend upon the choice of decomposition  $\{P^k\}$  (or orthonormal basis  $\{|\phi_1^k\rangle\}$ ). Overlooking this fact can give rise to confusion, because different decompositions may be incompatible with each other, and assigning probabilities simultaneously to noncommuting properties or projectors does not make sense.

- So what is the *right* set of properties  $\{P^k\}$  to use at time  $t_1$ ? This question has no right answer. Typically a decomposition is chosen because the corresponding properties are interesting for some reason. One reason they might be interesting is that the decomposition is associated with some physical variable  $V$  that one is interested in; see the discussion below.

★ A particular case: at  $t_1$  use the decomposition  $P^1 = |\psi_1\rangle\langle\psi_1|$ ,  $P^2 = I - |\psi_1\rangle\langle\psi_1|$ . The Born rule then tells us that  $P^1$  is certain (probability 1) at time  $t_1$ , given  $|\psi_0\rangle$  at  $t_0$ . Thus a measurement arranged to determine this particular property at  $t_1$  will always show that the system was, just before the measurement, in (the ray corresponding to)  $|\psi_1\rangle$ , rather than in the subspace corresponding to its orthogonal complement.

□ Exercise. Suppose that the orthonormal basis  $\{|\phi_1^k\rangle\}$  includes  $|\psi_1\rangle$ , i.e.,  $|\psi_1\rangle$  is in the same ray as one of the basis vectors. What probability does the Born rule assign to each  $|\phi_1^k\rangle$ ?

## 2.2 Physical variables

★ let  $V = V^\dagger$  be the Hermitian operator corresponding to a physical variable or “observable”. There is a unique decomposition of the identity  $\{P^k\}$  associated with  $V$  in the sense that

$$V = \sum_k v'_k P^k; \quad j \neq k \text{ implies that } v'_j \neq v'_k. \quad (36)$$

- The probability that  $V$  takes on one of its eigenvalues, say  $V = v_k$ , is then just the probability of the projector  $P^k$ .

★ A physical variable  $V$  is like a random variable in ordinary probability theory, and hence it makes sense to talk about its average value  $\langle V \rangle$  and its variance  $\langle V^2 \rangle - \langle V \rangle^2$  (the square of the standard deviation  $\Delta V$ ).

- In particular, we can use (34) to write

$$\langle V \rangle = \sum_k v'_k \Pr(P^k) = \sum_k v'_k \langle\psi_1|P^k|\psi_1\rangle = \langle\psi_1|\sum_k v'_k P^k|\psi_1\rangle = \langle\psi_1|V|\psi_1\rangle \quad (37)$$

◦ And in exactly the same way,  $\langle V^2 \rangle = \langle \psi_1 | V^2 | \psi_1 \rangle$ .

★ Formulas (37) is a very convenient way to calculate  $\langle V \rangle$  starting from a pre-probability  $|\psi_1\rangle$ , and it should be memorized. By setting  $V = P^k$  one obtains (51), since  $\text{Pr}(P^k) = \langle P^k \rangle$

• As in the case of other extremely convenient and simple formulas, it is wise to keep in mind some limitations.

• First, if  $V$  can take on more than two values,  $\langle V \rangle$  does not determine the probability distribution for  $V$ , so the latter contains additional information not found in  $\langle V \rangle$ .

□ Exercise. Show that if  $V$  can only take on two values, the two probabilities are uniquely determined if  $\langle V \rangle$  is known.

• Second, suppose that  $V$  and  $W$  are two Hermitian operators that *do not commute*. Then because the average defined in (37) is linear in its argument, it follows that

$$\langle V + W \rangle = \langle V \rangle + \langle W \rangle. \quad (38)$$

There is nothing wrong with this as a mathematical equation; it holds both when  $VW = WV$  and also when  $VW \neq WV$ . However, in the latter case it is difficult to give it a physical interpretation, because  $V$  and  $W$  cannot (at least in general) be assigned values simultaneously, and neither of them commute with their sum  $S = V + W$ . Consequently, (38) is a relationship among the averages of three operators to which one cannot ascribe simultaneous values. One may, however, be tempted by the simplicity of (38) to suppose that such simultaneous values exist.

• The assumption that physical variables (observables) can simultaneously possess definite values even when the operators do not commute is one form of what is known as a *hidden variables theory*: supplementing the quantum Hilbert with additional stuff because it allows what the Hilbert space does not.

◦ Despite an enormous amount of time expended on them, it seems safe to say that hidden variables theories have not yet produced any useful resolution of any of the conceptual difficulties of quantum mechanics.

### 2.3 Probabilities and measurements

★ It is often said that (34) will give the probabilities for the different outcomes of a measurement designed to measure the decomposition  $\{P^k\}$  or, equivalently, designed to measure the physical variable  $V$  with which  $\{P^k\}$  is associated through (36).

◦ Measuring  $V$  is the same thing as measuring the decomposition  $\{P^k\}$ , in the sense that each eigenvalue  $v'_k$  of  $V$  is associated with a unique projector  $P^k$ , and vice versa.

• Identifying  $\text{Pr}(P^k)$  with the probability of a measurement outcome is correct if one keeps in mind that a somewhat idealized type of measurement is in view, one in which each  $P^k$  in the decomposition leads to a distinct measurement outcome. Imagine that the measuring apparatus has a pointer pointing at a scale on which  $k$  (or  $v'_k$ ) is indicated after the measurement is complete. Keep in mind that measurements tend to have significant effects upon the measured system, and the measured system may even disappear during the measurement process. Thus the measurement outcome (pointer position) is telling one something about properties of the system *just before* the measurement took place.

◦ Matters become clearer when one sets up models for quantum measurements and analyzes (in quantum terms, of course) what happens.

• Incompatible properties such as the  $V$  and  $W$  considered in connection with (38) cannot be simultaneously measured. The reason is that there are no values to be simultaneously measured; even the most competent experimentalist cannot design apparatus to measure what is not there.

◦ Keeping this in mind avoids falling into the hidden variables trap discussed above.

• In fact, from the operational point of view checking the equality in (38) requires a large number of repeated measurements. To determine  $\langle V \rangle$  one needs several repeated measurements. For each one the system is prepared in the same  $|\psi_0\rangle$  at the time  $t_0$ , allowed to evolve to the time  $t_1$ , and then a measurement is carried out yielding one of the values of  $k$  in (36) (equivalently, one of the eigenvalues of  $V$ ). Since successive measurements will in general yield different values, it is necessary to carry out a sufficiently large number of measurements so that one can be reasonably confident that  $\langle V \rangle$  has been determined with the



desired accuracy. After this has been done another independent series of measurements, in each case starting with  $|\psi_0\rangle$  and measuring  $W$  (or the associated decomposition of  $I$ ) at  $t_1$ , is required in order to determine  $\langle W \rangle$ . Each time a measurement is made the system must be thrown away after the measurement because even an ideal measurement can produce nonnegligible changes in the measured system, so there is no way of combining the  $V$  and  $W$  measurements. Finally, a third series of measurements is required to determine the average value of  $S = V + W$ . Thus a long, time consuming process.

## 2.4 Averages as a function of time

★ It is sometimes of interest to discuss how the average of some physical variable  $V$  as given by (37), rewritten as

$$\langle V(t) \rangle_t = \langle \psi(t) | V(t) | \psi(t) \rangle, \quad (39)$$

depends upon the time  $t$ , assuming that  $|\psi(t)\rangle$  is a solution to Schrödinger's equation with a fixed initial state  $|\psi_0\rangle$  at an initial time  $t_0$  (which could be  $T_0 = 0$ ). We also allow for the possibility that the physical variable  $V$  depends upon the time, i.e., has time-dependent matrix elements in a fixed orthonormal basis, see Sec. 1.2.

★ In particular, we can ask for the *time derivative*  $d\langle V(t) \rangle_t / dt$ . If one is not familiar with taking derivatives of an expression like that found on the right side of (39) it is helpful to write it out using a fixed (time-independent) orthonormal basis:

$$\langle V(t) \rangle_t = \langle \psi(t) | V(t) | \psi(t) \rangle = \sum_{j,k} \langle \psi(t) | j \rangle \cdot \langle j | V(t) | k \rangle \cdot \langle k | \psi(t) \rangle. \quad (40)$$

• When written in this form it is evident that we can take the time derivative of  $\langle V(t) \rangle_t$  by applying the usual rule for derivatives of products to each of the summands on the right side of (40). The time derivatives  $d\langle \psi(t) | j \rangle / dt$  and  $d\langle k | \psi(t) \rangle / dt$  can be written in terms of the Hamiltonian by using (11) and its adjoint (take the complex conjugate of both sides). And  $d\langle j | V(t) | k \rangle / dt = \langle j | V'(t) | k \rangle$ , see (6). After some rewriting one arrives at

$$\frac{d\langle V(t) \rangle_t}{dt} = \frac{i}{\hbar} \langle \psi(t) | [H(t), V(t)] | \psi(t) \rangle + \langle \psi(t) | V'(t) | \psi(t) \rangle, \quad (41)$$

where the last term is sometimes written as  $\langle \psi(t) | \partial V / \partial t | \psi(t) \rangle$ ; see the comments in Sec. 1.2.

• The same result can be obtained more quickly by writing

$$\frac{d}{dt} \langle \psi(t) | V(t) | \psi(t) \rangle = (d\langle \psi(t) | / dt) V(t) | \psi(t) \rangle + \langle \psi(t) | dV/dt | \psi(t) \rangle + \langle \psi(t) | V(t) (d|\psi(t)\rangle / dt), \quad (42)$$

and evaluating the derivatives of the ket and bra using Schrödinger's equation (1) and its adjoint.

★ If  $V$  is independent of the time, which does *not* by itself mean that  $\langle V \rangle_t$  is independent of the time, then the last term in (41) is absent, and the time derivative of the average of  $V$  is equal to  $(i/\hbar)$  times the average of its commutator with the Hamiltonian.

$$d\langle V \rangle / dt = (i/\hbar) \langle [H(t), V] \rangle. \quad (43)$$

• In the case where both  $H$  and  $V$  are independent of time and the two operators commute one refers to the physical variable  $V$  as a *constant of the motion*. In this case  $d\langle V \rangle / dt = 0$ , as one might expect for something that could be called a constant of the motion. One can use the fact that  $H$  and  $V$  can be simultaneously diagonalized to prove a stronger result: not only  $\langle V \rangle$  but also the probability of each projector  $P^k$  in the associated decomposition (36) is independent of  $t$ .

□ Exercise. What are the constants of the motion of a classical particle moving in a spherically-symmetrical potential? What does this suggest in terms of operators that commute with the quantum Hamiltonian?

★ Despite its elegant appearance, giving a realistic physical interpretation to (41) is far from straightforward.

- Consider the case where  $V'(t) = 0$ , so the final term in (41) can be ignored, but assume that  $[H, V] \neq 0$ , so there is a nontrivial time dependence of  $\langle V \rangle_t$ . How would one check this experimentally by means of measurements? Here is what would be required.

- First fix a time  $t_1$  and by repeatedly preparing the quantum system in the same state at the initial time  $t_0$  determine the probability distribution for the  $P^k$ , and use this to find  $\langle V \rangle_{t_1}$ . To do this accurately may require many repeated measurements. Next fix a second time  $t_2 = t_1 + \Delta t$ , where  $\Delta t$  is a small but finite time difference. Carry out a large number of repeated experiments to find the probabilities of the  $P^k$  at this new time. From this find  $\langle V \rangle_{t_2}$ . Finally construct a numerical approximation

$$(\langle V \rangle_{t_2} - \langle V \rangle_{t_1}) / \Delta t \tag{44}$$

in order to estimate  $d\langle V \rangle / dt$  at  $t_1$ .

- Note that one *cannot* carry out a measurement at  $t_1$  and then let the *same* system evolve for an additional time  $\Delta t$  before carrying out a second measurement to determine whether  $V$  has changed; in general measurements produce nonnegligible perturbations on the measured system.

- An alternative way of thinking about (41) is to imagine a large number of identical but independent systems all prepared in the same initial state and allowed to evolve using identical Hamiltonians. Then  $\langle V \rangle$  might be interpreted as an average over all these systems, and the experimental check would consist in sacrificing a small fraction, a random sample, of the systems to measurement at a time  $t$  and throwing them away; then sacrificing additional systems at time  $t + \Delta t$  and throwing them away, and so forth.

- However, to do analyze this properly in quantum mechanical terms one should use the Hilbert space of the many different systems considered as a single (tensor product) Hilbert space. That analysis lies outside the scope of these notes.

### 3 Two-Level Systems (Spin Half)

- Reference: CQT Sec. 4.2

#### 3.1 Notation

- We are interested in simple examples of unitary time development in the simplest quantum systems, Hilbert space of dimension 2.

- ★ Any quantum two-level (two-state) system is “the same” as any other so far as the formal math is concerned. However, thinking of it as a spin-half particle gives a very nice geometrical picture of what is going on, and picture is realized physically in experiments in which such a particle is placed in a magnetic field and its spin precesses. Hence nowadays it is customary to discuss the dynamics of any two-level quantum system using what is often called the “Bloch sphere” picture

- The “qubit” in quantum information is a two-level system

- We choose an orthonormal basis

$$|z^+\rangle = |0\rangle, \quad |z^-\rangle = |1\rangle, \tag{45}$$

where the kets are eigenvectors of the operator  $S_z$  for the  $z$  component of spin angular momentum, with eigenvalues  $+\hbar/2$  and  $-\hbar/2$ , respectively.

- From now on we choose units with  $\hbar = 1$ , so these eigenvalues are  $\pm 1/2$ .

- The  $|0\rangle, |1\rangle$  notation is widely used in quantum information.

- Let  $w$  be a direction in space corresponding to angles  $(\theta, \phi)$  in spherical polar coordinates. Then a normalized state corresponding to  $S_w = +1/2$  can be written in the form

$$\begin{aligned} |w^+\rangle &= \cos(\theta/2)e^{-i\phi/2}|z^+\rangle + \sin(\theta/2)e^{i\phi/2}|z^-\rangle \\ &= \cos(\theta/2)e^{-i\phi/2} \left( |z^+\rangle + \tan(\theta/2)e^{i\phi}|z^-\rangle \right). \end{aligned} \tag{46}$$

- Remember that multiplying a ket by a nonzero complex number does not alter its physical significance. It is convenient to think of kets for spin half as being of the form  $|z^+\rangle + \gamma|z^-\rangle$ , or  $|0\rangle + \gamma|1\rangle$  in the terminology

of quantum information, where the “physics” is determined by the complex number  $\gamma$ . In particular, in terms of the Bloch sphere picture,  $\gamma = 0$  is the north pole,  $\gamma = \infty$  is the south pole, and  $\gamma = e^{i\phi}$  corresponds to the equator of the Bloch sphere,  $\theta = \pi/2$ , with  $\phi = 0$  the positive  $x$  axis.

- Matrices and column vectors will always be written using the  $\{|z^+\rangle, |z^-\rangle\}$  basis:

$$|z^+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |z^-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \sqrt{2}|x^+\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \sqrt{2}|x^-\rangle = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad (47)$$

and so forth. There is some arbitrariness in the choice of overall phase; e.g., multiplying the  $|x^+\rangle$  or  $|x^-\rangle$  column vectors by  $-1$  would be just as good.

□ Exercise. Write  $|y^+\rangle, |y^-\rangle$  and  $|w^+\rangle$  as column vectors, where  $w$  corresponds to  $\theta = 120^\circ$  and  $\phi = 145^\circ$ .

- Note that  $|z^\pm\rangle$  are eigenkets of  $S_z = \sigma_z/2$ , etc.; recall that the Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (48)$$

and the spin operators (when  $\hbar = 1$ ) are these times a factor of  $1/2$ :  $S_y = \frac{1}{2}\sigma_y$ .

- ★ Any  $2 \times 2$  matrix  $M$  can be written in the form

$$M = a_0 I + a_1 \sigma_x + a_2 \sigma_y + a_3 \sigma_z, \quad (49)$$

where the  $a_j$  are complex coefficients uniquely determined by  $M$ .

◦  $M$  is Hermitian if and only if all the  $a_j$  are real.

□ Exercise. Prove it.

### 3.2 Constant Hamiltonian

★ Let us work out the dynamics in the case in which—with  $\hbar = 1$ , so energy is the same as an angular frequency—the Hamiltonian is

$$H = \frac{1}{2}\vec{\omega} \cdot \vec{\sigma} = \frac{1}{2}(\omega_x \sigma_x + \omega_y \sigma_y + \omega_z \sigma_z), \quad (50)$$

where  $\vec{\omega}$  has three real coefficients, so  $H$  is Hermitian. One could add a constant times the identity, but this does nothing but add a time-dependent overall phase to solutions of the Schrödinger equation, which does not affect the physics.

– The factor of  $\frac{1}{2}$  is there to spare us a factor of 2 later on. It is “natural” if one thinks of  $H$  as  $\omega_x S_x + \omega_y S_y + \omega_z S_z$ .

◦ A Hamiltonian of the form (50) results when a magnetic field is applied in the direction  $\vec{\omega}$  (or the opposite direction, depending on the sign of the gyromagnetic ratio). It is thus rather natural, albeit somewhat careless, to refer to  $\omega_x, \omega_y, \omega_z$  as the “components of the magnetic field.” This terminology will be used frequently in the following discussion.

- ★ Consider the case  $\omega_x = \omega_y = 0$ , a magnetic field in the  $z$  direction. Then

$$H = \frac{\omega_z}{2} \sigma_z = \begin{pmatrix} \omega_z/2 & 0 \\ 0 & -\omega_z/2 \end{pmatrix}. \quad (51)$$

- As  $H$  is time independent, we can use (30):

$$U(t) = e^{-itH} = \begin{pmatrix} e^{-i\omega_z t/2} & 0 \\ 0 & e^{i\omega_z t/2} \end{pmatrix}. \quad (52)$$

- To see what this means, work out

$$U(t) \begin{pmatrix} 1 \\ ae^{i\phi} \end{pmatrix} = e^{-i\omega_z t/2} \begin{pmatrix} 1 \\ ae^{i(\phi + \omega_z t)} \end{pmatrix}. \quad (53)$$

◦ Thus ignoring the initial phase factor, which doesn't affect the physics, we see that the ket corresponding to  $w = (\theta, \phi)$  rotates into  $w = (\theta, \phi + \omega_z t)$ . The dynamics corresponding to (51) is a rotation by an angle  $\omega_z t$  about the  $z$  axis, which is “positive” (counterclockwise when looking down the  $z$  axis towards the Bloch sphere) when  $\omega_z t$  is positive. Thus in this case unitary dynamics means the Bloch sphere rotating at a uniform speed about the  $z$  axis.

• Any unitary transformation on a 2-dimensional Hilbert space can always be thought of as a rotation of the Bloch sphere by some amount around some axis. Only proper rotations are allowed (no reflections). Very useful geometrical picture.

★ For the most general time-independent Hamiltonian (50) of a two-state system (again, adding  $a_0 I$  to  $H$  does not change the dynamics, which is why we have omitted this term), the time development operator  $U(t)$  is constructed by writing

$$\vec{\omega} = \omega \hat{n}, \quad \omega = \sqrt{\omega_x^2 + \omega_y^2 + \omega_z^2}, \quad (54)$$

where  $\hat{n}$  is a unit vector in the direction of  $\vec{\omega}$ . Then  $U(t) = e^{-iHt}$  is the unitary corresponding to a rotation of the Bloch sphere by  $t\vec{\omega}$ , understood as a rotation (in a positive sense if  $t$  is positive) by  $\omega t$  radians about an axis given by the unit vector  $\hat{n}$ .

□ Exercise. Let  $\sigma$  be an operator such that  $\sigma^2 = I$ . Derive the formula

$$e^{i\theta\sigma} = (\cos\theta)I + i(\sin\theta)\sigma. \quad (55)$$

by expanding the exponential in a power series.

□ Exercise. Show that

$$\sigma_{\hat{n}} = \hat{n}_x \sigma_x + \hat{n}_y \sigma_y + \hat{n}_z \sigma_z, \quad (56)$$

where  $\hat{n}$  is a unit vector, is similar to  $\sigma_z$  in that it is Hermitian and its square is equal to  $I$ .

□ Exercise. Show that the unitary time development operator corresponding to  $H$  in (50) is given by:

$$U(t) = (\cos \omega t/2)I - i(\sin \omega t/2)\sigma_{\hat{n}}. \quad (57)$$

### 3.3 Time dependent Hamiltonian

★ The unitary time development of a 2-state system with a general  $H(t)$  is hard to work out in closed form, but the following intuitive picture is helpful. Let  $H$  be of the form (50), but with time-dependent coefficients  $\omega_x(t)$ ,  $\omega_y(t)$ ,  $\omega_z(t)$ . Then  $T(t + \Delta t, t)$  for small  $\Delta t$  corresponds to a rotation of the Bloch sphere about the axis defined by  $\vec{\omega}(t)$  by an angle  $|\vec{\omega}(t)|\Delta t$ .

• Suppose in particular that  $\vec{\omega}(t)$  is varying slowly in comparison to the precession rate  $|\vec{\omega}(t)|$ . Then it is plausible that the angle  $\theta'$  between the direction  $w$  defined by the ket (on the Bloch sphere) and the instantaneous direction of  $\vec{\omega}(t)$  will remain roughly constant.

– This *adiabatic approximation* is not perfect, but often provides a good approximation.

★ A case that is exactly solvable in closed form corresponds to a magnetic field of constant magnitude rotating at a uniform rate about a fixed axis.

• The “trick” for making progress is to use a “rotating coordinate system,” which is of interest in itself.

• In quantum mechanics a “coordinate transformation” usually means switching from one orthonormal basis to another for representing kets and operators as vectors and matrices. Such basis changes are associated with unitary operators or matrices. Thus let  $\{|b_j\rangle\}$  and  $\{|\bar{b}_k\rangle\}$  be two orthonormal bases and  $|\psi\rangle$  some ket. Then

$$\langle \bar{b}_k | \psi \rangle = \sum_j \langle \bar{b}_k | b_j \rangle \langle b_j | \psi \rangle. \quad (58)$$

□ Exercise. Show that  $U_{kj} = \langle \bar{b}_k | b_j \rangle$  is a unitary matrix.

◦ Thus in quantum mechanics a transformation to a *moving* coordinate system will be associated with a *time-dependent* unitary operator or matrix.

◦ Consider a particular example. The Hamiltonian  $H = \frac{1}{2}\omega_z \sigma_z$  in (51) leads to a precession of the Bloch sphere about the  $z$  axis, (52). So if we imagine ourselves in a coordinate system rotating along with the

Bloch sphere, the ket  $|\psi(t)\rangle$  on the right side of (53) will look as if it were constant. Thus if  $S(t)$  corresponds to a transformation to the rotating system, we expect

$$|\bar{\psi}\rangle = S(t)|\psi(t)\rangle, \quad (59)$$

to be independent of time, which can be achieved by letting  $S(t) = U^\dagger(t) = U(-t)$ .

★ Consider the general transformation

$$|\bar{\psi}(t)\rangle = S(t)|\psi(t)\rangle; \quad |\psi(t)\rangle = S^\dagger(t)|\bar{\psi}(t)\rangle, \quad (60)$$

with  $S(t)$  unitary for each  $t$ , but otherwise an arbitrary function of  $t$ .

• Construct the Schrödinger equation for  $|\bar{\psi}(t)\rangle$

$$\begin{aligned} i\frac{d}{dt}|\bar{\psi}(t)\rangle &= i\frac{dS(t)}{dt}|\psi(t)\rangle + S(t)\left(i\frac{d}{dt}|\psi(t)\rangle\right) \\ &= \left(i\frac{dS(t)}{dt}S^\dagger(t)\right)|\bar{\psi}(t)\rangle + \left(S(t)H(t)S^\dagger(t)\right)|\bar{\psi}(t)\rangle \\ &= \bar{H}_1(t)|\bar{\psi}(t)\rangle + \bar{H}_2(t)|\bar{\psi}(t)\rangle = \bar{H}(t)|\bar{\psi}(t)\rangle. \end{aligned} \quad (61)$$

◦ That is to say  $|\bar{\psi}(t)\rangle$  satisfies Schrödinger equation with a new Hamiltonian  $\bar{H}(t) = \bar{H}_1(t) + \bar{H}_2(t)$

□ Exercise. Show that both  $\bar{H}_1(t)$  and  $\bar{H}_2(t)$  are Hermitian operators, given that  $S(t)$  is at every time a unitary operator.

◦ The term  $\bar{H}_2(t)$  would be present even if the transformation were time independent, i.e.,  $S(t)$  a constant, whereas  $\bar{H}_1(t)$  is a consequence of the fact that  $S(t)$  depends on the time.

★ Now apply this to the case

$$H(t) = \frac{1}{2}\omega_z\sigma_z + \frac{1}{2}\omega_p[(\cos\omega_r t)\sigma_x + (\sin\omega_r t)\sigma_y], \quad (62)$$

which corresponds to a magnetic field with a constant component in the  $z$  direction along with a perpendicular component rotating in a counterclockwise direction in the  $x, y$  plane with an angular frequency  $\omega_r$ .

– Be careful to distinguish  $\omega_p$ , the magnitude of the transverse component, from  $\omega_r$ , the rate of rotation.

• Let us introduce a rotating coordinate system in which  $\bar{H}(t)$  is independent of time, as then we can employ the procedure of Sec. 3.2. The earlier discussion suggests using

$$S(t) = \begin{pmatrix} e^{i\omega_r t/2} & 0 \\ 0 & e^{-i\omega_r t/2} \end{pmatrix}, \quad (63)$$

since if the coordinate system is itself rotating at a rate  $\omega_r$ , in it the magnetic field will appear to be constant.

◦ The result, see (61), is

$$\bar{H}_1(t) = -\frac{1}{2}\omega_r\sigma_z, \quad \bar{H}_2(t) = \frac{1}{2}[\omega_z\sigma_z + \omega_p\sigma_x]. \quad (64)$$

There is no longer any time dependence, only a constant magnetic field in the  $x, z$  plane.

– In particular, if  $\omega_p = 0$  and  $\omega_r = \omega_z$  we have  $\bar{H} = 0$ , as expected.

□ Exercise. Derive (64).

★ A special but important case is that in which the rotation rate  $\omega_r$  of the magnetic field is set equal to the precession rate  $\omega_z$  due to the constant field in the  $z$  direction, so that the all that remains in  $\bar{H}$  is the perpendicular component  $\frac{1}{2}\omega_p\sigma_x$ .

• Then in the rotating frame the Bloch sphere precesses about the  $x$  axis at a rate  $\omega_p$ .

◦ In particular, if the initial state is  $|z^+\rangle$ , “spin in the  $z$  direction,” then in a time  $\tau_1 = (\pi/2)(1/\omega_p)$  it will precess into the  $y$  (or  $-y$ ) direction. But when viewed in the laboratory coordinate system the spin direction is rotating rapidly in the  $x, y$  plane. In the terminology of magnetic resonance, turning on a perpendicular oscillating component of the magnetic field for the time  $\tau_1$  is referred to as a “ $\pi/2$  pulse.”

◦ In practice one does not try and produce a rotating magnetic field that is actually of the form (62). Instead use

$$H(t) = \frac{1}{2}\omega_z\sigma_z + \omega_p(\cos\omega_r t)\sigma_x. \quad (65)$$

A simple oscillating field in the  $x$  direction is much easier to produce than a field rotating in the  $x, y$  plane. One can think of the oscillating field as a superposition of two rotating fields, one rotating clockwise and the other counterclockwise. Only the one which is nearly constant in the rotating coordinate system has a significant effect; the other can (typically, at least) be ignored because it is “far off resonance.”

## 4 Toy Models

### 4.1 Introduction

◦ Reference: CQT Sec. 7.4

• Basic strategy: set up as simple a model as possible, but with properties that are “genuinely quantum mechanical.”

• Toy models are most useful in *time-dependent* situations where solving Schrödinger’s (time-dependent) equation requires some effort.

– Even for force-free ( $V(x) = 0$ ) motion of a particle in one dimension, solving Schrödinger’s equation is not trivial.

★ Strategy is to *discretize time*, and we will assume that it takes on integer values:  $t = -1, 0, 1, 2, \dots$

◦ One could use  $t = n\Delta t$  where  $\Delta t = 10^{-35}$  s, so time discretization is not in itself a particular limitation.

• Time development operator will be

$$T(t, t') = U(t - t') = T^{t-t'} \quad (66)$$

where  $T$  is a single (time-independent) unitary operator, and  $t - t'$  is an integer.

– Make  $T$  as simple as possible; we want to be able to work out the dynamics on the back of an envelope.

★ When using discrete time and a simple  $T$  we typically *cannot* think of  $T$  as coming about by solving a continuous-time Schrödinger equation with a Hamiltonian  $H$ . Or, if there is a Hamiltonian it is something quite complicated, and using it would defeat the purpose for which the toy model was introduced: having something simple and easy to analyze.

• Toy models are particularly useful for understanding the stochastic or probabilistic aspects of quantum time evolution.

• They are also of considerable help in resolving some of the paradoxes of quantum mechanics, conceptual difficulties which are ignored or swept under the rug in typical textbook treatments.

### 4.2 One-dimensional hopping model

★ Label the sites of the toy model by  $m$ ,  $-M_a \leq m \leq M_b$ . The finite integers  $M_a$  and  $M_b$  can be as large as you want. Keeping them finite makes the Hilbert space finite. The kets  $|m\rangle$  with  $m$  in this range form an orthonormal basis of the Hilbert space:

$$\langle m|m'\rangle = \delta_{mm'}. \quad (67)$$

★ Simple hopping dynamics:  $T = S$  where  $S$  is the *shift* operator:

$$S|m\rangle = |m+1\rangle, \quad S|M_b\rangle = |-M_a\rangle. \quad (68)$$

We are using periodic boundary conditions.

•  $S$  (therefore  $T = S$ ) is unitary, since it maps an orthonormal basis onto an orthonormal basis.

□ Exercise. Prove that mapping an orthonormal basis onto an orthonormal basis is a necessary and sufficient condition for a linear operator  $U$  on a finite-dimensional Hilbert space to be unitary.

□ Exercise. (Advanced). And what might go wrong with this if we have an infinite-dimensional Hilbert space?

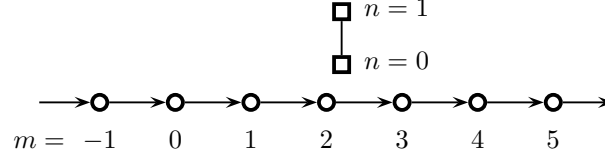


Figure 1: One-dimensional toy model with detector

### 4.3 Hopping model with detector

- ★ See Fig. 1. The detector has two states  $n = 0$  (ready) and  $n = 1$  (particle detected).
- Combined system is a tensor product  $\mathcal{H}_p \otimes \mathcal{H}_d$ . Unitary dynamics for the combination is

$$T = SR = (S \otimes I)R \quad (69)$$

where

$$R|m, n\rangle = |m, n\rangle \text{ for } m \neq 2; \quad R|2, n\rangle = |2, 1 - n\rangle. \quad (70)$$

◦  $T$  is unitary because  $S = S \otimes I$  (physicists use both) is unitary and  $R$  is unitary, and the product of two unitary operators is unitary.

□ Exercise. Convince yourself that  $R$  is unitary.

- With the particle initially at  $m = 0$  and the detector in the ready state  $n = 0$ , the unitary time development is

$$|0\rangle_p \otimes |0\rangle_d = |0, 0\rangle \mapsto |1, 0\rangle \mapsto |2, 0\rangle \mapsto |3, 1\rangle \mapsto |4, 1\rangle \mapsto \dots, \quad (71)$$

where  $|\psi\rangle_t \mapsto |\psi\rangle_{t+1}$  indicates what happens during a single time step.

□ Exercise. One could just as well have written  $T = RS$  in place of  $SR$ , but the result would be a bit different. Discuss.

□ Exercise. Work out the time development starting with the following different initial states of the particle at  $t = 0$ , assuming that the detector always starts off in the state  $n = 0$ .

(i)  $|m = 1\rangle$ . (ii)  $|m = 0\rangle + |m = 2\rangle$ . (iii)  $|m = 0\rangle + |m = 4\rangle$ .

- Using initial superpositions, (ii) or (iii) in the preceding exercise, allows one at certain times to have superpositions of the toy detector in different states: a Schrödinger kitten. (Many standard quantum paradoxes have toy counterparts.)

- ★ Born rule. Suppose that the initial state is

$$|\psi_0\rangle = (1/\sqrt{2})(|0\rangle + |1\rangle) \otimes |0\rangle = (1/\sqrt{2})(|0, 0\rangle + |1, 0\rangle) \quad (72)$$

Then after applying  $T^2$  one arrives at

$$|\psi_2\rangle = (1/\sqrt{2})(|2, 0\rangle + |3, 1\rangle) \quad (73)$$

- From this one can calculate various probabilities, e.g., for the detector:

$$\text{Pr}_2(n = 0) = \langle \psi_2 | (I_p \otimes |0\rangle_d) | \psi_2 \rangle = 1/2, \quad \text{Pr}_2(n = 1) = \langle \psi_2 | (I_p \otimes |1\rangle_d) | \psi_2 \rangle = 1/2, \quad (74)$$

where the subscript on Pr indicates the time ( $t = 2$ ). For the particle position

$$\text{Pr}_2(m = 2) = \langle \psi_2 | ([2]_p \otimes I_d) | \psi_2 \rangle = 1/2, \quad \text{Pr}_2(m = 3) = \langle \psi_2 | ([3]_p \otimes I_d) | \psi_2 \rangle = 1/2. \quad (75)$$

with vanishing probability for other values of  $m$ .

- ★ More interesting are the joint probabilities:

$$\text{Pr}_2(m = 2, n = 0) = \langle \psi_2 | ([2]_p \otimes |0\rangle_d) | \psi_2 \rangle = 1/2 = \text{Pr}_2(m = 3, n = 1), \quad (76)$$

and 0 for other choices of  $m$  and  $n$ .

- From the result (76) one can calculate conditional probabilities, e.g.,

$$\Pr_2(m = 2 | n = 0) = 1 = \Pr_2(m = 3 | n = 1), \quad (77)$$

which is to say: if at  $t = 2$  the detector has not triggered one can be sure that the particle is at  $m = 2$ , whereas if it has triggered one can be sure that the particle is at  $m = 3$ .

□ Exercise. Show that (77) is a consequence of (76) using the usual definition of conditional probabilities:  $\Pr(A | B) = \Pr(A, B) / \Pr(B)$ , assuming that  $\Pr(B) \neq 0$ .

- Although derived in the context of a toy model, (77) is an example of the sort of thing which can give meaning to the somewhat vague notion of “measurement” presented in many quantum textbooks. When properly analyzed in quantum mechanical terms it is possible to understand how measurements reveal (or fail to reveal) physical properties of measured systems.

- The use of conditional probabilities is what allows reasonable inferences from measurements without invoking the notion of “wavefunction collapse.” (Or, to turn it around, “wavefunction collapse” as employed in quantum textbooks is never a physical process, but instead a tool for calculating conditional probabilities.)

#### 4.4 Alpha particle decay

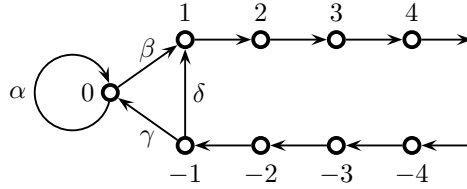


Figure 2: Toy model for alpha decay

★ Radioactive decay is a common phenomenon. Figure 2 represents a toy model of such a decay process. While labeled “alpha decay” it could equally well be a toy model of beta decay or gamma decay or an atom emitting a photon. When the alpha particle is at  $m = 0$  it is inside the nucleus, whereas the other  $m$  values represent possible locations outside the nucleus.

- The unitary time transformation in this case is a modified shift operator  $S_a$ , compare (68),

$$\begin{aligned} S_a|m\rangle &= |m+1\rangle \text{ for } m \neq 0, -1, M_b; & S_a|M_b\rangle &= |-M_a\rangle \\ S_a|0\rangle &= \alpha|0\rangle + \beta|1\rangle; & S_a|-1\rangle &= \gamma|0\rangle + \delta|1\rangle. \end{aligned} \quad (78)$$

□ Exercise. Show that  $S_a$  is a unitary operator provided the coefficients  $\alpha, \beta, \gamma, \delta$  form a unitary matrix

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}. \quad (79)$$

★ Unitary time development with the alpha particle initially inside the nucleus is given by:

$$\begin{aligned} |0\rangle &\mapsto \alpha|0\rangle + \beta|1\rangle \mapsto \alpha^2|0\rangle + \alpha\beta|1\rangle + \beta|2\rangle \\ &\mapsto \alpha^3|0\rangle + \alpha^2\beta|1\rangle + \alpha\beta^2|2\rangle + \beta^3|3\rangle \mapsto \dots, \end{aligned} \quad (80)$$

- The coefficient of  $|0\rangle$  at time  $t$  is  $\alpha^t$ . The Born rule then gives

$$\Pr_t(m = 0) = |\alpha|^2 t = e^{-\lambda t}, \text{ with } \lambda = -2 \ln(1/|\alpha|). \quad (81)$$

That is, an exponential decay with time (note that  $t$  is an integer), similar to what is observed experimentally for radioactive substances.

★ It is possible to add to the arrangement in Fig. 2 a detector similar to that in Fig. 1, and then work out various probabilities. This is left as a (somewhat nontrivial) exercise.