Problem Set 1

Due Tuesday October 1, 9:30 AM.
Submit in class or in TA's mailbox in the Physics office.

1. Begin immediately setting yourself up with access to Mathematica, probably for most of you by using NUIT's free access. I say "immediately" because there is an activation with Wolfram which sometimes takes up a week, and you will need access for next week's problem set. We will use Mathematica's numerical differential equation solver, its plotting, and possibly some of its other tools. You are also free to use a different software package if you are confident that it provides an equivalent suite of tools.

2. For fun, check out this wavefunction dynamics simulator. You might look at the infinite square well and/or other potentials. http://www.falstad.com/qm1d/

3. Shankar 1.1.5

4. Shankar 1.3.4

5. Shankar 1.6.6

6. Shankar 1.8.1

7. Shankar 1.8.11

8. Shankar 1.8.12

9. Shankar 1.10.4

As a second example, consider all functions $f(x)$ defined in an interval $0 \le x \le L$. We define scalar multiplication by a simply as $af(x)$ and addition as pointwise addition: the sum of two functions f and g has the value $f(x)+g(x)$ at the point x. The null function is zero everywhere and the additive inverse of f is $-f$.

Exercise 1.1.3. Do functions that vanish at the end points $x=0$ and $x=L$ form a vector space? How about *periodic functions* obeying $f(0)=f(L)$? How about functions that obey $f(0)=4$? If the functions do not qualify, list the things that go wrong.

The next concept is that of *linear independence* of a set of vectors $|1\rangle, |2\rangle \ldots |n\rangle$. First consider a linear relation of the form

$$\sum_{i=1}^{n} a_i |i\rangle = |0\rangle \tag{1.1.1}$$

We may assume without loss of generality that the left-hand side does not contain any multiple of $|0\rangle$, for if it did, it could be shifted to the right, and combined with the $|0\rangle$ there to give $|0\rangle$ once more. (We are using the fact that any multiple of $|0\rangle$ equals $|0\rangle$.)

Definition 3. The set of vectors is said to be *linearly independent* if the only such linear relation as Eq. (1.1.1) is the trivial one with all $a_i=0$. If the set of vectors is not linearly independent, we say they are *linearly dependent*.

Equation (1.1.1) tells us that it is not possible to write any member of the linearly independent set in terms of the others. On the other hand, if the set of vectors is linearly dependent, such a relation will exist, and it must contain at least two nonzero coefficients. Let us say $a_3 \neq 0$. Then we could write

$$|3\rangle = \sum_{i=1,\neq 3}^{n} \frac{-a_i}{a_3} |i\rangle \tag{1.1.2}$$

thereby expressing $|3\rangle$ in terms of the others.

As a concrete example, consider two nonparallel vectors $|1\rangle$ and $|2\rangle$ in a plane. These form a linearly independent set. There is no way to write one as a multiple of the other, or equivalently, no way to combine them to get the null vector. On the other hand, if the vectors are parallel, we can clearly write one as a multiple of the other or equivalently play them against each other to get 0.

Notice I said 0 and not $|0\rangle$. This is, strictly speaking, incorrect since a set of vectors can only add up to a vector and not a number. It is, however, common to represent the null vector by 0.

Suppose we bring in a third vector $|3\rangle$ also in the plane. If it is parallel to either of the first two, we already have a linearly dependent set. So let us suppose it is not. But even now the three of them are *linearly dependent*. This is because we can write one of them, say $|3\rangle$, as a linear combination of the other two. To find the combination, draw a line from the tail of $|3\rangle$ in the direction of $|1\rangle$. Next draw a line antiparallel to $|2\rangle$ from the tip of $|3\rangle$. These lines will intersect since $|1\rangle$ and $|2\rangle$ are not parallel by assumption. The intersection point P will determine how much of $|1\rangle$ and $|2\rangle$ we want: we go from the tail of $|3\rangle$ to P using the appropriate multiple of $|1\rangle$ and go from P to the tip of $|3\rangle$ using the appropriate multiple of $|2\rangle$.

Exercise 1.1.4. Consider three elements from the vector space of real 2×2 matrices:

$$|1\rangle = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \quad |2\rangle = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \quad |3\rangle = \begin{bmatrix} -2 & -1 \\ 0 & -2 \end{bmatrix}$$

Are they linearly independent? Support your answer with details. (Notice we are calling these matrices vectors and using kets to represent them to emphasize their role as elements of a vector space.)

Exercise 1.1.5. Show that the following row vectors are linearly dependent: (1, 1, 0), (1, 0, 1), and (3, 2, 1). Show the opposite for (1, 1, 0), (1, 0, 1), and (0, 1, 1).

Definition 4. A vector space has *dimension n* if it can accommodate a maximum of n linearly independent vectors. It will be denoted by $\mathbb{V}^n(R)$ if the field is real and by $\mathbb{V}^n(C)$ if the field is complex.

In view of the earlier discussions, the plane is two-dimensional and the set of all arrows not limited to the plane define a three-dimensional vector space. How about 2×2 matrices? They form a four-dimensional vector space. Here is a proof. The following vectors are linearly independent:

$$|1\rangle = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad |2\rangle = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \quad |3\rangle = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \quad |4\rangle = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

since it is impossible to form linear combinations of any three of them to give the fourth any three of them will have a zero in the one place where the fourth does not. So the space is at least four-dimensional. Could it be bigger? No, since any arbitrary 2×2 matrix can be written in terms of them:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = a|1\rangle + b|2\rangle + c|3\rangle + d|4\rangle$$

If the scalars a, b, c, d are real, we have a *real four-dimensional space*, if they are complex we have a *complex four-dimensional space*.

Theorem 1. Any vector $|V\rangle$ in an n-dimensional space can be written as a linear combination of n linearly independent vectors $|1\rangle \ldots |n\rangle$.

The proof is as follows: if there were a vector $|V\rangle$ for which this were not possible, it would join the given set of vectors and form a set of $n+1$ linearly independent vectors, which is not possible in an n-dimensional space by definition.

Exercise 1.3.2. Show how to go from the basis

$$|I\rangle=\begin{bmatrix}3\\0\\0\end{bmatrix}\quad |II\rangle=\begin{bmatrix}0\\1\\2\end{bmatrix}\quad |III\rangle=\begin{bmatrix}0\\2\\5\end{bmatrix}$$

to the orthonormal basis

$$|1\rangle=\begin{bmatrix}1\\0\\0\end{bmatrix}\quad |2\rangle=\begin{bmatrix}0\\1/\sqrt{5}\\2/\sqrt{5}\end{bmatrix}\quad |3\rangle=\begin{bmatrix}0\\-2/\sqrt{5}\\1/\sqrt{5}\end{bmatrix}$$

When we first learn about dimensionality, we associate it with the number of perpendicular directions. In this chapter we defined it in terms of the maximum number of linearly independent vectors. The following theorem connects the two definitions.

Theorem 4. The dimensionality of a space equals $n_\perp$, the maximum number of mutually orthogonal vectors in it.

To show this, first note that any mutually orthogonal set is also linearly independent. Suppose we had a linear combination of orthogonal vectors adding up to zero. By taking the dot product of both sides with any one member and using the orthogonality we can show that the coefficient multiplying that vector had to vanish. This can clearly be done for all the coefficients, showing the linear combination is trivial.

Now $n_\perp$ can only be equal to, greater than or lesser than n, the dimensionality of the space. The Gram–Schmidt procedure eliminates the last case by explicit construction, while the linear independence of the perpendicular vectors rules out the penultimate option.

Schwarz and Triangle Inequalities

Two powerful theorems apply to any inner product space obeying our axioms:

Theorem 5. The Schwarz Inequality

$$|\langle V|W\rangle|\leq|V||W| \tag{1.3.15}$$

Theorem 6. The Triangle Inequality

$$|V+W|\leq|V|+|W| \tag{1.3.16}$$

The proof of the first will be provided so you can get used to working with bras and kets. The second will be left as an exercise.

Before proving anything, note that the results are obviously true for arrows: the *Schwarz inequality* says that the dot product of two vectors cannot exceed the product of their lengths and the *triangle inequality* says that the length of a sum cannot exceed the sum of the lengths. This is an example which illustrates the merits of thinking of abstract vectors as arrows and guessing what properties they might share with arrows. The proof will of course have to rely on just the axioms.

To prove the Schwarz inequality, consider axiom $\langle Z|Z\rangle\geq 0$ *applied to*

$$|Z\rangle=|V\rangle-\frac{\langle W|V\rangle}{|W|^2}|W\rangle \tag{1.3.17}$$

We get

$$\begin{aligned}\langle Z|Z\rangle&=\langle V-\frac{\langle W|V\rangle}{|W|^2}W|V-\frac{\langle W|V\rangle}{|W|^2}W\rangle\\&=\langle V|V\rangle-\frac{\langle W|V\rangle\langle V|W\rangle}{|W|^2}-\frac{\langle W|V\rangle^*\langle W|V\rangle}{|W|^2}\\&\quad+\frac{\langle W|V\rangle^*\langle W|V\rangle\langle W|W\rangle}{|W|^4}\\&\geq 0\end{aligned} \tag{1.3.18}$$

where we have used the antilinearity of the inner product with respect to the bra. Using

$$\langle W|V\rangle^*=\langle V|W\rangle$$

we find

$$\langle V|V\rangle\geq\frac{\langle W|V\rangle\langle V|W\rangle}{|W|^2} \tag{1.3.19}$$

Cross-multiplying by $|W|^2$ and taking square roots, the result follows.

Exercise 1.3.3. When will this equality be satisfied? Does this agree with your experience with arrows?

Exercise 1.3.4. Prove the triangle inequality starting with $|V+W|^2$. You must use $\mathrm{Re}\langle V|W\rangle\leq|\langle V|W\rangle|$ and the Schwarz inequality. Show that the final inequality becomes an equality only if $|V\rangle=a|W\rangle$ where a is a real positive scalar.

1.4. Subspaces

Definition 11. Given a vector space $\mathbb{V}$, a subset of its elements that form a vector space among themselves‡ is called a *subspace*. We will denote a particular subspace i of dimensionality n_i by $\mathbb{V}_i^{n_i}$.

‡ Vector addition and scalar multiplication are defined the same way in the subspace as in $\mathbb{V}$.

Definition 15. An operator U is *unitary* if

$$UU^\dagger = I \tag{1.6.19}$$

This equation tells us that U and $U^\dagger$ are inverses of each other. Consequently, from Eq. (1.5.12),

$$U^\dagger U = I \tag{1.6.20}$$

Following the analogy between operators and numbers, unitary operators are like complex numbers of unit modulus, $u = e^{i\theta}$. Just as $u^* u = 1$, so is $U^\dagger U = I$.

*Exercise 1.6.3.** Show that a product of unitary operators is unitary.

Theorem 7. Unitary operators preserve the inner product between the vectors they act on.

Proof. Let

$$|V_1'\rangle = U|V_1\rangle$$

and

$$|V_2'\rangle = U|V_2\rangle$$

Then

$$\begin{aligned}\langle V_2'|V_1'\rangle &= \langle UV_2|UV_1\rangle \\ &= \langle V_2|U^\dagger U|V_1\rangle = \langle V_2|V_1\rangle\end{aligned} \tag{1.6.21}$$

(Q.E.D.)

Unitary operators are the generalizations of rotation operators from $\mathbb{V}^3(R)$ to $\mathbb{V}^n(C)$, for just like rotation operators in three dimensions, they preserve the lengths of vectors and their dot products. In fact, on a real vector space, the unitarity condition becomes $U^{-1} = U^T$ (T means transpose), which defines an *orthogonal* or rotation matrix. [$R(\frac{1}{2}\pi\mathbf{i})$ is an example.]

Theorem 8. If one treats the columns of an $n \times n$ unitary matrix as components of n vectors, these vectors are orthonormal. In the same way, the rows may be interpreted as components of n orthonormal vectors.

Proof 1. According to our mnemonic, the jth column of the matrix representing U is the image of the jth basis vector after U acts on it. Since U preserves inner products, the rotated set of vectors is also orthonormal. Consider next the rows. We now use the fact that $U^\dagger$ is also a rotation. (How else can it neutralize U to give $U^\dagger U = I$?) Since the rows of U are the columns of $U^\dagger$ (but for an overall complex conjugation which does not affect the question of orthonormality), the result we already have for the columns of a unitary matrix tells us the rows of U are orthonormal.

Proof 2. Since $U^\dagger U = I$,

$$\begin{aligned}\delta_{ij} &= \langle i|I|j\rangle = \langle i|U^\dagger U|j\rangle \\ &= \sum_k \langle i|U^\dagger|k\rangle\langle k|U|j\rangle \\ &= \sum_k U_{ik}^\dagger U_{kj} = \sum_k U_{ki}^* U_{kj}\end{aligned} \tag{1.6.22}$$

which proves the theorem for the columns. A similar result for the rows follows if we start with the equation $UU^\dagger = I$. Q.E.D.

Note that $U^\dagger U = I$ and $UU^\dagger = I$ are not independent conditions.

*Exercise 1.6.4.** It is assumed that you know (1) what a *determinant* is, (2) that $\det \Omega^T = \det \Omega$ (T denotes transpose), (3) that the determinant of a product of matrices is the product of the determinants. [If you do not, verify these properties for a two-dimensional case

$$\Omega = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

with $\det \Omega = (\alpha\delta - \beta\gamma)$.] Prove that the determinant of a unitary matrix is a complex number of unit modulus.

*Exercise 1.6.5.** Verify that $R(\frac{1}{2}\pi\mathbf{i})$ is unitary (orthogonal) by examining its matrix.

Exercise 1.6.6. Verify that the following matrices are unitary:

$$\frac{1}{2^{1/2}}\begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix}, \qquad \frac{1}{2}\begin{bmatrix} 1+i & 1-i \\ 1-i & 1+i \end{bmatrix}$$

Verify that the determinant is of the form $e^{i\theta}$ in each case. Are any of the above matrices Hermitian?

1.7. Active and Passive Transformations

Suppose we subject all the vectors $|V\rangle$ in a space to a unitary transformation

$$|V\rangle \to U|V\rangle \tag{1.7.1}$$

Under this transformation, the matrix elements of any operator Ω are modified as follows:

$$\langle V'|\Omega|V\rangle \to \langle UV'|\Omega|UV\rangle = \langle V'|U^\dagger \Omega U|V\rangle \tag{1.7.2}$$

It is clear that the same change would be effected if we left the vectors alone and subjected all operators to the change

$$\Omega \to U^\dagger \Omega U \tag{1.7.3}$$

The first case is called an *active transformation* and the second a *passive transformation*. The present nomenclature is in reference to the vectors: they are affected in an active transformation and left alone in the passive case. The situation is exactly the opposite from the point of view of the operators.

Later we will see that the physics in quantum theory lies in the matrix elements of operators, and that active and passive transformations provide us with two equivalent ways of describing the same physical transformation.

*Exercise 1.7.1.** The *trace* of a matrix is defined to be the sum of its diagonal matrix elements

$$\mathrm{Tr}\,\Omega = \sum_i \Omega_{ii}$$

Show that

(1) $\mathrm{Tr}(\Omega\Lambda) = \mathrm{Tr}(\Lambda\Omega)$
(2) $\mathrm{Tr}(\Omega\Lambda\theta) = \mathrm{Tr}(\Lambda\theta\Omega) = \mathrm{Tr}(\theta\Omega\Lambda)$ (The permutations are *cyclic*).
(3) The trace of an operator is unaffected by a unitary change of basis $|i\rangle \to U|i\rangle$. [Equivalently, show $\mathrm{Tr}\,\Omega = \mathrm{Tr}(U^\dagger \Omega U)$.]

Exercise 1.7.2. Show that the determinant of a matrix is unaffected by a unitary change of basis. [Equivalently show $\det \Omega = \det(U^\dagger \Omega U)$.]

1.8. The Eigenvalue Problem

Consider some linear operator Ω acting on an arbitrary *nonzero* ket $|V\rangle$:

$$\Omega|V\rangle = |V'\rangle \tag{1.8.1}$$

Unless the operator happens to be a trivial one, such as the identity or its multiple, the ket will suffer a nontrivial change, i.e., $|V'\rangle$ will not be simply related to $|V\rangle$. So much for an arbitrary ket. Each operator, however, has certain kets of its own, called its *eigenkets*, on which its action is simply that of rescaling:

$$\Omega|V\rangle = \omega|V\rangle \tag{1.8.2}$$

Equation (1.8.2) is an eigenvalue equation: $|V\rangle$ is an *eigenket* of Ω with *eigenvalue* ω. In this chapter we will see how, given an operator Ω, one can systematically determine all its eigenvalues and eigenvectors. How such an equation enters physics will be illustrated by a few examples from mechanics at the end of this section, and once we get to quantum mechanics proper, it will be eigen, eigen, eigen all the way.

Example 1.8.1. To illustrate how easy the eigenvalue problem really is, we will begin with a case that will be completely solved: the case $\Omega = I$. Since

$$I|V\rangle = |V\rangle$$

for all $|V\rangle$, we conclude that

(1) the only eigenvalue of I is 1;
(2) all vectors are its eigenvectors with this eigenvalue. □

Example 1.8.2. After this unqualified success, we are encouraged to take on a slightly more difficult case: $\Omega = \mathbb{P}_V$, the projection operator associated with a *normalized* ket $|V\rangle$. Clearly

(1) any ket $\alpha|V\rangle = |\alpha V\rangle$, parallel to $|V\rangle$ is an eigenket with eigenvalue 1:

$$\mathbb{P}_V|\alpha V\rangle = |V\rangle\langle V|\alpha V\rangle = \alpha|V\rangle|V|^2 = 1\cdot|\alpha V\rangle$$

(2) any ket $|V_\perp\rangle$, perpendicular to $|V\rangle$, is an eigenket with eigenvalue 0:

$$\mathbb{P}_V|V_\perp\rangle = |V\rangle\langle V|V_\perp\rangle = 0 = 0|V_\perp\rangle$$

(3) kets that are neither, i.e., kets of the form $\alpha|V\rangle + \beta|V_\perp\rangle$, are simply not eigenkets:

$$\mathbb{P}_V(\alpha|V\rangle + \beta|V_\perp\rangle) = |\alpha V\rangle \neq \gamma(\alpha|V\rangle + \beta|V_\perp\rangle)$$

Since every ket in the space falls into one of the above classes, we have found all the eigenvalues and eigenvectors. □

Example 1.8.3. Consider now the operator $R(\frac{1}{2}\pi\mathbf{i})$. We already know that it has one eigenket, the basis vector $|1\rangle$ along the x axis:

$$R(\tfrac{1}{2}\pi\mathbf{i})|1\rangle = |1\rangle$$

Are there others? Of course, any vector $\alpha|1\rangle$ along the x axis is also unaffected by the x rotation. This is a general feature of the eigenvalue equation and reflects the linearity of the operator:

if

$$\Omega|V\rangle = \omega|V\rangle$$

then

$$\Omega\alpha|V\rangle = \alpha\Omega|V\rangle = \alpha\omega|V\rangle = \omega\alpha|V\rangle$$

(1) Solve the eigenvalue problem of Ω.
(2) Construct the propagator U in terms of the eigenvalues and eigenvectors.
(3) $|x(t)\rangle = U(t)|x(0)\rangle$.

The Normal Modes

There are two initial states $|x(0)\rangle$ for which the time evolution is particularly simple. Not surprisingly, these are the eigenkets $|\mathrm{I}\rangle$ and $|\mathrm{II}\rangle$. Suppose we have $|x(0)\rangle = |\mathrm{I}\rangle$. Then the state at time t is

$$\begin{aligned} |\mathrm{I}(t)\rangle &\equiv U(t)|\mathrm{I}\rangle \\ &= (|\mathrm{I}\rangle\langle\mathrm{I}| \cos\omega_{\mathrm{I}} t + |\mathrm{II}\rangle\langle\mathrm{II}| \cos\omega_{\mathrm{II}} t)|\mathrm{I}\rangle \\ &= |\mathrm{I}\rangle \cos\omega_{\mathrm{I}} t \end{aligned} \tag{1.8.42}$$

Thus the system starting off in $|\mathrm{I}\rangle$ is only modified by an overall factor $\cos\omega_{\mathrm{I}} t$. A similar remark holds with $\mathrm{I} \to \mathrm{II}$. These two modes of vibration, in which all (two) components of a vector oscillate in step are called *normal modes*.

The physics of the normal modes is clear in the $|1\rangle, |2\rangle$ basis. In this basis

$$|\mathrm{I}\rangle \leftrightarrow \frac{1}{2^{1/2}}\begin{bmatrix}1\\1\end{bmatrix}$$

and corresponds to a state in which both masses are displaced by equal amounts. The middle spring is then a mere spectator and each mass oscillates with a frequency $\omega_{\mathrm{I}} = (k/m)^{1/2}$ in response to the end spring nearest to it. Consequently

$$|\mathrm{I}(t)\rangle \leftrightarrow \frac{1}{2^{1/2}}\begin{bmatrix}\cos[(k/m)^{1/2}t]\\ \cos[(k/m)^{1/2}t]\end{bmatrix}$$

On the other hand, if we start with

$$|\mathrm{II}\rangle \leftrightarrow \frac{1}{2^{1/2}}\begin{bmatrix}1\\-1\end{bmatrix}$$

the masses are displaced by equal and opposite amounts. In this case the middle spring is distorted by *twice* the displacement of each mass. If the masses are adjusted by Δ and $-\Delta$, respectively, each mass feels a restoring force of $3k\Delta$ ($2k\Delta$ from the middle spring and $k\Delta$ from the end spring nearest to it). Since the effective force constant is $k_{\mathrm{eff}} = 3k\Delta/\Delta = 3k$, the vibrational frequency is $(3k/m)^{1/2}$ and

$$|\mathrm{II}(t)\rangle \leftrightarrow \frac{1}{2^{1/2}}\begin{bmatrix}\cos[(3k/m)^{1/2}t]\\ -\cos[(3k/m)^{1/2}t]\end{bmatrix}$$

If the system starts off in a linear combination of $|\mathrm{I}\rangle$ and $|\mathrm{II}\rangle$ it evolves into the corresponding linear combination of the normal modes $|\mathrm{I}(t)\rangle$ and $|\mathrm{II}(t)\rangle$. This is the content of the propagator equation

$$\begin{aligned} |x(t)\rangle &= U(t)|x(0)\rangle \\ &= |\mathrm{I}\rangle\langle\mathrm{I}|x(0)\rangle \cos\omega_{\mathrm{I}} t + |\mathrm{II}\rangle\langle\mathrm{II}|\, x(0)\rangle \cos\omega_{\mathrm{II}} t \\ &= |I(t)\rangle\langle\mathrm{I}|x(0)\rangle + |\mathrm{II}(t)\rangle\langle\mathrm{II}|x(0)\rangle \end{aligned}$$

Another way to see the simple evolution of the initial states $|\mathrm{I}\rangle$ and $|\mathrm{II}\rangle$ is to determine the matrix representing U in the $|\mathrm{I}\rangle$, $|\mathrm{II}\rangle$ basis:

$$U \underset{\substack{\mathrm{I,II}\\ \text{basis}}}{\longleftrightarrow} \begin{bmatrix}\cos\omega_{\mathrm{I}} t & 0\\ 0 & \cos\omega_{\mathrm{II}} t\end{bmatrix} \tag{1.8.43}$$

You should verify this result by taking the appropriate matrix elements of $U(t)$ in Eq. (1.8.41b). Since each column above is the image of the corresponding basis vectors ($|\mathrm{I}\rangle$ or $|\mathrm{II}\rangle$) after the action of $U(t)$, (which is to say, after time evolution), we see that the initial states $|\mathrm{I}\rangle$ and $|\mathrm{II}\rangle$ evolve simply in time.

The central problem in quantum mechanics is very similar to the simple example that we have just discussed. The state of the system is described in quantum theory by a ket $|\psi\rangle$ which obeys the Schrödinger equation

$$i\hbar|\dot{\psi}\rangle = H|\psi\rangle$$

where $\hbar$ is a constant related to Planck's constant h by $\hbar = h/2\pi$, and H is a *Hermitian* operator called the Hamiltonian. The problem is to find $|\psi(t)\rangle$ given $|\psi(0)\rangle$. [Since the equation is first order in t, no assumptions need be made about $|\dot{\psi}(0)\rangle$, which is determined by the Schrödinger equation to be $(-i/\hbar)H|\psi(0)\rangle$.]

In most cases, H is a time-independent operator and the algorithm one follows in solving this initial-value problem is completely analogous to the one we have just seen:

Step (1). Solve the eigenvalue problem of H.

Step (2). Find the propagator $U(t)$ in terms of the eigenvectors and eigenvalues of H.

Step (3). $|\psi(t)\rangle = U(t)|\psi(0)\rangle$.

You must of course wait till Chapter 4 to find out the physical interpretation of $|\psi\rangle$, the actual form of the operator H, and the precise relation between $U(t)$ and the eigenvalues and eigenvectors of H. □

Exercise 1.8.11. Consider the coupled mass problem discussed above.
(1) Given that the initial state is $|1\rangle$, in which the first mass is displaced by unity and the second is left alone, calculate $|1(t)\rangle$ by following the algorithm.
(2) Compare your result with that following from Eq. (1.8.39).

Exercise 1.8.12. Consider once again the problem discussed in the previous example. (1) Assuming that

$$|\ddot{x}\rangle = \Omega|x\rangle$$

has a solution

$$|x(t)\rangle = U(t)|x(0)\rangle$$

find the differential equation satisfied by $U(t)$. Use the fact that $|x(0)\rangle$ is arbitrary.

(2) Assuming (as is the case) that Ω and U can be simultaneously diagonalized, solve for the elements of the matrix U in this common basis and regain Eq. (1.8.43). Assume $|\dot{x}(0)\rangle = 0$.

1.9. Functions of Operators and Related Concepts

We have encountered two types of objects that act on vectors: scalars, which commute with each other and with all operators; and operators, which do not generally commute with each other. It is customary to refer to the former as c numbers and the latter as q numbers. Now, we are accustomed to functions of c numbers such as $\sin(x)$, $\log(x)$, etc. We wish to examine the question whether functions of q numbers can be given a sensible meaning. We will restrict ourselves to those functions that can be written as a power series. Consider a series

$$f(x) = \sum_{n=0}^{\infty} a_n x^n \tag{1.9.1}$$

where x is a c number. We define the same function of an operator or q number to be

$$f(\Omega) = \sum_{n=0}^{\infty} a_n \Omega^n \tag{1.9.2}$$

This definition makes sense only if the sum converges to a definite limit. To see what this means, consider a common example:

$$e^{\Omega} = \sum_{n=0}^{\infty} \frac{\Omega^n}{n!} \tag{1.9.3}$$

Let us restrict ourselves to Hermitian Ω. By going to the eigenbasis of Ω we can readily perform the sum of Eq. (1.9.3). Since

$$\Omega = \begin{bmatrix} \omega_1 & & & \\ & \omega_2 & & \\ & & \ddots & \\ & & & \omega_n \end{bmatrix} \tag{1.9.4}$$

and

$$\Omega^m = \begin{bmatrix} \omega_1^m & & & \\ & \omega_2^m & & \\ & & \ddots & \\ & & & \omega_n^m \end{bmatrix} \tag{1.9.5}$$

$$e^{\Omega} = \begin{bmatrix} \sum_{m=0}^{\infty} \frac{\omega_1^m}{m!} & & & \\ & & \ddots & \\ & & & \sum_{m=0}^{\infty} \frac{\omega_n^m}{m!} \end{bmatrix} \tag{1.9.6}$$

Since each sum converges to the familiar limit e^{ω_i}, the operator e^{Ω} is indeed well defined by the power series in this basis (and therefore in any other).

*Exercise 1.9.1.** We know that the series

$$f(x) = \sum_{n=0}^{\infty} x^n$$

may be equated to the function $f(x) = (1-x)^{-1}$ if $|x| < 1$. By going to the eigenbasis, examine when the q number power series

$$f(\Omega) = \sum_{n=0}^{\infty} \Omega^n$$

of a Hermitian operator Ω may be identified with $(1-\Omega)^{-1}$.

*Exercise 1.9.2.** If H is a Hermitian operator, show that $U = e^{iH}$ is unitary. (Notice the analogy with c numbers: if θ is real, $u = e^{i\theta}$ is a number of unit modulus.)

Exercise 1.9.3. For the case above, show that $\det U = e^{i\mathrm{Tr}H}$.

Derivatives of Operators with Respect to Parameters

Consider next an operator $\theta(\lambda)$ that depends on a parameter λ. Its derivative with respect to λ is defined to be

$$\frac{d\theta(\lambda)}{d\lambda} = \lim_{\Delta\lambda \to 0} \left[\frac{\theta(\lambda+\Delta\lambda) - \theta(\lambda)}{\Delta\lambda} \right]$$

If $\theta(\lambda)$ is written as a matrix in some basis, then the matrix representing $d\theta(\lambda)/d\lambda$ is obtained by differentiating the matrix elements of $\theta(\lambda)$. A special case of $\theta(\lambda)$ we

If we project $|\psi(t)\rangle$ on the $|m\rangle$ basis, in which K is diagonal with eigenvalues $(m\pi/L)^2$, the components $\langle m|\psi(t)\rangle$ will obey the decoupled equations

$$\frac{d^2}{dt^2}\langle m|\psi(t)\rangle = -\left(\frac{m^2\pi^2}{L^2}\right)\langle m|\psi(t)\rangle, \qquad m=1, 2, \ldots \tag{1.10.53}$$

in analogy with Eq. (1.8.33). These equations may be readily solved (subject to the condition of vanishing initial velocities) as

$$\langle m|\psi(t)\rangle = \langle m|\psi(0)\rangle \cos\left(\frac{m\pi t}{L}\right) \tag{1.10.54}$$

Consequently

$$\begin{aligned}|\psi(t)\rangle &= \sum_{m=1}^{\infty} |m\rangle\langle m|\psi(t)\rangle \\ &= \sum_{m=1}^{\infty} |m\rangle\langle m|\psi(0)\rangle \cos\omega_m t, \qquad \omega_m = \frac{m\pi}{L}\end{aligned} \tag{1.10.55}$$

or

$$U(t) = \sum_{m=1}^{\infty} |m\rangle\langle m| \cos\omega_m t, \qquad \omega_m = \frac{m\pi}{L} \tag{1.10.56}$$

The propagator equation

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

becomes in the $|x\rangle$ basis

$$\begin{aligned}\langle x|\psi(t)\rangle &= \psi(x, t) \\ &= \langle x|U(t)|\psi(0)\rangle \\ &= \int_0^L \langle x|U(t)|x'\rangle\langle x'|\psi(0)\rangle\, dx'\end{aligned} \tag{1.10.57}$$

It follows from Eq. (1.10.56) that

$$\begin{aligned}\langle x|U(t)|x'\rangle &= \sum_m \langle x|m\rangle\langle m|x'\rangle \cos\omega_m t \\ &= \sum_m \left(\frac{2}{L}\right)\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{m\pi x'}{L}\right)\cos\omega_m t\end{aligned} \tag{1.10.58}$$

Thus, given any $\psi(x', 0)$, we can get $\psi(x, t)$ by performing the integral in Eq. (1.10.57), using $\langle x|U(t)|x'\rangle$ from Eq. (1.10.58). If the propagator language seems too abstract, we can begin with Eq. (1.10.55). Dotting both sides with $\langle x|$, we get

$$\begin{aligned}\psi(x, t) &= \sum_{m=1}^{\infty} \langle x|m\rangle\langle m|\psi(0)\rangle \cos\omega_m t \\ &= \sum_{m=1}^{\infty} \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{m\pi x}{L}\right)\cos\omega_m t\langle m|\psi(0)\rangle\end{aligned} \tag{1.10.59}$$

Given $|\psi(0)\rangle$, one must then compute

$$\langle m|\psi(0)\rangle = \left(\frac{2}{L}\right)^{1/2}\int_0^L \sin\left(\frac{m\pi x}{L}\right)\psi(x, 0)\, dx$$

Usually we will find that the coefficients $\langle m|\psi(0)\rangle$ fall rapidly with m so that a few leading terms may suffice to get a good approximation. □

Exercise 1.10.4. A string is displaced as follows at $t=0$:

$$\begin{aligned}\psi(x, 0) &= \frac{2xh}{L}, && 0\le x\le\frac{L}{2} \\ &= \frac{2h}{L}(L-x), && \frac{L}{2}\le x\le L\end{aligned}$$

Show that

$$\psi(x, t) = \sum_{m=1}^{\infty} \sin\left(\frac{m\pi x}{L}\right)\cos\omega_m t\cdot\left(\frac{8h}{\pi^2 m^2}\right)\sin\left(\frac{\pi m}{2}\right)$$