Quantum Theory for the Computer Age

Unit 4

Wave Equations in Potentials
Unit 4 Wave Equations in Potentials
Unit 3 introduced the Schrodinger time equation using Fourier analysis and applied it to discrete systems with Fourier $C_n$ symmetry. Unit 4 begins by relating the discrete wave analysis to difference equations and then differential equations. The best known such equations are Schrodinger’s wave equation and time-independent potential equation. Such equations apply to systems of an arbitrary symmetry whose interaction with the environment is usually determined by a spatial potential function $V(x)$. Having such a potential goes against the relativistic symmetry and therefore Schrodinger theory is a low-energy approximation that treats time as an external parameter. In this Unit 4, the external environment is further approximated by representing the potential as a sequence of piecewise constant steps. Wave scattering depends on transmission and reflection amplitudes in crossing and scattering matrices ($C$-matrices and $S$-matrices) whose singularities represent resonances or bound states.

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Chapter 11
Differential Wave Equations

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REVIEW TOPICS & FORMULAS FOR UNIT 4

One way to “tame” continuous differential operators and differential equations is to discretize them so they become matrix equations. Such “coarse-graining” is required for numerical computer solution. In Chapters 9 and 10, quantum wave equations were written as matrix equations. In this Chapter 11, the connection is made between matrix theory with Dirac notation and the continuum theory of differential wave equations and operator analysis. The most famous of the quantum wave equations are Schrödinger’s equations, one of the foundations of non-relativistic quantum theory. Again, coupled pendulum analogies as in Chapter 10 help us understand what is happening.
Chapter 11. Introduction to Wave Equations

We have waited until now, the fourth unit, to introduce the differential wave equations of quantum mechanics. Chief among these is the Schrödinger differential equation, which in 1927 revolutionized the existing Einstein-Bohr-Kellar semiclassical quantization theory. Bohr quantization seemed full of seemingly unavoidable approximations that the differential approach avoided easily. Also, the Schrödinger equation was welcomed by a generation of physicists trained in Newtonian, Hamiltonian, Maxwellian, and Lorentzian formalism for mechanics, electrodynamics, thermodynamics, and hydrodynamics, all of which had differential equations as the main course, indeed, their identifying icons.

We can only imagine how mysterious the non-classical aspects of the then-new quantum theory must have seemed then if we still find them mysterious scores of years later. Therefore, it is understandable why the appearance of a differential equation from which, in principle, all quantum phenomena could be deduced, would seem like a good and familiar thing. Since space and time had always been treated as a continuum, the use of differential equations came naturally, and still does today. The chances are good that as you read this page, even years after its copyright date, you will be holding one of just a few quantum texts that do not start off with Schrödinger differential equations. Most new texts are like old military manuals that forever fight the last war.

However, proactive researchers need to focus on the future engagements. New tools will be required to deal effectively with new problems. For one thing it is the solutions to the differential equations that we seek to understand, not just the equations themselves. While the Schrödinger equation is easy to solve for some old textbook problems, it turns out to be rather clumsy in much of modern research. For example, the full Euler-coordinate Schrödinger equation for a rotating asymmetric molecule like water (H$_2$O) would cover this page for just a rigid-rotor approximation; for the next small-vibration-approximation it would fill this chapter, and with all the electronic and nuclear degrees of freedom included it might fill a library. That's just the equations; not their solutions!

One goal of this chapter is to show connections between differential equations and the analogous discrete bra-ket matrices introduced in the preceding Chapters. Another goal is to use the differential equations and operators for the problems in which they are most suitable, namely, unbounded ones with open boundary conditions. Finally, a most important goal is to point the way toward more powerful analytical and computational techniques that replace differential analysis when it becomes impractical.

Modern digital computational techniques require a course-grain discretizing of the continuum. This fact, alone, requires satisfactory connection between finite-discrete spaces and ones that are infinite or continuous. However, there are also fundamental reasons for clarifying the relations between discrete and continuos spaces. Some of the resulting insights will be discussed in what follows.
11.1 Discrete versus Continuous x and k Variables

Let us review some of the types of quantum base-state systems studied so far. The latter part of Chapter 7 (Sec. 7.3a and 7.3b) introduced a finite discrete and bounded N-position coordinate $|x_p\rangle$-state basis system for $N$ discrete lattice points $x_0=0, x_1=a, x_2=2a, x_3=3a, ... , x_{N-1}=(N-1)a$. 

\{ $|0\rangle, |1\rangle, |2\rangle, |3\rangle, ... |p\rangle, ... , |N-1\rangle \}$ or \{ $|x_0\rangle, |x_1\rangle, |x_2\rangle, |x_3\rangle, ... , |x_p\rangle, ... , |x_{N-1}\rangle \}$

This so-called Hilbert $x_p$-space is indexed by state index numbers $p = 0, 2, 3, ..., N-1$, which are discrete ("quantized") and bounded by $N$ (finite). But, they could be made unbounded by letting $N = \infty$.

At the other extreme, Sec.7.1 and 7.2 introduced infinite-state systems of continuous x-coordinate $x$. \{ $|-1.001\rangle,... |4.17\rangle, ... |x'\rangle, |x''\rangle, ... , |x\rangle, ... \}.

These so-called Banach x-spaces are indexed by a real variable $x$ which may be bounded to range only from $x = a$ to $x = b$ (typically from $x = 0$ to $x = L$) or may be unbounded and range from $x = -\infty$ to $x = +\infty$.

The wavevector or momentum base states $|k_m\rangle$ or $|k\rangle$ also came in four flavors. First there are the Bohr orbital states $|k_m\rangle$ that are indexed by a quantum number $m = 0, 1, 2, ... , \infty$ that is discrete but unbounded. (Integer $m$ is the number of $2\pi$-waves in the Bohr circumference bounded by $x = 0$ to $x = L$).

Then there are the Bloch wave states $|k_m\rangle$ similarly indexed except $m = 0, 1, 2, ... , N-1$ is bounded.

Then there are the two kinds of $|k\rangle$ states with continuous wavevector $k$ obtained from the above by letting $L = \infty$ as in the Bohr system or by letting $N = \infty$ (with $L$ fixed) as in the Bloch system. It might seem that this would lead to a large number of possible transformation matrix combinations beginning with $\langle x_p|k_m\rangle$ and ending with four kinds of $\langle x|k\rangle$. However, just four distinct types of transformations are possible overall. This is diagrammed in Fig. 11.1.1.

The X's mark off systems that are incompatible because their dimensions are different; obviously an $N$-dimensional basis cannot be transformed into an $\infty$-dimensional one by a "square" transformation matrix. Neither can an unbounded continuum be mapped one-to-one onto its sub-set of integers that skip all the irrational numbers. Similarly, a bounded continuum is a subset of the whole (unbounded) continuum. Transformation matrices must satisfy orthonormality-completeness axioms-2 and 3. These have a unitary symmetry that makes them two sides of one coin, so to speak.

The O's mark off systems that have incompatible boundary conditions. A bounded $x$-continuum leads to unbounded but discrete $k$-set of Bohr orbitals through conditions (7.1.3) repeated below

$0 < x \leq L$; leads to: $k_m = \frac{2\pi}{L} m$, where: $m = 0, \pm 1, \pm 2, \pm 3, ... , \pm \infty$ (7.1.3) repeated

Similarly, an unbounded but discrete set of $x$-points (the infinite lattice: (7.1.3) with $L = a N = \infty$) leads to a bounded Bloch $k$-continuum, that is, the Brillouin zone bounded by $\pm k_{BZB}$ as defined in (9.3.9a).

$x_p = p a = p L/N$, where: $p = 0, 1, 2, 3, ... , \infty$; leads to: $-k_{BZB} \leq k < k_{BZB} = \pi/a$ (11.1.1)

It is remarkable that a bounded continuum, irrationals and all, can be "counted" discretely by an infinite set of integers. Finer and finer wave zeros must eventually land close to all the numbers, rational or irrational.
### Fig. 11.1.1 Comparison of discrete versus continuum systems

What we are discussing here is known as the **point-set topology** of our possible quantum spaces. This just means we're viewing the empty terrain or "real estate" and its effect on a quantum particle wave adding any structures such as potentials or force fields. Potentials are introduced later in this Chapter.
11.2 Difference versus differential operators in coordinate space

Most treatments of quantum mechanics (including Bohr's and Schrödinger's original development) begin with the x-continuum side of Fig. 11.1.1. Here we finally consider the x-differential equations that result from an x-continuum. However, the connection between the corresponding discrete x_p side of Fig. 11.1.1 will be maintained. The discrete side involves x_p-differential equations. If you plan to simulate continuum systems on a computer then this connection is essential.

(a) First differences and derivatives

The first difference \((\Delta \psi)_p\) of a discrete function \(\psi(x_p)\) is usually defined by
\[
(\Delta \psi)_p = \psi(x_{p+1}) - \psi(x_p).
\]
A matrix representation of \(\Delta\) acting on a \(|\psi\rangle\) ket column of amplitudes
\[
\{x_0|\psi\rangle, x_1|\psi\rangle, \ldots, x_p|\psi\rangle, \ldots\} = \{\psi(x_0), \psi(x_1), \ldots, \psi(x_p), \ldots\} = \{\psi_0, \psi_1, \ldots, \psi_p, \ldots\}
\]
is the following.
\[
\Delta |\psi\rangle = \begin{pmatrix}
\langle x_0 | \Delta |\psi\rangle \\
\langle x_1 | \Delta |\psi\rangle \\
\langle x_2 | \Delta |\psi\rangle \\
\vdots
\end{pmatrix} = \begin{pmatrix}
-1 & 1 & 0 & 0 & 0 & \ldots \\
0 & -1 & 1 & 0 & 0 & \ldots \\
0 & 0 & -1 & 1 & 0 & \ldots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix} \begin{pmatrix}
\langle x_0 | \psi \rangle \\
\langle x_1 | \psi \rangle \\
\langle x_2 | \psi \rangle \\
\vdots
\end{pmatrix} = \begin{pmatrix}
\psi_1 - \psi_0 \\
\psi_2 - \psi_1 \\
\psi_3 - \psi_2 \\
\vdots
\end{pmatrix}.
\]
(11.2.3)

This operation is analogous to the first differential \(df(x)\) in continuum calculus.
\[
df(x) = f(x+dx) - f(x).
\]
While this is an infinitesimal, the following first derivative is finite in a suitable limit sequence.
\[
\lim_{dx \to 0} \frac{d\psi}{dx} = \frac{\psi(x+dx) - \psi(x)}{dx}.
\]
(11.2.4)

By analogy, the finite difference "derivative" or first differencitive is defined
\[
\left(\frac{\Delta \psi}{\Delta x}\right)_p = \frac{\psi(x_{p+1}) - \psi(x_p)}{\Delta x} = \frac{\psi(x_{p+1}) - \psi(x_p)}{a}.
\]
(11.2.5)

Finite differences have no problems with infinitesimal limits, but there is still a question of lattice location. One could define another operator \(\tilde{\Delta}\) that is the negative transpose of \(\Delta\) in (11.2.3).
\[
\tilde{\Delta} \psi = \psi(x_p) - \psi(x_{p-1})\quad \text{where:} \quad \tilde{\Delta} = -\Delta^T.
\]
(11.2.6)

Its representation is
\[
\tilde{\Delta} |\psi\rangle = \begin{pmatrix}
\langle x_0 | \tilde{\Delta} |\psi\rangle \\
\langle x_1 | \tilde{\Delta} |\psi\rangle \\
\langle x_2 | \tilde{\Delta} |\psi\rangle \\
\langle x_3 | \tilde{\Delta} |\psi\rangle \\
\vdots
\end{pmatrix} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & \ldots \\
-1 & 1 & 0 & 0 & 0 & \ldots \\
-1 & 1 & 0 & 0 & 0 & \ldots \\
-1 & 1 & \ldots & \ddots & \ddots & \ddots
\end{pmatrix} \begin{pmatrix}
\langle x_0 | \psi \rangle \\
\langle x_1 | \psi \rangle \\
\langle x_2 | \psi \rangle \\
\langle x_3 | \psi \rangle \\
\vdots
\end{pmatrix} = \begin{pmatrix}
\psi_0 - \psi_{-1} \\
\psi_1 - \psi_0 \\
\psi_2 - \psi_1 \\
\psi_3 - \psi_2 \\
\vdots
\end{pmatrix}.
\]
(11.2.7)
In continuum calculus no one would quibble about the difference between \( \vec{\Delta} \) and \( \Delta \) since they could not differ by more than an infinitesimal. Indeed, the derivative could just as well be defined using the average \( \vec{\Delta} \) of these two operators which is an \emph{anti-symmetric} operator

\[
\vec{\Delta} = \frac{\Delta + \Delta^T}{2} = -\Delta^T
\]  

(11.2.7a)

\[
\vec{\Delta}|\psi\rangle = \left( \begin{array}{c}
\langle x_0 | \vec{\Delta} | \psi \rangle \\
\langle x_1 | \vec{\Delta} | \psi \rangle \\
\langle x_2 | \vec{\Delta} | \psi \rangle \\
\vdots
\end{array} \right) = \left( \begin{array}{c}
0 \\
-\frac{1}{2} \\
-\frac{1}{2} \\
\vdots
\end{array} \right)
\]

\[
\left( \begin{array}{c}
\langle x_1 | \psi \rangle \\
\langle x_2 | \psi \rangle \\
\langle x_3 | \psi \rangle \\
\vdots
\end{array} \right) = \left( \begin{array}{c}
\frac{1}{2} \\
-1 \\
0 \\
\vdots
\end{array} \right)
\]

\[
\left( \begin{array}{c}
\psi_1 - \psi_{-1} \\
\psi_2 - \psi_0 \\
\psi_3 - \psi_1 \\
\vdots
\end{array} \right)
\]

(11.2.7b)

as follows.

\[
(D\psi)_p = \left( \begin{array}{c}
\Delta \psi \\
\Delta \psi \\
\Delta \psi \\
\vdots
\end{array} \right)_p = \frac{\psi(x_{p+1}) - \psi(x_{p-1})}{2\Delta x} = \frac{\psi(x_{p+1}) - \psi(x_{p-1})}{2a} \rightarrow \Delta x \rightarrow 0 \frac{d\psi}{dx} \quad (11.2.7c)
\]

While the alternative finite difference operator definitions all lead to the same limit in calculus, they only give slightly different results for unbounded or large-\( N \) discrete wave amplitudes. However, they give very different results for small-\( N \) discrete systems, particularly, near end points or boundaries.

The discrete and continuum representations of a derivative operator \( D \rightarrow \frac{d}{dx} \) are compared here.

\[
\langle x | D | y \rangle = \sum_{q=a}^{b} D_{p,q} \psi_q \quad (11.2.8)
\]

The continuum matrix element or \emph{kernal} \( D(x,y) = \langle x | D | y \rangle \) of the \( D \) operator follows from definition

\[
\langle x | D | y \rangle = \frac{d\psi(x)}{dx} = \frac{d\langle x | \psi \rangle}{dx} \quad (11.2.9a)
\]

with \( |\psi\rangle \) replaced by \( |y\rangle \) and use Dirac's delta \( \langle x | y \rangle = \delta(x,y) \). Anti-symmetry (11.2.7a) is added.

\[
\langle x | D | y \rangle = \frac{d\langle x | y \rangle}{dx} = \frac{d\delta(x,y)}{dx} = -\langle y | D | x \rangle = -\frac{d\delta(y,x)}{dy} \quad (11.2.9b)
\]

Now we check this strange kernal by substituting it into the integral (11.2.8) and integrating by parts.

\[
\int_{y=a}^{b} dy \langle x | D | y \rangle \psi(y) = \left. \int_{y=a}^{b} dy \frac{d\delta(y,x)}{dy} \psi(y) \right|_{y=a}^{b} + \int_{y=a}^{b} dy \frac{d\psi(y)}{dy} \delta(y,x) = \frac{d\psi(x)}{dx} \quad (11.2.10)
\]

This shows some more of the power of Dirac's notation and shows why the derivative of a Dirac delta function would cause an integral of a function to yield its derivative! The discrete-space versions of the \( \delta \)-forms show that two neighboring function points need to be subtracted.

\[
(D\psi)_p = \frac{\psi_{p+1} - \psi_p}{a} = \sum_{q=a}^{b} \delta_{p+1,q} \psi_q - \delta_{p,q} \psi_q = \sum_{q=a}^{b} (D\delta)_{p,q} \psi_q
\]
Indeed, that is analogous to a Dirac-delta derivative. If the Dirac delta is a spike sticking up, as in Fig. 11.2.1a then its derivative is two spikes, as shown in Fig. 11.2.1b; the first one sticking up and the second one sticking down and moved infinitesimally forward to \( x+dx \). It is actually the negative of this that must be integrated since we want the difference \(-\psi(x)+\psi(x+dx)\) as (11.2.9-10) tells us, not \( \psi(x) - \psi(x+dx) \).

(b) Second differences and derivatives

The second difference \((\Delta^2 \psi)_p\) of a discrete function \(\psi(x_p)\) is defined using two first differences by

\[
(\Delta^2 \psi)_p = (\tilde{\Delta} \tilde{\Delta} \psi)_p = \tilde{\Delta} \left( \psi(x_{p+1}) - \psi(x_p) \right) = \psi(x_{p+1}) - 2 \psi(x_p) + \psi(x_{p-1}).
\]  

(11.2.11a)

A matrix representation of \(\Delta^2\) acting on a ket column of amplitudes

\[
\begin{pmatrix}
\langle x_0 | \psi \\
\langle x_1 | \psi \\
\langle x_2 | \psi \\
\vdots
\end{pmatrix} =
\begin{pmatrix}
-2 & 1 & 0 & \cdots \\
1 & -2 & 1 & \cdots \\
0 & 1 & -2 & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\begin{pmatrix}
\langle x_0 | \psi \\
\langle x_1 | \psi \\
\langle x_2 | \psi \\
\vdots
\end{pmatrix}
\]

is the following

\[
\Delta^2|\psi\rangle = 
\begin{pmatrix}
\langle x_0 | \Delta^2 | \psi \rangle \\
\langle x_1 | \Delta^2 | \psi \rangle \\
\langle x_2 | \Delta^2 | \psi \rangle \\
\vdots
\end{pmatrix} = 
\begin{pmatrix}
-2 & 1 & 0 & \cdots \\
1 & -2 & 1 & \cdots \\
0 & 1 & -2 & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\begin{pmatrix}
\langle x_0 | \psi \\
\langle x_1 | \psi \\
\langle x_2 | \psi \\
\vdots
\end{pmatrix}
\]

(11.2.11b)

Now three points are taken from the function space and the kernal will be a second derivative of the Dirac delta which has three spikes; two up spikes surrounding a down spike of twice the area. (See Fig. 11.2.1c)

\[
\frac{\langle x | \Delta^2 | y \rangle}{dx^2} = \frac{d^2 \langle x | y \rangle}{dx^2} = \frac{d^2 \delta(x,y)}{dx^2} = \frac{d^2 \delta(x,y)}{dy^2}.
\]

(11.2.12a)

It is easy to verify that the integral representation of \(\Delta^2\) is the usual second derivative.

\[
\int_{y=a}^{y=b} dy \langle x | \Delta^2 | y \rangle \psi(y) = \int_{y=a}^{y=b} dy \frac{d^2 \delta(x,y)}{dy^2} \psi(y) = \frac{d^2 \psi(x)}{dx^2}.
\]

(11.2.12b)

Furthermore, it is easy to see that \(f(x) \cdot \Delta^2\) for any function \(f(x)\) gives a similar result. In Dirac notation we need to think of a function as a one-point functional evaluation. It is represented by left-multiplying \(\mathbf{D}\) by an abstract operator \(f(x)\) that is diagonal in the \(|x\rangle\) position state basis. That is,

\[
f(x) |x\rangle = f(x) |x\rangle \quad \text{and} \quad \langle y | f(x) | x \rangle = f(x) \langle y | x \rangle = f(x) \delta(y,x) = f(x) \delta(x,y)
\]

(11.2.13)

Then the following integral representations follow and correspond to the three parts of Fig. 11.2.1.

\[
\int_{y=a}^{y=b} dy \langle x | h(x) \mathbf{1} | y \rangle \psi(y) = \int_{y=a}^{y=b} dy \ h(x) \delta(y,x) \psi(y) = h(x) \psi(x)
\]

(11.2.14a)

\[
\int_{y=a}^{y=b} dy \langle x | g(x) \mathbf{D} | y \rangle \psi(y) = \int_{y=a}^{y=b} dy \ g(x) \frac{d \delta(y,x)}{dy} \psi(y) = g(x) \frac{d\psi(x)}{dx}
\]

(11.2.14b)

\[
\int_{y=a}^{y=b} dy \langle x | f(x) \mathbf{D}^2 | y \rangle \psi(y) = \int_{y=a}^{y=b} dy \ f(x) \frac{d^2 \delta(y,x)}{dy^2} \psi(y) = f(x) \frac{d^2 \psi(x)}{dx^2}
\]

(11.2.14c)

The first derivative is a bit more troublesome since the delta-derivative is anti-symmetric.

\[
\delta'(x,y) = \delta'(x-y) = -\delta'(y-x) = -\delta'(y,x), \quad \text{or} \quad \delta'(x,y) = \frac{d\delta(x-y)}{dx} = -\frac{d\delta(x-y)}{dy} = -\frac{d\delta(y-x)}{dx}
\]
Odd derivatives are represented as asymmetric matrices or anti-symmetric matrices like (11.2.7b). So the delta-derivative is similarly lopsided.

**Fig. 11.2.1 Delta function derivatives and function evaluation**

(a) **Dirac delta function** $\delta(x, 2.0)$
(measures value $\psi(2.0)$ at $x=2.0$)

(b) **Delta 1st derivative** $\delta'(x, 2.0)$
(measures slope $\psi'(2.0)$ at $x=2.0$)

(c) **Delta 2nd derivative** $\delta''(x, 2.0)$
(measures $\psi''(2.0)$ at $x=2.0$)

---

$\psi(2.0) = \int dx \delta(x-2.0)\psi(x)$

$\psi'(2.0) = \frac{\psi(2.0+dx)-\psi(2.0)}{dx}$

$\psi''(2.0) = \frac{\psi(2.0+dx)-2\psi(2.0)+\psi(2.0-dx)}{(dx)^2}$

$\psi''(2.0) = \int dx \delta''(x-2.0)\psi(x)$

$d\int dx \delta(x-a)\psi(x) \bigg|_{a=2.0}$

$\psi''(2.0) = \frac{d^2\int dx \delta(x-a)\psi(x)}{da^2} \bigg|_{a=2.0}$
(c) Differential equations in Dirac notation: Green’s operator

Summing (11.2.14) up gives a general linear second order differential equation and its integral operator representation

\[ \int_{y=a}^{b} dy \langle x | L | y \rangle \psi (y) = L \cdot \psi (x) = \langle x | L | \psi \rangle \]  \hspace{1cm} (11.2.15a)

where an inhomogeneous differential equation

\[ L \cdot \psi (x) = f(x) \frac{d^2 \psi (x)}{dx^2} + g(x) \frac{d \psi (x)}{dx} + h(x) \psi (x) = s(x) \]  \hspace{1cm} (11.2.15b)

has the following kernal or matrix element

\[ \langle x | L | y \rangle = f(x) \frac{d^2 \delta (y,x)}{dy^2} + g(x) \frac{d \delta (y,x)}{dy} + h(x) \delta (y,x) \]  \hspace{1cm} (11.2.15c)

and is written in abstract Dirac notation as follows.

\[ L | \psi \rangle = | \psi \rangle \]  \hspace{1cm} (11.2.15d)

The source function \( s(x) \) or inhomogeneity is just another ket-vector represented in \( x \)-space by \( s(x) = \langle x | s \rangle \). (11.2.15e)

The solution(s) to the equation \( L \cdot \psi = s \) have the form

\[ | \psi \rangle = | \phi \rangle + G | s \rangle , \]  \hspace{1cm} (11.2.15f)

where ket \( | \phi \rangle \) is a solution to a homogeneous equation (True Schrödinger equations are homogeneous.)

\[ L | \phi \rangle = 0 , \]  \hspace{1cm} (11.2.15g)

and \( G \) is called the Green’s operator and is a quasi-inverse to operator \( L \). In abstract operator notation

\[ L \cdot G = 1 , \]  \hspace{1cm} (11.2.15h)

which in Dirac notation using completeness expands to the following integral representation

\[ \int_{x=a}^{b} dx' \langle x | L | x' \rangle \langle x' | G | y \rangle = \langle x | 1 | y \rangle = \delta (x,y) \]  \hspace{1cm} (11.2.15i)

or converting back to a differential form using (11.2.15b-c), Green’s differential equation.

\[ L \cdot G (x,y) = f(x) \frac{d^2 G(x,y)}{dx^2} + g(x) \frac{d G(x,y)}{dx} + h(x) G(x,y) = \delta (x,y) \]  \hspace{1cm} (11.2.15j)

The latter is an "almost homogeneous" equation with just one isolated delta "spike" source. The general solution sums Green’s function \( G(x,x') = \langle x | G | x' \rangle \) over a source distribution \( s(x) = \langle x | s \rangle \) of delta spikes to give a complete representation of general solution (11.2.15f).

\[ \langle x | \psi \rangle = \langle x | \phi \rangle + \int_{x=a}^{b} dx' \langle x | G | x' \rangle \langle x' | s \rangle , \text{ or: } \psi (x) = \phi (x) + \int_{x=a}^{b} dx' G(x,x') s(x') \]  \hspace{1cm} (11.2.15k)

This ten-part equation shows many ways to represent a differential equation, which in Dirac notation are fairly easy to connect. Dirac’s powerful notation goes a long way toward taking some of the mathematical mystery out of differential analysis. At the same time it begins to show how the equations can be related to discrete space analogs and course-grained numerical simulations. Linear differential equations and integral equations all boil down to (or up from) matrix operator equations in Dirac notation.
We don’t need Green’s function for solving the standard form \( L |\psi\rangle = 0 \) of Schrodinger’s equations because the source term is zero \( \langle \mathbf{s} | = 0 \). However, approximation schemes exist which remove part of the Schrodinger operator and put it on the right hand side of the equation so it acts like a source or forcing term of a driven oscillator equation. Then the full solution (11.2.15k) is used.

**(d) Adjoint differential operator**

It is convenient for differential operators \( L \) to be Hermitian or self-conjugate \( (L^\dagger = L) \). For Hamiltonian generators (Recall (9.2.8a)) \( H^\dagger = H \) is mandated by axioms 1-4. The problem is: How do we define the "dagger" (\( \dagger \)) of a differential operator?

The key is in the matrix element or kernel (11.2.15c). The operator will have matrix elements that are transpose conjugates of the original matrix.

\[
\langle \mathbf{x} | L^\dagger | \mathbf{y} \rangle = \langle \mathbf{y} | L | \mathbf{x} \rangle^* \quad (11.2.17)
\]

Combining this with (11.2.15c) gives

\[
\langle \mathbf{x} | L^\dagger | \mathbf{y} \rangle = \int_{y=a}^{y=b} dy \langle \mathbf{x} | L^\dagger | y \rangle \psi(y)
\]

Putting this kernel into the integral (11.2.15a) gives

\[
L^\dagger \cdot \psi(x) = \int_{y=a}^{y=b} dy \left[ f^*(y) \frac{d^2 \delta(x,y)}{dx^2} + g^*(y) \frac{d \delta(x,y)}{dx} + h^*(y) \delta(x,y) \right] \psi(y)
\]

Using (11.2.9a) and (11.12a) and integrating by parts yields the adjoint differential operator \( L^\dagger \).

\[
L^\dagger \cdot \psi(x) = \frac{d^2 \left( f^*(x) \psi(x) \right)}{dx^2} - \frac{d \left( g^*(x) \psi(x) \right)}{dx} + h^*(x) \psi(x)
\]

(11.2.20a)

Assuming only real coefficient functions and expanding gives

\[
L^\dagger \cdot \psi(x) = f(x) \frac{d^2 \psi(x)}{dx^2} + \left( \frac{2 df(x)}{dx} - g(x) \right) \frac{d \psi(x)}{dx} + \left( \frac{d^2 f(x)}{dx^2} - \frac{dg(x)}{dx} + h(x) \right) \psi(x)
\]

(11.2.20b)

**1) Self-Adjoint differential operator: Sturm-Liouville form**

For many quantum applications we must equate the adjoint (11.2.20b) to the original operator in (11.2.15b) so that the coefficient functions for a quantum operator are restricted.

\[
g(x) = 2 \frac{df(x)}{dx} - g(x) \quad \text{and} \quad h(x) = \frac{d^2 f(x)}{dx^2} - \frac{dg(x)}{dx} + h(x)
\]

(11.2.21)

Either restriction gives

\[
\frac{df(x)}{dx} = g(x)
\]

(11.2.22)

So the second order real Hermitian or self-adjoint operator must have the following form

\[
L \cdot \psi(x) = f(x) \frac{d^2 \psi(x)}{dx^2} + \frac{df(x)}{dx} \frac{d \psi(x)}{dx} + h(x) \psi(x) = L^\dagger \cdot \psi(x) = \frac{d}{dx} \left( f(x) \frac{d \psi(x)}{dx} \right) + h(x) \psi(x)
\]

(11.2.23)
The self-adjoint \((\mathbf{L}^\dagger = \mathbf{L})\) operator is also called a **Sturm-Liouville operator**.

Because \(L\) is self-adjoint or Hermitian, it must have real eigenvalues, unitary diagonalizing transformations (d-trans), Hermitian projectors, and, of course, orthonormal and complete eigenfunctions. It must also have Hermitian Green's operators.

**Higher order difference and differential operators**

Higher derivatives have integral forms similar to (11.2.14). Higher difference operators can be generalized a number of(490,621),(879,772)

\[
\begin{pmatrix}
\vdots & & \\
-1 & 0 & 1 \\
0 & 1 & 0 \\
-1 & 0 & 1 \\
-1 & 0 & 0 \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
\vdots & & \\
-1 & 0 & 1 \\
0 & 1 & 0 \\
-1 & 0 & 1 \\
-1 & 0 & 0 \\
\end{pmatrix}
\]

This gives the following Pascal triangle with alternating ± signs along its diagonals. Using this you should be able to construct matrix representations of any \(\Delta^n\).

\[
\begin{pmatrix}
1 & \\
1 & -2 & 1 \\
1 & -3 & 3 & -1 \\
1 & -4 & 6 & -4 & 1 \\
1 & -5 & 10 & -10 & 5 & -1 \\
\end{pmatrix}
\]

(11.2.25)

Indeed, \(-\Delta^2\) is the Bloch's Hamiltonian set to give zero energy for zero-\(k_m\) and positive energy values (9.3.5g) for all other states and leads to the discrete Schrodinger's wave equation as we will see later.

The tunneling parameter \(S\) is inversely proportional to the effective mass \(M\) of the wave-particle motion, according to the matrix analysis of Bohr-Bloch waves after (9.3.11). This must show up in a wave differential equation, as well.
11.3 Momentum and coordinate space operators: Fourier transforms

First, we need to review the meaning of coordinate bases \(\{ |x\rangle \} \) and operators associated with them. Then we will make the Fourier change of basis (7.2.4) and see how all this plays out in the new wavevector or momentum space basis \(\{ |k\rangle \} \).

(a) Coordinate space and operators

Anything that is done to a function \(\psi(x) = \langle x | \psi \rangle\) should be thought of as a matrix operation \(M\) on its ket vector \(|\psi\rangle\) that maps it into a new vector \(|\varphi\rangle = M |\psi\rangle\),

\[
|\varphi\rangle = M |\psi\rangle, \tag{11.3.1}
\]

which is represented as a new function \(\varphi(x) = \langle x | \varphi \rangle = \langle x | M |\psi\rangle\).

Even just multiplying \(\psi(x)\) by the \(x\)-coordinate to give \(x \psi(x)\), or by a function \(f(x)\) of the \(x\)-coordinate to give \(f(x) \psi(x)\) is a mapping operation and is designated by bold-face type.

\[
x \psi(x) = \langle x | \mathbf{x} | \psi \rangle \quad \quad \quad f(x) \psi(x) = \langle x | f(\mathbf{x}) | \psi \rangle \tag{11.3.3}
\]

You might wonder, "How can I go through umpteen years of algebra and calculus and never see this?"

The reason is that in the continuum of coordinate bases \(\{ |x\rangle \} \) are eigenvectors ("own-vectors") of the \(x\)-operator and all its functions \(f(x)\).

\[
\mathbf{x} |x\rangle = x |x\rangle, \quad \text{or} \quad f(\mathbf{x}) |x\rangle = f(x) |x\rangle \tag{11.3.4a}
\]

Furthermore, the eigenbras \(\langle x | \mathbf{x} = |x\rangle \) have the same eigenvalue since \(x\) is real. (Recall (2.2.5).)

\[
\langle x | \mathbf{x} = \langle x | x = \langle x | \quad \text{or} \quad \langle x | f(\mathbf{x}) = f(x) \langle x | \tag{11.3.4b}
\]

So \(\mathbf{x}\) and \(f(\mathbf{x})\) are Hermitian (self-† conjugate) operators if the function \(f(x)\) is real, too.

\[
\mathbf{x} \dagger = \mathbf{x}, \quad \text{and} \quad f(\mathbf{x}) \dagger = f(\mathbf{x}) \tag{11.3.4c}
\]

This immediately gives (11.3.3).

\[
\langle x | \mathbf{x} | \psi \rangle = \langle x | \psi \rangle x = \langle x | \psi \rangle = x \psi(x), \quad \text{or} \quad \langle x | f(\mathbf{x}) | \psi \rangle = f(x) \langle x | \psi \rangle = f(x) \psi(x) \tag{11.3.4d}
\]

All \(\mathbf{x}\)-operators are diagonal in their own eigen-basis. (Oops, there's that bilingual redundancy again!) Matrix operator multiplication is reduced to plain old numerical multiplication.

You might wonder about a product like \(f(x) \psi(x)\), "Which is the vector and which is the operator?" Good question! The answer can be both, one of them, or neither, depending on what you are doing! As you become more familiar with Dirac functional analysis notation, it will be easier to see how various operators and operatees (Is "operatee" a word yet. It should be.) play many different roles and switch them often. That will be a sign that you're getting proficient in your chosen career as a quantum mechanic!
(b) Wavevector operator $k$

The empty infinite $x$-continuum is like the universe's most perfectly boring desert; miles and miles of nothing so much as a pop stand. That's what we call $C_\infty$-symmetry. No matter where you go, every point looks exactly the same as the last one. (Recall Sec. 8.2d which discussed the “roots” of $e^{ikx}$.) The analysis of $C_N$ in Sec. 8.2 suggests how $C_\infty$-symmetry gives a diagonalizing transformation matrix

$$\langle x | k \rangle = \psi_k(x) = e^{ikx} \sqrt{2\pi}$$

also known as a 1-D plane-wave function or Fourier transform kernel (7.2.4). The discussion in Sec. 7.2b listed some roles that this all-important exponential plays. Now we are using it as a transformation $\langle x | k \rangle$ or "ticket" to momentum space continuum bases $\{ \ldots | k \rangle \ldots \}$.

The seemingly magic feature of symmetry analysis is that it gives the diagonalizing transformation (11.3.5) for the time evolution operator $U$, or the Hamiltonian $H$ (Recall Sec. 9.3a) which describe physics in a $C_\infty$-symmetric desert. It does this without explicit knowledge of operators $U$ or $H$. More will be said about this later. For now it is easier to see the diagonalization by simpler arguments.

To do this, let a wavevector operator $k$ play the same role in wavevector space $\{ \ldots | k \rangle \ldots \}$ that the position operator $x$ plays in position space $\{ \ldots | x \rangle \ldots \}$. That is, let $k$ be a diagonal operator satisfying

$$k | k \rangle = k | k \rangle$$

in analogy to (11.3.4) the eigenbras $| k \rangle = | k \rangle^\dagger$ have the same real eigenvalue $k$.

$$\langle k | k = \langle k | k = k \langle k | \text{ , or } \langle k | f(k) = f(k) \langle k |$$

So $k$ and $f(k)$ are Hermitian (self-$\dagger$ conjugate) operators for any real function $f(k)$.

$$k^\dagger = k \text{ , and } f(k)^\dagger = f^*(k^\dagger) = f(k)$$

This immediately gives the $k$-space version of (11.3.3).

$$\langle k | k | \psi \rangle = \langle k | \psi \rangle = k \langle k | \psi \rangle = k \psi(k) \text{ , or } \langle k | f(k) | \psi \rangle = f(k) \langle k | \psi \rangle = f(k) \psi(k)$$

(c) Momentum operator $p$

The De Broglie relation (5.2.5c) equates momentum $p$ with wavevector $k$ times $\hbar$. The same applies to the operators:

$$p = \hbar k$$

A word of caution about notation: Boldface type $k$ here means a quantum operator for one-dimensional wavevector or momentum. Similar bold type is used in Chapter 6 to designate classical three-dimensional wavevectors $\mathbf{k}$. This is a common notation and may be an unfortunate source of confusion. Our solution is to denote quantum operators by a sans-serif $k$ and $p$ wherever they might be confused. Of course, this will be a real problem when we need to label three-dimensional quantum vector operator. One solution is "super-arrows" as in $\mathbf{k}$. Fortunately, there is more elegant and powerful notation based on the theory of quantum tensor operators which will be treated in later chapters.
(d) Coordinate to momentum change-of-basis

There is another notational caveat. You must be extremely careful when using such powerful notation as Dirac has given us. The last line in (11.3.6a) gives a $k$-wavefunction as

$$\langle k | \psi \rangle = \psi(k)$$

in analogy to the usual $x$-wavefunction $\langle x | \psi \rangle = \psi(x)$ . Does this mean just replace $x$ with $k$ in $\psi(x)$ ? The answer is no! no! no! No! NO-OOOO! This would be another example of "Dirac abuse" mentioned in Sec. 7.2. Instead, it means the Fourier transform (7.2.4c) of $\psi(x)$ repeated below.

$$\langle k | \psi \rangle = \int_{-\infty}^{+\infty} dx \, \langle k | x \rangle \langle x | \psi \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx \, e^{-ikx} \psi(x) , \quad (11.3.7)$$

You see the trouble is not with Dirac. We get in trouble when we convert back to that old function notation of those musty Newtonian calculus books! Avoid using $\psi(k)$ for $\langle k | \psi \rangle$ and use $\psi(x)$ with care.

Now this change of basis between $\{...|k\}...$ and $\{...|x\}...$ needs to be applied to the wavevector (or momentum) operators. We ask, "How do $\mathbf{k}$ and $\mathbf{p}$ , which are diagonal in momentum space $\{...|k\}...$ , get represented in the position coordinate basis $\{...|x\}..."?" A related question asks, "How does position operator $\mathbf{x}$ look when represented in momentum $k$-space?"

First, the effect of $\mathbf{k}$ on a general state, as represented in $x$-space, is found using $x$-completeness.

$$\langle x | k | \psi \rangle = \int_{-\infty}^{+\infty} dx' \langle x | k \rangle \langle k | \psi \rangle = \int_{-\infty}^{+\infty} dx' \langle x | k \rangle \psi(x') \quad (11.3.8)$$

Then the kernel $\langle x | k | x' \rangle$ is expanded using the $k$-basis in which $\mathbf{k}$ is diagonal (11.3.6a).

$$\langle x | k | x' \rangle = \int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} dk' \langle x | k \rangle \langle k | k' \rangle \langle k' | x' \rangle$$

$$= \int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} dk' \langle x | k \rangle \langle k | k' \rangle \langle k' | x' \rangle \quad \text{k-eigenvalue: } k \langle k | k \rangle$$

Fourier transformation matrix (11.3.5) and orthonormality $\langle k | k' \rangle = \delta(k-k')$ gives

$$\langle x | k | x' \rangle = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \frac{e^{ikx}}{\sqrt{2\pi}} \delta(k-k') \frac{e^{-ikx'}}{\sqrt{2\pi}} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \frac{e^{ik(x-x')}}{2\pi}$$

This can be written as an $x$-derivative of a Dirac delta $\langle x | x' \rangle = \delta(x-x')$.

$$\langle x | k | x' \rangle = \frac{1}{2\pi} \int \frac{d}{dx} \frac{e^{ik(x-x')}}{2\pi} = \frac{1}{2\pi} \int \frac{d}{dx} \frac{e^{ik(x-x')}}{2\pi} = \frac{1}{2\pi} \int \frac{d}{dx} \langle x | k \rangle \langle k | x' \rangle$$

$$= \frac{1}{2\pi} \int \frac{d}{dx} \langle x | k \rangle \langle k | x' \rangle = \frac{1}{2\pi} \int \frac{d}{dx} \langle x | x' \rangle$$

(11.3.9)

Putting the kernel $\langle x | k | x' \rangle$ back into the integral (11.3.8) gives the following.

$$\langle x | k | \psi \rangle = \int_{-\infty}^{+\infty} dx' \frac{1}{2\pi} \int \frac{d}{dx} \langle x | x' \rangle \psi(x') = \frac{1}{2\pi} \int \frac{d}{dx} \int_{-\infty}^{+\infty} dx' \delta(x-x') \psi(x')$$

(11.3.10a)

For momentum operator, multiply by the DeBroglie-Planck $\hbar$ to make $\mathbf{k}$ into $\mathbf{p} = \hbar \mathbf{k}$. 


\( \langle x|p|\psi \rangle = \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x) \) \hspace{1cm} (11.3.10b)

This is the desired coordinate representation of the momentum operator \( p \).

To test the operator \( p \) apply it to the plane wave function \( \langle x|k \rangle = \psi_k(x) = e^{ikx}/\sqrt{2\pi} \) from (11.3.5)

\[
\langle x|p|k \rangle = \frac{\hbar}{i} \frac{\partial}{\partial x} \psi_k(x) = \frac{\hbar}{i} \frac{\partial}{\partial x} e^{ikx}/\sqrt{2\pi} = \hbar k e^{ikx}/\sqrt{2\pi} = p\psi_k(x)
\]

\hspace{1cm} (11.3.10c)

So plane wavefunction \( \psi_k(x) \) is indeed an eigenfunction of the \( p \) operation. A matrix representation of the \( p \) operator is not diagonal in the \( x \)-basis. Rather it is represented by (1)'s and (-1)'s off-diagonal as shown in (11.2.3), (11.2.6) or (11.2.24).

Without doing any more calculation it is easy to answer the question about the momentum or \( k \)-representation of the position operator \( x \) in (11.3.4). The following

\[
\langle k|x|\psi \rangle = i \frac{\partial}{\partial k} \psi(k)
\]

is the desired wavevector or momentum representation of the position operator \( x \). To test the operator \( x \) apply it to the kernal function \( \langle k|x \rangle = e^{ikx}/\sqrt{2\pi} = \psi_x(k) \) which from (11.3.5) is an eigenfunction of \( x \).

\[
\langle k|x|\psi \rangle = i \frac{\partial}{\partial k} \psi_x(k) = i \frac{\partial}{\partial k} e^{-ikx}/\sqrt{2\pi} = x e^{-ikx}/\sqrt{2\pi} = x\psi_x(k)
\]

\hspace{1cm} (11.3.11b)

This is correct, apart from the terrible notation \( \psi_x(k) \) for the kernal \( \langle k|x \rangle = \langle x|k \rangle^* = e^{-ikx}/\sqrt{2\pi} \). (Avoid such bad form that can enable "Dirac abuse" in Fourier transforms!) So the \( x \)-operator is non-diagonal in the momentum representation.

Notice how both the \( x \) and \( k \) operator representations have imaginary \( (i) \) attached to their derivative definition. This is necessary to make them Hermitian self-conjugate operators \( x^\dagger = x \) and \( k^\dagger = k \) in (11.3.4c) and (11.3.6c), respectively, and thereby assure that their eigenvalues are real. A first derivative is an anti-symmetric operator \( \Delta = -\Delta^\dagger \) matrix as pointed out in (11.2.7a) so the \( (i) \) is needed to "fix" it.

Now we are prepared to give a more rigorous derivation of the Schrodinger wave equations that were first obtained by semi-classical arguments in Chapter 5. (Recall equations (5.4.10) and (5.4.15).)
11.4 Differential Wave Equations of Schrodinger

In Sec. 9.2 there was introduced the abstract time evolution operator $U(t;0)$ and its representation (9.1.3) in a discrete $N$-state basis. We now consider how it will be represented in a continuum basis such as the coordinate basis {...$|x\rangle$...}. This will be done by appealing to the Hamiltonian generating operator $H$ which generates the $U(t;0)$ operator according to Schrodinger's fundamental time equations (9.2.5)

$$i\hbar \frac{\partial}{\partial t} U(t,0) = -iH U(t,0), \quad (11.4.1a) \quad i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle \quad (11.4.1b)$$

and satisfies the energy eigenvalue equation (9.3.1)

$$H |\epsilon\rangle = E |\epsilon\rangle = \hbar \omega |\epsilon\rangle. \quad (11.4.2)$$

The development of $U(t;0)$ and $H$ shows from Planck's hypothesis that eigenvalues $E_k = \hbar \omega_k$ of $H$ are system energies, that is, $H$ is the quantum energy operator. We now develop a representation of energy operator $H$ in both the coordinate $|x\rangle$-basis and in a momentum $|k\rangle$-basis, just as we have already done for the position and momentum operators $x$ and $p = \hbar k$, respectively, in the preceding sections.

(a) Schrodinger Wave Equations in coordinate representation

Except for a brief description of classical analogies, it has been differences between classical and quantum mechanics that we have emphasized. In spite of all this a wonderfully simple axiom holds.

The quantum Hamiltonian energy operator $H(x,p)$ is obtained directly from the classical Hamiltonian function $H(x,p)$ by replacing $x \rightarrow x$ and $p \rightarrow p$.

In other words (or equations), it is only necessary to replace the coordinate $q=x$ and momentum $p$ in a classical Hamiltonian function $H(q,p)$ with the corresponding operators $x$ and $p$ and "Presto!" you have a correct working Hamiltonian operator $H$ to use in Schrodinger's time equation (11.4.1). Given classical

$$H(q,p) = H(x,p) = p^2/2M + V(x) \quad (11.4.3)$$

where $V(x)$ is a potential energy PE function $V(x)$, we immediately have

$$H(q,p) = H(x,p) = p^2/2M + V(x) \quad (11.4.4)$$

Sounds simple enough! Let us try it out using the coordinate $|x\rangle$-basis first.

According to (11.3.10) the kinetic energy operator

$$T = p^2/2M = \hbar^2 k^2/2M \quad (11.4.5a)$$

is $|x\rangle$-represented by

$$\langle x | T | x \rangle = \langle x | \frac{p^2}{2M} | x \rangle \equiv \frac{-\hbar^2}{2M} \frac{\partial^2}{\partial x^2} \Psi(x) \quad (11.4.5b)$$

so (11.4.1b) becomes Schrodinger's time-dependent $\Psi(x,t) = \langle x | \Psi(t) \rangle$ wave equation.

$$i\hbar \langle x | \frac{\partial}{\partial t} | \Psi \rangle = \langle x | \frac{p^2}{2M} + V(x) | \Psi \rangle \quad , \quad i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \frac{-\hbar^2}{2M} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x) \Psi(x,t) \quad (11.4.5c)$$

Also, (11.4.2) becomes Schrodinger's time-independent $\psi_E(x) = \langle x | \epsilon \rangle$ wave eigenequation.

$$\langle x | H | \epsilon \rangle = E \langle x | \epsilon \rangle \quad , \quad -\frac{\hbar^2}{2M} \frac{\partial^2 \Psi_E(x)}{\partial x^2} + V(x) \Psi_E(x) = E \Psi_E(x) \quad (11.4.5d)$$

where the latter also follows from a simple substitution of the time-dependent wavefunction

$$\Psi(x,t) = e^{-i\omega t} \Psi_E(x) = e^{-iEt/\hbar} \Psi_E(x) = e^{-iEt/\hbar} \Psi(x,0) \quad (11.4.5e)$$
The time-independent wave $\psi_\varepsilon(x)$ is a stationary state wave. Recall that eigenstates do not appear to move as far as mortals like us can tell; the absolute square of (11.4.5c) is, to us, dead as a doornail. However, most of the general wavefunctions $\Psi(x,t) = \langle x | \Psi(t) \rangle$ arising from (11.4.5c) will have a life! That is, their probability distributions $P(x,t) = |\Psi(x,t)|^2 = |\langle x | \Psi(t) \rangle|^2$ can easily dance the night away. The following chapters will show many examples.

(b) Free space wavefunction solutions

Without any potential function ($V(x)=0$) the Schrödinger wave equations are

\[
i \hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2M} \frac{\partial^2 \psi(x,t)}{\partial x^2}, \quad \text{and:} \quad -\frac{\hbar^2}{2M} \frac{\partial^2 \psi_E(x)}{\partial x^2} = \varepsilon \psi_E(x)
\]  

(11.4.7)

They should give the types of waves that are our old friends starting in Chapter 4. Indeed, substituting the plane moving wave (4.2.1a)

\[
\psi_k(x,t) = A e^{-i\omega t} \psi_k(x) = A e^{-i\omega t} e^{ikx} = A e^{i(kx - \omega t)}
\]

(11.4.8)

into (11.4.7) along with $\psi_k(x) = e^{ikx}$ yields the following

\[
-i\hbar \omega \frac{\partial e^{i(kx - \omega t)}}{\partial t} = -\frac{\hbar^2}{2M} \frac{\partial^2 e^{i(kx - \omega t)}}{\partial x^2}, \quad \text{and:} \quad -\frac{\hbar^2}{2M} \frac{\partial^2 e^{ikx}}{\partial x^2} = \varepsilon e^{ikx}
\]

with frequency and energy eigenvalues that are just Planck and DeBroglie's rules.

\[
\hbar \omega = \frac{\hbar^2 k^2}{2M} = \varepsilon
\]

(11.4.9a)

Either sign of the wavevector $k$ gives the same energy $\varepsilon$ or frequency $\omega$.

\[
k = \pm \sqrt{\frac{2ME}{\hbar^2}} = \pm \sqrt{\frac{2M\omega}{\hbar}}
\]

(11.4.9b)

So a more general set of solutions are the monochromatic galloping waves (4.2.5) which have both $\pm ikx$.

\[
\psi_{\text{gallop}}(x,t) = A_\rightarrow e^{i(kx - \omega t)} + A_\leftarrow e^{i(-kx - \omega t)}
\]

(11.4.10)

We insist on clockwise ($-i\omega t$) phasors as in Chapter 4 (Fig. 4.1.2). The two complex amps $A_\rightarrow$ and $A_\leftarrow$ define a general one-dimensional (1D) free-space energy eigenfunction.

The 1D wave (11.4.10) for a given energy $\varepsilon=\hbar \omega$, constitutes a two-state system with base states $|k\rangle$ and $|-k\rangle$. It is a $U(2)$ system like the many analogous ones discussed in Chapter 1 and 4. The two complex parameters $A_\rightarrow$ and $A_\leftarrow$ amount to four real parameters including normalization, which is yet to be set. In Fig. 11.4.1 are several waves made by the program BandIt. The wave is set by adjusting two "master phasors" representing the constants $A_\rightarrow$ and $A_\leftarrow$ at an arbitrary point of origin, and they determine the magnitude, shape, and direction of a "galloping" wave. Having ($A_\rightarrow=1, A_\leftarrow=0$) gives right moving wave (11.4.8) shown on top. A typical galloping wave setting ($A_\rightarrow=0.8 e^{i\pi/4}, A_\leftarrow=0.2$) produces a galloping wave with $SWR= (0.8-0.2)/(0.8+0.2) = 0.6$ shown in the center. At the bottom is a 50-50 standing wave with"master phasors" set to ($A_\rightarrow=0.5 e^{i\pi/4}, A_\leftarrow=0.2 e^{i\pi/12}$).
In spite of all the frantic phase galloping motion, these waves are actually stationary; their envelopes or interference moduli do not move since they are single-frequency (monochromatic) waves. Still the first two have a current. The current is proportional to $|A_{\to}|^2 - |A_{\leftarrow}|^2$ and is manifested by the relative phase between neighboring phasors in the time plots on the right hand side of Fig. 11.4.1. As (10.2.16) states, (See problem 10.2.1) the power factor for coupled oscillators is proportional to the sine of their relative phase lag. Each phasor in the upper right hand plot is about $45^\circ$ ahead of its neighbor to the right, so it is continuously passing $\sin 45^\circ$ of "work" to the right. The phase lag and SWR is less for each of the two plots below, and it is zero for the standing wave, which has no current at all.

Fig. 11.4.1 Three general types of monochromatic free-space waves. (Plots by BandIt)

With any constant potential function ($V(x)=V$) the Schrödinger $x$-eigen-equation (11.4.5d) is
\[ \frac{\partial^2 \psi_E(x)}{\partial x^2} + \frac{2M}{\hbar^2} (E - V) \psi_E(x) = 0. \] (11.4.7)

If energy \( E \) is above potential \( V \), it has the sinusoidal wave form \( \psi'' + k^2 \psi = 0 \) with real wavevector \( k \).

\[ \psi = A e^{ikx} + B e^{-ikx} \]

\[ k = \pm \sqrt{\frac{2M}{\hbar^2} (E - V)} \quad (E > V) \] (11.4.8)

(c) Exponential and evanescent wavefunctions

But, if energy \( \epsilon \) is below potential \( V \), the Schrodinger \( x \)-equation has the hyperbolic or exponential wave form \( \psi'' - \kappa^2 \psi = 0 \) with an imaginary wavevector \( k = i\kappa \) or exponential extinction constant \( \kappa = -i k \).

\[ \psi = A e^{-\kappa x} + B e^{+\kappa x} \]

\[ \kappa = \pm \sqrt{\frac{2M}{\hbar^2} (V - E)} \quad (E < V) \] (11.4.9)

If \( B = 0 \) you get an exponential wave \( \exp(-\kappa x) \) that dies in a potential barrier as shown in Fig. 11.4.2. Note that all phasors are synchronized to the same phase, but their area (probability) dies exponentially.

\[ \psi = \alpha \cosh \kappa x + \beta \sinh \kappa x \]

\[ \kappa = \pm \sqrt{\frac{2M}{\hbar^2} (V - E)} \quad (E < V) \] (11.4.10)

Fig. 11.4.2 Exponential waves \( \exp(-\kappa x) \) dying to the right

Generally \((E < V)\)-waves are hyperbolic sine-cosine combinations known as evanescent waves.
Phasors in evanescent waves have regions where their phase varies with $x$ so that they may communicate matter or energy through classically forbidden barriers in what is called a tunneling process. Tunneling paths between the quantum dots were hypothesized in Chapter 9. In Fig. 11.4.3, the relative phase between the two ends of a tunneling path may vary as shown in the following Chapter 12. The simple exponential waves in Fig. 11.4.2 have the same phase everywhere and therefore incapable of transmission.

Waves with above-barrier energy ($E>V$), such as in Fig. 11.4.1, curve toward the $x$-axis while the sub-barrier ($E<V$)-waves in Fig. 11.4.2-3 curve away from $x$. Grazing ($E=V$)-waves are straight lines.

(d) Schrodinger Wave Equations in momentum representation

The abstract time-independent Schrodinger eigenvalue equation (11.4.5) has the following form

$$
\mathbf{H}\varepsilon = E\varepsilon
$$

(11.4.11a)

based on the non-relativistic Hamiltonian or energy operator

$$
\mathbf{H}(q,p) = \mathbf{H}(x,p) = \frac{p^2}{2M} + V(x)
$$

(11.4.11b)

to give

$$
(p^2/2M + V(x))\varepsilon = E\varepsilon
$$

(11.4.11c)

where:

$$
p = \hbar \mathbf{k}
$$

is the momentum or $\hbar$ times the wavevector operator.

Now (11.4.11) in the momentum or wavevector-$k$ basis is found by $k$-completeness.

$$
\frac{\hbar^2}{2M} \langle k | k^2 | \varepsilon \rangle + \int dk \langle k | V(x) | k' \rangle \langle k' | \varepsilon \rangle = E \langle k | \varepsilon \rangle
$$

(11.4.12)

The kinetic term is very simple but the potential $V(x)$ requires an $x$-completeness expansion.

$$
\frac{\hbar^2}{2M} k^2 \langle k | \varepsilon \rangle + \int dk' \int dx \langle k | x | k' \rangle \langle x | V(x) | k' \rangle = E \langle k | \varepsilon \rangle
$$

(11.4.13a)

$$
\frac{\hbar^2}{2M} k^2 \langle k | \varepsilon \rangle + \int dk' \int dx V(x) \langle k | x | k' \rangle \langle x | \varepsilon \rangle = E \langle k | \varepsilon \rangle
$$

(11.4.13b)

Inserting transformation kernal $\langle x|k \rangle = e^{ikx}/\sqrt{2\pi}$ gives Schrodinger's integral eigen-equation.

$$
\frac{\hbar^2}{2M} k^2 \langle k | \varepsilon \rangle + \int dk' V(k-k') \langle k' | \varepsilon \rangle = E \langle k | \varepsilon \rangle
$$

(11.4.13c)

Here

$$
V(k-k') = \langle k | V(k') | k' \rangle = \frac{1}{2\pi} \int dx e^{-i(k-k')x} V(x)
$$

(11.4.13c)

is a Fourier transform of the potential operator $V(x)$. 
The momentum-space form of Schrödinger's equations is clearly more complicated unless the potential has a form that is easily Fourier transformed and simplifies the integral equation. The momentum representation becomes most useful for cases where the potential is isotropic or nearly so, that is, a constant almost everywhere. This is the situation in so-called scattering theory. More is said about this later when the \( k \)-equation returns with a vengeance of a jilted suitor in Chapter 16!

Many applications of Schrödinger equation involve a mass \( M \) hindered, trapped, or imprisoned in a more or less deep potential structure. This is the setting for the following chapter 12 that begins the saga of prisoner \( M \)! But first, some classical analogies will be discussed to help with physical intuition regarding differences between trapped, propagating, and evanescent waves.

### 11.5 Classical-Wave Analogies for Schrödinger equations

An analogy between 2-state quantum systems and two coupled pendulums was shown in Chapter 10. Now we generalize the mechanical analogy to show that \( N \)-state continuous wave systems if you have an infinite number of pendulums. As was the case for \( N=2 \), the correspondence is appropriate in the absence of complex \( C \)-type chiral or "gauge" couplings such as the Coriolis or cyclotron magnetic field effects discussed in Sec. 10.2c.

Classical (Newton's or Hamilton's) oscillator equations are second order (acceleration) differential equations in time \( (m \ddot{x} + K \cdot x = 0) \), while Schrödinger's equation \( (i\hbar \dot{\Psi} + H \cdot \Psi = 0) \) is first order in time. So the eigenvalues \( k_j \) of the classical \( K \)-spring matrix (divided by mass-\( m \) ) are squares of the eigenmode frequencies. Classical mode frequencies have a square root form \( \omega_j = \sqrt{(k_j/m)} \) as shown by comparing quantum frequencies \( (A\pm B) \) in (10.2.7a) to mode eigenfrequencies \( \sqrt{(A\pm B)} \) in (10.2.7b).

In contrast, the eigenvalues \( \varepsilon_j \) of the quantum Hamiltonian \( H \)-matrix (divided by Planck's \( \hbar \) ) are directly the eigenstate frequencies \( \omega_j = \varepsilon_j/\hbar \); no square root needed. The eigenvalues \( A\pm B \) in (10.2.7a) or \( H\pm S \) in (10.3.5) for \( C_2^B \)-symmetry \( (pE=0) \) are special cases of \( C_N \)-symmetry eigenvalues (9.3.5g).

\[
\hbar \omega_m = \varepsilon_m = H - 2S \cos(k_m a) \quad (11.5.1)
\]

These are eigenvalues of a the \( H \)-matrix in an \( N \)-by-\( N \) Schrodinger equation

\[
\begin{pmatrix}
\vdots \\
\langle 0 | \Psi \rangle \\
\langle 1 | \Psi \rangle \\
\langle 2 | \Psi \rangle \\
\langle 3 | \Psi \rangle \\
\langle 4 | \Psi \rangle \\
\vdots \\
\end{pmatrix}
= \frac{i\hbar}{\partial t}
\begin{pmatrix}
\vdots \\
\langle 0 | \Psi \rangle \\
\langle 1 | \Psi \rangle \\
\langle 2 | \Psi \rangle \\
\langle 3 | \Psi \rangle \\
\langle 4 | \Psi \rangle \\
\vdots \\
\end{pmatrix}
\begin{pmatrix}
\hat{H}
\end{pmatrix}
\]

(11.5.2a)

We let \( H=2S \) so the right hand side becomes \(-S \) times the \( \Delta^2 \) difference operator (11.2.11) in a matrix version of Schrödinger's wave equation with zero potential \( (V(x)=0) \). Recall that \( \lim_{a \to 0} \frac{\Delta^2 \psi}{a^2} = \frac{\partial^2 \psi}{\partial x^2} \).

\[
\begin{align*}
\frac{\partial \Psi(x,t)}{\partial t} & = -\hbar \frac{\partial^2 \Psi(x,t)}{2M \partial x^2}, \text{where: } S = \frac{\hbar^2}{2Ma^2} \\
\end{align*}
\]

(11.5.2b)

This relates the tunneling parameter \( S = \hbar^2/(2Ma^2) \) to mass \( M \), \( \hbar \), and inter-pendulum lattice space \( a=L/N \).
(a) Classical wave equation: “Phonon-like” to “photon-like” dispersion

In contrast, the classical wave equation with phase velocity \( C \) has a second order time derivative.

\[
\frac{\partial^2 Y}{\partial t^2} = sa^2 \nabla^2 Y
\]

\[\rightarrow \quad \frac{\partial^2 Y(x,t)}{\partial t^2} = C^2 \frac{\partial^2 Y(x,t)}{\partial x^2}, \quad \text{where: } s = \frac{k_{12}}{m} = \frac{C^2}{a^2} \quad (11.5.3a)
\]

The finite-difference-matrix form is Newton's equations for \( N \)-coupled mass-\( m \) oscillators or \( N \) gravity-free pendulums of inertia \( m \) connected by springs of constant \( k_{12} \) where \( k_{12}/m = s = C^2/a^2 \).

\[
\begin{align*}
\frac{\partial^2}{\partial t^2} & \begin{pmatrix}
\langle 0|Y \\
\langle 1|Y \\
\langle 2|Y \\
\langle 3|Y \\
\langle 4|Y \\
\vdots
\end{pmatrix} \\
& = C^2 \begin{pmatrix}
2s & -s & 0 & 0 & 0 & | 0|Y \\
-s & 2s -s & 0 & | 1|Y \\
0 & -s & 2s -s & | 2|Y \\
0 & 0 & -s & 2s -s & | 3|Y \\
0 & 0 & 0 & -s & 2s -s & | 4|Y \\
\vdots
\end{pmatrix}
\end{align*}
\quad (11.5.3b)
\]

The classical pendulum mode eigenfrequencies are the square roots of quantum \( \omega_m \) in (11.5.1) and give what is called a phonon dispersion relation between frequency and wavevector.

\[
\omega_m = \sqrt{2s \cdot 2s \cos \left( \frac{k_m a}{a} \right)} = 2 \sqrt{s} \frac{\sin \left( \frac{ka}{a} \right)}{2} \rightarrow \sqrt{s} |ka| \quad (11.5.3c)
\]

Fig. 11.5.1 is a plot of the phonon dispersion. For low \( k \) (|\( ka | << \pi \)), \( \omega_m(k) \) is linear in wavevector \( k \). Wave phase and group velocity of long-wavelength phonons are constant, like photons, but slower. \( (C << c) \)

\[
\frac{\omega_m}{k} \rightarrow \sqrt{s} |a| = \left| \frac{C^2}{a} \right| |a| = C \quad (11.5.3d)
\]

A \( k=-1 \) wave for \( N=12 \) pendulums at time \( t = 0 \) is plotted above the dispersion function. Twelve phasors, one for each mass, point to successive clock positions of 12 PM, 1 PM, 2 PM, ..., all the way around to 11 PM at the 11-th phasor. The pendulum displacement coordinate is the real part Re\( Y(x_p,t=0) \) and is indicated by dots and a cosine wave. A ring of dots shows a top view of the swinging pendulum masses. They are constrained to move only radially normal to their supporting ring. Each phasor is \( 30^\circ \) ahead of its neighbor to the left, so the wave is a 100% left-moving \((k=-1)\)-mode.

\[
\omega = \frac{2c \sin ka}{a} \quad \text{low-}k \text{ phase velocity } c=\text{const.} \\
\text{low-}k \text{ group velocity } c=\text{const.}
\]

Fig. 11.5.1 Phonon dispersion for \( N = 12 \) classical coupled-oscillators. Mode has wavevector \( k=-1 \).
(b) Classical gravity-waves: “Exciton-like” dispersion

The diagonal constant $H$ in the Schrödinger equation sets the zero-value of the energy and frequency but has no observable effect in quantum experiments. (Remember: overall phase cancels out of $\Psi^*\Psi$.) Adding $H$ to each diagonal element $2S$ shifts all eigenfrequencies upward together. But, since only differences (beats) between eigenfrequencies are observable, this change does not affect wave dynamics.

However, adding an $H$ to the classically analogous problem has a very great effect. It is equivalent to adding gravitational restoring acceleration $H = g/\ell$ to each classical pendulum which previously had only a restoring term $2k_{12}/m = 2s$ due to its two neighbors on either side. This changes their wave behavior entirely. It is first noticed in the eigenfrequencies because they are square roots of the force $K$-matrix eigenvalues. In place of (11.5.3c) we now have the following general "exciton" dispersion relation. At low wavevector $k \sim 0$, this resembles Bohr-Shrödinger dispersion $\omega \sim k^2$,

$$\omega_m = H + 4s \sin^2 \left(\frac{k_m a}{2}\right) \approx \sqrt{H + \frac{sa^2}{2H}} k_m^2 + . . . \quad (11.5.4a)$$

An example is plotted in Fig. 11.5.2 and should be compared to the phonon example in Fig. 11.5.1. An obvious new feature is a forbidden frequency gap of $\sqrt{H} = \sqrt{g/\ell}$ at $k = 0$. There the phase velocity is infinite. Phase velocity is not so ignorable a part of classical dynamics as it is for quantum waves!

$$\omega = \left(H + 4s \sin^2 ka\right)^{1/2}$$

Forbidden frequency gap $= \sqrt{H}$

The wave will not propagate in the gap where frequency is less than the individual frequency $\sqrt{(g/\ell)}$ of each uncoupled pendulum. This is true regardless of how strong we make the coupling $s = k_{12}/m$, the gap depends on the value of the local pendulum frequency $\sqrt{H} = \sqrt{g/\ell}$ only.

The low-$ka$ ($ka << \pi$) approximation to the gravity pendulum's dispersion function is the following

$$\omega_m = \sqrt{H + 4s \sin^2 \left(\frac{k_m a}{2}\right)} \equiv \sqrt{H + \frac{sa^2}{2H}} k_m^2 \quad (11.5.4b)$$

This has the same hyperbolic form as the waveguide dispersion function (6.3.5b) (Recall Fig. 6.3.2.)

$$\omega = \sqrt{c^2 k^2 + \omega_{\text{cutoff}}^2} \quad (6.3.5b)\text{repeated}$$

Each approximates the relativistic dispersion function (5.2.8) and the Bohr $\omega \sim k^2$, as in Fig. 11.5.3.
Relativistic Schrodinger Quantum System

\[ \frac{E}{\hbar} = \omega_{\text{rel}} = \sqrt{\left(\frac{Mc^2}{h}\right)^2 + \left(ck\right)^2} \]

\( k \ll Mc \Rightarrow \frac{Mc^2}{h} + \frac{hk^2}{2M} + ... \)

(a) Relativistic Dispersion

Classical Curtain of Coupled Pendulums

\[ \omega_{\text{curtain}} = \sqrt{(\omega_{\text{local}})^2 + 4s \sin^2 \frac{ka}{2}} \]

\( ka < \pi \Rightarrow \omega_{\text{local}} + \frac{s a^2 k^2}{2\omega_{\text{local}}} + ... \omega_{\text{local}} = \sqrt{\frac{g}{l}} \)

(b) Classical Curtain Dispersion

Fig. 11.5.3 Analogous dispersion functions at low k-values

(c) Shower-curtain model of Schrodinger equation

As stated in (5.2.5a) the cutoff or proper frequency \( \mu \) for a matter wave to propagate is related to its rest energy \( mc^2 \), that is \( \mu = \omega_{\text{cutoff}} = mc^2/h \). For the waveguide \( \omega_{\text{cutoff}} \) is related to the waveguide width \( W \): \( \omega_{\text{cutoff}} = \pi c/W \). For the coupled pendulums \( \omega_{\text{cutoff}} \) is equal to Galileo's pendulum frequency \( \omega_{\text{cutoff}} = \sqrt{H} = \sqrt{(g/l)} \). A wave below \( \omega_{\text{cutoff}} \) is evanescent and suffers exponential extinction away from its source. Suppose you grab a big stage curtain or a weighted shower curtain as sketched in Fig. 11.5.4. Swinging it back and forth slowly only moves the portion of the curtain closest to your hand; the response nearby is in phase with your hand but its amplitude dies off exponentially with distance as shown in Fig. 11.5.4a. (Note: The view here is, as usual, looking up from underneath the hanging pendulums or curtain.)

Fig. 11.5.4 Curtain motion around \( \omega_{\text{cutoff}} = \omega_{\text{local}} = \sqrt{g/l} \) (a) Below \( \omega_{\text{cutoff}} \), (b) At \( \omega_{\text{cutoff}} \), (c) Above \( \omega_{\text{cutoff}} \).
However, if you wiggle with frequency at or above $\omega_{\text{cutoff}} = \sqrt{g/\ell}$ you will make waves go as far as the curtain extends! At resonance frequency $\omega_{\text{cutoff}}$ the entire curtain will swing rigidly as shown in Fig. 11.5.4b. Above $\omega_{\text{cutoff}}$ the waves may propagate as in Fig. 11.5.4c, if your wiggle phase-lag is small.

To simulate a non-uniform potential $V(x)$ of a Schrodinger equation, we may vary the local frequency of each oscillator, that is, vary with $x$ of the pendulum lengths $\ell$ with position, that is pendulum length $\ell(x)$ goes up or down depending on location $x$ of the pendulum. The bottom edge of the curtain rises as $\ell$ is shortened in proportion to the value $V(x)$ of a potential barrier as sketched below in Fig. 11.5.5. In other words, higher $V(x)$ means higher local frequency $V(x)/\hbar$ which is modeled by shorter pendulum length $\ell(x)$ as sketched in Fig. 11.5.5b. Shorter $\ell$ means higher local frequency $\omega_{\text{local}} = \sqrt{g/\ell}$.

(a) Non-uniform potential... ANALOGOUS TO... (b) Non-uniform curtain...

Fig. 11.5.5 Schrodinger-curtain analogy (a) Potential barriers, (b) Equivalent curtain segments.

The Schrodinger-curtain analogy requires $ka << 1$ (Wavelength is much longer than inter-pendulum spacing $a$) as given by the corresponding dispersion relations above Fig. 11.5.3.

$$E - V = \frac{p^2}{2M} = \frac{\hbar^2 k^2}{2M}$$

$$\hbar \omega = E + V + \frac{\hbar^2 k^2}{2M}$$

(11.5.5a)

$$\omega - \omega_{\text{local}} = \frac{sa^2 k^2}{2\omega_{\text{local}}}$$

$$\omega = \omega_{\text{local}} + \frac{k^2}{2W}$$

$$k = \sqrt{2W \left( \omega - \omega_{\text{local}} \right)}$$

where $W = \frac{\omega_{\text{local}}}{sa^2}$

(11.5.5b)

Potential $V(x)$ or the analogous pendulum length $\ell(x)$ varies with $x$, but the factor $W = \sqrt{g/s^2 a^4 \ell}$ remains constant throughout. The $W$-factor is related to the Schrodinger mass factor $M/\hbar^2$ that is constant for all $x$. (The lattice spacing $a$ or spring coupling constant $s$ could vary in such a way to keep $W$ constant.)

This analogy helps to clarify the extinction effect of a barrier on a wave whose energy $E = 0.98$ is below the center barrier top $V_2 = 1.00$ in Fig. 11.5.5a but above the left or right hand plateau potentials $V_1 = 0.91$ or $V_3 = 0.96$. The analogous pendulaum system in Fig. 11.5.5b is oscillating at a frequency $\omega = 0.98$ (Planck scale factor $h$ relates the analogous systems) which is high enough to support wave propagation everywhere except in the $\omega_{\text{local}}$ barrier region where all the pendulums have a higher local frequency $\omega_{\text{local}} = 1.00$ which prevents them from responding enthusiastically to $\omega < 1$. Only evanescent waves (Recall Fig. 11.4.3.) are possible inside the barrier at frequency $\omega = 0.98$.

Difference-differential Schrodinger's equations with variable potential $V(x)$ follow from (11.2.11).
An energy operator is made from operator substitutions (11.3.10) as in the "crummy derivation" (5.4.10).

This equation was first presented by Schrodinger, Klein, and Gordon in 1926-1928 as a relativistic wave equation:

\[ \frac{\partial^2 \Psi(x,t)}{\partial t^2} = \frac{-\hbar^2}{2Mm} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) \] (11.5.6a)

Here the tunneling parameter \( S \) is the same as before. (Recall (9.3.11) and discussion of "effective" mass.)

\[ S = \frac{\hbar^2}{2Ma^2} \] (11.5.6b)

The matrix form has diagonal terms \( V_p \) at each discrete position \( x_p \) to approximate \( V(x) \) by \( V_p = V(x_p) \).

\[
\begin{bmatrix}
\langle 0 | \Psi \rangle \\
\langle 1 | \Psi \rangle \\
\langle 2 | \Psi \rangle \\
\langle 3 | \Psi \rangle \\
\langle 4 | \Psi \rangle \\
\vdots
\end{bmatrix}
\begin{bmatrix}
\frac{\partial \Psi}{\partial t} = i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2Mm} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi(x)
\end{bmatrix}
\]

It is instructive to compare the above with classically coupled pendulum equations,

\[
\frac{\partial^2 Y(x,t)}{\partial t^2} = \left( \frac{1}{2a^2} \right) \left( \frac{1}{2a^2} \right) K \right) Y \}
\]

\[
\frac{\partial^2 Y(x,t)}{\partial t^2} = C^2 \frac{\partial^2 Y(x,t)}{\partial x^2} + K(x)Y(x,t), \] (11.5.7a)

for \( N \)-coupled pendulums of inertia \( m \) connected by springs of constant \( k_{12} \) where, as before:

\[
k_{12}/m = s = C^2/a^2.
\] (11.5.7b)

\[
\begin{bmatrix}
\langle 0 | Y \rangle \\
\langle 1 | Y \rangle \\
\langle 2 | Y \rangle \\
\langle 3 | Y \rangle \\
\langle 4 | Y \rangle \\
\vdots
\end{bmatrix}
\begin{bmatrix}
\frac{\partial^2 Y(x,t)}{\partial t^2} = \left( \frac{1}{2a^2} \right) \left( \frac{1}{2a^2} \right) K \right) Y \}
\]

Spring term \( 2s \) adds to local Galilean gravity restoring acceleration \( K_p \) of each pendulum at point \( x=x_p \).

\[
K_p = k_p/m = g/l_p = K(x_p)
\] (11.5.7d)

(d.) Klein-Gordon equations: Relativistic dispersion?

If \( K(x) \) and \( K_p \) are set equal to proper frequency \( \mu^2=(mc^2)/h \) there results the **Klein-Gordon equation**.

\[
\frac{1}{c^2} \frac{\partial^2 Y(x,t)}{\partial t^2} = \frac{\partial^2 Y(x,t)}{\partial x^2} - \left( \frac{mc^2}{h} \right)^2 Y(x,t) \]

(11.5.8)

This equation was first presented by Schrodinger, Klein, and Gordon in 1926-1928 as a relativistic wave equation obtained from the energy momentum invariant (5.2.7).

\[
E^2 - c^2 p \cdot p = E^2 - c^2 p^2 = (mc^2)^2
\]

(5.2.7)repeated

An energy operator is made from operator substitutions (11.3.10) as in the "crummy derivation" (5.4.10).
So far, we have only dealt with zeroth and second Real constant coefficients.

Corresponding 

\[
\frac{\hbar}{i} \frac{\partial}{\partial \tau} = \frac{\hbar}{i} \nabla, \quad \frac{E}{c} \to \frac{\hbar}{c} \frac{\partial}{\partial t}, \quad \left( \frac{E}{\hbar} \right)^2 = \frac{c^2}{\hbar^2} \left( \frac{m c^2}{\hbar} \right)^2 \to \frac{-1}{c^2 \frac{\partial^2}{\partial t^2}} = -\nabla^2 + \left( m c^2 \right)^2 \]

It was proposed to add to this equation a non-constant potential \( V(x) \) energy as in the following.

\[
\frac{\hbar^2}{c^2} \frac{\partial^2 Y(x,t)}{\partial t^2} = \hbar^2 \frac{\partial^2 Y(x,t)}{\partial x^2} + \left( m c^2 + V \right)^2 Y(x,t)
\]

Such a scheme is flawed. A scalar potential \( V(x) \) can never be relativistically invariant, but must accompany an appropriately defined vector potential \( \mathbf{A}(x) \). Then the quantity \( V^2 - c^2 \mathbf{A}^2 \) is a relativistic invariant as in the case of electromagnetic theory. Vector potential \( \mathbf{A}(x) \) is introduced in Chapter 17.

(e) **“Hyper” Schrodinger equations and hyper-dispersion**

A general \( C_\lambda \)-symmetric “quantum-dot” Hamiltonian described in Chapter 9 (Recall (9.2.7) has tunneling amplitudes \(-S, -T, -U\), and so forth, from each point to neighboring points \( I, 2, 3, \ldots, N-1 \) steps away. Examples of \( STU\ldots \) “hyper-connectivity” are sketched in Fig. 9.2.1 and in Fig. 11.5.6 below.

Fig. 11.5.6 Hyper-connecting tunneling amplitudes and examples for \( N=8 \) quantum dot structure.

\[
\begin{bmatrix}
\vdots \\
\langle 0 | \Psi \rangle \\
\langle 1 | \Psi \rangle \\
\langle 3 | \Psi \rangle \\
\langle 4 | \Psi \rangle \\
\vdots \\
\end{bmatrix}
\begin{bmatrix}
\frac{i \hbar}{\partial t} \\
\end{bmatrix}
\begin{bmatrix}
\vdots \\
\langle 0 | \Psi \rangle \\
\langle 1 | \Psi \rangle \\
\langle 2 | \Psi \rangle \\
\langle 3 | \Psi \rangle \\
\vdots \\
\end{bmatrix}
= 
\begin{bmatrix}
\ddots \\
\ddots & -S & -T & -U \\
-\frac{1}{c^2} \nabla^2 & \ddots & -S & -T \\
-\frac{1}{c^2} \nabla^2 & \ddots & -S & -T \\
-\frac{1}{c^2} \nabla^2 & \ddots & -S & -T \\
\vdots & \ddots & -S & -T \\
\end{bmatrix}
\]

(11.5.10a)

If \( S, T, U, \ldots \) are real, discrete \( \Delta^k \) difference operators (11.2.24) could combine to give the matrix above.

\[
\frac{i \hbar}{\partial t} \frac{\partial \Psi}{\partial t} = \left( \delta_0 - \delta_2 \Delta^2 - \delta_4 \Delta^4 - \delta_6 \Delta^6 - \ldots \right) \Psi
\]

(11.5.10b)

Corresponding \( C_{\infty} \)-symmetric continuum differential equations involve a combination of higher order \( x \)-derivatives. **Bilateral** \( B \)-type symmetry (Sec. 10.2b) has real \( S, T, U \) and only even-order derivatives.

\[
\frac{i \hbar}{\partial t} \frac{\partial \Psi(x,t)}{\partial t} = d_0 \Psi(x,t) + d_2 \frac{\partial^2 \Psi(x,t)}{\partial x^2} + d_4 \frac{\partial^4 \Psi(x,t)}{\partial x^4} + d_6 \frac{\partial^6 \Psi(x,t)}{\partial x^6} + \ldots
\]

(11.5.10c)

Real constant coefficients \( d_k \) of derivatives are functions of tunnneling amplitudes \( STU\ldots \) and vice-versa. So far, we have only dealt with zeroth and second \( x \)-derivatives in the standard Schrodinger equation.
If potential \( V \) is constant, the dispersion function reduces to a quadratic (Bohr-ring!) \( \omega = (\hbar^2 / 2M)k^2 \).

If connectivity is \( C_\infty \)-symmetric so all \( S, T, U, \ldots \) or \( \delta_1, \delta_2, \delta_3, \ldots, \) or \( d_1, d_2, d_3, \ldots \) are independent of \( x \) or \( x_p \), then \( \Psi = e^{ikx} \) will be eigenfunctions for all \( d_k \) or \( d_k \). Real \( S, T, U, \ldots \) give \( B \)-type symmetry and \( B \)-\( \delta \)-hyperconnectivity allows us to make any even dispersion function \( (\omega_{m-n}(k)=\omega_{m}(k)) \). (Recall making revival Hamiltonians \( (9.4.6) \) where the objective was to recover a Bohr-ing \( \omega \sim k^2 \) dispersion.) Here, putting \( \Psi = e^{ikx} \) into the hyper-Schrodinger equation \( (11.5.10d) \) yields \( \omega(k) \) as a power series in \( k \).

\[
\omega(k) = d_0 + d_2 k^2 + d_4 k^4 + d_6 k^6 + \ldots \quad (11.5.10e)
\]

Equivalently, a quantum-dot equation yields \( \omega_{m}(k_m) \) as a Fourier cosine series \( (9.3.5d) \) in \( k_m \).

\[
\omega_m = H + 2|S| \cos(k_m a) + 2|T| \cos(2k_m a) + 2|U| \cos(3k_m a) + \ldots \quad (11.5.10f)
\]

In the high-\( N \) and low-\( k \) limit, the series \( (e) \) and \( (f) \) should converge on the same dispersion function.

Complex tunneling amplitudes \( S, T, U, \ldots \) correspond to \( C \)-type symmetry (Sec. 10.2c) and give anti-symmetric Hamiltonian matrix components and asymmetric dispersion functions. \( (\omega_{m-n}(k)=\omega_{m}(k)) \)

Cosine series are not sufficient. Complex \( e^{ikm\alpha} \) Fourier series dispersion functions \( (9.3.5c) \) arise.

\[
\hbar \omega_m = H + S e^{ikm\alpha} + S^* e^{ikm\alpha} + T e^{ikm\alpha} + T^* e^{ikm\alpha} + U e^{-ikm\alpha} + \ldots \quad (11.5.11)
\]

This has odd (sine) terms which give odd powers of \( k \) in the continuum dispersion function.

\[
\omega(k) = d_0 + d_2 k^2 + d_4 k^4 + d_6 k^6 + \ldots \quad (11.5.12)
\]

A \( C \)-type hyper-Schrodinger equation has odd-order derivatives. \( (Odd-k \ d_k \ are \ imaginary \ so \ H^\dagger = H.) \)

\[
\hbar \frac{\partial \Psi(x,t)}{\partial t} = d_0 \Psi(x,t) + d_1 \frac{\partial \Psi(x,t)}{\partial x} + d_2 \frac{\partial^2 \Psi(x,t)}{\partial x^2} + d_3 \frac{\partial^3 \Psi(x,t)}{\partial x^3} + d_4 \frac{\partial^4 \Psi(x,t)}{\partial x^4} + \ldots \quad (11.5.13)
\]

A first order Schrodinger derivative term arises from an electromagnetic vector potential \( A \).

\[
\hbar \frac{\partial \Psi(x,t)}{\partial t} = V \Psi(x,t) + \frac{\hbar^2}{2M} (p-eA)^2 \Psi(x,t)
\]

\[
= \left( V + \frac{\epsilon^2 \hbar^2}{2M} A^2 \right) \Psi(x,t) - i \frac{\hbar^2}{M} A \cdot \frac{\partial \Psi(x,t)}{\partial x} + \frac{\hbar^2}{2M} \frac{\partial}{\partial x} \frac{\partial \Psi(x,t)}{\partial x} \quad (11.5.14)
\]

The canonical electromagnetic momentum \( (p-eA) \) will be discussed in Chapter 17. This is a first step toward putting quantum theory back into its natural relativistic setting. (However, treating time as a separate parameter, as in any of these Schrodinger equations, can never yield fully relativistic theory.)

With no translation or \( C_x \)-symmetry, each coefficient \( d_k \), starting with \( d_0 = V(x) \), may be a function of \( x \). Having such \( asymmetric \) or \( A \)-type symmetry (Sec. 10.2a) destroys a Fourier-symmetry based dispersion \( (11.5.12) \). \( A \)-eigenfunctions localize or “puddle” around potential anisotopy due to \( d_0 = V(x) \) or kinetic anisotropy due to \( d_1 = -i(\hbar^2 / 2M)A(x) \) or higher kinetic \( d_k(x) \)-hyper-connectivity terms in \( (11.5.13) \).

In curved \((q_1, q_2, \ldots)\) coordinates, Schrodinger equations will have coordinate-\( q \)-dependent connectivity terms \( d_{k,l,\ldots}(q_m) \). Generally, these are restricted to second order \((k+l=2)\).
\[ i \hbar \frac{\partial \Psi(q_m, t)}{\partial t} = \sum_{k,l} d_{k,l} \frac{\partial^{k+l} \Psi(q_m, t)}{\partial q_k \partial q_l} \]

(11.5.15)

The two state systems avoid consideration of hyper-connectivity by having only nearest neighbors! So an \((N=2)\)-state mechanical analogy is much simpler than any of the Schrodinger equations or their discrete matrix versions considered above. The \(ABCD\) analogy for an \((N>2)\)-level system does not simply reduce to difference or differentials that are only second-order-in-\(x\). (See exercise 11.5.2.)
Problems for Chapter 11

Topology slopology

11.1.1. The Discrete Bloch Problem is the name we chose for a \( C_N \) “qudot” system. By changing number \( N \) of dots and lattice spacing \( a \) between them it is possible to approach each of the other three cases in Fig. 11.1.1.

Do so for each case (CBI) Continuous Bloch, (DBo) Discrete Bohr, and (CBo) Continuous Bohr.

Recycled differences

11.2.1. The differential-difference operators \( \Delta \) in (11.2.24) can be written so they apply to a cyclic \( C_N \) ring of \( N \)-qudots.

The key idea is that all such operators be invariant to \( C_N \) symmetry operator powers \( r^p \).

(a) Construct matrix \( \Delta \) for \( q=1 \) and \( N=6 \) so \( \Delta = (r^{q-1} - r)2 \) with \( r^2 = r^5 \) defined in discussion of \( C_6 \) after (8.1.5).

(b) Write the matrix for \( \Delta^2 \), that is \( \Delta \) for \( q=2 \). Is this definition consistent in that \( (\Delta^2)j^2 = \Delta^2 ? \)

(c) Derive similar \( N=6 \) matrix “derivatives” \( \Delta^q \) for \( q=3-6 \).

(d) Instead define \( \Delta^2 \) as in (11.2.26) and express it in terms of \( r^p \) from \( C_6 \). What \( \Delta^q \) matrices result from powers?

(e) Using results of (d) write Hamiltonian \( H \) in (9.2.7) in terms of \( \Delta^q \). Write as a “differential” equation (9.3.5b).

What adjoint

11.2.2. Consider a driven (by \( a(t) \)), damped (by \( \Gamma \)), harmonic (frequency \( \omega_0 \)) oscillator equation.

\[
H \cdot x = a \quad \text{or:} \quad H \cdot x(t) = \left( \frac{d^2}{dt^2} + 2\Gamma \frac{d}{dt} + \omega_0^2 \right) x(t) = a(t)
\]

(a) Under what conditions, if ever, is operator \( H \) self adjoint? Derive adjoint operator \( H^\dagger \).

(b) Find Green’s function such that \( H \cdot G(t) = \delta(t-0) \) or \( H \cdot G = 1 \).

(c) Represent equations in frequency basis (Fourier transform) and give frequency representation of \( G \). Hint: See Appendix 1.B.

\[
x \text{ Commute per } x
\]

11.3.1. Consider expressions and effects of the commutator \( C = [x, p] = xp - px \) or \( C/h = [x, k] = xk - kx \)

(a) Derive the coordinate representation of the operator \( C \) and apply it to a function \( \psi(x) \). Discuss.

(b) Derive the momentum representation of the operator \( C \) and apply it to a function \( \psi(p) \). Discuss.

Boosts and Roosts

11.3.2. We have noted that energy operator \( H \) is a generator of time translation or evolUtion operator \( U = \exp(-iHt) \). What do other operators such as \( x \) and \( p \) generate? (Here we take \( h = 1 \))

(a) Apply operator \( T = \exp(-ip\alpha) \) to a function \( \psi(x) \) of coordinate \( x \). Check for case of plane wave \( \psi(x) = e^{ikx} \).

(b) Apply operator \( B = \exp(ix\beta) \) to a function \( \psi(p) \) of momentum \( p = k \). Check for case of plane wave \( \psi(p) = e^{ikx} \).

Dying to keep the phase

11.4.1. Exponential and evanescent waves keep time (phase) differently as shown in Fig. 11.4.2-3.

(a) Consider an exponential “right-dying” plane wave \( \psi(x,t) = e^{ikx-i\alpha t} \). Are its phasors synchronized at each \( t \)?

(b) Consider an evanescent “growing-dying” plane wave \( \psi(x,t) = Ae^{ikx-i\alpha t} + Be^{-ikx+i\alpha t} \). Can its phasors be synchronized? For what \( A \) or \( B \)? Write the wave as a combination of hyper-cosine and hyper-sine functions.

(c) Consider the 50-50 cases of the “growing-dying” wave in (b). Derive “expo-hyperine” identities analogous to the expo-cosine or expo-sine identities used in Chapter 4.

Getting hyper

11.5.1. Compare qudot equations (11.5.10a), difference-eqs. (11.5.10b) and hyper Schrodinger eqs. (11.5.10c).

(a) Derive coefficients \( \delta_\epsilon \) in terms of \( S, T, \) and \( U \) and vice-versa.

(b) Derive coefficients \( \delta_k \) in terms of \( S, T, \) and \( U \) and vice-versa.

(c) Compare resulting dispersion relations (11.5.10e) and (11.5.10f). Relate them in the high-N-low-k limit.
Getting more hyper

11.5.2. Generalize the ABCD analogy in Ch. 10 between 2-state Schrodinger and 2-pendulum Hamilton equations.

(a) Write a general N-state Schrodinger equation (N=3 or 4 is a start) as real equations as in (10.1.2).
(b) Find a classical Hamiltonian would give the real equations (a).
(c) For an all real quantum Hamiltonian (Zero C-type components) find the Newton’s equations as in (10.1.5).
(d) Show how C<sub>N</sub> symmetry would simplify the results of (a-c).
(e) Write (a)-(d) equations as difference and differential equations as done, for example, in (11.5.10).

Curtain Call

11.5.3. This problem relates to the analogy between classical coupled pendulums and quantum waves which are evanescent or propagating. Suppose a curtain stretched by a tension of 1N across a 10 meter stage, connects a thousand loosely connected lead weights each hanging from the ceiling 9.8 meters above. (First, show that classical coupled pendulum equations give an approximate dispersion function of the form: \( \omega(k) \sim \omega_{\text{CUT}} + Ak^2 \).)

(a) You are holding one end while your partner stage-hand is at the other. You notice that if you swing your end at precisely \( \omega = 2 \text{ (radian)/sec.} \), the resulting waves take exactly 5 seconds to cross the stage to your partner who absorbs them. (Does this give \( V_{\text{phase}} \) or \( V_{\text{group}} \)? Explain. Note the word “precisely”.) Use this to find \( A \) and \( \omega_{\text{CUT}} \) in numeric dispersion formula and related formulas for the group and phase velocities and wave length as a function of angular frequency \( \omega \). Give the numerical values for these quantities for \( \omega = 1.0, 1.5, 2.0 \) and 3.0.
(b) Suppose you gently pull your end of the curtain toward the audience and hold it at one meter from its resting point. Describe the curve the curtain makes and tell how much of the curtain has been pulled more than 5 cm. from its resting point. \( e^{-2} = 0.05 \).
(c) If you gently swing your end at a steady frequency \( \omega \) with a 1 meter amplitude, what is the smallest frequency \( \omega \) needed to cause at least a 5 cm. swing amplitude at the location of your partner on the other side.