Eur. J. Phys. **23** (2002) 513–522 PII: S0143-0807(02)35666-6

The maze of quantum mechanics

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Received 9 April 2002, in final form 19 June 2002
Published 8 August 2002
Online at stacks.iop.org/EJP/23/513

Abstract

Students can explore quantum mechanics with a concept map that uses only the most elementary solutions to Schrödinger's equation. The content has been slightly modified from the traditional introduction to the subject because the issue of interpretation is postponed until Parseval's theorem is reached and used to postulate two fundamental equations of probability, simultaneously. A set of canonical but approximate equations can describe wavepacket motion for most linear waves. If restricted to certain special cases, these equations of wavepacket motion are easily derived and can serve as a temporary substitute for Ehrenfest's theorem. A number of exercises can be incorporated into this maze of quantum mechanics.

1. The map of quantum mechanics

If the primary bold-faced paths are followed, figure 1 depicts a concept map designed to help students organize the basic concepts of quantum mechanics [1]. The secondary paths, not bold-faced, can convert this into a bewildering maze that investigates why the theory is constructed as it is. Both the map and maze begin at the bold-faced box labelled '*Schrödinger's equation*'. Three exits are also shown as bold-faced boxes. The primary paths lead to two of these exits. The first concludes at the box labelled '*eigenfrequency represents energy*'. The second exit, in the lower left corner, normalizes the wavefunction, and also states equations of probability for energy, $P(E_n)$, and position, $P(x)\,\mathrm{d}x$. The third exit cryptically summarizes these equations in Dirac notation and cannot be reached without following the secondary paths. Two rules govern the paths of both map and maze. First, an exit is not fully mastered until all possible paths leading to it are understood. Second, one should refrain from using a concept until it has been encountered in the map. This requires that some topics be revisited after they have first been encountered.

We illustrate both rules with a tour of the map's bold-faced paths. Temporarily set aside all understanding of quantum mechanics gained *a priori* except for the insight that atomic spectral lines are associated with photon emission and absorption caused by transitions between atomic energy levels. Thus it is understood that $\hbar\omega = \Delta E$, where $\Delta E = E_n - E_m$. While this is a theoretical construction of quantum mechanics, experimental verification is essential. Therefore, experimental facts [2], such as the photoelectric effect, Compton scattering and

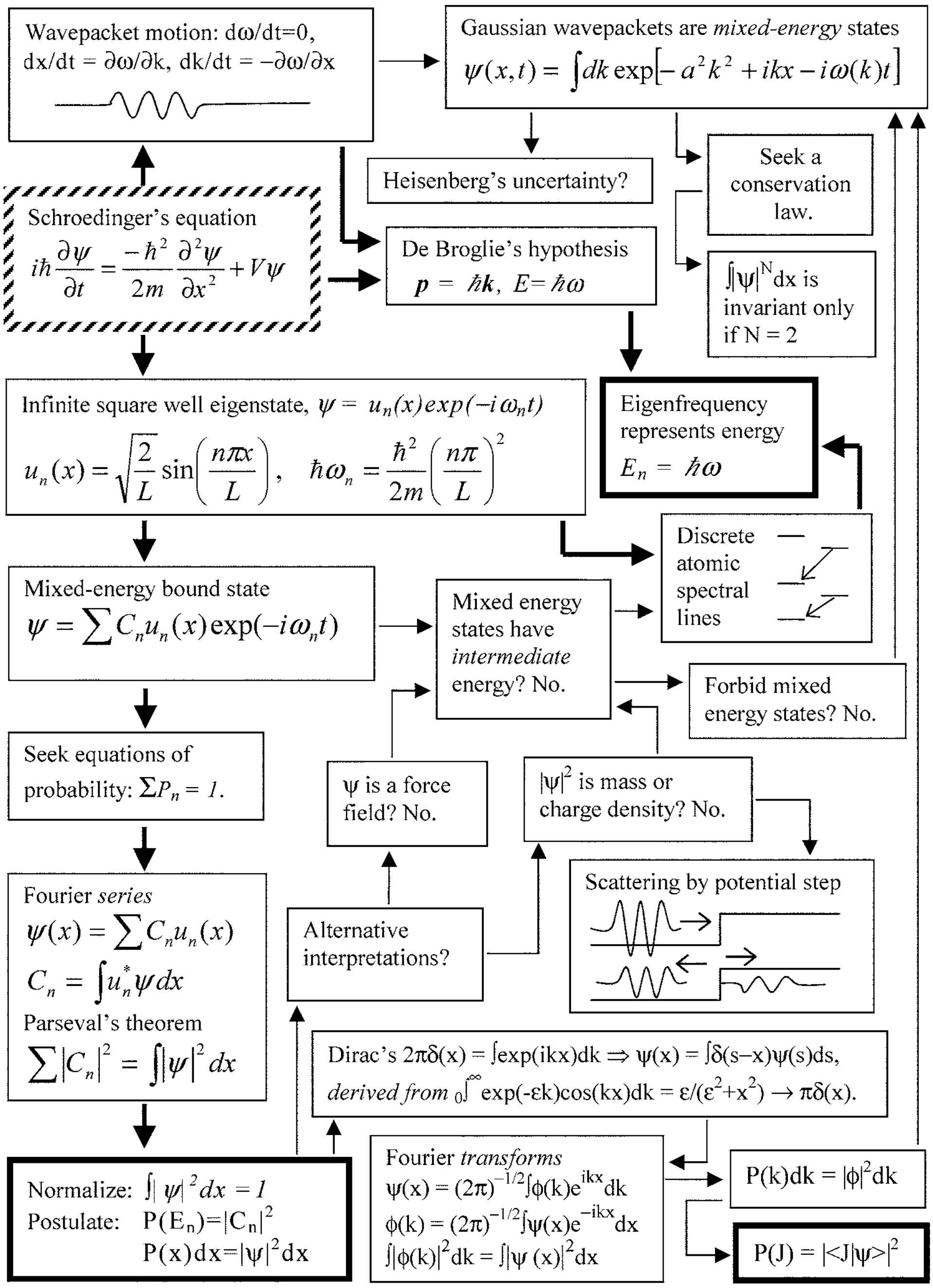

Figure 1. To convert this maze into a map, follow only the bold-faced arrows.

electron diffraction, might also be kept in mind, but not yet organized into a comprehensive theory. We seek to modify or replace Newtonian physics with a linear wave theory.

Begin with the box in figure 1 labelled *Schrödinger's equation* and enter the *infinite square well eigenstate*, $\psi(x, t) = u_n(x)\exp(-i\omega_n t)$, where $u_n = (2/L)^{1/2}\sin(n\pi x/L)$. The normalization constant has no significance or importance here and can only be justified on the grounds that it will later prove useful. The spectrum of eigenfrequencies associated with these solutions to Schrödinger's equation seems to explain the discrete nature of experimentally observed atomic spectral lines. Thus we complete our first path at the exit *eigenfrequency represents energy*. Two other primary paths to this same exit must also be mastered. Substitution of a plane wave, $\exp(\mathrm{i}kx - \mathrm{i}\omega t)$, into Schrödinger's wave equation yields a dispersion relation, $\omega = \omega(x, k)$:

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V(x). \tag{1}$$

Strictly speaking, the plane wave is a solution only if V is independent of x. In that case, substitution into (1) of de Broglie's relations, $E = \hbar\omega$ and $p = \hbar k$, recovers a statement of energy conservation. We now have a theoretical plausibility argument for de Broglie's hypothesis. This completes our second primary path to the exit *eigenfrequency represents energy*.

The third and final primary path to this same exit establishes that Newton's second law of motion represents a certain limit of this quantum theory. Wavepacket motion is usually introduced [2] via the concept of *group velocity*, $\mathrm{d}x/\mathrm{d}t = \partial\omega/\partial k$, where x can be defined loosely as some 'centre' or peak value. In the special case of a 'static' potential, it can be shown that $\mathrm{d}\omega/\mathrm{d}t = 0$. Though not rigorously proven to introductory students, this 'frequency conservation law' is often used in elementary discussions of the interaction of light with matter [3].

The dispersion relation (1) can only represent an exact plane wave solution in a strictly uniform potential. On the other hand, intuition suggests that a sufficiently localized wavepacket will experience a nearly uniform potential if the potential gradient is sufficiently weak. We seek to understand how the wavenumber of that localized wavepacket varies as time evolves. If this nearly uniform potential varies slowly over distance, it is reasonable to assume that x and k are constrained by the dispersion relation, which by (1) now expresses frequency as a function of both wavenumber and position, $\omega = \omega(k, x)$. Since ω is invariant, the dispersion relation stipulates how k and x must vary as the wavepacket moves through space. From the chain rule for a function of two variables,

$$\frac{\mathrm{d}\omega}{\mathrm{d}t} = \frac{\partial\omega}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial\omega}{\partial k}\frac{\mathrm{d}k}{\mathrm{d}t} = 0. \tag{2}$$

Using *group velocity* as $\partial\omega/\partial k = \mathrm{d}x/\mathrm{d}t$, one verifies that $\mathrm{d}k/\mathrm{d}t = -\partial\omega/\partial x$. It is helpful to organize these equations of wavepacket motion as follows:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\partial\omega}{\partial k}, \qquad \frac{\mathrm{d}k}{\mathrm{d}t} = -\frac{\partial\omega}{\partial x}, \qquad \frac{\mathrm{d}\omega}{\mathrm{d}t} = 0. \tag{3}$$

Here, the dispersion relation, $\omega = \omega(k, x)$, serves as a classical Hamiltonian, which suggests that (3) is a special case of Hamilton's well-known equations of motion [4]. This is further discussed in appendix A. Hamilton's elegant restatement of Newtonian mechanics can serve as a guide in the construction of the new quantum theory [1]. When applied to wavepackets, both (3) and its generalization (A.1) are approximations, valid in the 'eikonal' limit [4–6]. For our purposes, the eikonal limit might be defined as

$$\lambda \ll \Delta x \ll \Lambda. \tag{4}$$

Here, $\lambda = 2\pi/k$ is the wavelength, Δx is the size of the wavepacket and Λ is the spatial scale over which the medium supporting the wave varies. The word 'eikonal' comes from the Greek, $\varepsilon\iota\kappa\varpi\nu$ (icon) = 'image', probably because the approximation found early application in geometrical optics [6]. In optics, Δx might more appropriately represent the 'thickness' of a ray of light. Such a 'ray' must be many wavelengths wide in order to suppress diffraction. Yet it must be sufficiently small to serve as a one-dimensional curve through an optical device with dimensions Λ.

In our example of Schrödinger's equation, all variation in the medium occurs through the potential term, $V = V(x)$. Thus one might take $\Lambda^{-1} = V^{-1}\partial V/\partial x$ and the condition, $\Delta x \ll \Lambda$, guarantees that the wavepacket experiences a nearly uniform potential. This permits us to argue applicability of the dispersion relation (1) to what we treat as a plane wave in a homogeneous medium. By Heisenberg's uncertainty principle, $\lambda \ll \Delta x$ implies that the wavepacket may have a reasonably well-defined wavenumber [1, 2]. To emphasize the approximate nature of the Hamiltonian description of wavepackets, note that our wavepacket model eventually becomes meaningless as the wavepacket grows in size. Thus (3) can never truly replace Ehrenfest's theorem [1] in the teaching of introductory quantum mechanics. On the other hand, these Hamiltonian methods are useful in the study of waves outside quantum mechanics, as discussed in appendix A. Furthermore, since (3) can be derived before any interpretation of ψ is established, it is well suited for our purposes.

The primary arrows down the left side of the maze lead directly down to the second exit. By linearity, a superposition of infinite square well energy eigenstates also solves Schrödinger's equation, $\psi(x, t) = \Sigma C_n u_n(x) \exp(-\mathrm{i}\omega_n t)$. This solution is so central to later discussions that we shall henceforth refer to it as the 'mixed-energy bound state'. Orthonormality of the basis functions $u_n(x)$ can be verified by direct integration to be $\int u_m u_n \, \mathrm{d}x = \delta_{mn}$, where the symbol '$u$' is chosen to denote 'unit vector'. This orthonormality greatly facilitates the derivation of two fundamental equations [7] associated with the Fourier series expansion: $C_n = \int u_n{}^* \psi \, \mathrm{d}x$ and $\int |\psi|^2 \, \mathrm{d}x = \Sigma |C_n|^2$. The latter is *Parseval's theorem*, which can be used to establish the time invariance of $\int |\psi|^2 \, \mathrm{d}x$ directly from the obvious time invariance of $\Sigma |C_n|^2$. If the wavefunction is normalized, two fundamental equations of interpretation can be postulated: $P(x) = |\psi|^2 \, \mathrm{d}x$ and $P(E_n) = |C_n|^2$.

2. The maze quantum mechanics

If the primary paths of the map are intended to help a student understand quantum mechanics, then the secondary paths are for the soul that cannot rest until the theory is *believed*. The maze also demands multiple visits to certain topics. Nothing illustrates the need for this better than the stationary *Gaussian wavepacket*, at the top of figure 1. This solution is often introduced early in a course and for good reason. The Gaussian wavepacket displays both the particle-like properties of a wavepacket, as well as 'uncertainty' in position, wavenumber and energy [1]. The box '*Heisenberg's uncertainty principle?*' acknowledges certain 'spreads' in particle coordinates without intending to convey that a lack of knowledge is established. Hence the question mark, '?', is somewhat of a *double entendre*. A first visit to the Gaussian wavepacket might raise more questions than answers, but they are questions worth asking as soon as possible.

A stationary Gaussian wavepacket can be formed as a linear superposition of plane waves, $\exp(\mathrm{i}kx - \mathrm{i}\omega t)$, over a range of wavenumbers:

$$\psi(x, t) = A \int_{-\infty}^{\infty} \exp(-a^2 k^2) \mathrm{e}^{\mathrm{i}kx - \mathrm{i}\omega(k)t} \, \mathrm{d}k. \tag{5}$$

Appendix B shows how this can be integrated to obtain

$$|\psi(x, t)| = \left(\frac{A\pi^{1/2}}{a^{1/2}} \right) \frac{1}{w^{1/2}} \exp\left(\frac{-x^2}{4w^2} \right), \tag{6}$$

where

$$w = a\left(1 + \frac{t^2}{\tau^2}\right)^{1/2}, \tag{7}$$

is a time-dependent width and $\tau = 2ma^2/\hbar$ is a coherence time. On this first visit to the Gaussian wavepacket, (5)–(7) permit the identification of vaguely defined 'spreads', as $\Delta k = (2a)^{-1}$ and $\Delta x = w(t)$.

It would be idiosyncratic to construct a course that dwells on the integral $\int |\psi|^N \, \mathrm{d}x$ for arbitrary N. Fortunately, no one should be tempted to do this because an expression like (6) is easily put forth to students using the conventional approach [1]. Equation (6) strongly suggests that normalization be performed with the square of the modulus. Note that all time dependence in (6) is expressed through the parameter $w = w(t)$. Any loosely defined 'width' of $|\psi|$ is roughly equal to w. Since the 'height' is proportional to $w^{-1/2}$, only the square of the 'height' multiplied by 'width' is plausibly time independent. For a bit more rigour, introduce the change of variables, $\mathrm{d}\xi = \mathrm{d}x/w$, *before* integrating $\int |\psi|^N \, \mathrm{d}x$ over all space. Only the modulus squared, $|\psi|^2$, will remove $w(t)$ from the final result. Efforts such as this demonstration that N must equal 2 can help quantum mechanics seem more 'robust' against suggestions that the theory might require modification.

Recall the rule that concepts cannot be utilized until they have been encountered. This poses a dilemma because normalization cannot be justified until the meaning of ψ is established. One might imagine integrating $\int |\psi|^N \, \mathrm{d}x$ in order to find a mathematically conserved quantity, in the hope that the meaning of this quantity will later be discovered. The many physical quantities that $|\psi|^2$ might represent include the density of *charge, mass* and *probability*. The discovery that width grows as time evolves serves to provide one of many hints that $|\psi|^2$ represents probability. After this first visit to the *Gaussian wavepacket*, two other visits are possible from entirely different parts of the maze. One visit occurs when an effort to seek alternative interpretations of ψ leads to the suggestion that certain solutions of Schrödinger's equation be 'forbidden'. This will be discussed below. Another visit to the Gaussian *wavepacket* might follow the introduction of the integral Fourier transform, which finally attaches precise meaning to Δx and Δk as mean-square deviations, $(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle$ [1].

We now consider the third and final exit from the maze. It follows secondary paths via *Dirac's* delta function [1, 7], $\delta(x) = 2\pi \int \exp(\mathrm{i}kx) \, \mathrm{d}k$. While symmetry suggests that this integral is real, it has little meaning unless an infinitesimal amount of damping is introduced to convert the integral into $\varepsilon/(\varepsilon^2 + x^2)$. This approaches $\pi\delta(x)$ in the limit that ε vanishes. The identities in the box are sufficient to derive the integral Fourier transform using standard mathematical methods [1, 7]. These methods also convert an intuitively obvious formula for expectation value, $\langle k \rangle = \int |\phi|^2 k \, \mathrm{d}k$, into the operator form, $\langle k \rangle = \int \psi^* k_{op} \psi \, \mathrm{d}x$, where $k_{op} = -\mathrm{i}\partial/\partial x$ and $\hbar k$ is momentum. This develops quantum mechanics to the point where Ehrenfest's theorem can be introduced [1]. The advanced level required to reach Ehrenfest's theorem motivates the early introduction of approximate wavepacket motion at (3). This third exit cryptically summarizes three fundamental equations of interpretation with $P(J) = |\langle J|\psi\rangle|^2$. Here, $\langle J|\psi\rangle$ can represent any of the following:

$$\psi(s) = \int \delta(x - s)\psi(x) \, \mathrm{d}x \tag{8a}$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int \exp(-\mathrm{i}kx)\psi(x) \, \mathrm{d}x \tag{8b}$$

$$C_n = \int_0^L u_n(x)\psi(x) \, \mathrm{d}x. \tag{8c}$$

The annoying factor 2π seems to arise from the fact that the latter two eigenstates are not normalized.

Students either uncomfortable or fascinated with the role of probability in this theory may investigate '*alternative interpretations*', although, appropriately, this part of the maze has no exit. This discussion is somewhat superficial, intended not as the starting point for serious efforts to reconstruct quantum mechanics, but to help students appreciate the difficulties such a reconstruction might encounter. Two alternative interpretations are addressed, both representing attempts to construct quantum mechanics without appealing to probability. Could it be that $|\psi|^2$ *is mass or charge density?* A well-known solution to Schrödinger's equation makes this unlikely. Consider the *scattering by a potential step*. If the energy of the incident wave is sufficient, a single discontinuity in potential will scatter the outgoing wave into two opposite directions. Electrons cannot be split, created or destroyed (at non-relativistic energies).

Another alternative notion is more difficult to refute. Could ψ represent a *force field* not unlike the force electric field associated with the electron? This is not entirely inconsistent with the aforementioned splitting of a wavepacket due to a collision, because electromagnetic radiation is also generated by sudden accelerations of a classical point particle. If this force field is proposed in an effort to remove probability from the interpretation of Schrödinger's equation, it faces an important difficulty. Revisit the mixed-energy bound state, associated with an infinite square well. It is difficult to find an interpretation for this mixed-energy state that does not involve probability. If expectation value $\langle E\rangle = \Sigma E_n|C_n|^2$ is taken to be an atom's actual energy, then a complicated set of selection rules must be concocted to explain experimentally observed atomic spectral lines. It seems unnatural to forbid only unbound mixed-energy states. If all mixed-energy states were 'forbidden', then wavepackets would be forbidden, as can be seen by another revisit to the *Gaussian wavepacket*. Without wavepackets, quantum mechanics would lose its connection to the Newtonian regime.

3. How to use this map

If the map's notation or organization differs greatly from that of a given course, a copy of figure 1 might be given to students at the very end of the course for future reference and contemplation of the subject. To prevent discussion of the map from occupying an undue amount of time, it might be introduced to students late in the course, after most of the concepts have already been established. In this case, the map can be used to generate a large number of exercises simply by asking students to locate where concepts have already been encountered in the course or textbook. Elementary examples include verification that $u_n = (2/L)^{1/2}\sin(n\pi x/L)$ are orthonormal, and that this leads to Parseval's theorem. More challenging exercises that review material already covered might include integration of $\exp(-a^2k^2+\mathrm{i}kx-\mathrm{i}\omega t)$ to obtain the Gaussian wavepacket, the scattering of a wave by a potential step and the recovery of all important equations in integral Fourier transforms from the two integrals representing Dirac's delta function that are displayed in the map. Most courses somehow connect the de Broglie relations with Schrödinger's equation early in the course. The introduction of the map late in the course might motivate an assignment that reviews how this was accomplished.

The concept map also inspires three exercises not commonly found in textbooks. Each could be justifiably introduced into almost any course on quantum mechanics. The first involves appendix B, where the integration of $\int|\psi|^N\,\mathrm{d}x$ for the Gaussian wavepacket is no more difficult for arbitrary N than for $N = 2$. A second exercise involves the derivation of $\mathrm{d}k/\mathrm{d}t = -\partial\omega/\partial x$ from (2). A third exercise can inform students that equations of wavepacket motion extend beyond quantum mechanics, without taking the course far outside its intended scope. Given $\omega = ck/n$ for light in a simple dielectric material, derive $\mathrm{d}k/\mathrm{d}t = (\omega/n)\partial n/\partial x$. A number of advanced or peripheral exercises might be suggested by appendix A, which discusses Hamiltonian wavepacket motion outside the context of Schrödinger's equation.

The instructor who chooses to emphasize the maze with perhaps one lecture can assign, discuss or even test on a number of conceptual questions:

(1) What result from Fourier series analysis was used to postulate two simultaneous equations of probability?
(2) What equation(s) from the maze inform us that wavepackets (approximately) obey $F = ma$?
(3) Why would the postulate that probability density is actually $|\psi|^{2.1}$ require fundamental changes in the theory?
(4) Suppose one investigates the *Gaussian wavepacket* before the meaning of ψ is established. What might motivate an investigation of whether $\int|\psi|^2\,\mathrm{d}x$ is time invariant?

(5) What alternative interpretation of wave amplitude is rendered unlikely by the interaction of a wavepacket with a potential step?
(6) Why does it seem unnatural to 'forbid' the mixed-energy bound state?
(7) Why does it seem unnatural to attribute an 'averaged' energy to the mixed-energy bound state?
(8) The map suggests that a mixed-energy state cannot possess a 'known' energy, e.g. $\langle E\rangle = \Sigma E_n|C_n|^2$. However, such an assignment has precedence in Newtonian mechanics. If $|\psi|^2$ were to represent mass density, what would $\int |\psi|^2 x\, \mathrm{d}x$ represent?
(9) Suppose an attempt to remove probability from quantum mechanics leads to speculation that ψ represents a force field. What argument can render it difficult to use this idea to remove probability from the theory?
(10) Let any of the following wavefunctions represent $\psi(x,t)$ at $t=0$: $\delta(x-s)$, $\exp(\mathrm{i}kx)$ and $\sin(n\pi x/L)$. What do they have in common? Are any of them normalized?

Appendix A. Wavepacket motion in the eikonal approximation

The following equations are known to hold for wavepacket motion in the eikonal approximation for a wide variety of linear waves [4–6, 8, 9]:

$$\frac{\mathrm{d}x^j}{\mathrm{d}t} = \frac{\partial\omega}{\partial k^j}, \qquad \frac{\mathrm{d}k_j}{\mathrm{d}t} = -\frac{\partial\omega}{\partial x^j}, \qquad \frac{\mathrm{d}w}{\mathrm{d}t} = \frac{\partial\omega}{\partial t}. \tag{A.1}$$

Equation (A.1) is probably most familiar as Ehrenfest's theorem of quantum mechanics [1]. Here, $\omega = \omega(\boldsymbol{k}, \boldsymbol{r}, t)$ acts as a Hamiltonian, with $\boldsymbol{r}$ and $\boldsymbol{k}$ serving as coordinate variables and conjugate momentum variables, respectively. There is no restriction on the number of dimensions or on the metric. The mixed use of superscripts and subscripts is not required unless one employs non-orthogonal coordinate systems such as those found in solid-state physics [8] and general relativity [9]. It is convenient to define gradient operators as $\partial\omega/\partial\boldsymbol{k} = \partial\omega/\partial k_j$ and $\partial\omega/\partial\boldsymbol{r} = \partial\omega/\partial x^j = \nabla\omega$.

Application of (A.1) in two dimensions offers a wealth of applications in which the inhomogeneity bends the wave's path. Waves at the beach do not fully satisfy either the required condition of linearity or the eikonal approximation. Yet (A.1) seems to model certain wave processes, as shown in figure 2. Wavelength decreases with decreasing depth and this bends waves so that they approach the beach in a normal direction. The phenomenon of 'coastal straightening' has been attributed [10] to enhanced wave erosion in regions that jut out in the water, as shown in figure 2(b).

The reader should be cautioned against believing that group velocity, $\partial\omega/\partial\boldsymbol{k}$, is always parallel to wavenumber, $\boldsymbol{k}$. This only occurs when frequency is a function of magnitude, $k = |\boldsymbol{k}|$, but not direction. To verify this, apply the chain rule, $\partial\omega/\partial\boldsymbol{k} = (\partial\omega/\partial k)(\partial k/\partial\boldsymbol{k})$. In two dimensions, for example, $\partial k/\partial\boldsymbol{k} = \partial(k_1^2 + k_2^2)^{1/2}/\partial k_j = k_j/k$ is a unit vector parallel to $\boldsymbol{k}$. Figure 3 depicts a simple device in which wavenumber and group velocity are not parallel. It consists of a continuum of non-interacting strings arranged on a flat plane. Let transverse tension waves be polarized perpendicular to this plane so that the strings never touch. Neglecting the discrete spacing between the strings, we have a two-dimensional medium, upon which all wave energy is transmitted parallel to the strings. The dispersion relation is

$$\omega^2 = \frac{T}{\mu}k_x^2 \tag{A.2}$$

where T is tension and μ is the linear mass density of strings aligned parallel to x. To obtain real values of wave amplitude, it is necessary to superimpose branches with positive and negative values of frequency. From either branch of the dispersion relation, $\omega = \pm v_0 k_x$, we recover the expected result that group velocity can only point parallel to the x direction. What may not be expected is that $\boldsymbol{k}$ need not point along x. The three parallel lines in figure 3 depict three wave crests. Essentially a wavepacket on this device represents separate wavepackets on each

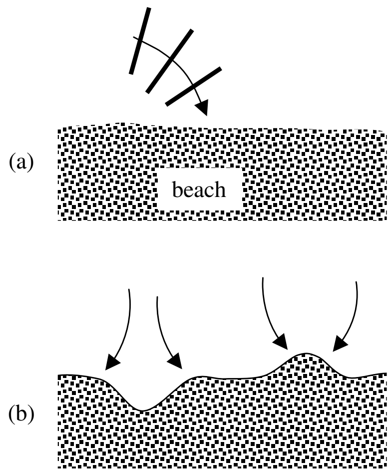

Figure 2. (a) Depicts wave refraction so as to approach a beach in the normal direction; (b) shows how the converging and diverging of waves cause an erosion pattern that tends to make beaches straight.

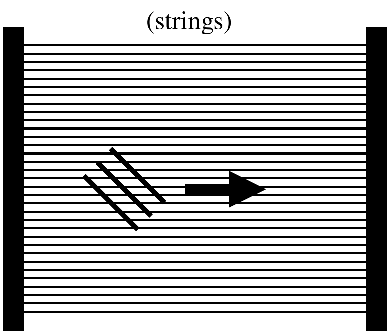

Figure 3. A continuum of independent parallel strings under tension. The large arrow depicts group velocity and the three bold lines depict wave crests.

of the non-interacting strings, synchronized so as to create a pattern from string to string that resembles a two-dimensional wavepacket in the limit that the strings become a continuum. Waves in this device resemble Alfvén waves in a sufficiently dense magnetized plasma [11].

Finally we consider a problem analogous to that of uniform circular motion, often encountered in introductory physics as centripetal acceleration, by equating a radially directed force to $ma = mv^2/r$. Let the dispersion relation be of the form $\omega = \omega(r, k)$, where, $r = |\boldsymbol{r}|$ and $k = |\boldsymbol{k}|$ are magnitudes. Assume k, r and $\partial\omega/\partial r$ to be such that the motion is circular and uniform. Figure 4 permits one to qualitatively verify how a nonzero value of $\partial\omega/\partial r$ might cause the wavelength to be smaller in regions closer to the origin. It depicts two consecutive wave crests of length δr and located a distance r from the origin. Also shown are the associated wavenumbers, as well as the vector difference, Δk. Frequency is a function of wavelength and distance to the origin, $\omega = \omega(r, \lambda)$. If $\partial\omega/\partial r$ is nonzero, then wavelength must change along a single crest. This will bend the wave in a manner seen on waves at the beach. As with the derivation at (2), we assume that frequency is invariant throughout the region.

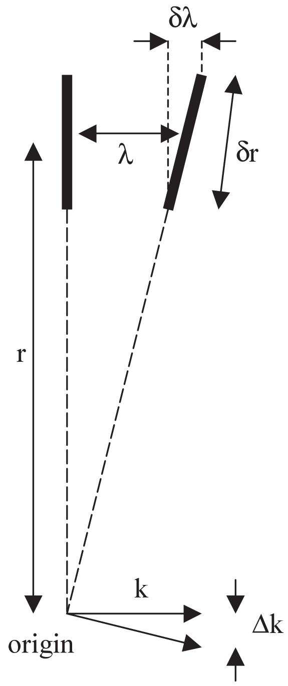

Figure 4. Two crests of a wavepacket undergoing uniform circular motion.

A quantitative calculation of uniform circular motion from figure 4 is somewhat complicated. The following argument is inspired by Born and Wolf's classic, *Principles of Optics* [6]. I find it helpful to distinguish between 'temporal' and 'spatial' differentials, denoted by Δ and δ, respectively. Using Δ to denote temporal variations, define $\Delta k = |\boldsymbol{k}_2 - \boldsymbol{k}_1|$ as a vector difference between two wavenumbers associated with two different times, separated by Δt. This vector variation Δk is shown in the figure. Note that $\Delta k/\Delta t = |\mathrm{d}\boldsymbol{k}/\mathrm{d}t|$ is not equal to $\mathrm{d}|\boldsymbol{k}|/\mathrm{d}t = 0$. The figure shows an entirely different differential associated with wavelength. It is a spatial differential, denoted by the symbol $\delta\lambda$, to represent the difference in wavelength at two different positions along a single wave crest. It might be helpful to visualize δr as the length of the wave crest depicted in figure 4. Since $k = 2\pi/\lambda$, elementary calculus yields $\delta k/k = -\delta\lambda/\lambda$. It is important to recognize that, in general, $\delta k \neq \Delta k$. Assuming that all parts of a wavepacket oscillate at the same frequency, we form the differential, $0 = \mathrm{d}\omega = (\partial\omega/\partial r)\delta r + (\partial\omega/\partial k)\delta k$, to derive $\delta k/\delta r = -(\partial\omega/\partial r)/(\partial\omega/\partial k)$. From two similar triangles in that figure, $\delta\lambda/\delta r = -\Delta k/k$. The negative sign represents the fact that the vector, $\Delta\boldsymbol{k}$, points downward, so that $\Delta k < 0$. The two wave crests shown in the figure can also be visualized as a single wavepacket at two different times. Therefore, the group velocity is $\partial\omega/\partial k = \lambda/\Delta k$. After a bit of algebra,

$$\frac{\mathrm{d}\vec{k}}{\mathrm{d}t} = -\vec{\nabla}\omega, \tag{A.3}$$

and one can verify from the figure that both vectors are directed parallel to the wave crests. Ironically, (A.3) could not be found in *Principles of Optics*. Instead, Born and Wolf derived

$$\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{c\vec{k}}{\omega}\right) = \vec{\nabla}n, \tag{A.4}$$

where n is the index of refraction and s is the path length along a light ray. Thus, $\mathrm{d}s/\mathrm{d}t = c/n$ is the magnitude of group velocity. Born and Wolf certainly knew that (A.3) holds and discussed its implication to quantum mechanics at some length. But they apparently saw little need to let this connection to classical mechanics dominate their notation in a book about geometric optics. Path length is often a more suitable parametrization to describe a ray's trajectory within an optical instrument. This is especially true if one is seeking analytic solutions without the aid of a computer.

Appendix B. Normalization of $|\psi(x,t)|^N$ for a Gaussian wavepacket

Here we integrate the Gaussian wavepacket (5) using traditional methods [1], but in such a way as to clarify the fact that suitable normalization only occurs with the modulus squared, $|\psi|^2$. Write (5) as $\psi = A\int \exp(-\varphi)\,\mathrm{d}k$, where $\varphi = a^2k^2 + \mathrm{i}kx - \mathrm{i}\omega t$ can be expressed using the dispersion relation $\hbar\omega(k) = \hbar^2k^2/2m$:

$$\varphi(k) = \left(a^2 + \frac{\mathrm{i}\hbar t}{2m}\right)k^2 - \mathrm{i}kx = b^2k^2 - \mathrm{i}kx, \tag{B.1}$$

where $b^2 = a^2 + \mathrm{i}\hbar t/(2m)$. To complete the square:

$$b^2k^2 - \mathrm{i}kx + \beta^2 - \beta^2 = (bk+\beta)^2 - \beta^2. \tag{B.2}$$

From the term proportional to the first power of k in (B.2), $\beta = -\mathrm{i}x/(2b)$. The integral over all k, $\int \exp(-\kappa^2)\,\mathrm{d}\kappa = \pi^{1/2}$, can be extended to certain contours in the complex plane [1, 7]. This inspires the change of variables from k to $\kappa = bk + \beta$. As we are interested in the absolute magnitude, we note that, for complex Z, $|\exp(Z)| = \exp[\mathrm{Re}\,(Z)]$:

$$|\psi(x,t)| = \left|\frac{A\pi^{1/2}}{b}\exp\left[\frac{-x^2}{4b^2}\right]\right| = \left(\frac{A\pi^{1/2}}{a^{1/2}}\right)\frac{1}{w^{1/2}}\exp\left(\frac{-x^2}{4w^2}\right), \tag{B.3}$$

where $w(t) = a(1+(t/\tau)^2)^{1/2}$. As mentioned above, it might be pedagogically better to follow custom and show students only the integral of the modulus squared. However, normalization for arbitrary N is easily achieved using the change of variables $\mathrm{d}\xi = \mathrm{d}x/w$:

$$\int_{-\infty}^{\infty} |\psi|^N\,\mathrm{d}x = 2A^N N^{-1/2}\pi^{\frac{N+1}{2}}a^{1-N}(1+t^2/\tau^2)^{\frac{2-N}{4}}. \tag{B.4}$$

Once it is recognized that $|\psi|^2$ represents probability density, we conclude that the appropriate normalization constant is $A = 2^{-1/4}\pi^{-3/4}a^{1/2}$.

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