The diffraction and spreading of a wavepacket

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The spreading of a one-dimensional wavepacket of Schrödinger's equation is related to the diffraction of light, as can be verified by considering the three-dimensional spreading of a wavepacket with arbitrary dispersion relation. This investigation uncovers a special property of Schrödinger's equation for a free particle: A wavepacket with initial spherical symmetry will preserve this symmetry in all Galilean reference frames. This leads to a 'derivation' of de Broglie's postulate that wavenumber is proportional to momentum (or velocity). Application to non-Gaussian wavepackets and to Fraunhoffer diffraction is also discussed.

I. INTRODUCTION

Many students encounter Heisenberg's 'uncertainty' principle through the Fraunhoffer diffraction of light by a single slit, taking de Broglie's hypothesis for momentum as a starting point, $p = \hbar k = 2\pi\hbar/\lambda$.[1] Passage through the slit yields information about the particle's position in the direction perpendicular to motion. The subsequent diffraction of the wave suggests uncertainty in that component of momentum. While this 'derivation' assumes that both light and particle waves diffract in essentially the same fashion, students should also know that pulses of light do not spread in the direction parallel to motion. This paper explores how arbitrary linear waves *spread* and/or *diffract*. It will show that both are governed by a symmetric tensor $\partial^2\omega/\partial k_i \partial k_j$, which is obtained directly from the dispersion relation $\omega = \omega(\boldsymbol{k}) = \omega(k_x, k_y, k_z)$.

Following the familiar study of a Gaussian wavepacket of Schrödinger's equation[1], we introduce a coherence time, τ: Let, $a = \langle (x - \langle x \rangle)^2 \rangle^{1/2}$, represent the initial standard deviation Δx of the wavepacket, and assume that $\Delta x \Delta k$ takes on its minimum possible value at time $t = 0$. As time evolves, the uncertainty (standard deviation) will grow as,

$$\Delta x = a \left[1 + \left(\frac{t}{\tau} \right)^2 \right]^{1/2}. \tag{1}$$

Under certain circumstances,(1) can be generalized for an arbitrary dispersion relation, and for higher dimensions:

$$\tau = \frac{(a/\Delta k)}{\|\partial^2\omega/\partial k^2\|} = \frac{(a/\Delta k)}{\|\partial v/\partial k\|}, \tag{2}$$

where, $v = \partial\omega/\partial k$, is group velocity, and Δk is the standard deviation in wavenumber. If the wavepacket has a Gaussian profile, then $a/\Delta k = 2a^2$. If the dispersion relation is Schrödinger's, $\hbar\omega = \hbar^2 k^2/2m + V$, this leads to the well-known result, $\tau = 2ma^2/\hbar$. Equation (2) might also be useful in understanding the spreading of a signal pulse as it propagates along a single mode optical fiber. It can be be understood as follows: The spread in group velocity is reasonably estimated as, $\Delta v = (\partial v/\partial k)\Delta k$. Under what might be called 'typical' or 'ideal' circumstances, a wavepacket of original size, a, will retain this size for a time, τ, where $\tau\Delta v \approx a$. Equation (2) follows directly, though only as an order-of-magnitude estimate. Sections II and III derive (1) and (2) for non-Gaussian wavepackets in three dimensions.

Throughout this paper, we assume the wavepacket to be of the form,

$$\psi(\boldsymbol{r}, t = 0) = \int d^3\boldsymbol{k}\ \eta(\boldsymbol{k}) \exp\left[i\boldsymbol{k}_0 \cdot \boldsymbol{r} + i\phi_0 \right], \tag{3}$$

where, $\eta = \eta(\boldsymbol{k})$, is a *real valued* function, and $\boldsymbol{k}_0 = \langle \psi | \boldsymbol{k}_{op} | \psi \rangle$ is the expectation value of the wavenumber. This expectation value may be taken either in $\boldsymbol{r}$-space, $\int d^3\boldsymbol{r}\ \psi^*(-i\boldsymbol{\nabla})\psi$, or in $\boldsymbol{k}$-space, $\int d^3\boldsymbol{k}\ \varphi^* \boldsymbol{k} \varphi$, where φ is the Fourier transform of ψ. As one might guess, generalization to higher dimensions is achieved by replacing $\partial^2\omega/\partial k^2$ in (2) by the eigenvalues of the 3×3 tensor, $\boldsymbol{\mathcal{D}} = \partial^2\omega/\partial\boldsymbol{k}\partial\boldsymbol{k} = \partial^2\omega/\partial k_i \partial k_j$. (See the discussion after (15) below.) What may not seem intuitive is that this tensor has non-zero elements even when the dispersion relation is of the so-called 'non-dispersive' form, $\omega = Ck$, where C is some constant (that need not be the speed of light).

The three-dimensional spreading of a wavepacket unveils a non-relativistic symmetry argument that essentially 'derives' Schrödinger's dispersion relation for a free particle. While the rigorous discussion of Sec. II requires tensor calculus, this symmetry argument can be intuitively understood as follows: Begin *without* knowledge of de Broglie's

relations ($E = \hbar\omega$ and $p = \hbar k$), but with the understanding that particles are the limiting form of wavepackets. We seek a non-relativistic dispersion relation. Consider first the familiar dispersion relation, $\omega(k) = Ck$. Since group velocity, $v = \partial\omega/\partial k = C$, never vanishes, this is obviously unsuitable as a model for Newtonian particles. The dispersion relation, $\omega(k) = Ck$, is also unsuitable due to the asymmetric manner in which wavepackets spread. Recall that *in vacuo* light has the peculiar property of (*diffracting*) in directions perpendicular to motion, while exhibiting no *spreading* (dispersion) in the direction parallel to motion. If the wavepacket is to represent a particle, an initially spherically symmetric Gaussian wavepacket must remain spherically symmetric for any (non-relativistic) velocity. The absence of such symmetry would suggest the existence of a preferred reference frame.

We therefore seek a dispersion relation for which the spreading is equal in all directions, temporarily restricting ourselves to those of the form, $\omega = Ck^n$. The *diffraction* of a beam of light arises from the fact it is a superposition of waves travelling in different *directions*. The *spreading* of a one-dimensional wavepacket arises from the various components of a wavepacket travelling at different *speeds*. Equation (2) implies that large n is associated with more spreading along the direction of propagation. Therefore it is plausible that for some unique n, the dispersion relation, $\omega = Ck^n$, might possess the required balance of dispersion and diffraction necessary to maintain spherical symmetry. While this plausiblility argument fails to suggest a specific value for n, Sec. II shows how Schrödinger's dispersion relation is uniquely suited for this purpose. De Broglie's relationship follows, $\hbar k = mv$, with $\hbar$ remaining as an undetermined constant of motion.

This symmetry argument seems to be unique among plausibility arguments leading to de Broglie's postulates. De Broglie's arguments were based largely on special relativity, a topic not yet fully grasped by students as they begin to learn about wave-particle duality.[2,3] An entirely different class of plausibility arguments[4] link the classical Hamiltonian to the dispersion relation via substitutions such as $p \to \hbar k \to -i\partial/\partial x$. While this argument leads directly to de Broglie's relationship, it requires a presumption that the classical free-particle Hamiltonian is $H(p,q) = p^2/2m$. Few people would object to this assumption, of course. Nevertheless it is fascinating to see the classical free-particle Hamiltonian 'derived' *solely* from the fact that it represents the limiting case of a wavepacket.

While most textbooks introduce coherence time for Schrödinger's equation as $\tau = 2ma^2/\hbar$, one advantage of the more general (2) is that numerical evaluation in terms of fundamental parameters is not always required, especially if one considers *coherence length*, defined as $v\tau = (\partial\omega/\partial k)\tau$. For any dispersion relations of Schrödinger's form, $\omega = A + Bk^2$, the coherence length for a Gaussian wavepacket is, $v\tau = 2a^2k = 4\pi Na$, where N is the number of wavelengths contained within the wavepacket's initial size (standard deviation). If this concept can be applied (at least qualitatively) to the atom, we immediately see that wavepackets constructed from the lowest order atomic eigenstates lose coherence after making approximately one orbit.

Strictly speaking, (1) and (2) do not describe the spreading of an electron wavepacket near an atomic nucleus because the spatial variation in potential energy, $V(\mathbf{r})$, violates the assumption of spatial homogeneity. By Ehrenfest's theorem, wavepackets of Schrödinger's equation obey Hamiltonian equations of motion, $\dot{\mathbf{r}} = \partial\omega/\partial\mathbf{k}$, $\dot{\mathbf{k}} = -\partial\omega/\partial\mathbf{r}$, $\dot{\omega} = \partial\omega/\partial t$.[1] Here the wavepacket's coordinates in $(\omega, \mathbf{k}, \mathbf{r}, t)$-space represent expectation values, and $\omega = \omega(\mathbf{k}, \mathbf{r}, t)$ is a classical Hamiltonian.[4] These same canonical equations of wavepacket motion also describe other situations in the 'eikonal' limit[4] that include solid-state physics[5], plasma waves[6], and general relativity[7]. Consideration of the spreading of a wavepacket when the dispersion relation exhibits such spatial inhomogeniety is beyond the scope of this paper.

II. SPREADING AND DIFFRACTION IN THREE DIMENSIONS

Taylor expand an arbitrary dispersion relation, assuming that the wavepacket is localized in $\mathbf{k}$-space, 'centered' at some wavenumber, k_0, and frequency, $\omega_0 = \omega(\boldsymbol{k}_0)$:

$$\begin{aligned}\omega(\mathbf{k}) &= \omega_0 + \mathbf{v}\cdot(\mathbf{k}-\mathbf{k}_0) \\ &\quad + \frac{1}{2}(\mathbf{k}-\mathbf{k}_0)\cdot\frac{\partial^2\omega}{\partial\mathbf{k}\partial\mathbf{k}}\cdot(\mathbf{k}-\mathbf{k}_0) + \cdots \\ &\equiv \omega_0 + \mathbf{v}\cdot\boldsymbol{\kappa} + \frac{1}{2}\boldsymbol{\kappa}\cdot\boldsymbol{\mathcal{D}}\cdot\boldsymbol{\kappa} + \cdots, \end{aligned} \tag{4}$$

where $\boldsymbol{\kappa} = (\mathbf{k} - \mathbf{k}_0)$. The symmetric 3×3 tensor $\boldsymbol{\mathcal{D}}$ may be expressed in a number of forms:

$$\mathcal{D}^{ij} = \frac{\partial^2\omega}{\partial k_i \partial k_j} = \frac{\partial^2\omega}{\partial\mathbf{k}\partial\mathbf{k}} = \partial\mathbf{v}/\partial\mathbf{k}. \tag{5}$$

The symmetry of this matrix ($\mathcal{D}^{ij} = \mathcal{D}^{ji}$) permits use of the compact but sometimes vague *dyadic* notation (e.g. $\partial\mathbf{v}/\partial\mathbf{k} \equiv \partial v^i/\partial k_j$). For example, the symmetry of $\mathcal{D}^{ij}$ implies that $(\partial/\partial\boldsymbol{\kappa})(\boldsymbol{\kappa}\cdot\boldsymbol{\mathcal{D}}\cdot\boldsymbol{\kappa}) = (\partial/\partial\kappa_i)(\kappa_j\mathcal{D}^{jk}\kappa_k) =$

$2\mathcal{D}^{ij}\kappa_j = 2\boldsymbol{\kappa}\cdot\boldsymbol{\mathcal{D}} = 2\boldsymbol{\mathcal{D}}\cdot\boldsymbol{\kappa}$ (written by hand as $2\underline{\underline{D}}\cdot\underline{\kappa}$). We sum over repeated indices (unless otherwise stated). The use of both superscripts and subscripts is optional, but facilitates transition to non-orthogonal coordinate systems.

The symmetry of $\mathcal{D}^{ij}$ also permits the coordinate system to be rotated so that the matrix is diagonal. Henceforth we shall assume that this rotation has taken place, and that $(\mathcal{D}^1, \mathcal{D}^2, \mathcal{D}^3)$ represent the eigenvalues of $\partial\omega^2/\partial\mathbf{k}\partial\mathbf{k}$ in the (x, y, z) directions, respectively. Further simplification occurs when the dispersion relation is such that angular frequency depends on the magnitude of wavenumber but not its direction, $\omega = \omega(|\mathbf{k}|) = \omega(k)$. The chain rule, $\partial\omega/\partial\mathbf{k} = (\partial\omega/\partial k)(\partial k/\partial\mathbf{k})$, implies:

$$v^i = \frac{\partial\omega}{\partial k}\frac{\partial}{\partial k_i}\left(k_1^2 + k_2^2 + k_3^2\right)^{1/2} = \frac{\partial\omega}{\partial k}\frac{k_i}{k}, \tag{6}$$

$$\begin{aligned}\mathcal{D}^{ij} &= \frac{\partial v^i}{\partial k_j} = \frac{\partial}{\partial k_i}\left(k^{-1}k^j v\right) \\ &= \left(\delta^{ij} - \frac{k^i k^j}{k^2}\right)\frac{v}{k} + \frac{k^i k^j}{k^2}\frac{\partial v}{\partial k},\end{aligned} \tag{7}$$

where δ^{ij} is the Kroniker (identity) matrix. If the medium supporting the wave is isotropic, we lose no generality by demanding that $\mathbf{k}$, and hence $\mathbf{v}$, both point in the x-direction. Hence, $k_i = 0$, unless $i = 1$. All terms in (7) proportional to $k_i k_j$ vanish, except the xx term corresponding to $i = j = 1$. However, nonzero yy and zz terms do arise from $(v/k)\delta^{ij}$ in (7). Thus $\partial^2\omega/\partial\mathbf{k}\partial\mathbf{k}$ is given by,

$$\mathcal{D}^{ij} = \begin{bmatrix} \partial v/\partial k & 0 & 0 \\ 0 & v/k & 0 \\ 0 & 0 & v/k \end{bmatrix}. \tag{8}$$

The three diagonal elements are the eigenvalues $\mathcal{D}^j$. A wavepacket is formed by multiplying the plane wave, $\exp[i\mathbf{k}\cdot\mathbf{r} - i\omega(\mathbf{k})t]$, by a wavenumber amplitude factor, $\phi(\mathbf{k})$, and then integrating over wavenumber. The integration is greatly facilitated by the change of variables, $\boldsymbol{\kappa} = \mathbf{k} - \mathbf{k}_0$, $\boldsymbol{\xi} = \mathbf{r} - \mathbf{v}t$, and $\eta(\boldsymbol{\kappa}) = \phi(\mathbf{k})$. This change of variables also facilitates the analysis of a one dimensional Gaussian wavepacket of Schrödinger's equation often encountered in introductory textbooks[1] because it converts the problem of a moving wavepacket into that of a stationary one:

$$\psi(\mathbf{r}, t) = \frac{e^{i\mathbf{k}_0\cdot\mathbf{r} - i\omega_0 t}}{(2\pi)^{3/2}}\int d^3\boldsymbol{\kappa}\ \eta(\boldsymbol{\kappa})\exp\left[i\kappa_j\xi^j - i\frac{\mathcal{D}^j\kappa_j^2}{2}t\right]. \tag{9}$$

If the amplitude $\eta(\boldsymbol{\kappa})$ represents a Gaussian wavepacket, $\eta \propto \exp[-(\boldsymbol{a}\cdot\boldsymbol{\kappa})^2]$, then the components, a^j, represent standard deviations (in ξ-space) along each of the three principle axes defined by the eigenvalues of $\boldsymbol{\mathcal{D}}$. As one might guess, an initially spherically symmetrical wavepacket ($a_1 = a_2 = a_3$) will spread in a spherically symmetrical fashion only if all three eigenvalues are equal ($\mathcal{D}^1 = \mathcal{D}^2 = \mathcal{D}^3$). This is easily verified because the three-dimensional integration (9) for a spherically symmetrical Gaussian wavepacket separates into a product of three integrals, each equivalent to the familiar one-dimensional Gaussian wavepacet. An initially spherical Gaussian wavepacket will retain its spherical symmetry only if $v/k = \partial v/\partial k$ in (8). Since $v = \partial\omega/\partial k$, this condition can be integrated to show that the dispersion relation must be of the form, $\omega = A + Bk^2$. This completes the argument that Schrodinger's equation for free particles (and hence de Broglie's relations) can be deduced from non-relativistic symmetry considerations.

III. NON-GAUSSIAN WAVEPACKETS

We now show how (1) and (2) can be generalized to include a certain class of non-Gaussian wavepackets. This class is defined by the constraint that η in (3) and (12) be real-valuded. Consider the integral Fourier transform pair inspired by (9):

$$\Psi(\boldsymbol{\xi}, t) = (2\pi)^{-3/2}\int d^3\boldsymbol{\kappa}\ \Phi(\boldsymbol{\kappa}, t)\exp[i\boldsymbol{\kappa}\cdot\boldsymbol{\xi}], \tag{10}$$

$$\Phi(\boldsymbol{\kappa}, t) = (2\pi)^{-3/2}\int d^3\boldsymbol{\xi}\ \Psi(\boldsymbol{\xi}, t)\exp[-i\boldsymbol{\kappa}\cdot\boldsymbol{\xi}], \tag{11}$$

$$\Phi(\boldsymbol{\kappa}, t) = \eta(\boldsymbol{\kappa})\exp\left[-i\frac{\mathcal{D}^j\kappa_j^2}{2}t\right] \equiv \eta(\boldsymbol{\kappa})e^{iS(\boldsymbol{\kappa}, t)}, \tag{12}$$

where we have identified the phase associated with wavepacket dispersion as $S = S(\boldsymbol{\kappa}, t) = -(t/2)(\boldsymbol{\kappa} \cdot \boldsymbol{\mathcal{D}} \cdot \boldsymbol{\kappa})$.

Following quantum mechanics, we treat $\boldsymbol{\kappa}$ and $\boldsymbol{\xi}$ as observables representing position and momentum, respectively. Here the expectation values are most conveniently taken in momentum space, where the components of $\boldsymbol{\kappa}$ act as a numbers, while $\boldsymbol{\xi} \to -i\partial/\partial\boldsymbol{\kappa}$ becomes an operator.[1] As the wavepacket has been tranformed to the origin in both $\mathbf{k}$ and $\mathbf{r}$ space, the expectation values vanish: $\langle\boldsymbol{\kappa}\rangle = 0 = \langle\boldsymbol{\xi}\rangle$. We seek the expectation value of the 'standard deviation tensor', $\langle\boldsymbol{\xi}\ \boldsymbol{\xi}\rangle = -\langle\partial/\partial\boldsymbol{\kappa}\ \ \partial/\partial\boldsymbol{\kappa}\rangle$. The diagonal components represent the size (variance) of the wavepacket, while the off-diagonal elements are correlation coefficients.

The careful reader will observe that the condition that $\eta(\boldsymbol{\kappa})$ must be real-valued in (12) is imposed as an extra constraint. Some justification for this constraint can be understood by considering three simple modifications whereby $\eta(\boldsymbol{\kappa})$ is not real: (i) Multiplication of η by a complex number has no consequence. (ii) Multiplication of η by $\exp[i\boldsymbol{\kappa}\cdot\boldsymbol{r}_0]$ is not permitted because it shifts the wavepacket away from the origin. (iii) On one dimension, multiplication by $\exp[i\boldsymbol{\kappa}\cdot\boldsymbol{\mathcal{M}}\cdot\boldsymbol{\kappa}]$ shifts the time when a Gaussian wavepacket converges to a minimum value of uncertainty, $\Delta x\Delta k = 1/2$. But in three dimensions, this simple interpretation holds only if strong restrictions are placed on $\boldsymbol{\mathcal{M}}$. In the special case that, $\boldsymbol{\mathcal{M}} = \frac{1}{2}\boldsymbol{\mathcal{D}}\, t_0$, the time of convergence is shifted from $t = 0$ to $t = t_0$. (Before that time, the wavepacket had been converging.) If $\boldsymbol{\mathcal{M}}$ is diagonal, but not proportional to $\boldsymbol{\mathcal{D}}$, then the three principle directions have different times of convergence. The so-called 'Gaussian wavepacket' is never achieved in this case. (In optics this would be associated with an astigmatic lens focusing a beam to different locations for each perpendicular direction.) We therefore see that non-real values of $\eta(\boldsymbol{\kappa})$ in (12) can greatly complicate the meaning of the wavepacket as a state of maximum compactness (minimum $\Delta x\Delta k$). To avoid such complications, we henceforth take $\eta(\boldsymbol{\kappa})$ to be real.

To evaluate the expectation values, $\langle\boldsymbol{\xi}\boldsymbol{\xi}\rangle$, we let the tensor operator $(\partial/\partial\boldsymbol{\kappa}\ \ \partial/\partial\boldsymbol{\kappa})$, act on Ψ in (12):

$$\frac{\partial^2\left(\eta\, e^{iS}\right)}{\partial\boldsymbol{\kappa}\partial\boldsymbol{\kappa}} = \frac{\partial}{\partial\boldsymbol{\kappa}}\left(\frac{\partial\eta}{\partial\boldsymbol{\kappa}}e^{iS} + i\eta\frac{\partial S}{\partial\boldsymbol{\kappa}}e^{iS}\right) = \frac{\partial^2\eta}{\partial\boldsymbol{\kappa}\partial\boldsymbol{\kappa}} - \frac{\partial S}{\partial\boldsymbol{\kappa}}\frac{\partial S}{\partial\boldsymbol{\kappa}}\eta + i\left\{2\frac{\partial S}{\partial\boldsymbol{\kappa}}\frac{\partial\eta}{\partial\boldsymbol{\kappa}} + \frac{\partial^2 S}{\partial\boldsymbol{\kappa}\partial\boldsymbol{\kappa}}\eta\right\}. \tag{13}$$

Upon multiplication by η^* and integrating over $\boldsymbol{\kappa}$-space, the term in curly brackets $\{\cdots\}$ vanishes if η is real. This is most quickly verified from the requirement that the Hermitian operators $\boldsymbol{\xi}\boldsymbol{\xi}$ must have real expectation values, but can also be proven using integration by parts, after using the reality of η to substitute η^2 for $\eta^*\eta$. Since $\boldsymbol{\mathcal{D}}$ is diagonal, the j-th component of, $\partial S/\partial\boldsymbol{\kappa} = -(\boldsymbol{\kappa}\cdot\boldsymbol{\mathcal{D}})t$, is $\kappa_j\mathcal{D}^j t$ (not summed over j). Therefore,

$$\begin{aligned}\langle\boldsymbol{\xi}\boldsymbol{\xi}\rangle &= \int d^3\boldsymbol{\kappa}\left\{-\eta^*\frac{\partial^2\eta}{\partial\boldsymbol{\kappa}\partial\boldsymbol{\kappa}} + |\eta|^2(\boldsymbol{\kappa}\cdot\boldsymbol{\mathcal{D}})(\boldsymbol{\mathcal{D}}\cdot\boldsymbol{\kappa})\, t^2\right\} \\ &= \left\{1 + (t/\tau_{ij})^2\right\}\langle\boldsymbol{\xi}\ \boldsymbol{\xi}\rangle_0\,,\end{aligned} \tag{14}$$

where the 0-subscript on, $\langle\boldsymbol{\xi}\ \boldsymbol{\xi}\rangle_0 = \langle\xi^i\xi^j\rangle_0$, represents the expectation value evaluated at $t = 0$, and

$$\tau_{ij}^2 = \left(\frac{1}{\mathcal{D}^i\mathcal{D}^j}\right)\frac{\langle\xi^i\xi^j\rangle_0}{\langle\kappa_i\kappa_j\rangle_0}. \tag{15}$$

Equation (14) is the generalization of (1). The diagonal elements of (15) represent the generalization of (2) since $\mathcal{D}^i$ is an eigenvalue of $\partial^2\omega/\partial k_i\partial k_j$, while $\langle\xi^2\rangle$ and $\langle\kappa^2\rangle$ represent variances in position and wavenumber, respectively. For a one-dimensional Gaussian distribution, $\Delta\xi \equiv \langle\xi^2\rangle^{1/2} = a$ and $\Delta\kappa \equiv \langle\kappa^2\rangle^{1/2} = (2a)^{-1}$.

IV. FRAUNHOFFER DIFFRACTION

To model the diffraction of a beam of light, take (8) as the dispersion matrix with x representing the direction of propagation, and $\mathcal{D} = v/k$ representing the eigenvalues along the other two (perpendicular) directions. Assume also that the (parallel) x-direction 'separates' as: $\eta(\boldsymbol{\kappa}) = \eta_\parallel(\kappa_x)\eta_\perp(\kappa_y, \kappa_z)$. It is sufficient to begin with only one of the perpendicular directions. Letting ξ represent either y or z, define a phase, F, in (10) and (12) :

$$\Psi(\xi, t) = (2\pi)^{-1/2}\int d\kappa\ \eta(\kappa)\ e^{iF(\kappa)} \tag{16}$$

$$\begin{aligned}F(\kappa) &= -\frac{1}{2}\mathcal{D}t\kappa^2 + \kappa\xi \\ &= -\frac{1}{2}\mathcal{D}t\left(\kappa - \frac{\xi}{\mathcal{D}t}\right)^2 + \frac{\xi^2}{2\mathcal{D}t}.\end{aligned} \tag{17}$$

At large time, $F(\kappa)$ oscillates so rapidly that $\exp(iF)$ acts as a Dirac delta function, $\delta(\kappa-\kappa_0)$. In (17) this occurs at $\kappa_0 = \xi/\mathcal{D}t$. The integrals over all K of $\int\cos(bK^2)dK$ and $\int\cos(bK^2)dK$ both equal $(\pi/2b)^{1/2}$. To the extent that extremely rapid oscillations causes a function to be effectively zero,

$$\lim_{b\to\infty} e^{ibK^2} = \left(\frac{\pi}{2b}\right)^{1/2}\delta(K). \tag{18}$$

Since the real part of the LHS is positive for any sign of b, one should choose the branch for which the real part on the RHS is positive. This yields an expression that can also be obtained using the method of steepest descent:[8]

$$\lim_{t\to\infty} e^{iF(\kappa)} = \exp\left(\frac{i\,\xi^2}{2\mathcal{D}t}\right)\,\sqrt{\frac{2i\pi}{\mathcal{D}t}}\,\delta\left(\kappa-\frac{\xi}{\mathcal{D}t}\right). \tag{19}$$

Consider diffraction by a slit of width, W, with Ψ_0 representing the uniform intensity at the slit. Hence, $\Psi(\xi, t=0) = \Psi_0$, and (12) suggests that $\eta(\kappa) = \Phi(\kappa, 0)$. Therefore (11) becomes an expression for η, which yields upon integration (at the slit):

$$\begin{aligned}\eta(\kappa) &= \Phi(\kappa,\ t=0)\\ &= \frac{1}{\sqrt{2\pi}}\int_{-W/2}^{W/2} d\xi'\ \Psi(\xi',0)\exp[-i\kappa\xi']\\ &= \frac{\Psi_0 W}{\sqrt{2\pi}}\frac{\sin(\kappa W/2)}{\kappa W/2}.\end{aligned} \tag{20}$$

To recover the single-slit diffraction pattern, combine (16), (19) and (20). Then make the substitutions, $\mathcal{D} = v/k$, and $x = vt$. We also make the approximation that, $\theta \approx \xi/x << 1$, is the angle with respect to the optical axis:

$$\begin{aligned}\Psi(\xi,t) &= \sqrt{\frac{i}{2\pi\mathcal{D}t}}\,\Psi_0 W\,\frac{\sin\left(\xi W/2\mathcal{D}t\right)}{\xi W/2\mathcal{D}t}\ \exp\left(\frac{i\,\xi^2}{2\mathcal{D}t}\right)\\ &\approx \sqrt{\frac{ik}{2\pi x}}\,\Psi_0 W\,\frac{\sin\left(kW\theta/2\right)}{kW\theta/2}\ \exp(ik\Delta\ell),\end{aligned} \tag{21}$$

where $\Delta\ell$ is a path length correction to the distance along the optical axis: $x + \Delta\ell \approx (x^2+\xi^2)^{1/2}$. The small-angle approximation, $\theta << 1$, is not demanded in traditional treatments of Fraunhoffer diffraction, where $\sin(\theta)$ would replace θ in (21).[4] The need for this approximation can be seen from the truncated Taylor expansion at (4). Light that has been diffracted by a large amount represents wavenumber far from the 'center' at $\mathbf{k_0}$, which is aligned along the x-direction. For light, the higher order terms in (4) do not vanish.

Diffraction by a rectangular aperture is obtained using the same methods outlined above. The result is the product of two terms such as given by (21). The same factor of $x^{-1/2}$ appears in both terms. In this small-angle approximation, x can be replaced by the distance to the slit, r. Thus the intensity of light far from a rectangular slit obeys the expected $1/r$ radiation law.

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[1] R. L. Liboff, *Introductory Quantum Mechanics* (Addison-Wesley, Reading, MA, 1992), 2nd ed.
[2] E. MacKinnon, Am. J. Phys. **44**, 1047 (1976).
[3] F. Crawford, Am. J. Phys. **50**, 269 (1982).
[4] M. Born and E. Wolf, *Principles of Optics* (Pergamon Press, New York, 1965), 3rd ed.
[5] C. Kittel, *Introduction to Solid State Physics* (Wiley, New York, 1976), 5th ed.
[6] S. Weinberg, Phys. Rev. **126**, 1899 (1962).
[7] R. Adler, M. Bazin, and M. Schiffer, *Introduction to General Relativity* (McGraw-Hill, New York, 1965).
[8] G. B. Arfken and H. J. Weber, *Mathematical Methods for Physicists* (Academic Press, San Diego, CA, 1995), 4th ed.