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UNCERTAINTY RELATION AND DIFFRACTION BY A SLIT*

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ABSTRACT

Rigorous diffraction theory is applied to the diffraction of a plane wave by a slit of arbitrary width and the uncertainties are studied as a function of the distance from the slit.

§1. The diffraction of a plane wave by a slit has often been discussed as an illustration of Heisenberg's uncertainty relations and their role in the process of measurement. Such a discussion involves two distinct steps: A) the solution of a well defined boundary value problem, representing schematically the example in question; B) the analysis of the connection between this

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solution and experimental results. Step B is connected with many apparently still unsettled questions. In the case of the above mentioned example, however, even the treatment of step A has not been satisfactory. It has been restricted to a wide slit[1], and only elementary diffraction theory has been employed; application of the results to a narrow slit has led to misunderstandings (see §5). The purpose of this paper is to give an improved treatment of step A, in the case of a slit of arbitrary width. We shall not attempt to enter into the discussion of step B.

§2. Let us consider a monochromatic plane wave of angular frequency ω, perpendicularly incident on an infinite slit of width $2a$ in a perfectly reflecting screen of vanishing thickness (the effect of non-zero thickness will be discussed later). We shall employ the coordinate system shown in Fig. 1. The time factor $\exp(-i\omega t)$ will be omitted throughout. The incident wave, $u_0 = A\exp(ikz)$, may represent either the Schrödinger wave function of a particle of mass m, in which case $\omega = \hbar k^2/2m$, or else it may represent the electric field amplitude of an electromagnetic wave (linearly polarized parallel to the edges), in which case $\omega = ck$. The rigorous formulation of the problem is the same in both cases. The total wave function $u(y,z)$ is given by

$$u(y,z) = \begin{cases} A\,[\exp(ikz) - \exp(-ikz)] + \phi(y,-z) & (z \leq 0) \\ \phi(y,z) & (z \geq 0) \end{cases} \qquad (1)$$

where $\phi(y,z)$, defined for $z \geq 0$, satisfies the following conditions[2]: (i) $(\Delta + k^2)\phi = 0$; (ii) $\phi(y,0) = 0$ ($|y| \geq a$); (iii) $\frac{\partial \phi}{\partial z}(y,0) = ikA$ ($|y| < a$); (iv) ϕ satisfies Sommerfeld's radiation condition at infinity; (v) ϕ is everywhere finite;

(vi) $\nabla\phi$ is quadratically integrable over any domain of three-dimensional space, including the edges of the slit.

If we express $\phi(y,0)$ as a Fourier integral,

$$\phi(y,0) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} \chi(k_y,0)\, \exp(ik_y y)\, dk_y \qquad (2)$$

we have, taking into account condition (ii),

$$\chi(k_y,0) = (2\pi)^{-1/2} \int_{-a}^{+a} \phi(y,0)\, \exp(-ik_y y)\, dy \qquad (3)$$

and, employing conditions (i) and (iv), we get[3]

$$\phi(y,z) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} \chi(k_y,z)\, \exp(ik_y y)\, dk_y \qquad (4)$$

where

$$\chi(k_y,z) = \chi(k_y,0)\, \exp(ik_z z) \qquad (5)$$

$$k_z = (k^2 - k_y^2)^{1/2} \; ; \quad \mathrm{Im}(k_z) \geqslant 0 \qquad (6)$$

The second member of (4) represents a superposition of plane waves, travelling in all directions (for $k_y < k$), and evanescent waves, exponentially attenuated in the z direction (for $k_y > k$).

In the case of non-relativistic particles, $|\phi(y,\zeta)|^2$ and $|\chi(k_y,\zeta)|^2$ (with suitable normalization factors) may be interpreted as probability distributions in y and in k_y, respectively, on a given plane $z = \zeta$. The physical interpretation is more involved in the electromagnetic case.

According to (5) and (6), we have

$$|\chi(k_y,\zeta)|^2 = \begin{cases} |\chi(k_y,0)|^2 & (k_y < k) \\ |\chi(k_y,0)|^2 \exp[-2(k_y^2-k^2)^{1/2}\zeta] & (k_y > k) \end{cases} \qquad (7)$$

Therefore, the distribution function in k_y for travelling waves does not depend on ζ, whereas it decreases exponentially with ζ for evanescent waves.

§3. According to (3), (4) and (5), it suffices to know $\phi(y,0)$ on the slit in order to determine the solution. It may be shown that[4]

$$\phi(y,0) = \sum_{n=1}^{\infty} C_n (1 - y^2/a^2)^{n-\frac{1}{2}} \tag{8}$$

In the case of a <u>very narrow slit</u> ($ka \ll 1$), the coefficients C_n decrease rapidly with n, and, for an incident wave of unit amplitude, $A = 1$, we may take[5]: $C_1 = -ika$; $C_2 = C_3 = \ldots = 0$, so that

$$\phi(y,0) = -ika\ (1 - y^2/a^2)^{1/2} \tag{9}$$

It follows from (9) that $\nabla\phi$ has a singularity at the edges, where it becomes infinitely large as $D^{-1/2}$ (D denotes the distance from the edge). The same type of singularity appears in Sommerfeld's well known theory of diffraction by a half-plane.

Replacing (9) in (3), we find

$$\chi(k_y,0) = -i(\pi/2)^{1/2}\ ka^2\ J_1(k_y a)/(k_y a) \tag{10}$$

where J_1 is Bessel's function of the first order. For $k_y a \gg 1$, we get

$$\chi(k_y,0) \approx -ika^2 (k_y a)^{-3/2} \sin(k_y a - \pi/4) \tag{11}$$

The asymptotic behaviour of $\chi(k_y,0)$, given by (11), is entirely determined by the singularity at the edges. This follows from a general theorem on the asymptotic behaviour of Fourier integrals whose integrands have singularities at both ends of the interval of integration[6].

The curves of $|\phi(y,0)|^2$ and $|\chi(k_y,0)|^2$, according to (9) and (10), are shown in Figs. 2a and 2b.

The wave function at large distances ρ from the origin is given by[7]

$$\phi \approx \frac{1}{4}(ka)^2 \cos\theta(2\pi/k\rho)^{1/2} \exp[i(k\rho - 3\pi/4)] \qquad (12)$$

where θ is the polar angle with respect to the z-axis. According to (12),

$$|\phi(y,\zeta)|^2 = (\pi/8k)(ka)^4\ \zeta^2\ (y^2+\zeta^2)^{-3/2} \text{ for } k\zeta \gg 1 \qquad (13)$$

The corresponding value of $|\chi(k_y,\zeta)|^2$ follows from (7) and (10). The results are shown in Figs. 3a and 3b. Fig. 4 shows the limiting form of $|\chi(k_y,\zeta)|^2$ for $\zeta \rightarrow \infty$.

Now let us consider the case of a <u>wide slit</u> ($ka \gg 1$). No simple rigorous expression for the wave function is known in this case. However, we can make the following assertions: A) $|\chi(k_y,0)|^2$ has a very large peak, located at $k_y = 0$; the width of this peak is of the order of $1/a$. This results from the proximity to "geometrical optics" conditions[8]. B) $|\chi(k_y,0)|^2$ decreases asymptotically as k_y^{-3}. This is shown by the considerations which follow (11).

§4. The preceding results will now be applied to the evaluation of the "uncertainties" in y and in k_y. In the quantitative derivation of the uncertainty relation[9], the uncertainties are defined as root mean square deviations from the mean values. While this definition may be convenient in some cases, there exist other cases in which it does not lead to physically meaningful results; as will be seen below, this happens in the present problem. It may be more suitable, then, to apply a different definition[10]. The uncertainty in a given variable may be defined, for instance, as the "half-width" of the probability distribution in that variable (assuming that the shape of the distribution allows a half-width to be defined). This definition has been applied in the theory of the natural line breadth[11]. We shall see that it should also be preferred in the present problem.

Let us denote by $\Delta y(\zeta)$, $\Delta k_y(\zeta)$, the root mean square deviations from the mean values of y and k_y, respectively, evaluated on the plane $z = \zeta$ [12]:

$$[\Delta y(\zeta)]^2 = \int_{-a}^{+a} y^2 |\phi(y,\zeta)|^2 \, dy \Big/ \int_{-a}^{+a} |\phi(y,\zeta)|^2 \, dy \qquad (14)$$

$$[\Delta k_y(\zeta)]^2 = \int_{-\infty}^{+\infty} k_y^2 |\chi(k_y,\zeta)|^2 \, dk_y \Big/ \int_{-\infty}^{+\infty} |\chi(k_y,\zeta)|^2 \, dk_y \qquad (15)$$

In the case of a narrow slit, it follows from (9), (10) and (11) that

$$\Delta y(0) = a/\sqrt{5} \qquad (16)$$

$$\Delta k_y(0) \to \infty \text{ logarithmically} \qquad (17)$$

$$\Delta y(0)\Delta k_y(0) \to \infty \text{ logarithmically} \qquad (18)$$

The logarithmic divergence of $\Delta k_y(0)$ is obviously due to the asymptotic behaviour (11) of $\chi(k_y, 0)$, which is determined by the singularity at the edges. For a screen of finite thickness having "rounded" edges, the singularity would disappear and Δk_y would no longer diverge[13].

On a plane $z = \zeta$ such that $k\zeta \gg 1$, we find, according to (13), (7) and (10),

$$\Delta y(\zeta) \to \infty \text{ logarithmically} \tag{19}$$

$$\Delta k_y(\zeta) \cong k/\sqrt{3} \tag{20}$$

$$\Delta y(\zeta)\Delta k_y(\zeta) \to \infty \text{ logarithmically} \tag{21}$$

The logarithmic divergence of $\Delta y(\zeta)$ also arises from the asymptotic behaviour of the probability distribution.

Both divergences, (17) and (19), reveal the inadequacy of the adopted definition of uncertainty. In fact, in both cases, the divergence arises, not from a lack of concentration of the probability distribution, but from the exaggerated weight which is attributed to large values of the variable, in spite of their extremely small probability.

On the other hand, inspection of Figs. 2-4 shows that the half-width will be a good measure of dispersion in the present case. Let us denote by $\delta y(\zeta)$, $\delta k_y(\zeta)$, the half-widths of the probability distributions in y and k_y, respectively, on the plane $z = \zeta$. Then, according to (9) and (10),

$$\delta y(0) = \sqrt{2}\, a \tag{22}$$

$$\delta k_y(0) \cong 3.24/a \tag{23}$$

$$\delta y(0)\, \delta k_y(0) \cong 4.58 \tag{24}$$

which satisfies the uncertainty relation. The small value of the uncertainty product (24), in contrast with (18), agrees with our expectation.

It follows from (13), (7) and (10) that, for $k\zeta \gg 1$,

$$\delta\, y(\zeta) \cong 1.53 \qquad (25)$$

$$\delta\, k_y(\zeta) \cong 2\, k \qquad (26)$$

$$\delta\, y(\zeta)\ \delta\, k_y(\zeta) \cong 3.06\, k\zeta \gg 1 \qquad (27)$$

The increase of $\delta\, y(\zeta)$ with ζ (25) reflects the linear spread of the beam in the region $k\zeta \gg 1$.

Let us consider now the case of a <u>wide slit</u>. Two properties of $|\chi(k_y,0)|^2$ in this case were given in p. 4. According to property B, (17) still holds for a wide slit (in a screen of vanishing thickness). On the other hand, according to property A,

$$\delta\, k_y(0) \sim 1/a \qquad (28)$$

whereas we obviously have

$$\delta\, y(0) \sim a \qquad (29)$$

so that

$$\delta\, y(0)\ \delta\, k_y(0) \sim 1 \qquad (30)$$

Since the large peak of $|\chi(k_y,0)|^2$ belongs to the spectrum of travelling waves, it follows from (7) that, in contrast with the case of a narrow slit, $\delta\, k_y$ does not depend on ζ :

$$\delta\, k_y(\zeta) = \delta\, k_y(0) \sim 1/a \text{ (for any } \zeta\text{)} \qquad (31)$$

§5. In the usual analysis of the connection between diffraction by a slit and the uncertainty relation[14], the uncertainty in k_y is evaluated as the width of the main peak in the Fraunhofer diffraction pattern (according to elementary diffraction theory). For a <u>wide slit</u>, the result corresponds, in our notation, to

$$\delta\, k_y(\infty) \sim 1/a \qquad (32)$$

It follows from (31) that, in (30), $\delta k_y(0)$ may be replaced by $\delta k_y(\infty)$ in the case of a wide slit.

From the physical point of view, (31) means that the wave function beyond a wide slit behaves approximately as a superposition of isochromatic plane waves in free space (for which the distribution function in k_y would be rigorously independent of ζ). This is no longer true for a narrow slit, because in this case border effects are predominant over the entire region of the slit, and the analogy with waves in free space breaks down.

On the other hand, for a slit of arbitrary width, we have

$$\delta k_y(\infty) \leqslant 2k \tag{33}$$

so that

$$\delta k_y(\infty)\ \delta y(0) \lesssim 2ka \tag{34}$$

It follows that, for a very narrow slit,

$$\delta y(0)\ \delta k_y(\infty) \ll 1 \tag{35}$$

If $\delta k_y(\infty)$ could be replaced by $\delta k_y(0)$, as in (32), (35) would contradict the uncertainty relation[15]. However, for a very narrow slit, this replacement is clearly not permissible (compare (23) and (26), and Figs. 2b and 4). Therefore, (35), which relates the uncertainties in two different planes, does not contradict the uncertainty relation.

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1. N. Bohr, Phys. Rev. 48, 696 (1935).

2. C.J. Bouwkamp, Rep. Progr. Physics 17, 35 (1954), p. 38.

3. Eq. (4) is equivalent to Eq. (2.23) of reference 2.

4. A. Sommerfeld, "Optics" (Academic Press, N. York, 1954), p. 278.

5. See reference 2, p. 74.

6. A. Erdélyi, "Asymptotic Expansions" (Dover Publ., N. York, 1956), p. 49. See also H.M. Nussenzveig, Thesis, S.Paulo, 1957 (to be published).

7. See reference 2, p. 74.

8. See H.M. Nussenzveig, reference 6. In the immediate neighbourhood of $k_y = 0$, the main term of $|\chi(k_y,0)|^2$ is given by Kirchhoff's approximation: $|\chi(k_y,0)|^2 \cong (2/\pi)\, a^2 \sin^2(k_y a)/(k_y a)^2$.

9. E.H. Kennard, Z. Physik 44, 326 (1927).

10. This was pointed out to us by Prof. Mário Schönberg.

11. See e. g. W. Heitler, "Quantum Theory of Radiation" (Oxford Univ. Press, Oxford, 1954), 3rd. ed., p. 184.

12. These quantities have to be distinguished from the corresponding values averaged over the whole space, which are not appropriate to this problem.

13. R. Gans and G. Beck, Rev. de la Un. Mat. Argent. 14, 425 (1950). Even for a screen of finite thickness having right angle corners at the edges Δk_y would no longer diverge. In fact, at such a corner, $\nabla\phi$ behaves as $D^{-1/3}$ (D = distance from the corner), and the probability distribution in k_y behaves asymptotically as $k_y^{-10/3}$ (see H.M. Nussenzveig, reference 6).

14. W. Heisenberg, "The Physical Principles of the Quantum Theory" (Univ. of Chicago Press, Chicago, 1930), p. 23.

15. D.I. Blochinzew, "Grundlagen der Quantenmechanik" (Deutscher Verlag Der Wissenschaften, Berlin, 1953), p. 50. According to Blochinzew, the solution of this paradox lies in the fact that one cannot ascribe a definite wavelength to the field beyond a very narrow slit. Plane waves of different wavelengths would indeed appear in the total (three-dimensional) Fourier representation of the wave function. In the present problem, however, only the Fourier representation in y can be employed. In this representation, $\lambda = 2\pi/k(\omega)$ is a well defined constant, and $k_y = k \sin\theta$ (where θ is no longer restricted to real values only).

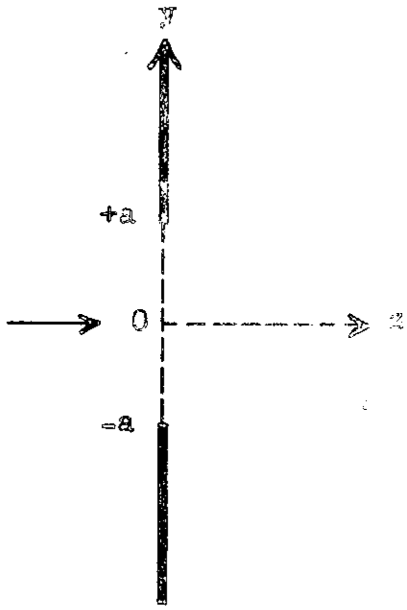

y
+a
0
z
-a

FIG. 1

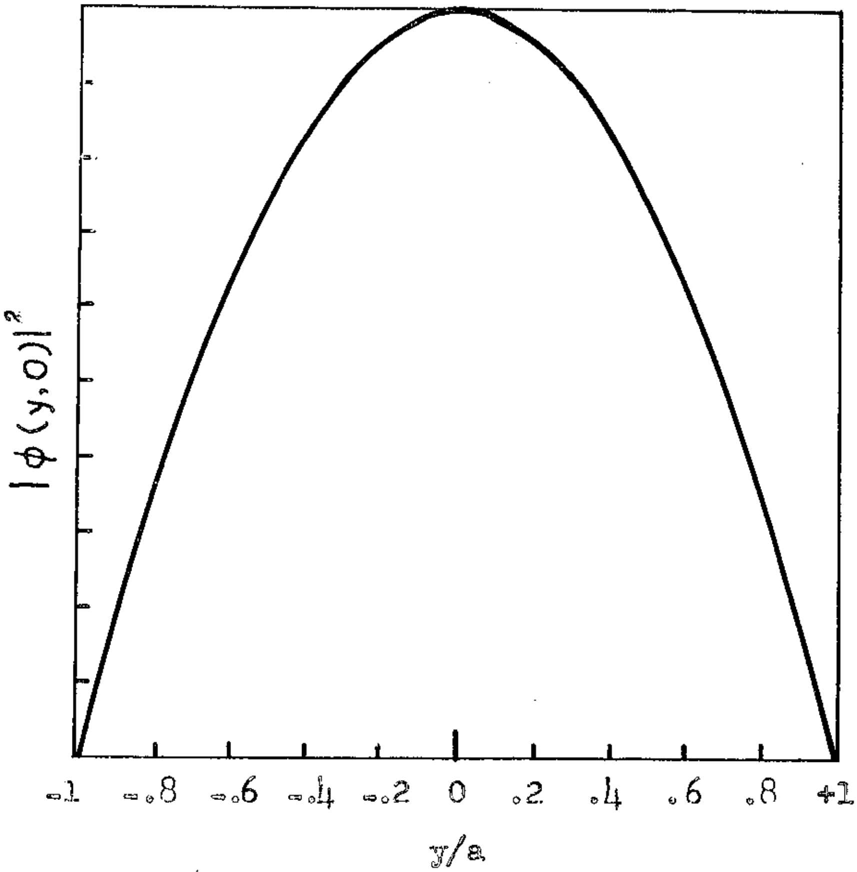
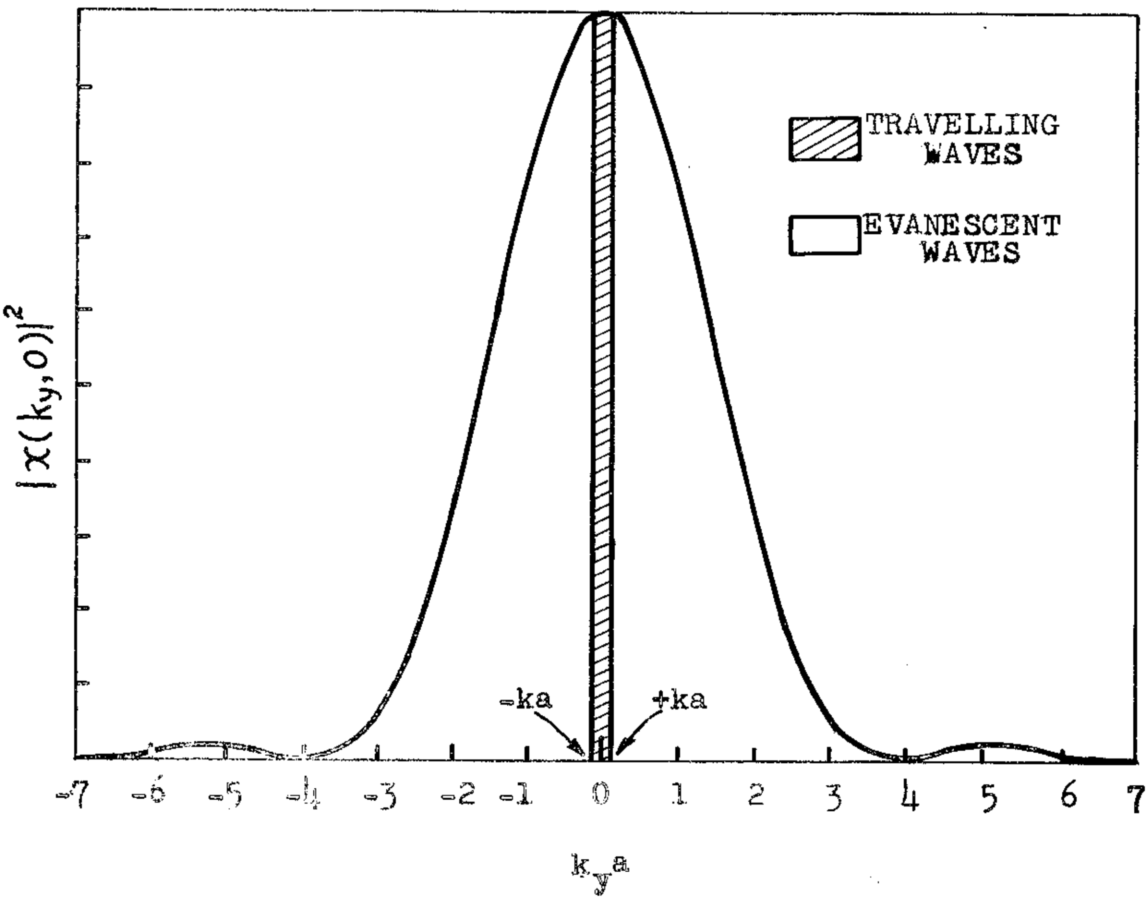

|φ(y,0)|²
-1
-.8
-.6
-.4
-.2
0
.2
.4
.6
.8
+1
y/a

FIG. 2a


|χ(k_y,0)|²
TRAVELLING WAVES
EVANESCENT WAVES
-ka
+ka
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
4
5
6
7
k_y a

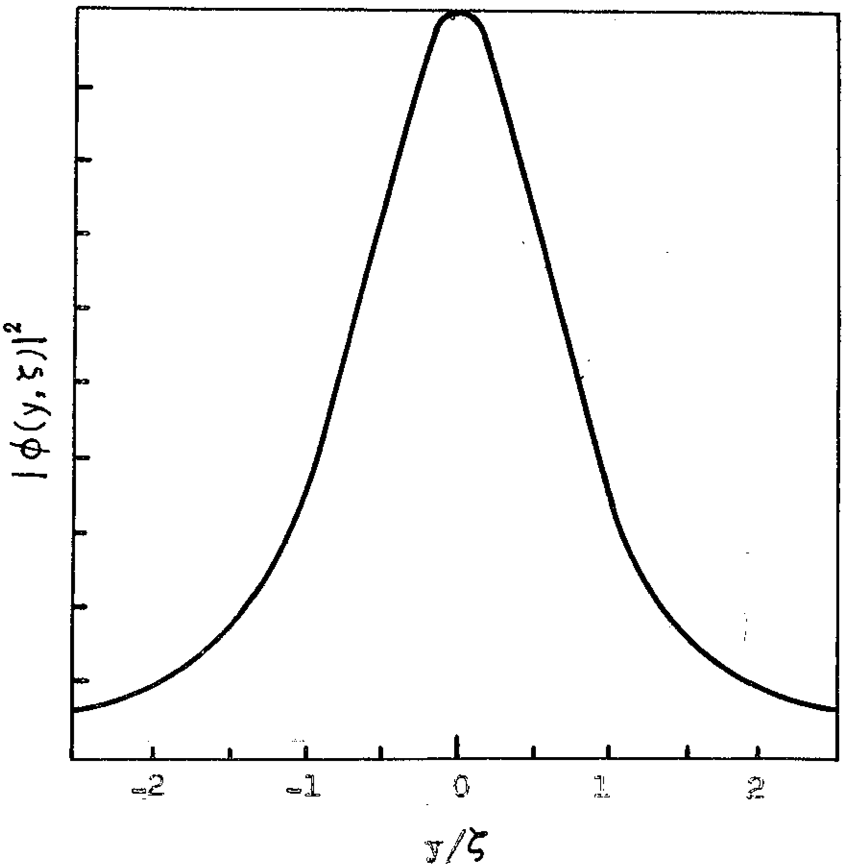


FIG. 3a

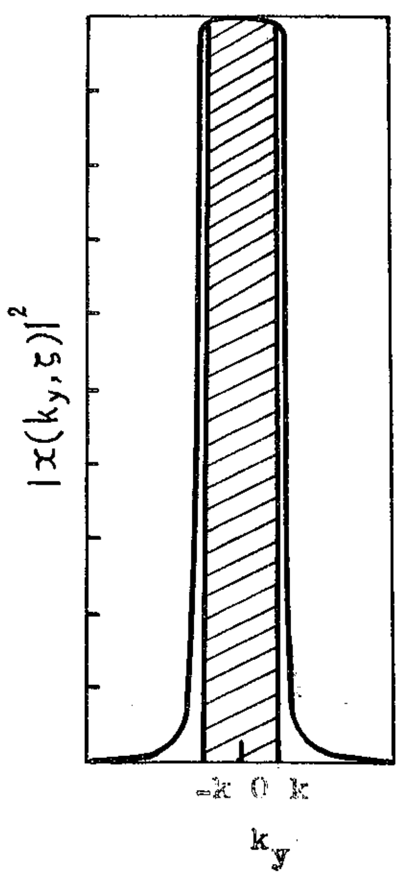


FIG. 3b

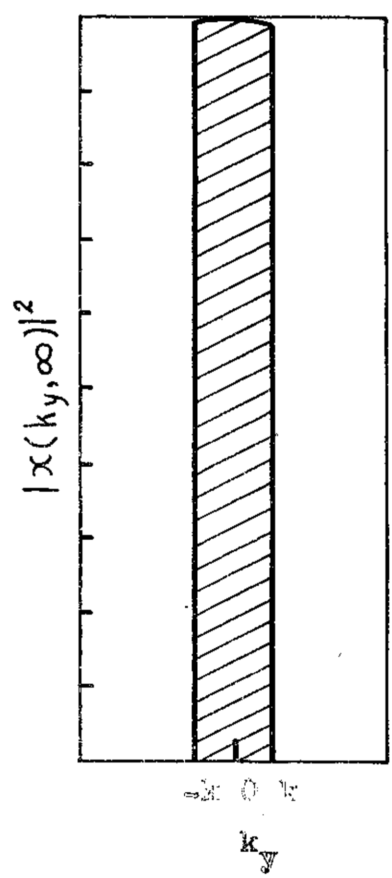


FIG. 4

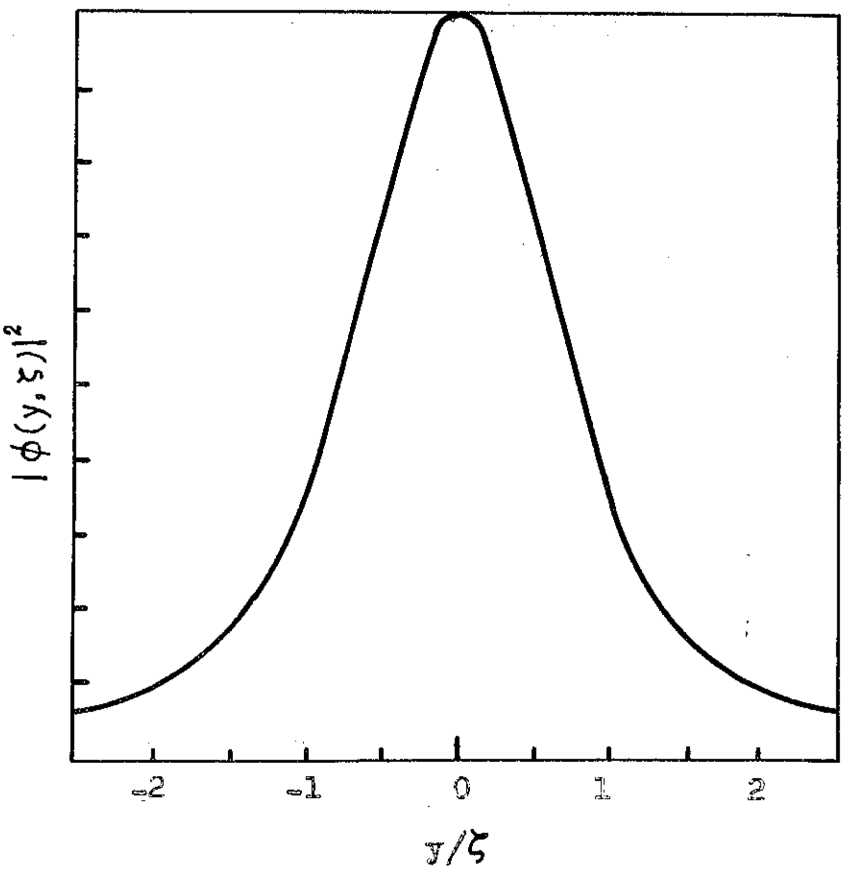


FIG. 3a

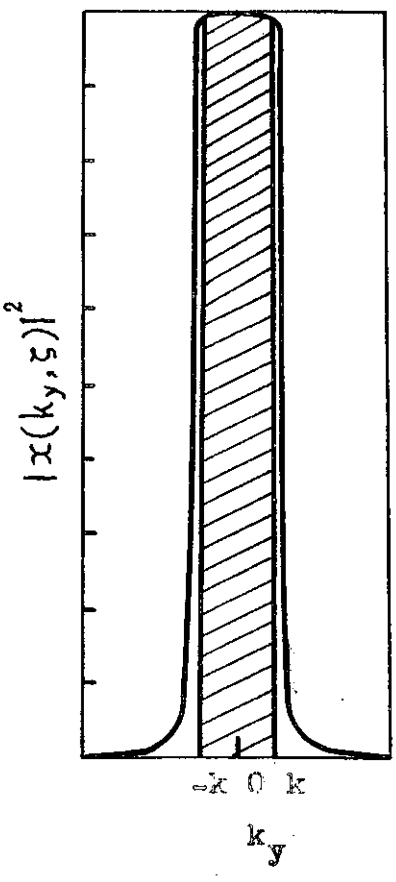


FIG. 3b

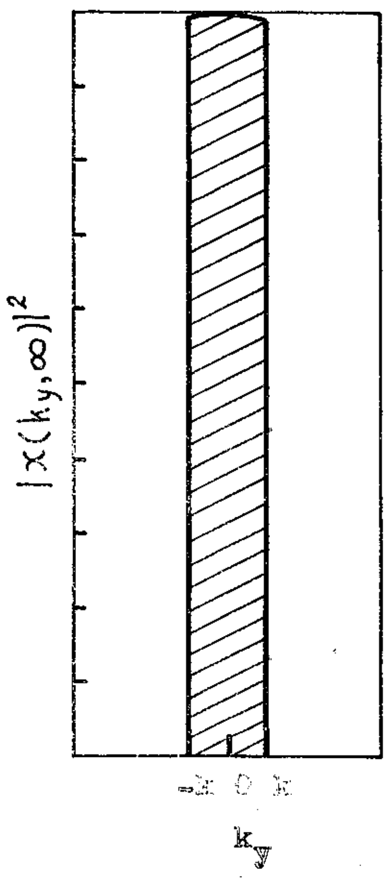


FIG. 4

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