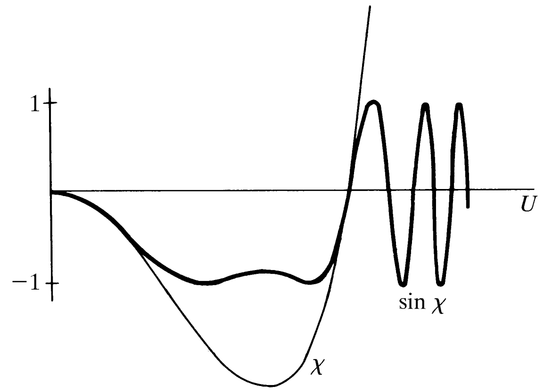

Fig. 2.5.2.3. The functions $\chi(U)$, the phase factor for the transfer function of a lens given by equation (2.5.2.33), and $\sin\chi(U)$ for the Scherzer optimum defocus condition, relevant for weak phase objects, for which the minimum value of $\chi(U)$ is $-2\pi/3$.

of (2.5.2.16). From (2.5.2.42), the image intensity (2.5.2.35) becomes

$$I(xy) = 1 + 2\sigma\varphi(xy) * s(xy), \qquad (2.5.2.43)$$

where the spread function $s(xy)$ is the Fourier transform of the imaginary part of $T(uv)$, namely $A(uv)\sin\chi(uv)$.

The optimum imaging condition is then found, following Scherzer (1949), by specifying that the defocus should be such that $|\sin\chi|$ is close to unity for as large a range of $U = (u^2 + v^2)^{1/2}$ as possible. This is so for a negative defocus such that $\chi(uv)$ decreases to a minimum of about $-2\pi/3$ before increasing to zero and higher as a result of the fourth-order term of (2.5.2.33) (see Fig. 2.5.2.3). This optimum, 'Scherzer defocus' value is given by

$$\frac{\mathrm{d}\chi}{\mathrm{d}u} = 0 \quad \text{for} \quad \chi = -2\pi/3$$

or

$$\Delta f = -\left(\tfrac{4}{3} C_s \lambda\right)^{1/2}. \qquad (2.5.2.44)$$

The resolution limit is then taken as corresponding to the value of $U = 1.51 C_s^{-1/4} \lambda^{-3/4}$ when $\sin\chi$ becomes zero, before it begins to oscillate rapidly with U. The resolution limit is then

$$\Delta x = 0.66 C_s^{1/4} \lambda^{3/4}. \qquad (2.5.2.45)$$

For example, for $C_s = 1$ mm and $\lambda = 2.51 \times 10^{-2}$ Å (200 keV), $\Delta x = 2.34$ Å.

Within the limits of the WPOA, the image intensity can be written simply for a number of other imaging modes in terms of the Fourier transforms $c(\mathbf{r})$ and $s(\mathbf{r})$ of the real and imaginary parts of the objective-lens transfer function $T(\mathbf{u}) = A(\mathbf{u}) \exp\{i\chi(\mathbf{u})\}$, where $\mathbf{r}$ and $\mathbf{u}$ are two-dimensional vectors in real and reciprocal space, respectively.

For dark-field TEM images, obtained by introducing a central stop to block out the central beam in the diffraction pattern in the back-focal plane of the objective lens,

$$I(\mathbf{r}) = [\sigma\varphi(\mathbf{r}) * c(\mathbf{r})]^2 + [\sigma\varphi(\mathbf{r}) * s(\mathbf{r})]^2. \qquad (2.5.2.46)$$

Here, as in (2.5.2.42), $\varphi(\mathbf{r})$ should be taken to imply the difference from the mean potential value, $\varphi(\mathbf{r}) - \bar{\varphi}$.

For bright-field STEM imaging with a very small detector placed axially in the central beam of the diffraction pattern (2.5.2.39) on the detector plane, the intensity, from (2.5.2.41), is given by (2.5.2.43).

For a finite axially symmetric detector, described by $D(\mathbf{u})$, the image intensity is

$$I(\mathbf{r}) = 1 + 2\sigma\varphi(\mathbf{r}) * \{s(\mathbf{r})[d(\mathbf{r}) * c(\mathbf{r})] - c(\mathbf{r})[d(\mathbf{r}) * s(\mathbf{r})]\}, \qquad (2.5.2.47)$$

where $d(\mathbf{r})$ is the Fourier transform of $D(\mathbf{u})$ (Cowley & Au, 1978).

For STEM with an annular dark-field detector which collects all electrons scattered outside the central spot of the diffraction pattern in the detector plane, it can be shown that, to a good approximation (valid except near the resolution limit)

$$I(\mathbf{r}) = \sigma^2\varphi^2(\mathbf{r}) * [c^2(\mathbf{r}) + s^2(\mathbf{r})]. \qquad (2.5.2.48)$$

Since $c^2(\mathbf{r}) + s^2(\mathbf{r}) = |t(\mathbf{r})|^2$ is the intensity distribution of the electron probe incident on the specimen, (2.5.2.48) is equivalent to the incoherent imaging of the function $\sigma^2\varphi^2(\mathbf{r})$.

Within the range of validity of the WPOA or, in general, whenever the zero beam of the diffraction pattern is very much stronger than any diffracted beam, the general expression (2.5.2.36) for the modifications of image intensities due to limited coherence may be conveniently approximated. The effect of integrating over the variables $\Delta f, u_1, v_1$, may be represented by multiplying the transfer function $T(u, v)$ by so-called 'envelope functions' which involve the Fourier transforms of the functions $G(\Delta f)$ and $H(u_1, v_1)$.

For example, if $G(\Delta f)$ is approximated by a Gaussian of width ε (at e^{-1} of the maximum) centred at Δf_0 and $H(u_1 v_1)$ is a circular aperture function

$$H(u_1 v_1) = \begin{cases} 1 & \text{if } u_1, v_1 < b \\ 0 & \text{otherwise,} \end{cases}$$

the transfer function $T_0(uv)$ for coherent radiation is multiplied by

$$\exp\{-\pi^2\lambda^2\varepsilon^2(u^2 + v^2)^2/4\} \cdot J_1(\pi B\eta)/(\pi B\eta)$$

where

$$\eta = f_0\lambda(u + v) + C_s\lambda^3(u^3 + v^3) + \pi i\varepsilon^2\lambda^2(u^3 + u^2 v + u v^2 + v^3)/2. \qquad (2.5.2.49)$$

(*b*) *The projected charge-density approximation.* For very thin specimens composed of moderately heavy atoms, the WPOA is inadequate. Within the region of validity of the phase-object approximation (POA), more complicated relations analagous to (2.5.2.43) to (2.5.2.47) may be written. A simpler expression may be obtained by use of the two-dimensional form of Poisson's equation, relating the projected potential distribution $\varphi(xy)$ to the projected charge-density distribution $\rho(xy)$. This is the PCDA (projected charge-density approximation) (Cowley & Moodie, 1960),

$$I(xy) = 1 + 2\Delta f \cdot \lambda\sigma\rho(xy). \qquad (2.5.2.50)$$

This is valid for sufficiently small values of the defocus Δf, provided that the effects of the spherical aberration may be neglected, *i.e.* for image resolutions not too close to the Scherzer