

3.3. MOLECULAR MODELLING AND GRAPHICS

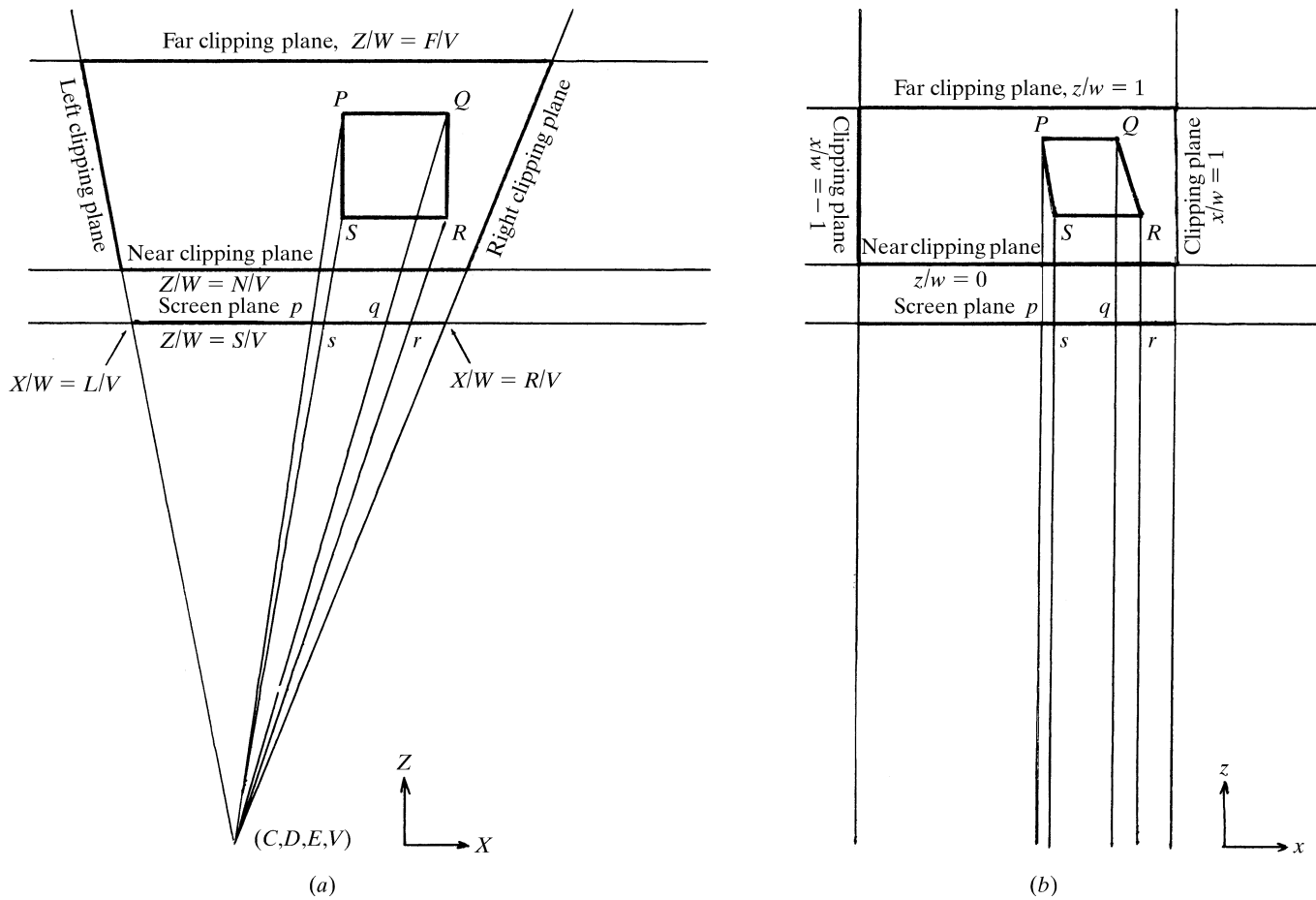


Fig. 3.3.1.1. The relationship between display-space coordinates ( $X, Y, Z, W$ ) and picture-space coordinates ( $x, y, z, w$ ) derived from them by the window transformation,  $U$ . (a) Display space (in  $X, Z$  projection) showing a square object  $P, Q, R, S$  for display viewed from the position  $(C, D, E, V)$ . The bold trapezium is the window (volume) and the bold line is the viewport portion of the screen. The points  $P, Q, R$  and  $S$  must be plotted at  $p, q, r$  and  $s$  to give the correct impression of the object. (b) Picture space (in  $x, z$  projection). The window is mapped to a rectangle and all sight lines are parallel to the  $z$  axis, but the object  $P, Q, R, S$  is no longer square. The distribution of  $p, q, r$  and  $s$  is identical in the two cases. Note that  $z/w$  values are not linear on  $Z/W$ , and that the origin of picture space arises at the midpoint of the near clipping plane, regardless of the location of the origin of display space. The figure is accurately to scale for coincident viewport positions. The words ‘Left clipping plane’, if part of the scene in display space, would currently be obscured, but would come into view if the eye moved to the right, increasing  $C$ , as the left clipping plane would pivot about the point  $L/V$  in the screen plane.

( $ZV/W - S$ ), respectively. This provides perspective because the weighted mean is at the point where the straight line from ( $X, Y, Z, W$ ) to the eye intersects the screen. This then has to be mapped into the  $L$ -to- $R$  interval, so that picture-space coordinates ( $x, y, z, w$ ) are given by

$$\begin{pmatrix} x \\ y \\ z \\ w \end{pmatrix} = \begin{pmatrix} \frac{2(S-E)V}{(R-L)} & 0 & \frac{(2C-R-L)V}{(R-L)} & \frac{(R+L)E-2SC}{(R-L)} \\ 0 & \frac{2(S-E)V}{(T-B)} & \frac{(2D-T-B)V}{(T-B)} & \frac{(T+B)E-2SD}{(T-B)} \\ 0 & 0 & \frac{(F-E)V}{(F-N)} & \frac{-N(F-E)}{(F-N)} \\ 0 & 0 & V & -E \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \\ W \end{pmatrix}$$

which provides for  $|x/w|$  and  $|y/w|$  to be unity on the picture boundaries, which is usually a requirement of the clipping hardware, and for  $0 < z/w < 1$ , zero being for the near-plane boundary. Even though  $z/w$  is not linear on  $Z/W$ , straight lines and planes in display space transform to straight lines and planes in picture space,

the non-linearity affecting only distances. Thus vector-drawing machines are not disadvantaged by the introduction of perspective.

Note that the dimensionality of  $X/W$  must equal that of  $S/V$  and that this may be regarded as length or as a pure number, but that in either case  $x/w$  is dimensionless, consistent with the stipulation that the picture boundaries be defined by the pure number  $\pm 1$ .

The above matrix is  $U$  and is suited to left-handed hardware systems. Note that only the last column of  $U$  (the translational part) is sensitive to the location of the origin of display space and that if the eye is on the normal to the picture centre then  $C = \frac{1}{2}(R+L)$ ,  $D = \frac{1}{2}(T+B)$  and simplifications result. If  $C, D$  and  $E$  can be continuously monitored then dynamic parallax as well as perspective may be obtained (Diamond *et al.*, 1982).

If data space is referred to right-handed axes, the viewing transformation  $T$  involves only proper rotations and the hardware uses a left-handed axial system then elements in the third column of  $U$  should be negated, as explained in the opening paragraph.

To provide for orthographic projection, multiply every element of  $U$  by  $-K/E$  and then let  $E \rightarrow -\infty$ , choosing some positive  $K$  to suit the word length of the machine [see Section 3.3.1.1.2 (iii)]. The