We first use the local HA potential to study the effects of different dielectric functions. When the exchange–correlation correction $f(q)$ to the dielectric function is neglected (line 1 in tables 2 and 3) the phonon frequencies are 25% larger than experiment, and the elastic constants at least as much in error. Inclusion of the Hubbard correction function (4) and (5) immediately halves these errors (line 2) and shows the essential nature of such corrections.

Altering the value of β to β_{AS} (equation (6)), which is a theoretically more probable value, decreases the errors again (line 3). Further, Shaw's form (7) for $f(q)$, with effectively the same value of β and same large q limit, gives significantly different results (line 4), while Kleinman's form (8), which has a different large q limit, decreases the frequencies still more (line 5). Theoretically, the most probable form for $f(q)$ that can be suggested now would differ from Shaw's form for large q and would produce results lying between those of lines 4 and 5.

We see, then, that the variations due to the different correction functions are almost as large as those due to neglecting it altogether. Thus it is important that the precise form of these corrections be known more accurately, particularly for intermediate q, before the bare model potential can be assessed conclusively.

Although Kleinman's $f(q)$ here produces the best agreement with the experimental phonon frequencies at the zone boundaries, the inclusion of effective mass corrections (see below) will alter the situation. The relative behaviour of the different forms for $f(q)$ is unlikely to be changed, however. Even when the L branches are close to experiment (line 4), the T branches are consistently about 20% too high. The elastic constants are sensitive to β rather than to the form of $f(q)$. C_{11} and its pressure derivative agree well with experiment, but the transverse branches are again far too large. Relative to the phonon frequency at the [100L] zone boundary the HA potential consistently predicts values of C_{11} which are too small. Overall, then, the dispersion curves and their pressure derivatives, calculated from the local HA potential, agree reasonably with experiment, but quite

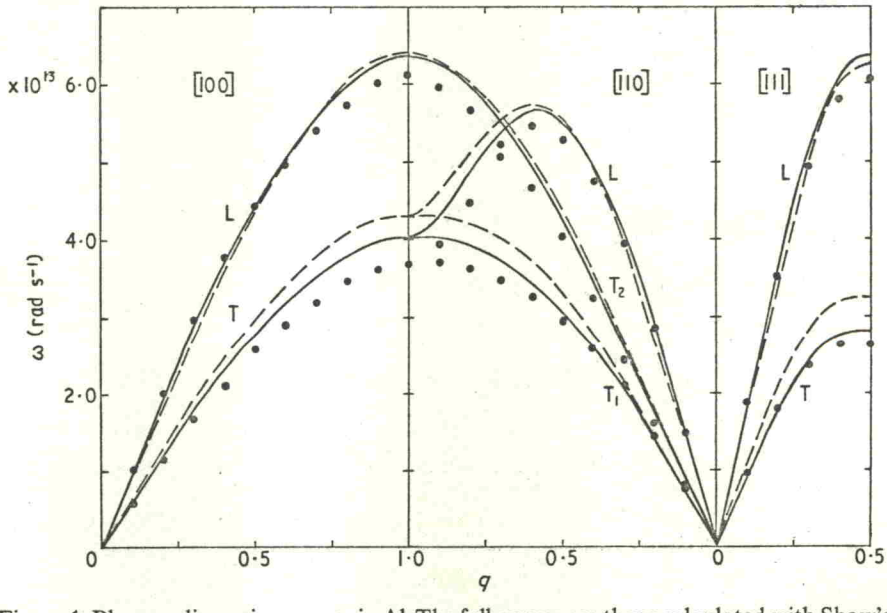

Figure 1. Phonon dispersion curves in Al. The full curves are those calculated with Shaw's potential screened by a dielectric function including his correction function (7). The broken curves are those calculated with the local HA potential, screened by the same dielectric function. The experimental points are taken from Stedman and Nilsson (1966). The wave vector q is plotted in units of $2\pi/a$, $(2)^{1/2}2\pi/a$ and $(3)^{1/2}2\pi/a$ in the [100], [110] and [111] directions respectively.