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

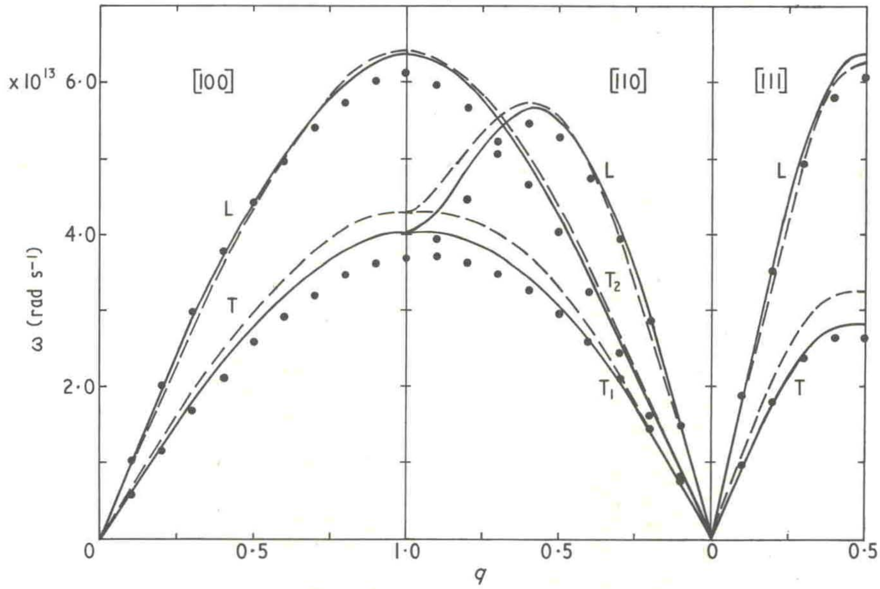

Figure 1. Phonon dispersion curves in Al. The full curves are those calculated with Shaw's potential screened by a dielectric function including his correction function (7). The broken curves are those calculated with the local HA potential, screened by the same dielectric function. The experimental 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.

large discrepancies exist in the T branches. The dispersion curves calculated using Shaw's correction function (7) in the screening of this potential are shown in figure 1, together with the experimental values, at 80 °K, of Stedman and Nilsson (1966).

The results can be quite sensitive to variations in the A_l parameters, a change of 1% in A_l altering the frequencies by 5%. This suggests that uncertainties in extrapolating the $A_l(E)$ to the energy of the solid may ultimately limit the reliability with which one could calculate dispersion curves from a model potential based on the HA method. By adjusting the A_l parameters slightly, (to 1·37, 1·635, 1·75 for $l = 0, 1, 2$ respectively, compared with the HA values of 1·38, 1·64 and 1·92) the phonon frequencies at the zone boundary can be brought much closer to experiment (line 6), although the elastic constants are not thereby improved greatly. Such a fitting adds little to our understanding of the fundamentals of the situation, however.

Calculations with the semi-non-local HA potential of Animalu (1966) agree closely with those for the local potential with the same dielectric function (line 1), so non-locality must be included fully for its effects to be evident.

The effects of changing the bare potential can be seen from the dispersion curves calculated with Shaw's potential, with exchange–correlation corrections (7) (Shaw and Pynn 1969). They are included in figure 1, with the results for the HA potential screened by the same dielectric function, and are also given in line 7 of the tables 2 and 3. Correcting the atomic volume Shaw used, from 300 to 80 °K, would marginally increase the frequencies. Shaw's L branches are almost identical with the HA ones (line 4) at the zone boundaries, but the predicted value of C_{11} is relatively closer to experiment. His T branches are also significantly closer to experiment, although errors of about 10% still exist. Similar errors, relative to the L branches, were also obtained by Vosko *et al.* (1965) and all appear to be due in part to uncertainties in the short range, that is large q, behaviour of the potential. This is suggested by the facts that the Kleinman $f(q)$ and the HA damping factor both affect the T frequencies more than the L, even though the cancellation of ω_c^2 by ω_E^2 is greater for the L branches.

The effects of the different forms for $f(q)$ on Shaw's potential can be studied by using equation (2.4) of Shaw and Pynn (1969). Neglect of the corrections increases the frequencies by 15–20%, so they are again essential, while the results are only slightly less sensitive to variations in $f(q)$ than for the HA potential. Modification of the correction function for large q via equation (8) again improves agreement with experiment.

Shaw has performed calculations of his potential at only one value of the volume for each metal, so we have not been able to calculate pressure derivatives of the elastic constants. We hope to do that later.

We have therefore confirmed Shaw and Pynn's conclusion that inclusion of exchange–correlation corrections in the screening is essential for all metals, and have shown that the precise form of these corrections is also very important. The relative trends using the different bare potentials are the same as those obtained by Shaw and Pynn for Mg, and indicate that the optimized non-local potential is a definite improvement over the local HA potential.

Two other refinements we should consider are the exchange overlap terms ω_R^2 and the effective mass corrections. In Al, the nearest neighbour distance is about 6 ionic radii, compared with 3 in Na. Therefore we expect the ω_R^2 to remain negligible, even though the cancellation of ω_c^2 and ω_E^2 is greater in Al. In fact, using plausible values for the overlap potential parameters, we find that these terms increase the phonon frequencies and pressure derivatives by less than 2%. The inclusion of effective mass corrections has been discussed by Shaw (1969 b). He gave approximate values for the resulting change in the energy–wavenumber characteristic $F(q)$ screened by a Hartree dielectric function. We find that these corrections decrease the L and T frequencies at the [100] zone boundary from 7·8 to 7·2 and 4·6 to 4·3 respectively, with similar changes in all branches. Such corrections should therefore improve still further the dispersion curves calculated with the properly screened Shaw potential (line 7).