

that their criticisms of Shaw's potential for Li do not apply to Na because Shaw modelled both the $l = 0$ and $l = 1$ components here.

Finally, we remark that the dispersion curves for K, calculated with Shaw's potential, agree exceptionally well with the experimental values, at 9°K, of Cowley *et al.* (1966) (see figure 3). The relative errors of the HA potential are the same as for Na and the exchange-correlation corrections have similar significant effects, so we need not discuss these curves further.

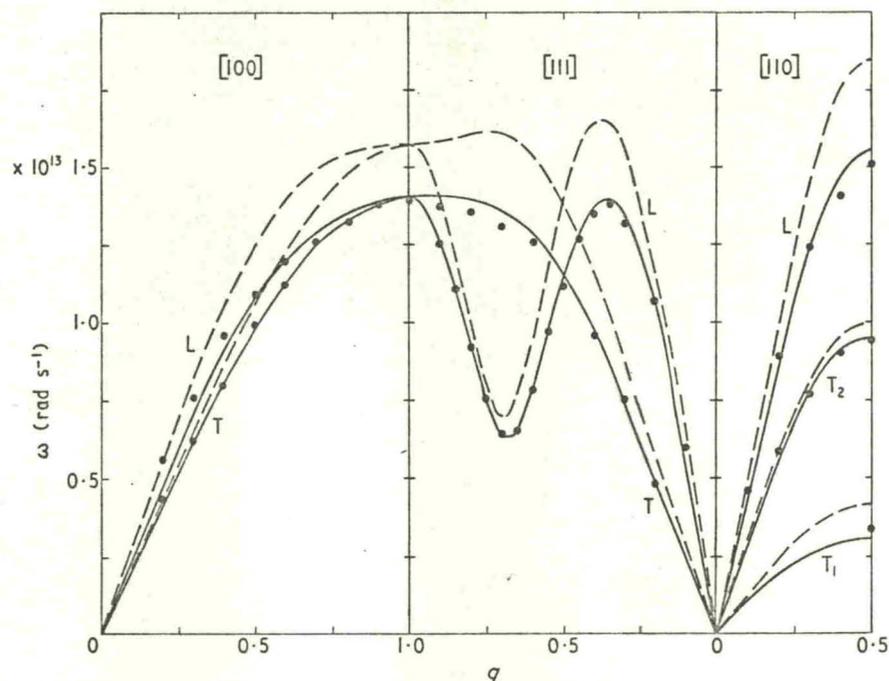


Figure 3. Phonon dispersion curves in K. The full and broken curves are again as in figure 1, and the experimental points are from Cowley *et al.* (1966). Units for the wave vector are as in figure 1.

3.3. Lead

The dispersion curves for Pb, calculated from the local HA potential, are, at best, in only qualitative agreement with experiment. Shaw has not calculated his potential for any element as heavy as Pb.

When the A_l parameters of Animalu and Heine (1965) are used, the lower part of the $[110T_1]$ branch is imaginary, the peaks in the $[100]$ branches are far too small and the phonon frequencies at the zone boundaries are too high, regardless of the dielectric function used. Because of the even greater cancellation of ω_c^2 and ω_E^2 than in Al, the effects of the different forms for $f(q)$ are greater, but the trends are much the same. The dispersion curves calculated with Animalu's semi-non-local potential have more pronounced peaks in the $[100]$ branches but are otherwise unaltered. The nearest neighbour distance in Pb is greater than four core radii, so we again expect the ω_R^2 contributions to be relatively unimportant. Effective mass corrections should be significant, but are unlikely to account for the differences from experiment.

Satisfactory agreement with experiment cannot be obtained even when the A_l parameters are varied arbitrarily, and the pressure derivatives of the elastic constants agree poorly with experiment (Miller and Schuele 1969). This form of potential therefore cannot be used to calculate reliably the phonon dispersion curves in Pb. Vosko *et al.* (1965) and