We cannot immediately compare our results with those of Animalu *et al.* (1966) since they set $A_2 = Z/R_M = 1{\cdot}50$ in their local HA potential. This change in A_2 decreases the magnitude of oscillations in the potential for large q and, as they remarked, does not affect greatly the values of the potential at the reciprocal lattice vectors. It does, however, change the phonon frequencies markedly, particularly in the 100T branch. As this change is almost ten times larger than that caused by the HA damping factor, we feel that our approach gives a better estimate of the reliability of the original HA method.

The only other calculation with which we can compare our elastic constants is that of Shyu and Gaspari (1969) who used a local Ashcroft potential, screened via Hubbard's $f(q)$, to obtain $C_{11} = 0{\cdot}78$ for Al. Our most reasonable value, as predicted by the local HA potential, was 1·02, while Shaw's potential gave 1·06. Even allowing for its overestimation of the rest of the [100L] branch, Shaw's result is better than the others, so we can hope to improve the pressure derivatives also by using his potential.

3.2. *Sodium*

The corresponding Shaw and HA dispersion curves for Na, together with the experimental values, at 80°K, of Woods *et al.* (1962), are shown in figure 2. Again the overall agreement of Shaw with experiment is good, and better than HA.

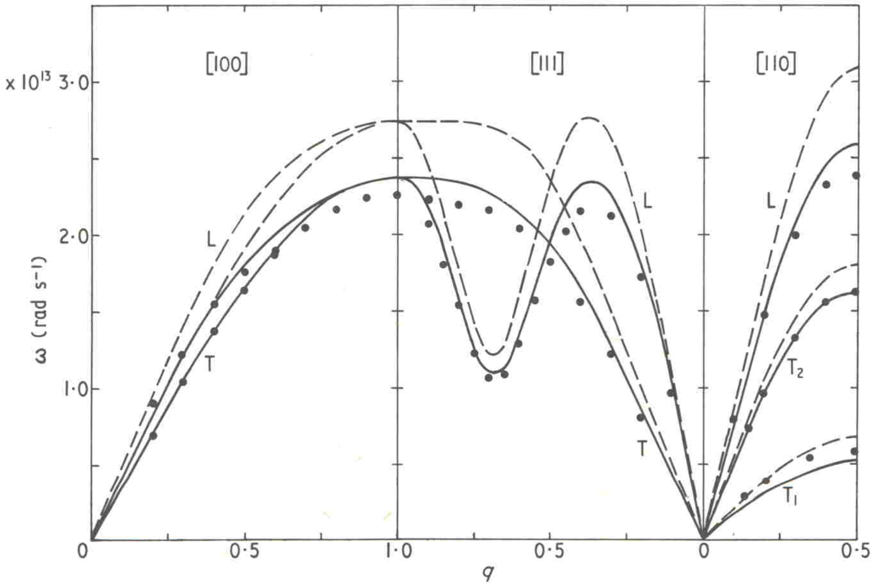

Figure 2. Phonon dispersion curves in Na. The full and broken curves represent calculations with the potentials corresponding to those in figure 1. The experimental points are taken from Woods *et al.* (1962). Units for the wave vector are also as in figure 1.

In Na, ω_c^2 and ω_E^2 do not cancel to the same degree as in Al, so the effects of any variations in the potential are not as pronounced. With both the Shaw and HA bare potentials, neglect of the exchange-correlation corrections in the dielectric function increases the L phonon frequency at the [110] zone boundary by 10% and the L elastic constants by 50%, but leaves the rest of the dispersion curves virtually unaltered (see tables 4 and 5). The different values of β yield results lying between these, with very little dependence on the actual form of $f(q)$. Therefore it is again necessary that these effects be included, while our results suggest that β_{AS} may again be preferable to β_H.

As in Al, Animalu's semi-non-local potential (1966) agrees closely with HA local. Comparing lines 1 and 2 in the tables 4 and 5, we see that Shaw's potential represents a distinct improvement, relative to experiment, over the local Ha potential. The elastic constants for

Table 4. Na phonon frequencies at the boundaries in units of 10^{13} rad s^{-1}

			100	110L	$110T_1$	$110T_2$
Experiment[a]			2·25	2·40	0·58	1·61
Calculations:						
potential	$f(q)$	β				
	(author and number of relevant equation in text)					
1. Shaw	Shaw (7)	Ashcroft and Shaw (6)	2·37	2·59	0·52	1·63
2. HA local	Shaw (7)	Ashcroft and Shaw (6)	2·73	3·11	0·68	1·81
3. HA local	none	—	2·73	3·32	0·67	1·80
4. HA + ω_R^2	Shaw (7)	Ashcroft and Shaw (6)	2·77	3·12	0·68	1·83

a, Woods *et al.* (1962), at 90 °K.

Table 5. Na elastic constants (in units of 10^9 Nm^{-2}) and pressure derivatives

		C_{11}	$\mathrm{d}C_{11}/\mathrm{d}P$	C_{44}	$\mathrm{d}C_{44}/\mathrm{d}P$	C'	$\mathrm{d}C'/\mathrm{d}P$
Experiment[a]		8·6	4·2	5·9	1·2	0·73	0·26
Calculations[b]	1.	8·1	—	5·9	—	0·58	—
	2.	11·4	4·8	7·3	1·6	1·00	0·3
	3.	17·7	6·2	7·2	1·6	0·97	0·3
	4.	10·6	4·9	7·5	1·8	1·00	0·3

a, Martinson (1969), at 80 °K; b, see table 4 for potential, $f(q)$ and β used for each set.

Shaw agree to within 5% with experiment, except for C' which is 20% too small. The HA potential, with Shaw's $f(q)$ in the screening, produces reasonably accurate elastic constants and pressure derivatives, considering the errors at the zone boundaries.

An estimate of the importance of the ω_R^2 can be obtained by using the Bleick–Mayer potential (Vosko 1964) for the exchange overlap interaction between Ne atoms. The results are given in line 4 of the tables 4 and 5. As Vosko argued, the interaction in metalic Na would be smaller by at least a factor $\frac{1}{16}$. Even without that reduction, the frequencies are altered by less than 2% and the pressure derivatives of the elastic constants by less than 5%, so we can certainly neglect the effect altogether. Effective mass corrections will probably have as small an effect in Na as the corrections to the dielectric function.

Compared with previous calculations, Shaw's phonons are rather closer to experiment than those of Vosko *et al.* (1965), but not quite as good as Ashcroft (1968) obtained with his local model potential. Ho (1968) fitted parameters in his local potential to reproduce the experimental elastic constants, but his errors at the zone boundaries are much the same as for the Shaw potential. Shyu and Gaspari (1969) obtained $C_{11} = 9{\cdot}6$ for Na, much the same as we have calculated with the HA potential, and also further from experiment than Shaw. Suzuki *et al.* (1968) fitted Ashcroft's potential to the experimental elastic constants and then found that their calculated pressure derivatives were less than 4% from experiment. Wallace (1968) fitted his potential to the measured crystal binding energy and its first two volume derivatives. His dispersion curves are then very good except for differences in the [110] branches of the same magnitude as Shaw's and Ho's.

Shaw's first-principles potential is thus as good as any of those which have been explicitly fitted to some experimental phonon data, and better than the local HA potential. We can therefore expect that it would also predict the pressure derivatives accurately. The calculations of Bortolani and Pizzichini (1969) for Li show that the inclusion of non-locality in the HA potential improves it significantly. This could also occur for Na. We should note