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}	dC_{11}/dP	C_{44}	dC_{44}/dP	C'	dC'/dP
Experiment[a]	8·6	4·2	5·9	1·2	0·73	0·26
	1. 8·1	—	5·9	—	0·58	—
Calculations[b]	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 $C_{11} = 9·6$ 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