

is used:

$$E_{\text{rep}} = \frac{1}{2} M \beta_{++} b_+^2 \exp \left(- \frac{A r_s}{\rho} \right)$$

where M is the number of nearest neighbors, and the parameters b_+ and ρ are from Fumi and Tosi's¹⁴ calculation. Although the value of E_{rep} is nearly negligible compared to the rest of the terms in the expression for the total energy, it becomes increasingly important after repeated differentiations with respect to r_s . Similar calculations of B_0 , B_0' and B_0'' with this repulsive term included have been carried out, and the results are listed in the third column of Tables II and III. However, the results are of questionable validity, because as remarked by Tosi¹⁵, there are uncertainties in these parameters b_+ and ρ arising from the uncertainties in the experimental values used in their determination.

Table III

	Expt'l	Theory (based on experimental B_0)	Theory (Born repulsive term included)
B_0^T	77 kb [*]	77 kb	77 kb
$B_0^{T'}$	3.904 ^{**}	3.945	4.092
$B_0^{T''}$	-0.0696 kb ^{-1**}	-0.0508 kb ⁻¹	-0.0519 kb ⁻¹

* extrapolated 0°K value

** 195°K value