where

$$B_{\mathrm{SC}}(L) = \frac{N}{18V}\sum_{k} (X_\alpha^k X_\beta^k \langle \phi_{\alpha\beta}^k \rangle_{\mathrm{SC}} - 2X_\alpha^k \langle \phi_\alpha^k \rangle_{\mathrm{SC}})$$

$$B_{\mathrm{SC}}(T) = \frac{1}{3MV}\sum_{k}\sum_{qs} S^k(q)\, X_\mu^k \langle \phi_{\alpha\beta\mu}^k \rangle_{\mathrm{SC}}\, e_\alpha^{qs} e_\beta^{qs}\, \frac{(U_{qs} + TC_{qs})}{\omega_{qs}^2}\, \gamma_{qs}^{\mathrm{SC}}$$

where $\gamma_{qs}^{\mathrm{SC}}$ is the self-consistent Grüneisen parameter discussed in Klein *et al.* (1970). $B_{\mathrm{SC}}(L)$ is recognizable as the smeared lattice contribution to B_{SC}. MK in their expression for the elastic constants gave the equivalent to this term only. $B_{\mathrm{SC}}(T)$ is the temperature-dependent part of B_{SC}. It involves an integral equation through its dependence on $\gamma_{qs}^{\mathrm{SC}}$, for if we write $\gamma_{qs}^{\mathrm{SC}}$ out fully we have

$$\begin{aligned}\gamma_{qs}^{\mathrm{SC}} = &-\frac{e_\alpha^{qs} e_\beta^{qs}}{3M\omega_{qs}^2}\sum_{k} S^k(q)\, X_\mu^k \langle \phi_{\alpha\beta\mu}^{\;k} \rangle_{\mathrm{SC}} - \frac{2e_\alpha^{qs} e_\beta^{qs}}{NM^2\omega_{qs}^2}\sum_{p\lambda}\sum_{k} S^k(p)\, S^k(q) \left(\frac{U_{p\lambda} + TC_{p\lambda}}{\omega_{p\lambda}^2}\right) \\ &\times e_\mu^{p\lambda} e_\nu^{p\lambda} \langle \phi_{\mu\nu\alpha\beta}^k \rangle_{\mathrm{SC}}\, \gamma_{p\lambda}^{\mathrm{SC}}. \end{aligned} \qquad (2.4)$$

This equation has been given and discussed in Klein *et al.* (1970). The integral equation arises out of the volume dependence of the correlation function Λ_k (see Klein *et al.*) occurring in the wave-function when the expectation values are taken.

3. Application and discussion

We have calculated the compressibility of solid ^{3}He and ^{4}He at 0 K in the molar volume range 12–18 cm^3. We used a Lennard-Jones (12–6) potential function ϕ.

$$\phi(r) = 4\varepsilon \left\{ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right\}$$

where $\varepsilon = 10{\cdot}22$ K and $\sigma = 2{\cdot}556$ Å. The parameters are the same as those used by MK and Horner (1970). The bulk modulus was calculated in two ways to give a check on numerical accuracy—firstly by numerical differentiation of the pressure using equation (2.2) and secondly using equation (2.3). The integral equation involved in the second calculation can be solved either by iteration or from frequencies calculated *ab initio* for different volumes. We used the latter method. Our results were further checked against an independent calculation made by V. V. Goldman (private communication). The compressibilities for ^{3}He and ^{4}He are displayed in figures 1 and 2 respectively together with the results of Horner (1970), MK and experiment.

Beyond 14 cm^3 molar volume our results are indicated by a dotted curve, because we found that for larger volumes there was appreciable penetration of the Gaussian wave function into the hard core of the potential. This resulted in the numerical integrations, needed to evaluate the expectation values, becoming sensitive to the cutoff in the repulsive part of the potential (see also MK). Thus at 12 cm^3 molar volume the free energy and bulk modulus changed by approximately 0·3% when the cutoff was varied over a distance of $0{\cdot}3\sigma$ inside the core. At 14 cm^3 the change was approximately 0·5% over a region of cutoff variation of $0{\cdot}2\sigma$. At 16 and 18 cm^3 molar volume the variation with cutoff is more pronounced and the actual values taken for the integrals become more uncertain. For this reason the results beyond 14 ccs are indicated by a dotted curve. Even with the uncertainty in these values it can be seen that our calculations, which included the explicit temperature dependent part of the bulk modulus $B_{\mathrm{SC}}(T)$, remove the major part of the difference between MK's compressibilities and experiment. At high pressures, where our results are more certain, they agree better with experiment than Horner's. The difference between Horner's and the values calculated here can be taken as a measure of the effect of numerical approximations, src, structure etc.

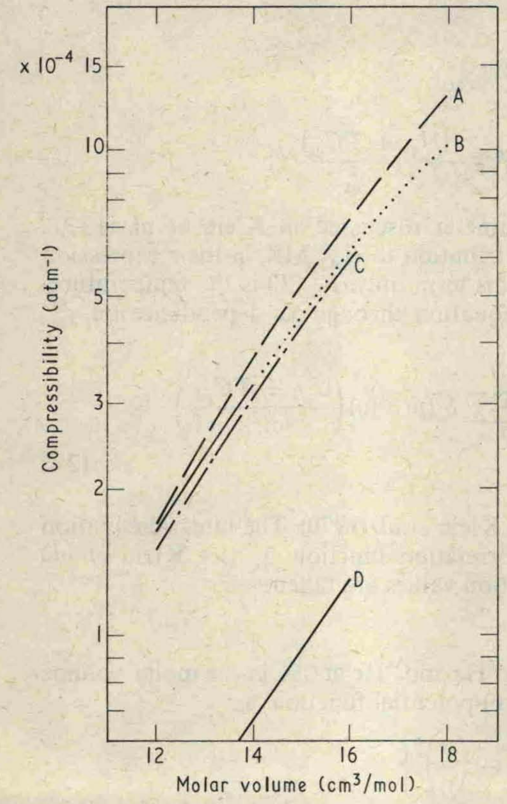

Figure 1. Compressibility of ^{3}He against molar volume. A, Horner (1970); B, present paper; C, experiment (Dugdale and Franck 1964); D, Morley and Kliewer (1969).

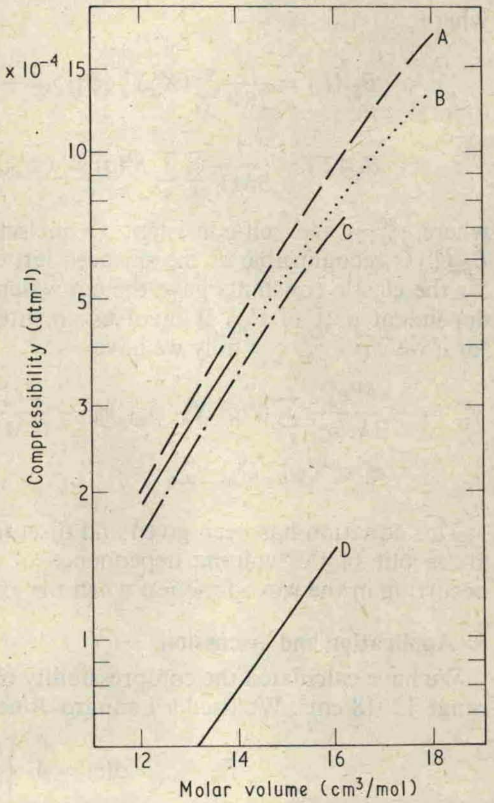

Figure 2. Compressibility of ^{4}He against molar volume. A, B, C, D, same references as in figure 1.

We summarize the results as follows. The present calculations illustrate three things: (i) the desirability of using the complete expression, equation (2.3), for calculating the bulk modulus and compressibility of helium; (ii) up to a molar volume of approximately 14 cm^3, compressibilities that are independent of cutoff are obtained without the use of src; (iii) the major difference between MK's compressibilities and experiment is due to the former's incomplete expressions for the SCP elastic constants and not their neglect of src.

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