

The energy-wavenumber characteristic  $F(q)$  is given, to second order in the HA model potential and in the 'semi-non-local' approximation, by (Animalu 1966).†

$$F(q) = \left\{ \frac{4\pi Z(1 + \alpha_{\text{eff}})}{\Omega q^2} \right\}^{-2} v(q) u_b(q) \frac{\epsilon(q) - 1}{1 - f(q)} \quad (2)$$

where  $\Omega$  is the atomic volume and  $Z$  the ionic charge. In the local approximation, the screened model potential  $v(q) = u_b(q)/\epsilon(q)$ , where the bare potential  $u_b(q)$  is given by Animalu and Heine (1965) and the dielectric function is

$$\epsilon(q) = 1 + \{1 - f(q)\} (1 + \alpha_{\text{eff}}) \frac{\lambda}{2y^2} \left\{ 1 + \frac{1 - y^2}{2y} \ln \left| \frac{1 + y}{1 - y} \right| \right\} \quad (3)$$

where  $y = q/2k_F$ ,  $\lambda = (\pi k_F)^{-1}$  and  $(1 + \alpha_{\text{eff}})$  is the orthogonalization hole correction factor introduced by Animalu and Heine (1965). In the theories of both Animalu *et al.* (1966) and Shaw (1969 a) a factor such as this appears in  $F(q)$  and in the plasma frequency because the ions are treated as having charge  $Z(1 + \alpha_{\text{eff}})$ . It appears in  $\epsilon(q)$  only when used with HA potentials, having been introduced by them to correct for an approximation in their treatment of the bare potential.

The function  $f(q)$  corrects for exchange and correlation effects among the conduction electrons. In the Hartree approximation  $f(q) = 0$ . From an approximate evaluation of higher order graphs, Hubbard (Falicov and Heine 1961) suggested that this correction could be approximated by

$$f_H(q) = \frac{1}{2} y^2 (y^2 + \beta)^{-1} \quad (4)$$

with

$$\beta_H = \frac{1}{4} (1 + 4\lambda). \quad (5)$$

More recently, Geldart and Vosko (1965) chose  $\beta$  to satisfy a fundamental relation between the compressibility of an interacting electron gas and its dielectric function for  $q \rightarrow 0$ . Ashcroft (1968) and Shaw and Pynn (1969) have obtained a slightly different value of  $\beta$  in a similar calculation based on the Nozières-Pines (1958) interpolation formula for the energy of an interacting electron gas:

$$\beta_{AS} = \frac{1}{2} (1 + 0.153\lambda)^{-1}. \quad (6)$$

Using the higher-order corrections to the exchange and correlation energies obtained by Ma and Brueckner (1968), Shaw found that an even better approximation for  $q \rightarrow 0$  was given by

$$f_S(q) = \frac{1}{2} \{1 - \exp(-2y^2)\} + \frac{4\gamma}{k_F} y^2 \exp\left(-\frac{4\alpha k_F}{\gamma} y^2\right) \quad (7)$$

with  $\alpha = 0.0538$  and  $\gamma = 0.0122$ . Each of (4) and (7) have also been designed so that  $\{1 - f(q)\} \rightarrow \frac{1}{2}$  as  $q \rightarrow \infty$ , implying that exchange corrections halve the effective interaction between electrons in this limit. However, Kleinman (1967, 1968) has argued that in fact  $f(q) = O(q^2)$  for  $q \rightarrow \infty$ , in agreement with the correction factor he obtained from both self-consistent field and diagrammatic techniques:

$$f_K(q) = \frac{1}{4} \left( \frac{y^2}{y^2 + \beta} + \frac{y^2}{\beta} \right). \quad (8)$$

Even more recent work by Langreth (1969) has confirmed this form for large  $q$ , but detailed calculations by Geldart and Taylor (1970 a, b) do not, so the subject is still open. In each case, the form of  $f(q)$  has simply been chosen to interpolate smoothly between the determined

† We use atomic units throughout.