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).†

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

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

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

where $y = q/2k_{\text{F}}$, $\lambda = (\pi k_{\text{F}})^{-1}$ 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

$$f_{\text{H}}(q) = \tfrac{1}{2}y^2(y^2+\beta)^{-1} \tag{4}$$

with

$$\beta_{\text{H}} = \tfrac{1}{4}(1+4\lambda). \tag{5}$$

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

$$\beta_{\text{AS}} = \tfrac{1}{2}(1+0{\cdot}153\lambda)^{-1}. \tag{6}$$

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 $q \to 0$ was given by

$$f_{\text{S}}(q) = \tfrac{1}{2}\{1 - \exp(-2y^2)\} + \frac{4\gamma}{k_{\text{F}}}y^2\exp\left(-\frac{4\alpha k_{\text{F}}}{\gamma}y^2\right) \tag{7}$$

with $\alpha = 0{\cdot}0538$ and $\gamma = 0{\cdot}0122$. Each of (4) and (7) have also been designed so that $\{1 - f(q)\} \to \frac{1}{2}$ as $q \to \infty$, implying that exchange corrections halve the effective interaction between electrons in this limit. However, Kleinman (1967, 1968) has argued that in fact $f(q) = \mathrm{O}(q^2)$ for $q \to \infty$, in agreement with the correction factor he obtained from both self-consistent field and diagrammatic techniques:

$$f_{\text{K}}(q) = \frac{1}{4}\left(\frac{y^2}{y^2+\beta} + \frac{y^2}{\beta}\right). \tag{8}$$

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.