

# Many-Body Interaction

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**Abstract**

Many-body interaction is a fundamental concept in quantum mechanics that describes the interaction between multiple particles. This phenomenon is crucial in understanding various physical systems, including solids, liquids, and gases. In this article, we provide an overview of many-body interaction, its significance, and its applications.

**Keywords:** Many-body interaction, quantum mechanics, quantum field theory, second quantization, Hartree-Fock method, density functional theory.

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## I. Introduction

The many-body interaction [A.K. Sarkar and S. Sengupta Phys. Stat.Solidi 36, 359 [1967], is given by

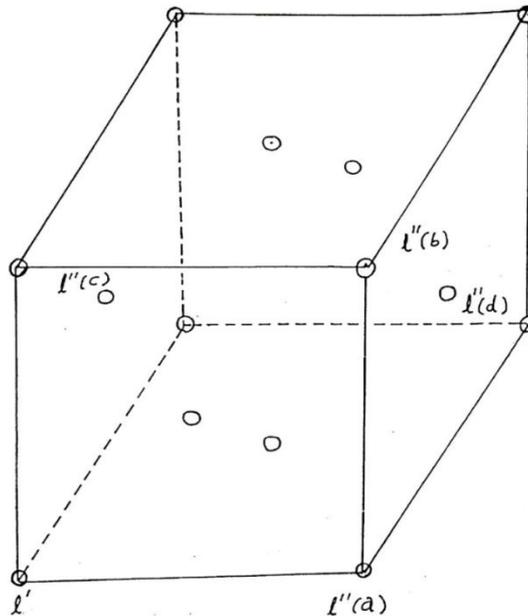
$$\phi^m = \frac{1}{2} \sum_{1'1''} \sum_{cnn} A \cdot \exp \left[ \frac{r(11') + r(11'')}{p} \right] \quad \dots(1)$$

Where p and A are the parameters for many-body interactions.

In the equation (1), the summation 1 runs over all the atoms which are common nearest neighbours of the atoms 1' and 1''  $\vec{r}(1)$  is the position vector of the atom in the 1<sup>th</sup> lattice and  $\vec{r}(u') = \vec{r}(1) - \vec{r}(1')$ .

We shall consider a FCC lattice of lattice-constant  $2r_0$  and nearest neighbour distance  $r = \sqrt{2} \cdot r_0$ . we shall calculate the force constant matrices for the many-body interactions given by equation(1). The force-constant between two atoms (1'1'') which have common nearest neighbours is given by

$$\begin{aligned} \phi_{1'1''}^m &= \frac{\partial^2 \phi}{\partial r_i(1') \partial r_{i'}(1'')} \\ &= \sum_{1(cnn)} A \cdot \frac{\exp\left(\frac{-2r}{p}\right)}{p^2 \cdot r^2} r_i(11') \cdot r_{i'}(11'') \quad \dots(2) \end{aligned}$$



**Fig. (1):** This figure shows the positions of the particles for which non-vanishing three body-force constants exist other particles are obtained by symmetry.

The force constant matrices for different types of atoms as shown in Fig.(1) are as follows-

$$\begin{aligned} \phi^m(1'a) &= p \begin{vmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} & \phi^m(1'b) &= -\frac{1}{2}p \begin{vmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{vmatrix} & \dots(3) \\ \phi^m(1'c) &= p \begin{vmatrix} 2 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{vmatrix} & \phi^m(1'd) &= -\frac{1}{2}p \begin{vmatrix} 1 & 0 & 1 \\ 2 & 1 & 1 \\ 1 & 1 & 0 \end{vmatrix} \end{aligned}$$

Where  $P = \left(\frac{A}{P^2}\right) \exp\left[-\frac{2r}{P}\right]$

In addition to the above, equation (1) gives a non-vanishing force constant between nearest neighbours which is essentially of the same form as that of a two-body interaction and is given by

$$\phi_{ii'}(11') = \Sigma_{1'' \neq 1'(n.n.of 1)} \phi_{ii'}[r(11'), r(11'')] + \Sigma_{1'' \neq 1(n.n.of 1')} \phi_{ii'}[r(11), r(1'1'')]$$

Where

$$\phi_{ii'}[r(11') \cdot r(11'')] = \frac{A}{P} \left[ -\frac{r_i(11') \cdot r_{i'}(11'')}{r(11')^3} + \frac{\partial_{ii'}}{r(11')} - \frac{r_i(11')r_{i'}(11'')}{P \cdot r(11')^2} - \frac{r_i(11') \cdot r_{i'}(11'')}{P \cdot r(11')r(11'')} \right] \exp\left[-\frac{r(11')+r(11'')}{P}\right] \dots(4)$$

This gives the force constant matrix between the atoms (001) and (010) as

$$\phi(1'n) = \begin{vmatrix} -10P + \frac{11}{\sqrt{2}}Q & 0 & -10P - \frac{11}{\sqrt{2}}Q \\ 0 & 11\sqrt{2}Q & 0 \\ -10P - \frac{11}{\sqrt{2}}Q & 0 & -10P + \frac{11}{\sqrt{2}}Q \end{vmatrix} \dots(5)$$

Where  $Q = \frac{A}{P \cdot r_o} \exp\left[-\frac{2r}{P}\right]$

Using the force constant matrices given in equations (3) and (5), we get the following elements of the dynamical matrix for the many-body interaction

$$\begin{aligned} D_{ii}^m(\vec{q}) &= \frac{1}{m} \left[ 8P \sin^2 q_1 \cdot \frac{a}{2} - 4P \left( \sin^2 q_j \cdot \frac{a}{2} + \sin^2 q_k \cdot \frac{a}{2} \right) - 2P \cos q_i \cdot a \left( \cos q_j \cdot a + \cos q_k \cdot a \right) \right. \\ &\quad + 8P \cos q_i \cdot \frac{a}{2} \cdot \cos q_j a \cdot \cos q_k a - (40P - 22\sqrt{2}Q) \cos q_i \frac{a}{2} \left( \cos q_j \frac{a}{2} + \cos q_k \frac{a}{2} \right) \\ &\quad + 44\sqrt{2}Q \cos q_j \frac{a}{2} \cos q_k \frac{a}{2} - 84P \\ &\quad \left. + 88\sqrt{2}Q \right] \dots(6) \end{aligned}$$

$$\begin{aligned} D_{ij}^m(\vec{q}) &= \frac{1}{m} \left[ 2P \cdot \sin q_i a \sin q_j a + 4P \sin q_i \frac{a}{2} \cdot \sin q_j \frac{a}{2} \right. \\ &\quad + 4P \left( \sin q_i a \cdot \sin q_j \frac{a}{2} + \sin q_i \frac{a}{2} \cdot \sin q_j a \right) \cos q_k \frac{a}{2} + 4P \sin q_i \frac{a}{2} \cdot \sin q_k \frac{a}{2} \\ &\quad \left. + (40P + 22\sqrt{2}Q) \sin q_i \frac{a}{2} \sin q_j \frac{a}{2} \right] \dots(7) \end{aligned}$$

Other elements of the dynamical matrix for the many-body interaction can be written by the cyclic permutation of the indices  $i, j$  and  $k$ .

## II. Elements Of Dynamical Matrix For Long-Rance Interaction

The matrix-elements corresponding to the ion-electron (long-range) interaction have been obtained by picturing the metallic crystal to consist of a series of point-ions immersed in a uniform compensation background of free-electron gas. The displacement  $\vec{u}(1'k')$  of  $(1'k')$  the ion from its equilibrium position,  $\vec{R}^o$  gives rise to a change in the electrostatic potential of the system at the point  $\vec{r}$  which can be written as

$$Z(1'k')e \left[ V^{I-E} \left\{ \vec{r} - \vec{R}(1'k') \right\} - V^{I-E} \left\{ \vec{r} - \vec{R}^o(1'k') \right\} \right] \dots(8)$$

Where  $\vec{R}(1'k') = \vec{R}^o(1'k') + \vec{u}(1'k')$  is the position of the  $(1'k')^{th}$  ion after displacement and  $[Z_{(1'k')}e]$  is the charge on this ion.  $V^{I-E}$  is the long range potential produced by a unit charge at the origin. The force exerted on the  $(1k)^{th}$  ion having charge  $[Z_{(1k)}e]$  is given by

$$\begin{aligned} \vec{F} &= [-Z_{(1k)}Z_{(1'k')}e^2] \nabla [V^{I-E} \left\{ \vec{r} - \vec{R}(1'k') \right\} - V^{I-E} \left\{ \vec{r} - \vec{R}^o(1'k') \right\}] \vec{R}(1'k') = \vec{R}^o(1'k') \\ &= \{-Z_{(1k)}Z_{(1'k')}e^2\} \nabla [\nabla V^{I-E} \left( \frac{\vec{r}}{R} \right)] \vec{u}(1'k') \\ &= -\nabla^2 \left[ \{Z_{(1k)}Z_{(1'k')}e^2\} V^{I-E} \left( \frac{\vec{r}}{R} \right) \right] \vec{u}(1'k') \\ &= -\nabla^2 \left[ V \left( \frac{\vec{r}}{R} \right) \right] \vec{u}(1'k') = -V_{ij}(1k, 1'k')u(1'k') \dots(9) \end{aligned}$$

Where  $\vec{R} = \left[ \vec{R}^o(1k) - \vec{R}^o(1'k') \right]$  is the equilibrium separation between  $(1k)^{th}$  ion and  $(1'k')^{th}$  ion.

$V(R) = \{Z_{(1k)}Z_{(1'k')}e^2\}V^{I-E}(\vec{R})$   
 = potential energy of the pair of ions (1k) and (1'k') and  $V_{ij}(1k, 1'k')$  is the force constant matrix.

For a screened charge the interaction potential is of the form  
 $V^{I-E} \sim R^{-1}e^{-\lambda R}$  ... (10)

Where  $\lambda$  is the screening parameter.

As the calculation of the force constant matrix is conveniently carried out in the momentum space, we work with the Fourier transform of the potential function  $V^{I-E}$  which is given by

$$V^{I-E} = \frac{4\pi}{(2\pi)^3} \int \frac{[\exp(i\vec{k} \cdot \vec{R})]d\vec{k}}{|\vec{k}|^2 + \lambda^2(|\vec{k}|)} \dots (11)$$

Here  $\vec{k}$  is the electron wave vector and  $\lambda(|\vec{k}|)$  a wave vector dependent screening parameter.

The long-range dynamical matrix representing the ion-electron interaction is therefore given by

$$D_{ij}^{I-E}(\vec{q}) = \sum_{1'} V_{ij}(1k, 1'k') \exp[-i\vec{q} \cdot \{R^o(1k) - R^o(1'k')\}] \dots (12)$$

From above equations matrix element is obtained which is written as

$$D_{ij}^{I-E}(\vec{q}) = \sum_{1'} \frac{4\pi Z_{(1k)}Z_{(1'k')}e^2}{(2\pi)^3} \left[ \int \frac{k_i k_j \exp(i\vec{k} \cdot \vec{R}) [\exp[-i\vec{q} \cdot \{R^o(1k) - R^o(1'k')\}]] d\vec{k}}{|\vec{k}|^2 + \lambda^2(|\vec{k}|)} \right]$$

$$= \frac{4\pi e^2 Z_{1k} Z_{1'k'}}{(2\pi)^3} \left[ \int \frac{k_i k_j d\vec{k} \sum_{1'} \exp[-i(\vec{q} - \vec{k}) \cdot R^o(1k) - R^o(1'k')]}{|\vec{k}|^2 + \lambda^2(|\vec{k}|)} \right] \dots (13)$$

Now we use the sum rule

$$\exp[-i(\vec{q} - \vec{k}) \cdot R^o(1k) - R^o(1'k')] = (2\pi)^3 \sum_{\vec{h}} \delta(\vec{q} - \vec{k} + \vec{h}) \dots (14)$$

Where  $\vec{h}$  is the reciprocal lattice vector.  $\delta$  is the usual Dirac delta function and  $\Omega$  is the atomic volume. Thus from equation (13) we get

$$D_{ij}^{I-E}(\vec{q}) = \frac{4\pi e^2 Z_{(1k)}Z_{(1'k')}}{\Omega} \frac{\sum_{\vec{h}} (\vec{q} + \vec{h})_i (\vec{q} + \vec{h})_j}{|\vec{q} + \vec{h}|^2 + \lambda^2(|\vec{q} + \vec{h}|)} + C \dots (15)$$

The constant C is determined by the boundary condition of infinitesimal displacement invariance which implies that  $D_{ij}^{I-E}(\vec{q})$  should vanish for non-vibrating lattice. From this we obtain

$$C = -\frac{4\pi e^2 Z_{(1k)}Z_{(1'k')}}{\Omega} \sum_{\vec{h} \neq 0} \frac{h_i h_j}{|\vec{h}|^2 + \lambda^2(|\vec{h}|)}$$

And equation (15) reduces to

$$D_{ij}^{I-E}(\vec{q}) = \frac{4\pi Z_{(1k)}Z_{(1'k')}e^2}{\Omega} \left[ \sum_{\vec{h}} \frac{(\vec{q} + \vec{h})_i (\vec{q} + \vec{h})_j}{|\vec{q} + \vec{h}|^2 + \lambda^2(|\vec{q} + \vec{h}|)} - \sum_{\vec{h} \neq 0} \frac{h_i h_j}{|\vec{h}|^2 + \lambda^2(|\vec{h}|)} \right]$$

$$= k_e \Omega \lambda^2(o) \left[ \sum_{\vec{h}} \frac{(\vec{q} + \vec{h})_i (\vec{q} + \vec{h})_j}{|\vec{q} + \vec{h}|^2 + \lambda^2(|\vec{q} + \vec{h}|)} - \sum_{\vec{h} \neq 0} \frac{h_i h_j}{|\vec{h}|^2 + \lambda^2(|\vec{h}|)} \right] \dots (16)$$

Where

$$K_e = \frac{4\pi e^2 Z_{(1k)}Z_{(1'k')}}{\Omega^2 \lambda^2(o)}$$

Is a constant depending upon the effective charge of the ions and the screening parameter  $\lambda(o)$ . Finally we obtain the following expression by substituting  $A$  For  $k_e \Omega \lambda^2(o)$  in equation (16)

$$D_{ij}^{I-E}(\vec{q}) = A \left[ \sum_{\vec{h}} \frac{(\vec{q} + \vec{h})_i (\vec{q} + \vec{h})_j}{|\vec{q} + \vec{h}|^2 + \lambda^2(|\vec{q} + \vec{h}|)} - \sum_{\vec{h} \neq 0} \frac{h_i h_j}{|\vec{h}|^2 + \lambda^2(|\vec{h}|)} \right] \dots (17)$$

The reciprocal vector  $\vec{h}$  determined by the structure of the crystal. In  $\vec{h}$  summation  $h_x + h_y + h_z$  should be even for BCC lattice and  $h_x + h_y + h_z$  should be all odd or all even in FCC lattices.

Langer and Vosko showed that the screening parameter in a high density electron gas was a function of electron wave number  $\vec{k}$  and so screening parameter should be multiplied by a function  $f(t)$ , where

$$f(t) = 0.5 + \frac{1-t^2}{4t} \log \frac{1+t}{1-t} \dots (18)$$

With  $t = \frac{\vec{k}}{2k_F}$ , where  $K_F$  is known as Fermi wave vector. Function  $f(t)$  goes to unity for  $t = 0$  and has a logarithmic singularity as  $t = 1$ , which gives rise to the so called Kohn anomalies in the dispersion curves.

The effective potential for large  $\vec{K}$  values corresponding to the core-region of the ion, consists of two parts viz. the potential energy of the nucleus which is negative and high kinetic energy associated with the rapid oscillations of the wave function within the core-region which is positive. The former is very nearly compensated by the later, and for large wave vector, there is, indeed, a tendency towards the exact cancellation of the two terms as shown by Phillips and Kleinman and Cohen et al and also by Sham and Ziman in the case of monoatomic metals in which the Fermi surface does not deviate much from the spherical symmetry and also does not approach close to a zone-boundary.

This cancellation effect was taken into account by introducing the decay function  $g^2(x)$  in the dynamical matrix such that

$$g^2(x) = \left[ \frac{3(\sin x - x \cos x)}{x^3} \right] \dots(19)$$

$$\text{Where } x = \left| \vec{q} + \vec{h} \right| \cdot r_e,$$

$$r_e = \text{inter electron spacing} = \left( \frac{3}{4\pi n_e} \right)^{\frac{1}{3}}, n_e \text{ being the electron density. In the case of monovalent metals}$$

$r_e$  is equal to the radius of atomic sphere  $r_o$ . In the case of polyvalent metals, however  $r_e = Z^{-\frac{1}{3}}(r_o)$ , where  $z$  represents the valency of metals.

Wall and Kohn have shown that introduction of  $g^2(x)$  is the essential modification of the free electron result which occurs if one assumes that the electron wave functions are of the Bloch-type. Some times this is referred to as the overlap integral or interference factor and follows from the wigner-Seitz model for the band structure. Krebs also suggested to insert this function in the expression of  $D_{ij}^{I-E}(\vec{q})$  to simulate the reducing effect of large  $h$  values. In the light of above facts the modified expressions for the matrix elements are given by

$$D_{ij}^{I-E}(\vec{q}) = A \left[ \sum_{\vec{h}} \frac{(\vec{q} + \vec{h})_i (\vec{q} + \vec{h})_j g^2(|\vec{q} + \vec{h}|) \cdot r_e}{|\vec{q} + \vec{h}|^2 + \lambda^2 (\vec{q} + \vec{h}) f(t_1)} - \sum_{\vec{h} \neq 0} \frac{h_e^2 g^2(|h| \cdot r_e)}{|\vec{h}|^2 + \lambda^2 (|\vec{h}|) f(t_2)} \right] \dots(20) \quad D_{ij}^{I-E}(\vec{q}) =$$

$$A \left[ \sum_{\vec{h}} \frac{(\vec{q} + \vec{h})_i (\vec{q} + \vec{h})_j g^2(|\vec{q} + \vec{h}|) \cdot r_e}{|\vec{q} + \vec{h}|^2 + \lambda^2 (\vec{q} + \vec{h}) f(t_1)} - \sum_{\vec{h} \neq 0} \frac{h_i h_j g^2(|\vec{h}| \cdot r_e)}{|\vec{h}|^2 + \lambda^2 (|\vec{h}|) f(t_2)} \right] \dots(21)$$

If we take wigner-Seitz spheres and assume a uniform charge distribution of conduction electrons in the spheres, the boundary conditions on the ion-electron pseudopotential  $V^{I-E}$  are

$$V^{I-E} = \frac{Ze^2}{r} \quad r > r_o$$

$$= \frac{3Ze^2}{2r_o} - \frac{Ze^2 r^2}{2r_o^3} \quad r < r_o$$

Using this expression for ion-electron pseudopotential Fielek has obtained the following expression for the matrix elements.

$$D_{ij}^{I-E}(\vec{q}) = A \sum_{\vec{h}} \left[ \frac{(\vec{q} + \vec{h})_i (\vec{q} + \vec{h})_j g^2(\vec{q} + \vec{h}) r_o}{|\vec{q} + \vec{h}|^2 + \theta (\vec{q} + \vec{h}) \lambda_{TF}} - \frac{\vec{h} \cdot \vec{h} g^2(|\vec{h}| r_o)}{|\vec{h}|^2 + \lambda \theta (|\vec{h}|) \lambda_{TF}} \right] \dots(22)$$

Where  $\theta$  is the dielectric function,  $\lambda_{TF}$  is the Thomas-Fermi screening parameter, is the Bohm-Pines screening parameter and  $r_o$  is the Wigner-Seitz radius obtained from the unit cell volume.

It may be noted that Krebs expressions can be obtained from the first principle by considering the ion to be a uniformly spherical charge distribution of radius  $r_o$ . As mentioned earlier  $r_o$  is equal to  $r_e$  is equal to  $r_e$ , the inter electron spacing for mono-valent metals.

### III. Elastic Constants And Model Parameters

The secular determinants can be expanded in the long wavelength limit ( $q \rightarrow 0$ ) because the wavelength of the plane wave in this case is much longer than the lattice spacing and medium behaves just like a continuous medium for the propagation of waves.

Comparing the expanded determinants for long waves with the christoffel's equation for the elastic waves in ordinary elastic continuum, we get the following expressions for the three elastic constants in terms of model parameters.

$$A[C_{11} - K_e] = 2\alpha_1 + 4\alpha_2 + 72P - 22\sqrt{2}Q \dots(23)$$

$$a[C_{12} - K_2] = \alpha_1 + 36P + 35\sqrt{2}Q \dots(24)$$

$$aC_{44} = \alpha_1 + 32P - 33\sqrt{2}Q \dots(25)$$

Where  $K_e$  is the Bulk-modulus of electron gas.

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