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Two Body and Central-Interaction

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Abstract: ***This study presents a comprehensive analysis of the two-body central-interaction problem in quantum mechanics. We investigate the Schrödinger equation for two particles interacting through a central potential, and derive the radial and angular parts of the wave function. The energy eigenvalues and Eigen functions are obtained for various central potentials, including the Coulomb, harmonic oscillator, and square well potentials.***

Keywords: Two-body central-interaction, quantum mechanics, Schrödinger equation, central potential, energy eigenvalues, Eigen functions

1. Introduction

When the forces between atoms act along the line joining the two atoms they are called central forces. Let A and B [Fig. (1)] denote the equilibrium position of the 1^{th} *and* $1'^{th}$ atoms separated by a distance d. Let θ_1, denote the unit vector along the line A to B and α the force constant $\vec{u}(1)$ and $\vec{u}(1')$ denote displacements of the two atoms from their equilibrium positions. These displacements are assumed to be much smaller than the interatomic distance. Thus even in the displaced positions the restoring force may be assumed to be in the direction $\vec{\theta}_{1'}$ Now the distance between the two atoms in their displaced position is

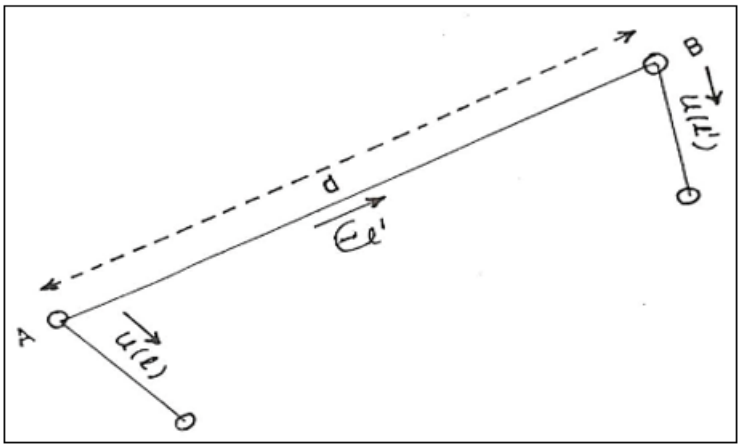

Figure 1: in this fig. A and B shows the equilibrium position of 1^{th} *and* $1'^{th}$ atoms.

$$\left|d\vec{\theta}_{1'} + \vec{u}(1') - \vec{u}(1)\right| \sim \left[d^2 + 2d\vec{\theta}_{1'}\left[\vec{u}(1') - \vec{u}(1)\right]\right]^{\frac{1}{2}} - d + \vec{\theta}_{1'}\left[\vec{u}(1') - \vec{u}(1)\right]$$

Thus, the increase in the interatomic distance is approximately $\vec{\theta}_{1'}\left[\vec{u}(1') - \vec{u}(1)\right]$.

Assuming the restoring force to be central with force constant a we must have

$$\vec{F}(1') = \alpha\left[\vec{\theta}_{1'}\left[\vec{u}(1') - \vec{u}(1)\right]\right]\theta_1 \quad \ldots(1)$$

Here $\vec{F}(1')$ is the force acting on the 1^{th} atom due to displacement of the $1'^{th}$ atom.

Let $\lambda_\beta(1')\ [\beta = 1,2,3]$ be the direction cosines of $\vec{\theta}_{1'}$. Denoting $F_\alpha(1)$ as the α-components of vec $\vec{F}(1')$, where α =1,2,3 for x, y, and z directions respectively, we have

$$F_1(1') = \alpha \bullet \lambda_1(1')\{\lambda_1(1')[u_1(1') - u_1(1)] + {}_2(1')[u_2(1') - u_2(1)] + {}_3(1')[u_3(1') - u_3(1)]\}$$
$$= \alpha \bullet \lambda_1(1') \sum_{\beta=1,2,3} \lambda \bullet_\beta (1')\left[u_\beta(1') - u_\beta(1)\right] \quad \ldots(2)$$

Thus, in general,

$$F_\alpha(1') = \alpha \bullet \lambda_\alpha(1') \sum_\beta \lambda_\beta(1')\left[u_\beta(1') - u_\beta(1)\right] \quad \ldots(3)$$

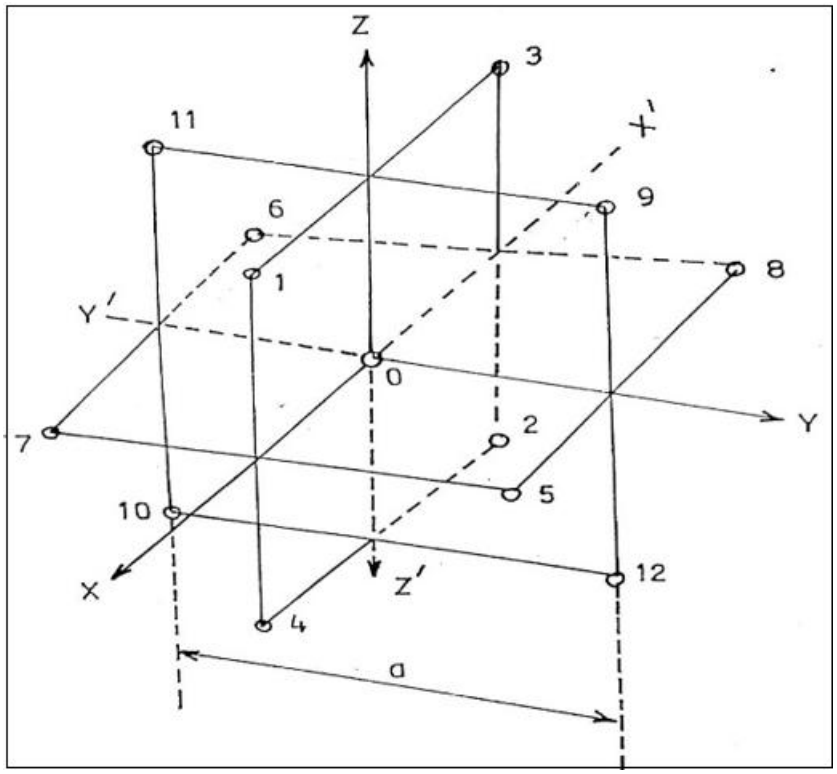

Figure 2: The 12 nearest neighbours of atom (o) of FCC lattice.

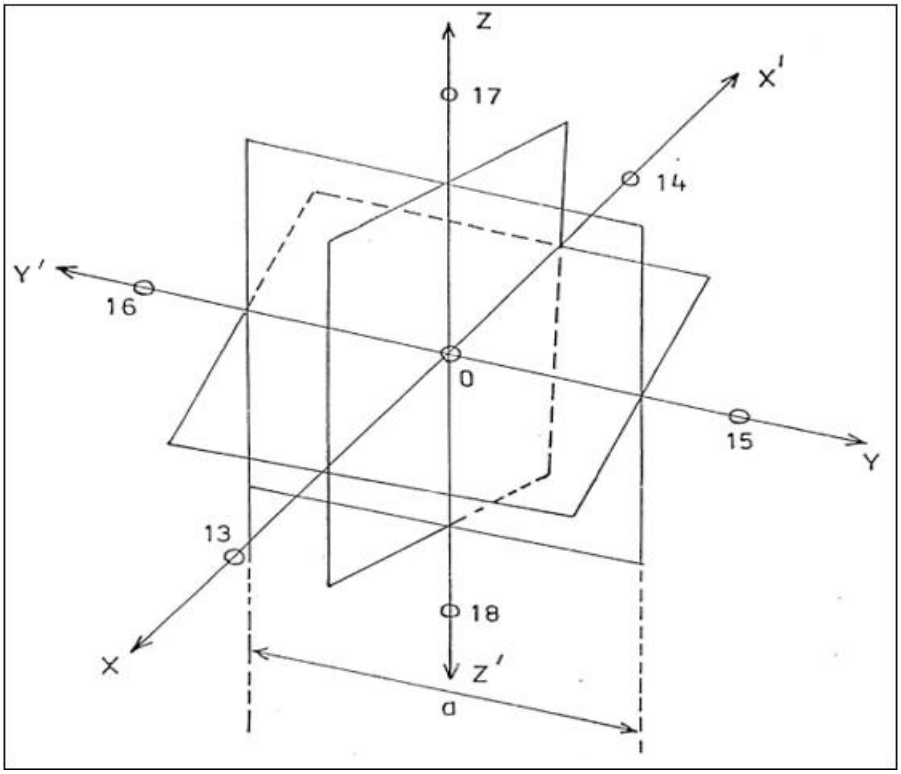

Figure 3: The six next nearest neighbours of atom (o) of FCC lattice.

Table

1	X_1	Y_1	Z_1	$1^{(1)}$	$2^{(1)}$	$3^{(1)}$	X_l	Y_l	Z_l
1	$\frac{a}{2}$	0	$\frac{a}{2}$	$\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	$-\frac{\alpha_1}{2}[u_1(0)-u_1(1)+u_3(0)-u_3(1)]$	0	$-\frac{\alpha_1}{2}[u_3(0)-u_3(1)+u_1(0)-u_1(1)]$
2	$-\frac{a}{2}$	0	$-\frac{a}{2}$	$-\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	$-\frac{\alpha_1}{2}[u_1(0)-u_1(2)+u_3(0)-u_3(2)]$	0	$-\frac{\alpha_1}{2}[u_3(0)-u_3(2)+u_1(0)-u_1(2)]$
3	$-\frac{a}{2}$	0	$\frac{a}{2}$	$-\frac{1}{\sqrt{2}}$	0	$\frac{1}{\sqrt{2}}$	$-\frac{\alpha_1}{2}[u_1(0)-u_1(3)-u_3(0)+u_3(3)]$	0	$-\frac{\alpha_1}{2}[u_3(0)-u_3(3)-u_1(0)+u_1(3)]$
4	$\frac{a}{2}$	0	$-\frac{a}{2}$	$\frac{1}{\sqrt{2}}$	0	$-\frac{1}{\sqrt{2}}$	$-\frac{\alpha_1}{2}[u_1(0)-u_1(4)-u_3(0)+u_3(4)]$	0	$-\frac{\alpha_1}{2}[u_3(0)-u_3(4)-u_1(0)+u_1(4)]$
5	$\frac{a}{2}$	$\frac{a}{2}$	0	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	0	$-\frac{\alpha_1}{2}[u_1(0)-u_1(5)+u_2(0)-u_2(5)]$	$-\frac{\alpha_1}{2}[u_2(0)-u_2(5)+u_1(0)-u_1(5)]$	0
6	$-\frac{a}{2}$	$-\frac{a}{2}$	0	$-\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	0	$-\frac{\alpha_1}{2}[u_1(0)-u_1(6)+u_2(0)-u_2(6)]$	$-\frac{\alpha_1}{2}[u_2(0)-u_2(6)+u_1(0)-u_1(6)]$	0
7	$\frac{a}{2}$	$-\frac{a}{2}$	0	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	0	$-\frac{\alpha_1}{2}[u_1(0)-u_1(7)-u_2(0)+u_2(7)]$	$-\frac{\alpha_1}{2}[u_2(0)-u_2(7)-u_1(0)+u_1(7)]$	0
8	$-\frac{a}{2}$	$\frac{a}{2}$	0	$-\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	0	$-\frac{\alpha_1}{2}[u_1(0)-u_1(8)-u_2(0)+u_2(8)]$	$-\frac{\alpha_1}{2}[u_2(0)-u_2(8)-u_1(0)+u_1(8)]$	0
9	0	$\frac{a}{2}$	$\frac{a}{2}$	0	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	0	$-\frac{\alpha_1}{2}[u_2(0)-u_2(9)+u_3(0)-u_3(9)]$	$-\frac{\alpha_1}{2}[u_3(0)-u_3(9)+u_2(0)-u_2(9)]$
10	0	$-\frac{a}{2}$	$-\frac{a}{2}$	0	$-\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	0	$-\frac{\alpha_1}{2}[u_2(0)-u_2(10)+u_3(0)-u_3(10)]$	$-\frac{\alpha_1}{2}[u_3(0)-u_3(10)+u_2(0)-u_2(10)]$
11	0	$-\frac{a}{2}$	$\frac{a}{2}$	0	$-\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	0	$-\frac{\alpha_1}{2}[u_2(0)-u_2(11)-u_3(0)+u_3(11)]$	$-\frac{\alpha_1}{2}[u_3(0)-u_3(11)-u_2(0)+u_2(11)]$
12	0	$\frac{a}{2}$	$-\frac{a}{2}$	0	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	0	$-\frac{\alpha_1}{2}[u_2(0)-u_2(12)-u_3(0)+u_3(12)]$	$-\frac{\alpha_1}{2}[u_3(0)-u_3(12)-u_2(0)+u_2(12)]$
13	a	0	0	1	0	0	$-\alpha_2[u_1(0)-u_1(13)]$	0	0
14	$-a$	0	0	-1	0	0	$-\alpha_2[u_1(0)-u_1(14)]$	0	0
15	0	a	0	0	1	0	0	$-\alpha_2[u_2(0)-u_2(15)]$	0
16	0	$-a$	0	0	-1	0	0	$-\alpha_2[u_2(0)-u_2(16)]$	0
17	0	0	a	0	0	1	0	0	$-\alpha_2[u_3(0)-u_3(17)]$
18	0	0	$-a$	0	0	-1	0	0	$-\alpha_2[u_3(0)-u_3(18)]$

For obtaining the secular determinants for the metallic crystals having FCC structure we assume central forces between nearest and next nearest neighbours. Figs. (2) and (3) show the nearest and next nearest neighbours of the atoms, which is taken as the reference atom. The equilibrium position of atom is taken as origin.

Let the interaction between the nearest and next nearest neighbours be represented by force constants α_1 and α_2 respectively. The coordinates and the direction-cosines of the first neighbours and the second neighbours are given in tables.

From equations (3) and using the tables, we have

$$m\frac{d^2u_1(0)}{dt^2} = \Sigma_{1=1}^{18}F_1(1) = -\frac{\alpha_1}{2}[8u_1(0) - \Sigma_{1=1}^{8}u_1(1) - u_2(5) - u_2(6) + u_2(7) + u_2(8) - u_3(2) - u_3(1) + u_3(3) + u_3(4)] - \alpha_2[2u_1(0) - u_1(13) - u_1(14)] \quad \ldots(4)$$

Similarly,

$$m\frac{d^2u_2(0)}{dt^2} = -\frac{\alpha_1}{2}[8u_2(0) - \Sigma_{1=5}^{12}u_2(1) - u_1(5) - u_1(6) + u_1(7) + u_1(8) - u_3(9) - u_3(10) + u_3(11) + u_2(12)] - \alpha_2[2u_2(0) - u_2(15) - u_2(16)] \quad \ldots(5)$$

$$m\frac{d^2u_3(0)}{dt^2} = -\frac{\alpha_1}{2}[8u_3(0) - \Sigma_{1=1}^{4}u_3(1) - u_1(1) - u_1(2) + u_1(3) + u_1(4) - u_2(9) - u_2(10) + u_2(11) + u_2(12)] - \alpha_2[2u_3(0) - u_3(17) - u_3(18)] \quad \ldots(6)$$

we new compare equations (4), (5), (6) with equation 1.17. for α=1,2,3 and we obtain the various coefficients of $\phi\alpha\beta$. For $\alpha = \beta = 1$, we have

$$\phi_{11}(0) = 4\alpha_1 + 2\alpha_2 \quad \ldots(7)$$

$$\phi_{11}(1) = \phi_{11}(2) = - - - = \phi_{11}(8) = -\frac{\alpha_1}{2} \quad \ldots(8)$$

$$\phi_{11}(9) = \phi_{11}(10) = \phi_{11}(11) = \phi_{11}(12) = 0 \quad \ldots(9)$$

$$\phi_{11}(13) = \phi_{11}(14) = -\alpha_2 \quad \ldots(10)$$

$$\phi_{11}(15) = \phi_{11}(16) = \phi_{11}(17) = \phi_{11}(18) = 0 \quad \ldots(11)$$

Thus we have

$$D_{11}\left(\vec{q}\right) = \frac{1}{m}\Sigma_{1=0}^{18}\phi_{11}(1) \bullet \exp\left[-\mathrm{i}\vec{q}\,\vec{r}\,(1)\right]$$

$$= \frac{1}{m}[\phi_{11}(0) - \frac{\alpha_1}{2}\Sigma_{1=1}^{8}e^{-i\vec{q}\,\vec{r}\,(1)} - \alpha_2\Sigma_{1=13}^{14}e^{-i\vec{q}\,\vec{r}\,(1)}$$

Substituting the coordinates of various atoms from tables and on simplification we get

$$m \bullet D_{11}\left(\overrightarrow{q}\right) = (4\alpha_1 + 2\alpha_2) - \alpha_1\left[\cos q_1 \bullet \frac{a}{2}\left(\cos q_2 \bullet \frac{a}{2} + \cos q_3 \bullet \frac{a}{2}\right)\right] - 2\alpha_2 \cos q_1\, a$$

Writing $C_1 = \cos q_1 \bullet \frac{a}{2};\ C_2 = \cos q_2 \bullet \frac{a}{2};\ C_3 = \cos q_3 \bullet \frac{a}{2}$

$S_1 = \sin q_1 \bullet \frac{a}{2};\ S_2 = \sin q_2 \bullet \frac{a}{2};\ S_3 = \sin q_3 \bullet \frac{a}{2}$

and rearranging the terms we get,

$$D_{11}\left(\overrightarrow{q}\right) = \frac{1}{m}[4\alpha_1 - 2\alpha_1 \bullet\ C_1(C_2 + C_3) + 4\alpha_2 S_1^2] \ldots(12)$$

Similarly,

$$D_{22}\left(\overrightarrow{q}\right) = \frac{1}{m}[4\alpha_1 - 2\alpha_1 \bullet\ C_2(C_1 + C_3) + 4\alpha_2 S_2^2] \ldots(13)$$

And

$$D_{33}\left(\overrightarrow{q}\right) = \frac{1}{m}[4\alpha_1 - 2\alpha_1 \bullet\ C_3(C_1 + C_2) + 4\alpha_2 S_3^2] \ldots(14)$$

In similar manner the non-diagonal elements are obtained. We have,

$$D_{12}\left(\overrightarrow{q}\right) = \frac{2\alpha_1}{m}\ S_1 \bullet S_2 \ldots(15)$$

In general

$$D_{ij}\left(\overrightarrow{q}\right) = \frac{2\alpha_1}{m} S_i \bullet S_j\ i \neq j \ldots(16)$$

Thus, for a two body central interaction the elements the diagonal and non-diagonal elements are given by

$$D_{11}^{(c)}\left(\overrightarrow{q}\right) = \frac{1}{m}\left[4\alpha_1 - 2\alpha_1 \bullet C_1\left(C_j + C_k\right)\alpha_1\alpha_2 S_i^2\right] \ldots(17)$$

$$D_{ij}^{(c)}\left(\overrightarrow{q}\right) = \frac{2\alpha_1}{m}\ S_i \bullet S_j\ i \neq j \ldots(18)$$

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