Chapter 4

An su(1,1) Algebraic Approach To Periodic Potential

In this chapter we use a different realization of su(1,1) algebra and use it to obtain the Schrödinger equation for a one dimensional periodic potential. By different realization, we mean different set of operators (not same as that used in chapter3) which obey su(1,1) commutation relations as discussed in chapter 1. In this chapter Scraf potential has been considered as it is a periodic potential having real period.

4.1 Schrödinger Equation For a Particle in One Dimensional Scraf Potential:

Numerous instances of fruitful applications of SU(1,1) group theoretical methods have encouraged us to use a different set of operators obeying su(1,1) Lie algebra. Lie algebraic methods has been used extensively to study both bound (Arima and Iachello, 1976, 1978; Iachello, 1981; Roosmalen et al., 1982; Iachello and Levine, 1982; Levine and Wulfman, 1979; Roy et al., 2010, 2011) and scattering states (Alhassid et al., 1983a, 1983b, 1986; Frank and Wolf, 1984; Alhassid and Wu, 1984; Alhassid et al., 1984) of some potentials. Schrödinger equation for some asymmetric double well potentials have also been studied by R. Koc and D. Haydargil using Lie algebra (Koc and Haydargil, 2004). But hardly any attempts were being made to exercise this method in case of a periodic potential having real period. So, in this chapter we use su(1,1) algebra to obtain the Schrödinger equation for a one dimensional Scraf potential which is a periodic potential having real period.

To begin with we reproduce a construction of the su(1,1) Lie algebra by three (angular momentum) operators $\hat{J}_+$, $\hat{J}_-$ and $\hat{J}_z$ defined by

$$\hat{J}_+ = e^{+i\phi}\left(-\sin\theta\frac{\partial}{\partial\theta} + i\cos\theta\frac{\partial}{\partial\phi}\right) \tag{4.01}$$

$$\hat{J}_- = e^{-i\phi}\left(+\sin\theta\frac{\partial}{\partial\theta} + i\cos\theta\frac{\partial}{\partial\phi}\right) \tag{4.02}$$

and

$$\hat{J}_z = -i\frac{\partial}{\partial\phi} \tag{4.03}$$

The respective commutation relations are as follows:

$$\left[\hat{J}_z, \hat{J}_+\right] = \hat{J}_z\hat{J}_+ - \hat{J}_+\hat{J}_z$$

$$= \left(-i\frac{\partial}{\partial\phi}\right)\left[e^{+i\phi}\left(-\sin\theta\frac{\partial}{\partial\theta} + i\cos\theta\frac{\partial}{\partial\phi}\right)\right] - \left[e^{+i\phi}\left(-\sin\theta\frac{\partial}{\partial\theta} + i\cos\theta\frac{\partial}{\partial\phi}\right)\right]\left(-i\frac{\partial}{\partial\phi}\right)$$

$$= \left(-i\frac{\partial}{\partial\phi}\right)\left[e^{i\phi}\left(-\sin\theta\frac{\partial}{\partial\theta} + i\cos\theta\frac{\partial}{\partial\phi}\right)\right] + i\left[e^{i\phi}\left(-\sin\theta\frac{\partial}{\partial\theta} + i\cos\theta\frac{\partial}{\partial\phi}\right)\right]\left(\frac{\partial}{\partial\phi}\right)$$

$$= -i(i)\left[e^{i\phi}\left(-\sin\theta\frac{\partial}{\partial\theta} + i\cos\theta\frac{\partial}{\partial\phi}\right)\right] + ie^{i\phi}\cancel{\sin\theta\frac{\partial^2}{\partial\phi\partial\theta}} + e^{i\phi}\cancel{\cos\theta\frac{\partial^2}{\partial\phi^2}}$$
$$- ie^{i\phi}\cancel{\sin\theta\frac{\partial^2}{\partial\theta\partial\phi}} - e^{i\phi}\cancel{\cos\theta\frac{\partial^2}{\partial\phi^2}}$$

$$= e^{+i\phi}\left(-\sin\theta\frac{\partial}{\partial\theta}+i\cos\theta\frac{\partial}{\partial\phi}\right)=\hat{J}_+$$

$$\therefore \qquad \left[\hat{J}_z,\hat{J}_+\right]=\hat{J}_+$$

$$\left[\hat{J}_z,\hat{J}_-\right]=\hat{J}_z\hat{J}_- - \hat{J}_-\hat{J}_z$$

$$=\left(-i\frac{\partial}{\partial\phi}\right)\left[e^{-i\phi}\left(\sin\theta\frac{\partial}{\partial\theta}+i\cos\theta\frac{\partial}{\partial\phi}\right)\right] - \left[e^{-i\phi}\left(\sin\theta\frac{\partial}{\partial\theta}+i\cos\theta\frac{\partial}{\partial\phi}\right)\right]\left(-i\frac{\partial}{\partial\phi}\right)$$

$$=\left(-i\frac{\partial}{\partial\phi}\right)\left[e^{-i\phi}\left(\sin\theta\frac{\partial}{\partial\theta}+i\cos\theta\frac{\partial}{\partial\phi}\right)\right]+\left[ie^{-i\phi}\left(\sin\theta\frac{\partial}{\partial\theta}+i\cos\theta\frac{\partial}{\partial\phi}\right)\right]\left(\frac{\partial}{\partial\phi}\right)$$

$$=-i(-i)\left[e^{-i\phi}\left(\sin\theta\frac{\partial}{\partial\theta}+i\cos\theta\frac{\partial}{\partial\phi}\right)\right]-\cancel{ie^{-i\phi}\sin\theta\frac{\partial^2}{\partial\phi\partial\theta}}+\cancel{e^{-i\phi}\cos\theta\frac{\partial^2}{\partial\phi^2}}$$

$$+\cancel{ie^{-i\phi}\sin\theta\frac{\partial^2}{\partial\theta\partial\phi}}-\cancel{e^{-i\phi}\cos\theta\frac{\partial^2}{\partial\phi^2}}$$

$$=-e^{-i\phi}\left(\sin\theta\frac{\partial}{\partial\theta}+i\cos\theta\frac{\partial}{\partial\phi}\right)=-\hat{J}_-$$

$$\therefore \qquad \left[\hat{J}_z,\hat{J}_-\right]=-\hat{J}_-$$

Now, $\hat{J}_+\hat{J}_-=\left[e^{+i\phi}\left(-\sin\theta\frac{\partial}{\partial\theta}+i\cos\theta\frac{\partial}{\partial\phi}\right)\right]\left[e^{-i\phi}\left(\sin\theta\frac{\partial}{\partial\theta}+i\cos\theta\frac{\partial}{\partial\phi}\right)\right]$

$$=\cancel{-\sin\theta\cos\theta\frac{\partial}{\partial\theta}}-\sin^2\theta\frac{\partial^2}{\partial\theta^2}+i\sin^2\theta\frac{\partial}{\partial\phi}-\cancel{i\sin\theta\cos\theta\frac{\partial^2}{\partial\theta\partial\phi}}+\cancel{\sin\theta\cos\theta\frac{\partial}{\partial\theta}}$$

$$+i\cos^2\theta\frac{\partial}{\partial\phi}+\cancel{i\sin\theta\cos\theta\frac{\partial^2}{\partial\phi\partial\theta}}-\cos^2\theta\frac{\partial^2}{\partial\phi^2}$$

$$=-\sin^2\theta\frac{\partial^2}{\partial\theta^2}+i\frac{\partial}{\partial\phi}-\cos^2\theta\frac{\partial^2}{\partial\phi^2} \qquad (4.04)$$

$$\hat{J}_-\hat{J}_+ = \left[e^{-i\phi} \left(\sin\theta \frac{\partial}{\partial\theta} + i\cos\theta \frac{\partial}{\partial\phi} \right) \right] \left[e^{i\phi} \left(-\sin\theta \frac{\partial}{\partial\theta} + i\cos\theta \frac{\partial}{\partial\phi} \right) \right]$$

$$= \cancel{-\sin\theta\cos\theta \frac{\partial}{\partial\theta}} - \sin^2\theta \frac{\partial^2}{\partial\theta^2} - i\sin^2\theta \frac{\partial}{\partial\phi} + \cancel{i\sin\theta\cos\theta \frac{\partial^2}{\partial\theta\partial\phi}} + \cancel{\sin\theta\cos\theta \frac{\partial}{\partial\theta}}$$

$$- i\cos^2\theta \frac{\partial}{\partial\phi} - \cancel{i\sin\theta\cos\theta \frac{\partial^2}{\partial\phi\partial\theta}} - \cos^2\theta \frac{\partial^2}{\partial\phi^2}$$

$$= -\sin^2\theta \frac{\partial^2}{\partial\theta^2} - i\sin^2\theta \frac{\partial}{\partial\phi} - i\cos^2\theta \frac{\partial}{\partial\phi} - \cos^2\theta \frac{\partial^2}{\partial\phi^2}$$

$$= -\sin^2\theta \frac{\partial^2}{\partial\theta^2} - i \frac{\partial}{\partial\phi} - \cos^2\theta \frac{\partial^2}{\partial\phi^2}$$

$$\therefore \left[\hat{J}_+, \hat{J}_- \right] = \hat{J}_+\hat{J}_- - \hat{J}_-\hat{J}_+$$

$$= \left(-\sin^2\theta \frac{\partial^2}{\partial\theta^2} + i \frac{\partial}{\partial\phi} - \cos^2\theta \frac{\partial^2}{\partial\phi^2} \right) - \left(-\sin^2\theta \frac{\partial^2}{\partial\theta^2} - i \frac{\partial}{\partial\phi} - \cos^2\theta \frac{\partial^2}{\partial\phi^2} \right)$$

$$= 2i \frac{\partial}{\partial\phi} = -2\hat{J}_z$$

So the obtained commutation relations are given by

$$\left[\hat{J}_z, \hat{J}_+ \right] = \hat{J}_+, \quad \left[\hat{J}_z, \hat{J}_- \right] = -\hat{J}_-, \quad \left[\hat{J}_+, \hat{J}_- \right] = -2\hat{J}_z \qquad (4.05)$$

Also these three operators $\hat{J}_+$, $\hat{J}_-$ and $\hat{J}_z$ obey the Jacobi identity as

$$\left[[\hat{J}_z, \hat{J}_+], \hat{J}_- \right] + \left[[\hat{J}_+, \hat{J}_-], \hat{J}_z \right] + \left[[\hat{J}_-, \hat{J}_z], \hat{J}_+ \right]$$

$$= \left[\hat{J}_+, \hat{J}_- \right] + \left[-2\hat{J}_z, \hat{J}_z \right] + \left[\hat{J}_-, \hat{J}_+ \right]$$

$$= -2\hat{J}_z + 0 + 2\hat{J}_z$$

$$= 0$$

The above commutation relations and the Jacobi identity confirms the correct choice of the operators of su(1,1) Lie algebra.

Now as the choosen algebra is su(1,1) so the Casimir operator of the algebra can be written as

$$\hat{C} = \hat{J}^2 = -\hat{J}_+\hat{J}_- + \hat{J}_z{}^2 - \hat{J}_z \tag{4.06}$$

The eigen value equation for $\hat{J}^2$ and $\hat{J}_z$ are given by

$$\left.\begin{aligned} &\hat{C}\left| j,m\right\rangle = \hat{J}^2\left| j,m\right\rangle = j\left(j+1\right)\left| j,m\right\rangle \\ &\hat{J}_z\left| j,m\right\rangle = m\left| j,m\right\rangle \end{aligned}\right] \tag{4.07}$$

Now putting values of $\hat{J}_+\hat{J}_-$ as given by Eq. (4.04) and values of $\hat{J}_z$ as given by Eq. (4.03) in Eq. (4.06) we get,

$$\begin{aligned} \hat{C} = \hat{J}^2 &= -\hat{J}_+\hat{J}_- + \hat{J}_z{}^2 - \hat{J}_z \\ &= \sin^2\theta\frac{\partial^2}{\partial\theta^2} - i\frac{\partial}{\partial\phi} + \cos^2\theta\frac{\partial^2}{\partial\phi^2} + \left(-i\frac{\partial}{\partial\phi}\right)^2 - \left(-i\frac{\partial}{\partial\phi}\right) \\ &= \sin^2\theta\frac{\partial^2}{\partial\theta^2} + \cos^2\theta\frac{\partial^2}{\partial\phi^2} - i\frac{\partial}{\partial\phi} - \frac{\partial^2}{\partial\phi^2} + i\frac{\partial}{\partial\phi} \\ &= \sin^2\theta\frac{\partial^2}{\partial\theta^2} + \frac{\partial^2}{\partial\phi^2}\left(\cos^2\theta - 1\right) \\ &= \sin^2\theta\left(\frac{\partial^2}{\partial\theta^2} - \frac{\partial^2}{\partial\phi^2}\right) \end{aligned}$$

$$\therefore \qquad \hat{C} = \hat{J}^2 = \sin^2\theta\left(\frac{\partial^2}{\partial\theta^2} - \frac{\partial^2}{\partial\phi^2}\right) \tag{4.08}$$

In this realization the basis states takes the form

$$\psi = \psi_{jm}(\theta) e^{+im\phi} \tag{4.09}$$

where $\psi_{jm}(\theta) = P_j^m(i\cot\theta)$; $P_j^m(i\cot\theta)$ is the associated Legendre polynomial.

Combining Eq. (4.07), Eq. (4.08) and Eq. (4.09) we can write

$$\hat{J}^2\psi = \sin^2\theta\left(\frac{\partial^2}{\partial\theta^2} - \frac{\partial^2}{\partial\phi^2}\right)\psi_{jm}(\theta)\ e^{im\phi} = j(j+1)\ \psi_{jm}(\theta)\ e^{im\phi}$$

$$\Rightarrow e^{im\phi}\sin^2\theta\ \frac{\partial^2}{\partial\theta^2}\ \psi_{jm}(\theta) - \sin^2\theta\ \psi_{jm}(\theta)\ \frac{\partial^2}{\partial\phi^2}\ e^{im\phi} = j(j+1)\ \psi_{jm}(\theta)\ e^{im\phi}$$

$$\Rightarrow e^{im\phi}\sin^2\theta\ \frac{\partial^2}{\partial\theta^2}\ \psi_{jm}(\theta) - \sin^2\theta\ \psi_{jm}(\theta)\ (-m)^2 e^{im\phi} = j(j+1)\ \psi_{jm}(\theta) e^{im\phi}$$

$$\Rightarrow \sin^2\theta\ \frac{d^2}{d\theta^2}\ \psi_{jm}(\theta) + \sin^2\theta\ \psi_{jm}(\theta)\ m^2 = j(j+1)\ \psi_{jm}(\theta)$$

$$\Rightarrow\left[\frac{d^2}{d\theta^2} - \frac{j(j+1)}{\sin^2\theta}\right]\ \psi_{jm}(\theta) = -\ m^2\ \psi_{jm}(\theta)$$

$$\Rightarrow\left[-\frac{d^2}{d\theta^2} + \frac{j(j+1)}{\sin^2\theta}\right]\ \psi_{jm}(\theta) = \ m^2\ \psi_{jm}(\theta) \tag{4.10}$$

4.2 Results and Discussions:

This Eq. (4.10) is the Schrödinger equation for a particle in one dimensional Scraf potential. The strength of the potential is proportional to $j(j+1)$. Eq. (4.10) shows that energy of the particle is given by $E = m^2$. Also this potential is a periodic potential with period *2π* which is relevant so far one dimensional crystal is considered.

As the strength of the potential is given by $j(j+1)$, a given strength of potential corresponds to a fixed representation *'j'* and hence **a single representation 'j' accounts for the spectral properties given by m²**.

4.2.1 Periodicity of the Scraf Potential:

Periodicity of the Scraf potential is checked by following method:

Consider, $$f(\theta)=\frac{1}{\sin^2(\theta)}$$

Now let us put $a=2\pi$, then

$$f(\theta+a)=f(\theta+2\pi)$$

$$\Rightarrow f(\theta+2\pi)=\frac{1}{\sin^2(\theta+2\pi)}=\frac{1}{\sin^2\theta}=f(\theta)$$

The above calculation confirms the periodicity of the Scraf potential.

4.2.2 The Graphical Form of the Scraf Potential:

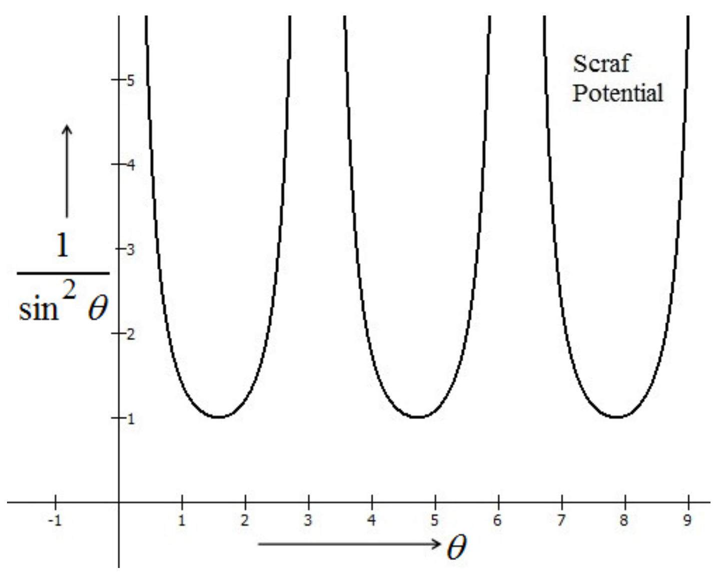

Figure 4.1: Graphical Form of the Scraf Potential

4.3 Conclusion:

In this chapter a completely different set of operators which obey su(1,1) Lie algebra is used to obtain the Schrödinger equation for one dimensional Scraf potential. The period of this potential is found to be 2π which is quite feasible for a crystal.

The form of the operators used in chapter 3 obeying su(1,1) Lie algebra are different from that used in this chapter. Earlier realization lead to Scattering states of Pöschl-Teller potential but this realization led to Schrödinger equation for a particle in one dimensional Scraf potential. This explains how just by varying the suitable set of operators satisfying a Lie algebra, completely different physical states can be achieved.

In the next chapter we exercise these results and use the unitary representation of su(1,1) to obtain the energy bands.