Dynamical Symmetry Approach to Periodic Hamiltonians

Hui Li and Dimitri Kusnezov

Center for Theoretical Physics, Sloane Physics Laboratory, Yale University, New Haven, CT 06520-8120

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ABSTRACT

We show that dynamical symmetry methods can be applied to Hamiltonians with periodic potentials. We construct dynamical symmetry Hamiltonians for the Scarf potential and its extensions using representations of \( su(1,1) \) and \( so(2,2) \). Energy bands and gaps are readily understood in terms of representation theory. We compute the transfer matrices and dispersion relations for these systems, and find that the complementary series plays a central role as well as non-unitary representations.

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I. Introduction

Lie-algebraic techniques have found wide application to physical systems and generally provide descriptions of bound states or scattering states\[1, 2, 3\]. Once an algebraic structure is identified, such as a spectrum generating algebra, exactly solvable limits of the theory, or dynamical symmetries, can be constructed\[4\]. Here representation theory provides a full classification of states and often transitions\[5\]. These dynamical symmetry limits can be intuitive guides to the more general structure and behavior of solutions of the problem. Quantum systems can be characterized by three types of spectra: discrete (bound states), continuous (scattering states) and bands (periodic potentials). The third case corresponds to spectra with energy bands and gaps. Up to now, however, dynamical symmetry treatments have focused only on the first two, leaving the case of band structure and its connection to representation theory unclear.

In this article, we extend the dynamical symmetry approach to quantum systems by showing that Lie algebras and representation theory can also be used to treat Hamiltonians with periodic potentials, allowing the calculation of dispersion relations and transfer matrices\[6\]. We will focus our attention here on the Scarf potential\[7\] and its generalizations and show how representations of $so(2, 1)$ and $so(2, 2)$ can be used to explain energy bands and gaps. The representations which will be necessary are the projective representations of $su(1, 1) \sim so(2, 1)$. These have three families, known as the discrete, principal, and complementary series. The discrete and principal series have found much application in physics. For instance, the Pöschl-Teller Hamiltonian, $H = -d^2/dx^2 + g/\cosh^2 x$, can be expressed as an $su(1, 1)$ dynamical symmetry\[8\], with the discrete and principal series describing the bound and scattering states. The complementary series, however, with $-1/2 < j < 0$, has found little application in physics and is considered to be more of a curiosity. We will see that this series is precisely what is needed to describe band structure in certain periodic potentials, and further, that the unitary representations correspond to the energy gaps, rather than the bands.

II. Scarf Potential

The Scarf potential\[7\] provides a convenient starting point for the dynamical symmetry analysis of periodic systems. It was originally introduced as an example of an exactly solvable crystal model. The starting point is the Hamiltonian

$$H_{sc} = -\frac{d^2}{dx^2} + \frac{g}{\sin^2 x}. \quad (1)$$

The potential is shown in Fig. 1. (We choose units with mass $M = 1/2$ and $\hbar = 1$.) The strength of the potential $g$ is usually expressed as $g = s^2 - 1/4$ since for $g \leq -1/4$, 

one can no longer define a Hilbert space for which the Hamiltonian is self-adjoint[9]. The
dispersion relation for this Hamiltonian was found to be

\[ E(k) = \frac{1}{\pi^2} \left( \cos^{-1}(\sin \pi s \cos k\pi) \right)^2 \]  

with the band edges for the \( n \)-th band:

\[ E_n^\pm = (n + \frac{1}{2} \pm s)^2. \]  

The bands become degenerate as \( s \to 0 \). For \( s = 1/2 \), the motion is that of a free particle
with \( E(k) = k^2 \). While Scarf originally showed that the potential admits band structure
for \( 0 < s \leq 1/2 \), it was demonstrated more recently that the Hamiltonian has bands for
\( 1/2 \leq s < 1 \)[9]. In our analysis, we will see that the entire range of \( 0 < s < 1 \) arises
naturally from representation theory.

In order to realize the Scarf problem as a dynamical symmetry, we consider the Lie
algebras isomorphic to \( so(3) \). We will see that while different constructions are possible,
not all are fruitful.

### A. \( so(3) \) Realization

The relationship of the Scarf Hamiltonian to \( so(3) \) was noted some time ago by Gürsey[10]. Consider the realization of \( so(3) \) given by the generators:

\[
I_\pm = e^{\pm i \phi} \left[ \sin \frac{1}{2} \frac{\partial}{\partial \theta} + \cot \theta \left( \frac{\partial^2}{\partial \phi^2} - \frac{1}{4} \right) \right] \\
I_3 = -i \frac{\partial}{\partial \phi} \\
I^2 = I_+ I_- + I_3^2 - I_3 \\
= -\frac{\partial^2}{\partial \theta^2} - \frac{1}{\sin^2 \theta} \left( \frac{\partial^2}{\partial \phi^2} + \frac{1}{4} \right) - \frac{1}{4}
\]

which satisfy the usual commutation relations:

\[
[I_3, I_+] = I_+, \quad [I_3, I_-] = -I_-, \quad [I_+, I_-] = 2I_3.
\]

Then, using the basis \( \psi_j^m = \sqrt{\sin \theta} \ P_j^m(\cos \theta) \), with the unitary representations of \( so(3) \)
labeled by \((j, m)\), the Casimir invariant \( I^2 \) can be rewritten as the Schrödinger equation:

\[
\left[ -\frac{d^2}{d\theta^2} + \frac{m^2 - \frac{1}{4}}{\sin^2 \theta} \right] \psi_j^m(\theta) = (j + \frac{1}{2})^2 \psi_j^m(\theta).
\]

While this is Scarf’s Hamiltonian with \( g = m^2 - 1/2 \) (similar to \( g = s^2 - 1/2 \) in \( (1) \)),
it is not a useful realization for several reasons. For instance, one cannot obtain any
band structure from the discrete representations of \( so(3) \). Here the spectrum is labeled
by \((j + 1/2)\), which identifies only bound states. Further, the strength of the potential,
$m^2 - 1/4$, is only negative for $m = 0$. In this case $g = -1/4$ and the Hamiltonian is no longer self-adjoint. Finally, since $m$ appears in the strength $g$ of the potential, a given representation $j$ would correspond to different forms of the Hamiltonian, rather than the spectrum of a single Hamiltonian. For this reason, the previous realizations of $H_{Sc}$ are not useful for the discussion of band structure.

B. $so(2,1)$ realization

A more suitable realization of the Scarf Hamiltonian can be found using $so(2,1) \sim su(1,1)$. To obtain this form, we perform the following transformations of the $so(3)$ algebra: (i) scaling the wavefunction by $\frac{1}{\sqrt{\sin \theta}}$, (ii) changing $\cos \theta \rightarrow \tanh \theta$ and (iii) taking $\theta \rightarrow i \theta$. The result is the $so(2,1)$ realization

$$I_\pm = e^{\pm i \phi} \left( \mp \sin \theta \frac{\partial}{\partial \theta} + i \cos \theta \frac{\partial}{\partial \phi} \right)$$

$$I_3 = -i \frac{\partial}{\partial \phi}$$

$$I^2 = -I_+ I_- + I_3^2 - I_3$$

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

which satisfies the commutation relations

$$[I_3, I_+] = I_+, \quad [I_3, I_-] = -I_-, \quad [I_+, I_-] = -2I_3.$$  

The Casimir operator, using the basis states $\psi_j^m(\theta) = P_j^m(i \cot \theta), 0 < \theta < \frac{\pi}{2}$, reduces to Scarf’s Hamiltonian in the dynamical symmetry form:

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

While this Hamiltonian is more pleasing than Eq. (8) in the sense that a single representation $j$ will account for the spectral properties, given by $m^2$, the standard unitary representations (given in Appendix A) are not yet sufficient to describe the bands. These come in three series. The principal series with $j = -1/2 + i \rho$, $\rho > 0$, the discrete series $D_j^\pm$ where $j = -n/2$ for $n = 1, 2, ...$, and the complementary series, $-1/2 < j < 0$.

In order to realize band structure as a dynamical symmetry, it is clear that we must consider slightly more general representations. For Hamiltonians with periodic potentials, $V(x + a) = V(x)$, Bloch’s theorem requires the form of the wavefunctions to be

$$\Psi_k(x) = e^{ikx} u_k(x), \quad u_k(x + a) = u_k(x),$$

so that $\Psi_k(x + a) = \exp(ik a) \Psi_k(x)$ is not single valued. To obtain multi-valued functions, we pass to the projective unitary representations of $su(1,1) \sim so(2,1)$ [12, 13]. In contrast to the more familiar representations of $so(3)$ which are related to the orthogonal symmetries in the vector space $\mathcal{R}^3$, the projective representations are associated with equivalence
classes of vectors defined up to a phase (as in Eq. 14). The action of a group on the projective space (rather than a vector space), defined by this equivalence class of states, leads to the projective representations. While these are multi-valued representations of the group, they are proper representations of the algebra and are hence suitable. Consequently, the single-valued representations of this covering group of $su(1,1)$ are infinitely many-valued representations of $su(1,1)$. Such representations have been used to describe bound and scattering states in the Pöschl-Teller potential\[8\]. They fall into the same three series as the usual unitary representations of $su(1,1)$ discussed above (see Appendix A).

We will see that for our Scarf dynamical symmetry (13), the discrete series corresponds to the band edges, the complementary series provides the bands and gaps, while the principal series is unphysical, corresponding to the regime where the Hamiltonian is not self-adjoint.

Consider first the complementary series of the projective unitary representations of $so(2,1)$. Here we must have

$$-\frac{1}{2} < j < 0, \quad \text{or} \quad -\frac{1}{4} < j(j+1) < 0. \quad (15)$$

This is precisely the range of $g = j(j+1)$ studied initially by Scarf in Eq. (1). The states are labeled by two quantum numbers $j, m$, with unitary representations given by the range of quantum numbers:

$$m = m_0 \pm n \ (n = 0, 1, \cdots), \quad 0 \leq m_0 < 1, \quad m_0(1-m_0) < -j(j+1) < -\frac{1}{4}. \quad (16)$$

The last condition provides the range:

$$0 < m_0 < -j, \quad \text{and} \quad 1 + j < m_0 < 1, \quad (17)$$

which is illustrated in Fig. 2. For a given value of $j$, $j(j+1)$ (dots) separates unitary from non-unitary representations. The unitary representations are given by values of $m$ for which the periodically continued parabola (dashes and solid) are above $j(j+1)$. One can now see that these unitary representations correspond to the band gaps rather than the bands by taking $j \to 0$. In this case the Hamiltonian (13) is that of a free particle, so that the spectrum is $E = m^2 \geq 0$. From Eqs. (16)-(17) and Fig. 2, we see that as $j \to 0$ the allowed values of $m$ become restricted to $m = 0, \pm 1, \pm 2, \ldots$. Therefore, for a specific $j$, $E = m^2$ has band structure, with the range of $m$ from unitary projective representations giving the energy gaps. The non-unitary projective representations of the complementary series give the energy bands

$$(-j+n)^2 < E < (1+j+n)^2, \quad n-j < m < 1+j+n. \quad (18)$$

The band edges are not contained in the complementary series. In contrast to the states in the band, the edge states are periodic. They form a discrete set of states which are associated with the discrete series. These series $D_j^\pm$ have the representations $j < 0$ with $m$ given by

$$D_j^+: \ m = -j, 1-j, 2-j, \ldots \quad (19)$$

$$D_j^-: \ m = j, j-1, j-2, \ldots \quad (20)$$
When we restrict to the range of physical interest, $-\frac{1}{2} < j < 0$, this series provides the upper and lower band edges (compare to Eq. (18)):

\begin{align*}
D^+_j(\text{lower}) & : E = (n - j)^2 \\
D^-_{j-1}(\text{upper}) & : E = (n + j + 1)^2.
\end{align*}

Eq. (22) arises from the invariance of our Hamiltonian (13) under $j \rightarrow -1 - j$, allowing both discrete series $D^+_j$ and $D^-_{1-j}$. Other discrete representations with $j < -1$ are not useful for band structure. The band spectrum of the Scarf potential which includes both the discrete and complementary series is shown in Fig. 3. The shaded region corresponds to the bands (non-unitary) and the unshaded to the gaps (unitary).

The remaining representations, the principal series, has $j = -\frac{1}{2} + i\rho$ ($\rho > 0$). This gives a potential with strength $g = j(j + 1) < -\frac{1}{4}$, for which the Hamiltonian is no longer self-adjoint and is of no physical interest.

Note that we have explained the band structure for strengths of the potential $-1/4 < g = j(j + 1) < 0$ and found agreement with Scarf\cite{7}. More recently it was noted that for $0 \leq g < 3/4$, there is also band structure\cite{9}. In this range the potential is strictly positive. (The origin of the band structure here is that the matching conditions on the wavefunctions around the singularity in the potential, needed to have a self-adjoint Hamiltonian, in a sense ‘dilute’ the infinite potential at these points and allow bands.) While our $so(2,1)$ realization above cannot account for this range of $g$, we will see in Section III, that a limiting case of an $so(2,2)$ dynamical symmetry will account for this range using the same complementary series. For $g \geq 3/4$, there is no band structure and the discrete projective representation then describe the bound state spectrum.

C. Transfer matrix

The transfer matrix $T$ for the period $x \in (-\frac{\pi}{2}, \frac{\pi}{2})$ can be computed directly from wave functions. However, the quadratic singularity of the potential requires some care. There are two approaches one can consider, but both are equivalent\cite{7, 8, 9}. In the first, we compute the transfer matrix at $x = \pm \varepsilon$. We then match the transfer matrices on both sides of the singularity as $\varepsilon \rightarrow 0$, which results in matching conditions on the wavefunctions. This procedure is not equivalent to an analytical continuation around the origin. The second arises in the construction of the Hilbert space of functions for which $H$ is self-adjoint. This gives rise to equivalent matching conditions around the origin\cite{9}. The matrix elements of the transfer matrix are related to the values of the even and odd solutions and their first derivatives at $\frac{\pi}{2}$ (see Appendix B). We find

\begin{equation}
T = \begin{pmatrix}
\alpha & \beta \\
\beta^* & \alpha^*
\end{pmatrix}
\end{equation}

where $\alpha$ and $\beta$ are determined by the representations of the complementary and discrete series $j, m$ as:
\[
\alpha = e^{-im\pi} \left[ \frac{\cos \pi m}{\sin \pi (j + \frac{1}{2})} + i \left( -\frac{2}{m} \frac{\Gamma(\frac{1-j+m}{2})\Gamma(\frac{1-j-m}{2})}{\Gamma(-\frac{j+m}{2})\Gamma(-\frac{j-m}{2})} m \frac{\Gamma(\frac{1+j+m}{2})\Gamma(\frac{1+j-m}{2})}{2 \Gamma(\frac{2+j+m}{2})\Gamma(\frac{2+j-m}{2})} \right) \frac{\cos \frac{j+m}{2}}{\sin \pi (j + \frac{1}{2})} \right] \tag{24}
\]

\[
\beta = ie^{im\pi} \frac{\cos \frac{j+m}{2}}{\sin \pi (j + \frac{1}{2})} \left[ \frac{2}{m} \frac{\Gamma(\frac{1-j+m}{2})\Gamma(\frac{1-j-m}{2})}{\Gamma(-\frac{j+m}{2})\Gamma(-\frac{j-m}{2})} + m \frac{\Gamma(\frac{1+j+m}{2})\Gamma(\frac{1+j-m}{2})}{2 \Gamma(\frac{2+j+m}{2})\Gamma(\frac{2+j-m}{2})} \right]. \tag{25}
\]

Although the Scarf Hamiltonian can be obtained from the Pöschl-Teller potential \( V(x) = g / \cosh^2 x \) through a transformation, the above transfer matrix is not related to that of the Pöschl-Teller in any simple manner.

The Bloch form of the \( so(2,1) \) wave functions for the \( n \)-th period, \( (n - \frac{1}{2})\pi < x \leq (n + \frac{1}{2})\pi \), of the Scarf Hamiltonian are readily found to be

\[
\Psi_k(x) = f_k(x - n\pi)e^{ikx} \tag{26}
\]

where:

\[
f_k(z) = e^{-ik(z + \frac{\pi}{2})}[aP_m(i \cot z) + bP_{-m}(i \cot z)] \tag{27}
\]

and:

\[
a = (-)^{-j/2} \frac{\sqrt{\pi} 2^{-m}}{\sin m\pi} \left[ \cos k\pi \frac{\Gamma(\frac{1-j-m}{2})}{\Gamma(\frac{1-j+m}{2})} - \sin k\pi \frac{\Gamma(\frac{2+j-m}{2})}{\Gamma(\frac{2+j+m}{2})} \right] \tag{28}
\]

\[
b = (-)^{-j/2} \frac{\sqrt{\pi} 2^m}{\sin m\pi} \left[ \cos k\pi \frac{\Gamma(\frac{1+j-m}{2})}{\Gamma(\frac{1+j+m}{2})} - \sin k\pi \frac{\Gamma(\frac{2-j-m}{2})}{\Gamma(\frac{2-j+m}{2})} \right]. \tag{29}
\]

Since \(-\frac{\pi}{2} < z \leq \frac{\pi}{2}\), \( f_k(z) \) is made periodic, and \( \Psi_k(x) \) satisfies Bloch’s theorem.

D. Dispersion relation

Once we have the transfer matrix, the dispersion relation is obtained from \( \alpha \) by the condition [11, 13]:

\[
\cos \pi k = Re(\alpha e^{im\pi}) = \frac{\cos \pi m}{\sin \pi (j + \frac{1}{2})}. \tag{30}
\]

Solving for the energy \( E = m^2 \), we find:

\[
E(k) = m^2 = \frac{1}{\pi^2} \left[ \cos^{-1}(\sin \pi (j + \frac{1}{2}) \cos \pi k) \right]^2. \tag{31}
\]

This is precisely the result (2) obtained by Scarf. Again, the values of \( j \) and \( m \) are determined from the representations given in (18) and (21)-(22). From the dispersion
relation, we can also compute the group velocity $V$ and the effective mass $M^*$. These will depend only upon the representation labels $j$ and $m$. We have:

$$V(j, m) = \frac{\partial E}{\partial k} = 2m \frac{\sqrt{\cos^2 \pi j - \cos^2 \pi m}}{\sin \pi m}.$$  \hspace{1cm} (32)

This is plotted in Fig. 4(a) for selected values of $j$. $V(j, m)$ vanishes on the band edges. For $j = 0$, the Hamiltonian (13) describes free motion, and we expect $V = \pm k/M = \pm 2k$ (dots), while for $j \to -1/2$, we have degenerate bands, and $V \to 0$ at half-integer values of $m$. For the effective mass:

$$\frac{1}{M^*(j, m)} = \frac{\partial^2 E}{\partial k^2} = 2 \left[ \frac{\cos^2 j \pi}{\sin^2 m \pi} - \cot^2 m \pi + m \pi \sin j \pi \cot m \pi \right].$$  \hspace{1cm} (33)

(Note that this differs slightly from the result derived in [4].) In Fig. 4(b), $1/M^*(j, m)$ is shown for selected values of $j$. For $j = 0$, $M^* = M = 1/2$, while for $j \to -1/2$, $1/M^* \to 0$.

E. Variation of Scarf potential

In the next section we will present a dynamical symmetry Hamiltonian for a variation of the Scarf potential using $so(2, 2)$. This potential will have several limits where the Hamiltonian reduces to the Scarf case, including the $1/cos^2 x$ potential. In order to compare the transfer matrix in this limit to the Scarf result, we consider the Scarf Hamiltonian translated by $\frac{\pi}{2}$:

$$\left[ -\frac{d^2}{d\theta^2} + \frac{j(j+1)}{cos^2 \theta} \right] \psi_j^m(\theta) = m^2 \psi_j^m(\theta).$$  \hspace{1cm} (34)

The dispersion relation $E(k)$ and the energy band structure will remain the same as before. The transfer matrix for $(-\frac{\pi}{2}, \frac{\pi}{2})$, on the other hand, will change. The new transfer matrix can be calculated easily from a translation of the solutions of Scarf case:

$$\alpha = e^{-im\theta} \left[ \frac{\cos \pi m}{\sin \pi (j + \frac{1}{2})} + i \left( -m \frac{\Gamma(j + \frac{1}{2}) \Gamma(\frac{1-j+m}{2}) \Gamma(\frac{1-j-m}{2})}{\Gamma(-j - \frac{1}{2}) \Gamma(\frac{2+j+m}{2}) \Gamma(\frac{2+j-m}{2})} + \frac{1}{m} \frac{\Gamma(-j - \frac{1}{2}) \Gamma(\frac{1-j+m}{2}) \Gamma(\frac{1-j-m}{2}) \cos \pi \frac{j+m}{2} \cos \pi \frac{j-m}{2}}{\Gamma(\frac{j+\frac{1}{2}+\frac{m}{2}}{2}) \Gamma(\frac{j+\frac{1}{2}-\frac{m}{2}}{2})} \right) \right].$$  \hspace{1cm} (35)

$$\beta = -ie^{im\theta} \left[ \frac{\cos \frac{j+m}{2} \cos \frac{j-m}{2}}{\sin \pi (j + \frac{1}{2})} \left[ \frac{m \Gamma(j + \frac{1}{2}) \Gamma(\frac{1-j+m}{2}) \Gamma(\frac{1-j-m}{2})}{\Gamma(-j - \frac{1}{2}) \Gamma(\frac{2+j+m}{2}) \Gamma(\frac{2+j-m}{2})} + \frac{1}{m} \frac{\Gamma(-j - \frac{1}{2}) \Gamma(\frac{1-j+m}{2}) \Gamma(\frac{1-j-m}{2}) \cos \pi \frac{j+m}{2} \cos \pi \frac{j-m}{2}}{\Gamma(\frac{j+\frac{1}{2}+\frac{m}{2}}{2}) \Gamma(\frac{j+\frac{1}{2}-\frac{m}{2}}{2})} \right] \right].$$  \hspace{1cm} (36)
III. Generalized Scarf Potential

We have now shown that band structure can arise naturally as a dynamical symmetry. We would like to build on the analysis of the Scarf problem and study a different class of periodic potentials. Consider an extension of the Scarf potential given by a generalized Pöschl-Teller Hamiltonian

\[\left[-\frac{d^2}{dx^2} + \frac{g_1}{\sin^2 x} + \frac{g_2}{\cos^2 x}\right]\Psi(x) = E\Psi(x), \quad (g_1, g_2 > -\frac{1}{4}) \]  

(37)

While this Hamiltonian is exactly solvable, we would like to see how band structure can be obtained from representation theory using dynamical symmetry considerations. We will relate this Hamiltonian to the $so(4)$ and $so(2, 2)$ algebras and develop the band structure from the complementary series. We plot some forms of this potential in Fig. 5 for several values of $g_1$ and $g_2$. Our study will be restricted to the range $-1/4 < g_1, g_2 \leq 0$.

A. $so(4)$ REALIZATION

We start with the realization of the $so(4)$ algebra:

\begin{align*}
A_\pm &= \frac{1}{2}e^{\pm i(\phi + \alpha)} \left[ \pm \frac{\partial}{\partial \theta} + \cot 2\theta \left(i \frac{\partial}{\partial \phi} + i \frac{\partial}{\partial \alpha} \mp 1\right) - i \sin 2\theta \left(\frac{\partial}{\partial \phi} - \frac{\partial}{\partial \alpha}\right)\right] \\
A_3 &= -\frac{i}{2} \left(\frac{\partial}{\partial \phi} + \frac{\partial}{\partial \alpha}\right) \\
B_\pm &= \frac{1}{2}e^{\pm i(\phi - \alpha)} \left[ \pm \frac{\partial}{\partial \theta} + \cot 2\theta \left(i \frac{\partial}{\partial \phi} - i \frac{\partial}{\partial \alpha} \mp 1\right) - i \sin 2\theta \left(\frac{\partial}{\partial \phi} - \frac{\partial}{\partial \alpha}\right)\right] \\
B_3 &= -\frac{i}{2} \left(\frac{\partial}{\partial \phi} - \frac{\partial}{\partial \alpha}\right)
\end{align*}

(38)

which have the commutation relations:

\begin{align*}
[A_3, A_+] &= A_+ , \quad [A_3, A_-] = -A_-, \quad [A_+, A_-] = 2A_3, \\
[B_3, B_+] &= B_+ , \quad [B_3, B_-] = -B_- , \quad [B_+, B_-] = 2B_3, \quad [A, B] = 0.
\end{align*}

(39)

Since this is the direct product of two $so(3)$ algebras, the quadratic Casimir invariant has the form:

\begin{align*}
C_2 &= 2(A^2 + B^2) \\
&= 2(A_+ A_- + A_3^2 - A_3 + B_+ B_- + B_3^2 - B_3) \\
&= -\frac{\partial^2}{\partial \theta^2} + \frac{1}{\cos^2 \theta} \left[ -\frac{\partial^2}{\partial \phi^2} - \frac{1}{4} \right] + \frac{1}{\sin^2 \theta} \left[ -\frac{\partial^2}{\partial \alpha^2} - \frac{1}{4} \right] - 1
\end{align*}

(40)
The representations of \( so(4) \) can be labeled by \((j_1, m; j_2, c)\), where \(j_1, j_2, m, c\) are non-negative integers or half integers and \(-j_1 \leq m \leq j_1, -j_2 \leq c \leq j_2\). It is easy to check that, as differential operators, \( A^2 = B^2 \). So for this realization, we only need to consider symmetric representations with \( j_1 = j_2 = j \). Hence, \( C_2 = 4j(j+1) \). The resulting Schrödinger equation is

\[
[- \frac{d^2}{d\theta^2} + \frac{(m+c)^2 - \frac{1}{4}}{\cos^2 \theta} + \frac{(m-c)^2 - \frac{1}{4}}{\sin^2 \theta}] \psi_j^{m,c}(\theta) = (2j+1)^2 \psi_j^{m,c}(\theta) \tag{41}
\]

While this is suitable for bound states, the discrete representation \( s \) of \( so(4) \) do not explain band structure, and the strength of the potential is not in the range of physical interest.

B. \( so(2,2) \) realization

We can derive a more suitable realization by passing to \( so(2,2) \). Starting with the above generators, we \((i)\) scale the wavefunctions by \( \frac{1}{\sqrt{\sin \theta}} \), \((ii)\) transform \( \cos \theta \rightarrow \tanh \theta \) and \((iii)\) take \( \theta \rightarrow i\theta \). This results in the \( so(2,2) \) realization:

\[
A_{\pm} = \frac{1}{2} e^{\pm i(\phi + \alpha)} \left[ \pm \cos \theta \frac{1}{\partial \theta} + i \frac{1}{\sin \theta} \left( \frac{\partial}{\partial \phi} + \frac{\partial}{\partial \alpha} \right) \right] \tag{42}
\]

\[
A_3 = -\frac{i}{2} \left( \frac{\partial}{\partial \phi} + \frac{\partial}{\partial \alpha} \right)
\]

\[
B_{\pm} = \frac{1}{2} e^{\pm i(\phi - \alpha)} \left[ \pm \cos \theta \frac{1}{\partial \theta} + i \frac{1}{\sin \theta} \left( \frac{\partial}{\partial \phi} - \frac{\partial}{\partial \alpha} \right) \right] \tag{43}
\]

\[
B_3 = -\frac{i}{2} \left( \frac{\partial}{\partial \phi} - \frac{\partial}{\partial \alpha} \right)
\]

with the commutation relations

\[
[A_3, A_+ = A_+, \quad [A_3, A_- = -A_-, \quad [A_+, A_-] = -2A_3, \quad [B_3, B_+ = B_+, \quad [B_3, B_- = -B_-, [B_+, B_-] = -2B_3, \quad [A, B] = 0. \tag{44}
\]

The quadratic Casimir invariant now has the form

\[
C_2 = 2(A^2 + B^2) = 2(-A_+A_- + A_3^2 - A_3 - B_+B_- + B_3^2 - B_3) = \cos^2 \theta \frac{\partial^2}{\partial \theta^2} - \cos^2 \theta \frac{\partial^2}{\partial \alpha^2} + \frac{\cos^2 \theta}{\sin^2 \theta} \left( \frac{\partial^2}{\partial \phi^2} + \frac{1}{4} \right) - \frac{3}{4}
\]

The states of the representations of \( so(2,2) \) can be labeled by a direct product of representations of \( so(2,1) \), denoted \((j_1, m; j_2, c)\). Again, as differential operators, \( A^2 = B^2 \) so that \( j_1 = j_2 = j \). Replacing \( \theta \) by \( x \), this leads to the Schrödinger equation:
\[
\left[-\frac{d^2}{dx^2} + \frac{(m+c)^2 - \frac{1}{4}}{\sin^2 x} + \frac{(2j+1)^2 - \frac{1}{4}}{\cos^2 x}\right] \psi_{j,m,c}^m(x) = (m-c)^2 \psi_{j,m,c}^m(x) \tag{45}
\]

Two independent solutions \[17, 18\] in the region \(0 < x < \frac{\pi}{2}\) are:

\[
\psi_1(x) = (\sin^2 x)^{\frac{1}{4} - \frac{m+c}{2}} (\cos^2 x)^{-j-\frac{1}{2}} F_1(-c-j, -m-j; 1-m-c; \sin^2 x) \tag{46}
\]

\[
\psi_2(x) = (\sin^2 x)^{\frac{1}{4} + \frac{m+c}{2}} (\cos^2 x)^{-j+\frac{1}{2}} F_1(m-j, c-j; 1+m+c; \sin^2 x)
\]

In order to develop the band structure of this Schrödinger equation, we must construct the complementary series of the projective representations of \(so(2,2) \sim su(1,1) \oplus su(1,1)\). This direct product structure allows us to simply use the results discussed in the Scarf dynamical symmetry.

The complementary series, labeled by \((j, m, c)\), is constructed as follows. For ranges of \(m\) and \(c\) which correspond to unitary representations of (projective) complementary series \(su(1,1)\), the resulting \(so(2,2)\) representation is also unitary. For ranges of \(m\) and \(c\) which are both non-unitary, the resulting direct product becomes unitary in the strip of physical interest, \(0 < |m+c| \leq 1/2\). The remaining cases when \(m\) is unitary and \(c\) is non-unitary and the case with \(m\) and \(c\) interchanged, result in non-unitary representations of the complementary series of \(so(2,2)\). These non-unitary representations correspond to the energy bands of the extended Scarf potential, which can be seen by taking limiting cases where (i) the potential reduces to the Scarf case (see below) and (ii) the potential vanishes and the spectrum is continuous.

Since the eigenvalue of our Hamiltonian is \(E = (m-c)^2\), and the strength of the potential is labeled by \(j\) and \(m+c\), it is convenient to plot the resulting unitary and non-unitary representations of \(so(2,2)\) versus \(m+c\) for selected values of \(j\). This is done in Fig. 6. Here the energy gaps correspond to the shaded regions and the bands to the unshaded regions. Three values of \(j\) are chosen: (a) \(j = -0.45\), (b) \(j = -0.35\) and (c) \(j = -0.25\). Case (c) corresponds to the Scarf potential limit. As \(j \to -1/2\) or \(|m+c| \to 0\), the bands become degenerate. On the other hand, when \(j \to -1/4\) and \(|m+c| \to 1/2\), the spectrum becomes continuous. For the band edges, one takes the direct product of \(su(1,1)\) discrete projective representations.

The bands \(E = (m-c)^2\) are given by the following ranges of quantum numbers in the \((m, c)\) plane:

\[
2n - (m_o + c_o) - 2j \leq m - c \leq 2n + 1 - |2j + 1 - m_o - c_o|, \tag{47}
\]

\[
2n + 1 - |2j + 1 - m_o - c_o| \leq m - c \leq 2n + 2 + 2j + m_o + c_o,
\]

where \(n = 0, 1, 2, \ldots\) and

\[
0 < |m + c| \leq \frac{1}{2}, \quad 0 < 2j + 1 \leq \frac{1}{2}. \tag{48}
\]

C. Transfer matrix
Due to the strong singularity structure of the potential, one again must introduce boundary conditions for the solutions at singularities such that the Schrödinger operator can be made self-adjoint. Such an analysis has been undertaken in Refs. [9, 17]. We can then easily compute the transfer matrix for the interval \( x \in (-\frac{\pi}{2}, \frac{\pi}{2}) \) using the boundary values and first derivatives at \( \frac{\pi}{2} \). The transfer matrix is:

\[
T = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} \tag{49}
\]

where

\[
\alpha = e^{-i(m-c)\pi} \left[ \frac{\cos \pi(m-c) + \cos \pi(2j+1)\cos \pi(m+c)}{\sin \pi(2j+1)\sin \pi(m+c)} \right. \\
+ i \left( \frac{1}{m-c} \frac{\Gamma(-2j-1)\Gamma(1+j-m)\Gamma(1+j-c)}{\Gamma(2j+1)\Gamma(-j-m)\Gamma(-j-c)} \\
- (m-c) \frac{\Gamma(2j+1)\Gamma(-j-m)\Gamma(-j+c)}{\Gamma(-2j-1)\Gamma(1+j+m)\Gamma(2+j+c)} \right) \\
\left. \frac{\sin \pi(j-m)\sin \pi(j-c)}{\sin \pi(2j+1)\sin \pi(m+c)} \right] \tag{50}
\]

\[
\beta = -i e^{i(m-c)\pi} \frac{\sin \pi(j-m)\sin \pi(j-c)}{\sin \pi(2j+1)\sin \pi(m+c)} \left[ \frac{1}{m-c} \frac{\Gamma(-2j-1)\Gamma(1+j-m)\Gamma(1+j-c)}{\Gamma(2j+1)\Gamma(-j-m)\Gamma(-j-c)} \\
+ (m-c) \frac{\Gamma(2j+1)\Gamma(-j-m)\Gamma(-j+c)}{\Gamma(-2j-1)\Gamma(1+j+m)\Gamma(2+j+c)} \right] \tag{51}
\]

D. Dispersion relation

The dispersion relation is computed as before, using \( \cos \pi k = Re(\alpha e^{i(m-c)\pi}) \):

\[
\cos \pi k = \frac{\cos \pi(m-c) + \cos \pi(2j+1)\cos \pi(m+c)}{\sin \pi(2j+1)\sin \pi(m+c)}. \tag{52}
\]

If we denote

\[
m_+ = m + c, \quad m_- = m - c, \tag{53}
\]

then \( E = (m-c)^2 = m_-^2 \), and we find:

\[
E(k) = m_-^2 \]

\[
= \frac{1}{\pi^2} \left[ \cos^{-1}(\cos \pi k \sin \pi(2j+1)\sin \pi m_+ - \cos \pi(2j+1)\cos \pi m_+) \right]^2 \tag{54}
\]
The band structure could be explained through the projective representations of $so(2, 2)$ when $0 < |m + c| \leq \frac{1}{2}$ and $-\frac{1}{2} < j \leq -\frac{1}{4}$. Again, non-unitary representations give the energy bands while unitary representations correspond to energy gaps.

The group velocity for this potential is

$$V(j, m, c) = \frac{\partial E}{\partial k} = \frac{2m_-}{\sin \pi m_-} \left[ \sin^2(2\pi j) - \cos^2 \pi m_+ - \cos^2 \pi m_- \right]$$

$$+ 2 \cos \pi m_- \cos \pi m_+ \cos 2\pi j \right]^{1/2}$$

The behavior is shown in Fig. 7 for selected values of $j$ and $m + c$ given by the dashed lines in Fig. 6. The effective mass $M^*(j, m, c)$ is given by:

$$\frac{1}{M^*} = \frac{\partial^2 E}{\partial k^2} = 2m_- \pi \left[ \cot \pi m_- - \cos 2\pi j \cos \pi m_+ \csc \pi m_- \right]$$

$$+ 2 \csc^2 \pi m_- (1 - m_- \pi \cot \pi m_-) \left( \sin^2 2\pi j - \cos^2 \pi m_+ \right)$$

$$- \cos^2 \pi m_- + 2 \cos \pi m_- \cos \pi m_+ \cos 2\pi j$$

E. Limiting cases

There are three cases where the extended Scarf potential reduces to the Scarf case:

(i) When $2j + 1 = \frac{1}{2}$, the potential becomes the Scarf potential and the transfer matrix is equivalent to Eqs. (24)-(25).

(ii) When $m + c = \frac{1}{2}$, Eq. (38) reduces to the potential

$$\frac{(2j + 1)^2 - \frac{1}{4}}{\cos^2 \theta}$$

and the transfer matrix is consistent with the results of Sec. II.E.

(iii) When $|m + c| = 2j + 1$, the Hamiltonian reduces to the Scarf potential with twice the period.

Of the three limiting cases, it is case (ii) which provides something new. To compare to the Scarf results, we let $2j + 1 = \tilde{j} + \frac{1}{2}$, so that the potential (57) becomes $\tilde{j}(\tilde{j} + 1)/\sin^2 x$.

For the full complementary series $-1/2 < j \leq 0$, we have $-1/2 < \tilde{j} \leq 1/2$ which corresponds to potentials $g/\sin^2 x$ with $-1/4 < g < 3/4$. From (47) we find that the energy bands are given by

$$2n - \tilde{j} \leq m - c \leq 2n + 1 + \tilde{j},$$

$$2n + 1 - \tilde{j} \leq m - c \leq 2n + 2 + \tilde{j}.$$
agrees with the more recent observation that the Scarf potential admits band structure for ranges of the strength which are positive[1]. It also exemplifies the fact that a dynamical symmetry does not necessarily exhaust all possible regimes of band structure, and that other realizations might provide additional regions. In principle we can extend our analysis of the generalized Scarf potential to $g_1, g_2 > 0$ as well, but we do not do so here.

IV. Conclusions

We have shown that dynamical symmetry techniques can be applied to Hamiltonians with periodic potentials, and band structure can arise naturally from representation theory. This fills a long-standing gap in the algebraic approach to quantum systems. We have constructed dynamical symmetry Hamiltonians in $so(2,1)$ and $so(2,2)$ which can be expressed as Schrödinger operators with periodic potentials. Using projective representations motivated by Bloch’s theorem, we have seen that the complementary series of $so(2,1)$ and $so(2,2)$ (and their non-unitary representations) are needed to explain band structure, while the discrete representations are important for band edges. As far as we know, this is the first application of the $su(1,1)$ complementary series to a physical problem. It now seems reasonable to loosely associate the three series of projective representations, discrete, principal and complementary, with the quantum problems of bound states, scattering states and energy bands.

Using our dynamical symmetries, Hamiltonians such as Scarf’s and its extension can be reduced to quadratic forms of the Cartan subalgebra generators, such as $H = J_z^2$, which are readily solved. We are then able to derive not only the band structure, but the dispersion relation and transfer matrix as well. It would be interesting to develop higher dimensional periodic Hamiltonians connected to representations of $u(n,m)$ or $so(n,m)$. In this case, the inclusion of additional discrete symmetries using point groups would be possible, and extensions to non-dynamical symmetry problems could be pursued.

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Appendix A: Representations of \( so(2, 1) \)

First, let us recall the presentation of \( so(3) \). The algebra can be realized as differential operators on the sphere \( x^2 + y^2 + z^2 = 1 \). The representations are labeled by \((j, m)\) where \( j \) is any non-negative half integer and \( -j \leq m \leq j \).

The \( so(2, 1) \) algebra can be realized as differential operators on the sphere \( x^2 + y^2 + z^2 = 1 \). The representations are labeled as \((j, m)\) where \( j \) is any non-negative half integer and \( -j \leq m \leq j \).

The unitary representations are [12]:

- The principal series \( j = -\frac{1}{2} + i\rho, \rho > 0, m = 0, \pm 1, \ldots \)
- The complementary series \( -\frac{1}{2} < j < 0, m = 0, \pm 1, \ldots \)
- The discrete series \( D^+_j \), where \( j \) is a negative integer or half integer and \( m = -j, -j + 1, \ldots \)
- The discrete series \( D^-_j \), where \( j \) is a negative integer or half integer and \( m = j, j - 1, \ldots \)

A more general form of the representations of the algebra are the projective representations. The projective unitary representations of \( so(2, 1) \) are [13]:

- The principal series \( j = -\frac{1}{2} + i\rho, \rho > 0, 0 \leq m_0 < 1, m = m_0 \pm n, n = 0, 1, 2, \ldots \)
- The complementary series \( -\frac{1}{2} < j < 0, 0 \leq m_0 < 1, m_0(m_0 - 1) > j(j + 1) \geq -\frac{1}{4}, m = m_0 \pm n, n = 0, 1, \ldots \)
- The discrete series \( D^+_j, j < 0, m = -j, -j + 1, \ldots \)
- The discrete series \( D^-_j, j < 0, m = j, j - 1, \ldots \)

Since we find that the non-unitary representations are important for the bands, we review their origin [13]. Assuming \( I_3 f = m_0 f \), with \( 0 \leq m_0 < 1 \), and using the commutation relations for \( so(2, 1) \), we have

\[
\begin{align*}
I_3 I_+ f &= (m_0 + 1)I_+ f \quad \text{(A1)} \\
I_3 I_- f &= (m_0 - 1)I_- f \quad \text{(A2)} \\
I_- I_+ f &= [-j(j + 1) + m_0(m_0 + 1)]f \quad \text{(A3)} \\
I_+ I_- f &= [-j(j + 1) + m_0(m_0 - 1)]f \quad \text{(A4)}
\end{align*}
\]

where \( I^2 = j(j + 1) \) is the Casimir, a constant for a specific representation. Replacing \( f \) by \( I_+^{n-1} f \) and \( I_-^{n-1} f \) \((n = 1, 2, \ldots)\) in the last two equations, we get

\[
\begin{align*}
I_- I_+^n f &= \alpha_n I_+^{n-1} f \quad \text{(A5)} \\
I_+ I_-^n f &= \beta_n I_-^{n-1} f \quad \text{(A6)}
\end{align*}
\]
where \( \alpha_n = -j(j+1) + (m_0 + n - 1)(m_0 + n) \) and \( \beta_n = -j(j+1) + (m_0 - n)(m_0 - n + 1) \). The above relations imply

\[
||I_{n+1}^n f||^2 = (I_{n+1}^n f, I_{n+1}^n f) = \alpha_{n+1}||I_{n+1}^n f||^2 \quad (A7)
\]

\[
||I_{n+1}^{-1} f||^2 = (I_{n+1}^{-1} f, I_{n+1}^{-1} f) = \beta_{n+1}||I_{n+1}^{-1} f||^2 \quad (A8)
\]

Starting with the initial state \( f \), we can generate the coefficients \( \alpha_k \) and \( \beta_k \) \((k > 0)\). Of these coefficients, only \( \beta_1 \) can be positive or negative. This distinguishes the unitary and non-unitary representations. For instance \( \beta_1 > 0 \) when \( m_0(m_0 - 1) > j(j+1) \), which gives the complementary series. When we are in the region \( -j < m_0 < 1 + j \), \( \beta_1 < 0 \). So if we start with a state \( f \) labeled by \((j, m_0)\) with \( -j < m_0 < 1 + j \), we find that all states obtained by operating with \( I_+ \) will have norms of the same sign. These are related to all the states \( I_n^m f \) by a sign change in the norm. Consequently, the states of the non-unitary representation can be divided into two families. In each family, the states have norms of the same sign, while the two families are related by a change in sign in the norm.

### Appendix B: A Formula for the Transfer Matrix

When the potential is symmetric about the center of each period, it is convenient to consider even and odd solutions \( g(E, x), u(E, x) \) such that

\[
g(E, 0) = 1, \quad g'(E, 0) = 0, \quad (B1)
\]

\[
u(E, 0) = 0, \quad u'(E, 0) = 1. \quad (B2)
\]

Let us define \([14]\)

\[
g(E, -\frac{a}{2}) = g(E, \frac{a}{2}) = g_0(E); \quad (B3)
\]

\[
g'(E, -\frac{a}{2}) = -g'(E, \frac{a}{2}) = g'_0(E); \quad (B4)
\]

\[
u(E, -\frac{a}{2}) = -u(E, \frac{a}{2}) = u_0(E); \quad (B5)
\]

\[
u'(E, -\frac{a}{2}) = u'(E, \frac{a}{2}) = u'_0(E); \quad (B6)
\]

According to the definition of transfer matrix \([15]\), we can derive a formula as follows:

\[
T = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} \quad (B7)
\]

where

\[
\alpha = e^{-ik\alpha}[(g_0u'_0 + g'_0u_0) + i(u'_0g'_0/k - u_0g_0k)] \quad (B8)
\]

\[
\beta = -ie^{ika}(u'_0g'_0/k + u_0g_0k) \quad (B9)
\]

and \( k = \sqrt{E}, a \) is the period.
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\[ E = m^2 \]
