Bound States and Band Structure - a Unified Treatment through the Quantum Hamilton-Jacobi Approach

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Abstract

We analyze the Scarf potential, which exhibits both discrete energy bound states and energy bands, through the quantum Hamilton-Jacobi approach. The singularity structure and the boundary conditions in the above approach, naturally isolate the bound and periodic states, once the problem is mapped to the zero energy sector of another quasi-exactly solvable quantum problem. The energy eigenvalues are obtained without having to solve for the corresponding eigenfunctions explicitly. We also demonstrate how to find the eigenfunctions through this method.

1 Introduction

Study of periodic potentials has evoked renewed interest in the literature in light of their appearance in Bose-Einstein condensates [1], [2] and photonic crystals [3], [4], [5], [6]. It has been possible to experimentally change structure of the potential, so as to produce superfluid - insulator transition [7], the former having delocalized states and the latter localized ones. In this context, traditional Kronig-Penny model [8] is used for illustrative purposes, wherein the known wave functions lead to transcendental equations involving energy and momentum, when appropriate boundary conditions are implemented. The possibility of investigating superfluid-insulator type transitions mentioned above does not arise here, due to the lack of any control parameter. Quite sometime back, Scarf showed that a solvable model exists, which exhibits both discrete bound states and band spectra [9], as a function of the coupling parameter. The group theoretical aspects of this problem have recently been investigated [10]. The fact that Scarf potential yields both bound states and band structure, as a function of a coupling parameter, makes this model an ideal one to study the interplay of these two types of distinct behavior in a given quantal problem.

The goal of this paper is to first map the Scarf eigenvalue problem into the zero energy sector of another quasi-exactly solvable (QES) problem. We then use the quantum Hamilton-Jacobi (QHJ) approach [11], which naturally takes advantage of the singularities of the new potential, to isolate the domains corresponding to discrete and band spectra. The subtle aspects of the boundary

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conditions in quantum mechanics, which lead to the existence of both bound states and band structure in the Scarf potential, come out naturally in this approach. We then proceed to obtain the eigenvalues and eigenfunctions, for both the cases. In this procedure, the energy eigenvalues can be obtained, without finding the eigenfunctions. The QHJ formalism, being formulated in the complex domain where the non-linear Riccati equation replaces the Schrödinger equation, makes use of powerful theorems in complex variable theory to obtain the solutions.

Apart from the fact that QHJ formalism is relatively new and requires detailed study, this approach may provide a different perturbative treatment for the traditional problems. As will be clear from the text, WKB approximation scheme is close to this method [12]. In the following section, we briefly describe the working principles of the QHJ formalism, which is then used for the analysis of the Scarf potential in Section 3. The origin of the bound and the band spectra is then illustrated, without getting into the explicit computation of the eigenvalues, whose details are given in Section 3.2. We obtain the solutions pertaining to both the spectra. We conclude in the final section after pointing out various directions for future investigations.

2 Quantum Hamilton-Jacobi formalism

The QHJ formalism, formulated as a theory analogous to the classical canonical transformation theory [13], [14], [15], was proposed by Leacock and Padgett in 1983. It has been applied to one dimensional bound state problems and separable problems in higher dimensions [11]. In our earlier studies, we have shown that one could use the QHJ formalism to analyze one dimensional exactly solvable (ES), quasi-exactly solvable models, consisting of both periodic and aperiodic potentials [16], [17], [18], [19], [20], [21] and the recently discovered PT symmetric potentials [22]. The advantage of this method lies in the fact that it requires a modest understanding of basic quantum mechanics and complex analysis as a prerequisite.

In this formalism, the logarithmic derivative of the wave function $\psi(x)$, given by

$$p = -i\hbar \frac{d}{dx} \ln \psi(x),$$

plays an important role. This is referred to as the quantum momentum function (QMF), since it is defined analogous to the classical momentum function as, $p = \frac{dS}{dx}$. Here, $S$ is the Hamilton’s characteristic function which is related to the wave function by $\psi(x) = \exp(iS/\hbar)$. Substituting $\psi(x)$ in terms of $S$ in the Schrödinger equation,

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x),$$

and using the relation between $p$ and $\psi$, one obtains the non-linear Riccati
\[ p^2 - i\hbar p' = 2m(E - V(x)). \] \hspace{1cm} (3)

The above equation is known as the QHJ equation; here \( x \) is treated as a complex variable, thereby extending the definition of \( p \) to the complex plane. We show that one can arrive at the required results by studying the singularity structure of the QMF.

**Singularity structure**

The QMF has two types of singularities, the moving and the fixed singularities. From (1) one can see that, the \( n \) nodes of the \( n^{th} \) excited state, whose locations depend on the initial conditions and energy, correspond to the singularities of \( p \). These are known as the moving singularities. It is a fact that only poles can appear as moving singularities in the solutions of the Riccati equation. One can calculate the residue at a moving pole \( x_0 \), where \( V(x) \) is analytic, by doing a Laurent expansion of \( p \) around \( x_0 \) as,

\[ p = \sum_{k=1}^{l} (x - x_0)^{-k} + \sum_{k=0}^{\infty} (x - x_0)^k. \] \hspace{1cm} (4)

Substituting this in (3) and comparing individually the coefficients of different powers of \( x - x_0 \), one obtains \( l = 1 \), with the corresponding residue equalling \(-i\hbar\).

The fixed singularities originate from the potential and are present in all the solutions of the Riccati equation. One can calculate the residue at the fixed poles in the same way, as is done for the moving poles. Owing to the quadratic nature of the QHJ equation, one obtains two solutions. In order to arrive at the right solution, one needs to choose the residue that gives the correct physical behavior. The right value of the residue is chosen by applying the appropriate boundary conditions, details of which will be given in the text, as and when required. Thus, knowing the singularity structure of QMF and the behavior of \( p \) at infinity, one gets the complete form of the QMF. In all the models studied so far, including the periodic potentials, the assumption that, the QMF has finite number of singularities, is equivalent to saying that the point at infinity is an isolated singular point, has been found to be true. We expect it to be valid for the present case also.

For most exactly solvable models, the QMF has been found to be a rational function. As is known, for a rational function the sum of all residues including that at infinity is zero. This result has been used to obtain the energy eigenvalues for all the models studied in the QHJ approach. It should be pointed out that, this condition is equivalent to the exact quantization condition satisfied by the action \( J \) [11]:

\[ J = \oint_C p \, dx = n\hbar. \] \hspace{1cm} (5)

Hence, for the case of Scarf potential, one first tries to bring the QMF into a rational form through a suitable change of variable, as discussed in the next
section. It is interesting to note that in the classical limit,
\[ p \to p_c = \sqrt{2m(E - V(x))}, \]  
(6)
where \( p_c \) is the classical momentum. The QHJ quantization condition then leads to the WKB approximation scheme. The boundary condition (6) was originally used by Leacock and Padgett to obtain the constraints on the residues [11].

3 The Scarf Potential

The Scarf potential is given by
\[ V(x) = -\left(\frac{(\frac{1}{4} - s^2)x^2}{2ma^2\sin^2\left(\frac{\pi x}{a}\right)}\right), \]  
(7)
where, \( a \) is the potential period. One finds that in the range \( s > 1/2 \), the potential is an array of infinite potential wells as shown in Fig 1. A quantum particle is then confined to only one well, implying that the wave function should vanish at \( x = \pm a \). Thus, in the above range, the potential exhibits bound state spectra. As shown in Fig.2, in the range \( 0 < s < 1/2 \), the potential is similar to that of a potential in a crystal lattice, leading to the possibility of energy bands. In this scenario, a particle can escape to infinity. Therefore the wave function need not vanish at \( x = \pm a \). However, \( \psi(x) \) should not diverge anywhere, on physical grounds.

The QHJ equation for the Scarf potential, with \( p = -iq \) and \( \hbar = 1 \) in (3), is given by,
\[ q^2 + q' + \frac{\pi^2}{a^2} \left( \lambda^2 + \frac{(\frac{1}{4} - s^2)}{\sin^2\left(\frac{\pi x}{a}\right)} \right) = 0, \]  
(8)
where \( \lambda^2 = 2mEa^2/\pi^2 \). We perform a change of variable using
\[ y = \cot\left(\frac{\pi x}{a}\right), \]  
(9)
In order to get all the coefficients in the above equation to a rational form, which in turn will easily yield the singularities of the QMF, we use the transformation equations

\[ q = -\frac{\pi h}{a}(1 + y^2)\phi ; \quad \phi = \chi - \frac{y}{1 + y^2}. \]  

This leads to the QHJ equation in terms of \( \chi \) as,

\[ \chi^2 + \frac{d\chi}{dy} + \frac{\chi^2 - 1}{(y^2 + 1)^2} + \frac{(1 - s^2)}{y^2 + 1} = 0. \]  

Henceforth, the above equation will be treated as the QHJ equation and \( \chi \) as the QMF. It is interesting to note that, substituting \( \chi = \frac{d}{dy}(\ln(\tilde{\psi}(y))) \) in the above equation, one gets a Schrödinger equation, which describes the zero energy sector of the potential, \((\lambda^2 - 1)/(y^2 + 1)^2 + (1 - s^2)/(y^2 + 1)\). By analyzing the singularity structure of this quasi-exactly solvable problem, we obtain the required results for the solvable Scarf potential, as shown below.

### 3.1 Form of the QMF \( \chi \)

The QMF has \( n \) moving poles with residue one on the real line, as is clear from the Riccati equation. From (12), one can see that \( \chi \) has fixed poles at \( y = \pm i \). Making use of the assumption that the QMF has finite number of moving poles, one can write \( \chi \) in the rational form, separating its analytical and singular parts as

\[ \chi = \frac{b_1}{y - i} + \frac{b'_1}{y + i} + \sum_{k=1}^{n} \frac{1}{y - y_k} + Q. \]  

Figure 2: Scarf potential, with \( s = 0.4, a = 1 \), allows band structure.
Here, $b_1$ and $b'_1$ are the residues at $y = i$ and $y = -i$ respectively and the summation term describes the sum of all the singular parts coming from the moving poles. Note that, $\sum_{k=0}^{n} \frac{1}{y - y_k} = \frac{P'_n(y)}{P_n(y)}$, where $P_n(y)$ is an $n^{th}$ degree polynomial. The quantity $Q$ represents the analytic part of $\chi$ and from (12) one can see that $\chi$ is bounded for large $y$. Thus, from Liouville’s theorem, $Q$ is a constant; denoting it as $C$, [13] can be written as,

$$\chi = \frac{b_1}{y - i} + \frac{b'_1}{y + i} + \frac{P'_n(y)}{P_n(y)} + C. \quad (14)$$

One can calculate the residues at the fixed poles $y = \pm i$, by making a Laurent expansion of $\chi$ around the pole. For example, to calculate the residue at $y = i$, we expand $\chi$ as,

$$\chi = \frac{b_1}{y - i} + a_0 + a_1(y - i) + \cdots. \quad (15)$$

Comparing the coefficients of different powers of $(y - i)$ individually, one obtains

$$b_1 = \frac{1 \pm \lambda}{2}. \quad (16)$$

Similarly the other residue at $y = -i$ is found to be

$$b'_1 = \frac{1 \pm \lambda}{2}. \quad (17)$$

To find the eigenvalues, we now make use of the fact that, for a rational function, the sum of all the residues equals zero. As noted earlier, this is equivalent to the quantization condition [13] of Leacock and Padgett. Thus, we obtain

$$b_1 + b'_1 + n = d_1, \quad (18)$$

where $d_1$ is the residue at infinity, which is calculated by taking Laurent expansion of $\chi$ around the point at infinity:

$$\chi = d_0 + \frac{d_1}{y} + \frac{d_2}{y^2} + \cdots. \quad (19)$$

Substitution of the above in the QHJ equation yields,

$$d_1^2 - d_1 + \left(\frac{1}{4} - s^2\right) = 0, \quad (20)$$

from which, the values of $d_1$ can be deduced:

$$d_1 = \frac{1 \pm 2s}{2}. \quad (21)$$

Substituting the values of the residues in (18), one obtains

$$n = -\frac{1}{2} \pm s \mp \lambda, \quad (22)$$

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which gives the degree of the polynomial $P_n(y)$ in (14). From the definition of $\lambda$, one can see that if $E < 0$, $\lambda$ becomes imaginary, in which case (22) will not be satisfied. Thus, from the above equation, we have the condition $E > 0$, which in turn implies $\lambda > 0$ and real. Hence, for any range of $s$, the energy eigenvalues are greater than zero. With this condition on $\lambda$, we now proceed to select the values of the residues at the fixed poles and at infinity, which will give us the physically acceptable results.

### 3.2 Choice of the residues

One needs to use the boundary conditions obeyed by the QMF [11] to choose the right value of residues. Although, there are several ways of implementing the boundary conditions in the QHJ formalism, we have chosen the one closest to the conventional approach for clarity. First, we shall fix the value of the residue at infinity. From the prior discussion of the potential, we know that the wave functions should not become infinite anywhere, in particular, for $x = \pm a$. From (11), one can obtain $\psi(x)$ in terms of the QMF. Writing $p = -iq$ and doing the change of variable, one obtains the wave function:

$$\psi(y) = \exp \left( -\int \frac{a}{\pi} \frac{q}{1 + y^2} \, dy \right).$$  \hspace{1cm} (23)

Using the transformation equations in (11), the above expression for the wave function becomes

$$\psi(y) = \exp \left( \int \left( \chi - \frac{y}{1 + y^2} \right) \, dy \right).$$  \hspace{1cm} (24)

For large $y$, the leading behavior of $\chi$ is obtained as $\chi \sim \frac{d_1}{y}$, which when substituted in (24), yields,

$$\psi(y) \sim \exp \left( \int \left( \frac{d_1}{y} - \frac{y}{1 + y^2} \right) \, dy \right)$$  \hspace{1cm} (25)

$$\sim \frac{y^{d_1}}{(y^2 + 1)^{1/2}}.$$  \hspace{1cm} (26)

Using the value of $d_1$ from (21) in the above equation, one obtains

$$\psi(y) \sim \frac{y^{\frac{1}{2} \pm s}}{(y^2 + 1)^{1/2}}.$$  \hspace{1cm} (27)

For $0 < s < \frac{1}{2}$, one can see that $\psi \rightarrow 0$, in the limit $y \rightarrow \infty, x \rightarrow ma$, with $m$ being an integer, for both the values of $d_1$. This range corresponds to the case where the potential exhibits band structure.

For $s > 1/2$, $\psi(y) \rightarrow 0$, in the limit $y \rightarrow \infty, x \rightarrow ma$, with $m$ being an integer, only if $d_1$ takes the value $1/2 - s$. In this way, the two different ranges of the potential parameter $s$ emerge simultaneously, while fixing the values of
In order to select the values of $b_1$ and $b'_1$, we note that the bound state and band edge wave functions of one dimensional potentials are non-degenerate and have definite parity. Parity operation requires that $\chi(-y) = -\chi(y)$, which in turn gives

$$b_1 = b'_1.$$  \hfill (28)

With the above constraint, (18) becomes

$$2b_1 + n = d_1.$$  \hfill (29)

Finiteness of the wave function as $x \to \infty$, gives the values of $d_1$ in the two ranges as

$$d_1 = \begin{cases} \frac{1+2s}{2} & \text{for } 0 < s < 1/2, \\ \frac{1-2s}{2} & \text{for } s > 1/2. \end{cases}$$ \hfill (30)

From the parity constraint, one obtains the restriction on the values of the residues at the fixed poles as $b_1 = b'_1$. Using these results, we proceed to calculate the solutions for the two ranges.

3.3 Case 1: Band spectrum

In the range $0 < s < 1/2$, we have seen that $d_1$ can take both the values of the residues. Taking all the possible combinations of the residues, with $b_1 = b'_1$ and substituting them in (18), we evaluate $n$, the degree of the polynomial $P_n(y)$. There are four combinations forming four different sets, as given in the fifth column of table I. Since $n$ needs to be positive, from table I, we pick only those sets which give a positive integral value for $n$. As seen earlier, $\lambda$ is a positive real constant. Thus, only the sets 1 and 2 will yield positive values for $n$ and hence; the other two sets are ruled out. Taking the values of $b_1$ and $d_1$ from the sets 1 and 2, substituting them in (29) and using the definition of $\lambda$ and $s$, we obtain the expressions for the energy eigenvalues corresponding to the two band edges of the $n^{th}$ band as,

$$E_n^\pm = \frac{\pi^2}{2ma^2} \left( n + \frac{1}{2} \pm s \right)^2.$$ \hfill (31)

Here, $E_n^\pm$ correspond to the upper and lower band energies of the $n^{th}$ band. These results match with the solutions given in [9] and [10].

The corresponding wave functions follow from (14) and (24):

$$\psi(y) = (y^2 + 1)^{b_1 - \frac{1}{2}} P_n(y).$$ \hfill (32)

To obtain the expression for the polynomial, we substitute $\chi$ from (14) in the QHJ equation, which gives a second order differential equation:

$$P_n''(y) + \left( \frac{4b_1y}{y^2 + 1} \right) P_n'(y) + \left( \frac{1/4 - s^2}{y^2 + 1} + \frac{4b_1^2y^2 + 2b_1(1 - y^2) + \lambda^2 - 1}{(y^2 + 1)^2} \right) P_n(y) = 0.$$ \hfill (33)

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$$P_n''(y) + \left( \frac{4b_1y}{y^2 + 1} \right) P_n'(y) + \left( \frac{1/4 - s^2}{y^2 + 1} + \frac{4b_1^2y^2 + 2b_1(1 - y^2) + \lambda^2 - 1}{(y^2 + 1)^2} \right) P_n(y) = 0.$$ \hfill (33)
The sets 1 and 2 have \( b_1 = (1 - \lambda)/2 \), which yields

\[
P'_n(y) + \left( \frac{2(1 - \lambda)y}{y^2 + 1} \right) P_n(y) + \frac{1}{y^2 + 1} s^2 - \lambda P_n(y) = 0. \tag{34}\]

From (31), one can see that \( \lambda \) has two values \( \lambda = n \pm s + \frac{1}{2} \). Substituting these in the above equation, one obtains two differential equations corresponding to the two energy eigenvalues \( E^\pm_n \):

\[
(y^2 + 1)P''_n(y) + (1 - 2n - 2s)yP'_n(y) + n(n + 2s)P_n(y) = 0. \tag{35}\]

Defining \( y = it \), the above equation takes the form of the well known Jacobi differential equation

\[
(1 - t^2)P''_n(t) + \left( \nu_1 - \nu_2 - t(\nu_1 + \nu_2 + 2) \right)P'_n(t) + n(n + \nu_1 + \nu_2 + 1)P_n(t) = 0, \tag{36}\]

with \( \nu_1 = \nu_2 = -n \pm s - 1/2 \), for the corresponding two \( \lambda \) values. The expression for the two band edge wave functions for the \( n \)th band are given by,

\[
\psi(y) = (y^2 + 1)^{-\frac{s}{2}} P_{s_1,s_2}^\nu (iy), \tag{37}\]

with their respective \( \nu \) values corresponding to \( \lambda = n \pm s + 1/2 \).

### 3.4 Case 2 : Bound state spectrum

We proceed in the same way as in case 1 i.e., take all possible combinations of \( b_1, b'_1 \) and \( d_1 \), keeping \( b_1 = b'_1 \) in (29). Since \( d_1 \) can take only one value \( 1 - s \), only two sets are possible here. Out of these, the set corresponding to \( b_1 = b'_1 = (1 - \lambda)/2 \) alone, will give a positive value for \( n \). Thus, substituting these values of residues in (29), one obtains the expression for the energy eigenvalue as

\[
E_n = \frac{\pi^2}{2ma^2} \left( \frac{1}{2} + n + \sqrt{1 - \frac{2mV_0a^2}{\pi^2 \hbar^2}} \right)^2, \tag{38}\]

where \( n \) can take positive integral values. Proceeding as above one obtains the Jacobi differential equation in terms of \( t \) for the polynomial part :

\[
(1 - t^2)P''_n(t) - 2t(-n - s + \frac{1}{2})P'_n(t) - n(n + 2s)P_n(t) = 0. \tag{39}\]

The expression for the wave function is then given by

\[
\psi(y) = (y^2 + 1)^{-\frac{s}{2}} P_{s_1,s_2}^\nu (iy), \tag{40}\]

where \( s_1 = s_2 = -n - s - 1/2 \).

Hence, as pointed out in the beginning, the two different sectors of the Hamiltonian, as a function of the coupling parameter and the eigenvalues emerge from general principles of QHJ formalism, relying on the singularity structure of
the QMF function. The wave functions corresponding to the definite eigenvalues are obtained at the end, which match with the known results [23].

Conclusions
We have mapped the entire Scarf problem, containing the bound state and energy bands, to the zero energy sector of a different Hamiltonian, which is quasi-exactly solvable. This was achieved through point canonical transformations which led to the redistribution of singularities in the complex domain. The singularity structure of this new Hamiltonian is transparent enough to clearly isolate two different regimes, as a function of the coupling constant. When related to the original problem, they turn out to represent discrete levels and the band edges. It will be interesting to carefully analyze the equilibrium structure of the classical electrostatics problem, associated with the QES system, which leads to both bound states and band structure in the quantum domain. In light of the current interest in periodic potentials in BEC and photonic crystals, we hope the quantum Hamilton-Jacobi based treatment presented here is not only illuminating, but may also lead to development of new perturbative treatments for non-exactly solvable problems.

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Table 1. All possible combinations of residues in the range $0 < s < 1/2$.

| Set | $b_1$ | $b'_1$ | $d_1$ | $n = d_1 - b_1 - b'_1$ | remark |
|-----|-------|-------|-------|-----------------|-------|
| 1   | $\frac{1-\lambda}{2}$ | $\frac{1-\lambda}{2}$ | $d_1 = 1/2 - s$ | $\lambda - s - \frac{1}{2}$ | $\lambda > (s + \frac{1}{2})$ |
| 2   | $\frac{1-\lambda}{2}$ | $\frac{1-\lambda}{2}$ | $d_1 = 1/2 + s$ | $\lambda + s - \frac{1}{2}$ | $\lambda > -(s - \frac{1}{2})$ |
| 3   | $\frac{1+\lambda}{2}$ | $\frac{1+\lambda}{2}$ | $d_1 = 1/2 - s$ | $-\lambda - s - \frac{1}{2}$ | not valid |
| 4   | $\frac{1+\lambda}{2}$ | $\frac{1+\lambda}{2}$ | $d_1 = 1/2 + s$ | $-\lambda + s - \frac{1}{2}$ | not valid |