

On the Dimensions of the Vector Space Generated by the Bound States for a Two Dimensional Schrödinger Equation with Anisotropic Interactions Confined in a Riemann Surface E^2

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Abstract

In this paper, we consider the dimensions of the vector space generated by the bound states for a 2-dimensional Schrödinger equation with an anisotropic potential $\sum_{j=1}^N v_j(r)\omega(\phi)\delta(r - a_j)$ bounded by two-dimensional Riemann surfaces of radius a_j , where δ is the usual Kronecker delta function. The variables r and ϕ are radial and angular coordinates respectively, $\omega(\phi)$ measures the interaction at angle ϕ on the Riemann surface. The Hamiltonian is the sum of the kinetic and the interaction part. The interactions are separable and are centered at arbitrary points on the surface. The dimension of the vector space generated by bound states is obtained using a general method suitable for the determination of energies and mean values of different operators corresponding to the normalized wave function. Conditions for the existence and for the number of bound states in finite linear chains are formulated in terms of the parameters of the interactions and intercentre distances. It is shown that for the model considered in this paper, the dimension of the vector space generated by the bound states reduces as the number of inter-particle interactions N in the surface increases.

1.0 Introduction

Hamiltonians based on point interactions are known to be fruitful in the mathematical development of solvable quantum mechanical models for a one particle system. The two dimensional model presents great features that enable us reduce bound state problems to the evaluation of finite matrices whose elements are known analytic functions while, at the same time, avoiding the complexity resulting from the algebra of angular momentum when dealing with the three dimensional case. Furthermore, a two dimensional model gives room for the possibility of introducing the effect of an exterior uniform magnetic field more easily than in the three-dimensional case. Models in two-dimensional spaces are relevant in surface physics.

2.0 The Hamiltonian

Hamiltonians based on point interactions are given as

$$H = \frac{p_x^2 + p_y^2}{2M} + \sum_{j=1}^N v_j(r)\omega(\phi)\delta(r - a_j) = H_0 + V \quad (2.1)$$

The kinetic part $\frac{p_x^2 + p_y^2}{2M}$ for a particle of mass M is taken as H_0 while the interaction is denoted by V and is a sum of the separable interactions $v_j\omega(\phi)\delta(r - a_j)$ resulting from the various particle actions centered at a point P_j located at a distance a_j from a point O , that is $a_j = \overline{OP_j}$

For the planar case, that is when the Riemannian surface is E^2 , cartesian coordinates x, y in the plane are related to polar coordinates by $x = r \cos(\phi)$ and $y = r \sin(\phi)$, where $0 \leq r < \infty$ and $0 \leq \phi \leq 2\pi$. The following assumptions shall be made

(i) There is a one to one correspondence between the number of interactions N and the points P_j at which the interactions are centered.

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(ii) Atomic units are employed where $\hbar = 1, e = 1$

(iii) The interaction is anisotropic and is a sum of separable interactions $V_j = \sum_k \lambda_j^k |\xi_j^k\rangle \langle \xi_j^k| \omega(\phi) \delta(r-a_j)$ where $|\xi_j^k\rangle = \exp(-i\mathbf{a}_j \cdot \mathbf{p}) r_j^k |r_j^k, m_j^k\rangle$.

The kets $|r_j^k, m_j^k\rangle$ are generalized eigenvectors (normalized with respect to a Dirac distribution) of the radial position operator r which has an eigenvalue r_j^k and the eigenvector of the angular momentum operator $l = xp_y - yp_x$ which has an eigenvalue m_j^k . Besides the kets already introduced, generalized eigenvectors of the position operator \mathbf{r} , of the momentum operator \mathbf{p} and of the radial momentum operator p shall be needed. The operator $\exp(-i\mathbf{a}_j \cdot \mathbf{p})$ rotates the state vectors by an amount \mathbf{a}_j , while λ_j^k is an overall strength parameter with energy as dimension and $\omega(\phi)$ measures the energy interaction at angular position ϕ which (for simplicity, but without loss of generality is assumed to be confined in E^2). If $\omega(\phi)$ is constant, we have an isotropic Hamiltonian. The isotropic case has been considered in [1]. In this paper, we shall be interested in only the anisotropic case where $\omega(\phi)$ is not constant. The Schrödinger equation in configuration space reads

$$-\frac{\nabla^2}{2M} \Psi(\mathbf{r}, \phi) + \sum_{j=1}^N v_j(r) \omega(\phi) \delta(r - a_j) \Psi(\mathbf{r}, \phi) = E \Psi(\mathbf{r}, \phi) \tag{2.2}$$

where $v_j(r) = \sum_k \lambda_j^k |\xi_j^k\rangle \langle \xi_j^k|$. In operator form, we can express the Hamiltonian corresponding to (2.2) as

$$H_\lambda = \frac{p_x^2 + p_y^2}{2M} + \sum_j \sum_k \lambda_j^k |\xi_j^k\rangle \langle \xi_j^k| a_j \int d\phi \omega(\phi) |a_j, \phi\rangle \langle a_j, \phi| \tag{2.3}$$

where the integration over ϕ is taken over the interval $0 \leq \phi \leq 2\pi$. V can be expressed as

$$V = \sum_j a_j \sum_k \lambda_j^k |\xi_j^k\rangle \langle \xi_j^k| \sum_{m_j^k=-\infty}^{\infty} \sum_{m_j^k=-\infty}^{\infty} c_q(\omega) |a_j, m_j^k\rangle \langle a_j, m_j^k| \tag{2.4}$$

where $q = m_j^k - m_j^{k'}$ and c_q is the Fourier coefficient of ω which can be written as

$$c_q(\omega) = \frac{1}{2\pi} \int_0^{2\pi} d\phi \omega(\phi) \exp[-i(m_j^k - m_j^{k'}) \phi] \tag{2.5}$$

where

$$\omega(\phi) = \sum_{l=-\infty}^{\infty} c_l(\omega) \exp(il\phi) \tag{2.6}$$

We assume $\omega(\phi)$ in (2.6) is real so that c_q satisfies

$$c_q = \overline{c_{-q}} \tag{2.7}$$

3.0 The Resolvent Equation

It is well known that bound state problems as well as scattering problems reduce to the calculations of matrix elements of the free resolvent

$$G_0(z) = \frac{1}{z - H_0} \tag{3.1}$$

Here H_0 is the kinetic part of the Hamiltonian H . The bound state energies for a finite number of centres $G(z)$, is then defined as

$$G(z) = \left\{ \left(z - \frac{p^2}{2M} \right) - V \right\}^{-1} \tag{3.2}$$

and is related to the free resolvent $G_0(z)$, by the equation

$$G(z) = G_0(z) + G_0(z) V G(z) \tag{3.3}$$

Equation (3.3) is an identity equation called the resolvent equation. The resolvent equation yields after some calculations the following equations

$$\Gamma(z) = \left([\Gamma_0(a_j, a_j z)]^{-1} - \sum_j a_j \sum_k \lambda_j^k |\xi_j^k\rangle \langle \xi_j^k| c(\omega) \right)^{-1} \tag{3.4}$$

where

$$[\Gamma_0(a_j, a_j z)]_{m_1 m} \equiv \delta_{m_1 m} \langle a_j, m_1 | G_0(z) | a_j, m \rangle \tag{3.5}$$

so that

$$\left\{ \left[\Gamma_0(a_j, a_j, z) \right]^{-1} \right\}_{m_1 m_1} = \delta_{m_1 m_1} \frac{1}{\langle a_j, m_1 | G_0(z) | a_j, m_1 \rangle} \quad (3.6)$$

According to the general formulation of quantum mechanics the values of z are

$$z = \lim_{\varepsilon \rightarrow 0^+} \frac{p^2}{2M} + i\varepsilon \quad (3.7)$$

The notation $\lim_{\varepsilon \rightarrow 0^+}$ means that ε goes to zero by positive values. It can be established that

$$\langle r_1, m_1 | G_0(z) | r_2, m_2 \rangle = \delta_{m_1, m_2} \int_0^\infty dp \, p \frac{J_{m_1}(pr_1) J_{m_1}(pr_2)}{z - \frac{p^2}{2M}} \quad (3.8)$$

Also

$$\begin{aligned} \langle r_1, m_1 | \exp(-i\mathbf{a}\cdot\mathbf{p}) G_0(z) | r_2, m_2 \rangle &= -(-1)^{m_1 - m_2} 2M \exp(i\varphi_a(m_1 - m_2)) \\ &\times \int_0^\infty dp \, p \frac{J_{m_1}(pr_1) J_{m_2}(pr_2) J_{m_1 - m_2}(ap)}{p^2 - 2Mz} \end{aligned} \quad (3.9)$$

The final expression for $\langle r_1, m_1 | G_0(z) | r_2, m_2 \rangle$ can be obtained by explicit determination of the integral on the right hand side of equation (3.9). To achieve this, we assume $a \geq r_1 + r_2$. This inequality corresponds to the non-overlapping interactions. Consider now the positive square root of the quantity $2Mz$, we denote this as

$$p_z \equiv \sqrt{2Mz} \quad (3.10)$$

When z is negative, (which is essential for a bound state to occur), p_z lies on the positive imaginary axis. When z is positive, we must then take into consideration the value of $\lim_{\varepsilon \rightarrow 0} z + i\varepsilon$ when evaluating the integral. The following results then suffices

$$\langle r_1, m_1 | G_0(z) | r_2, m_1 \rangle = \delta_{m_1, m_2} \left[-iM\pi J_{m_1}(p_z r_<) H_{m_1}^{(1)}(p_z r_>) \right] \quad (3.11)$$

$$\langle r_1, m_1 | \exp(i\mathbf{a}\cdot\mathbf{p}) G_0(z) | r_2, m_2 \rangle = \mu M \pi \exp(i\varphi_a(m_2 - m_1)) H_{m_1 - m_2}^{(1)}(ap_z) J_{m_1}(r_1 p_z) J_{m_2}(r_2 p_z) \quad (3.12)$$

$r_< = \min(r_1, r_2)$, $r_> = \max(r_1, r_2)$ and $\mu = -i(-1)^{m_1 - m_2 + 1}$. $H_m^{(1)}$ is the Hankel function irregular at the origin [4].

4.0 Bound State Problems

Depending on the nature of the interaction V , bound state may or may not exist. If they exist, their energies can be calculated from the relation $z = E$ for negative values of z . The bound state energies for a finite number of centres can be determined as the negative z values for which the determinant of a matrix $b(z)$ are zero [1]. The order of the matrix is equal to the number of projectors. The matrix $b(z)$ is defined by its elements

$$b_{s,n}(z) = \delta_{s,n} - \lambda_n \langle \xi_s | G_0(z) | \xi_n \rangle \quad (4.1)$$

This result follows from the identity (3.3). The unnormalized expression for the bound states is given as

$$|\Psi\rangle = \sum_j a_j \sum_k \lambda_j^k |\xi_j^k\rangle \langle \xi_j^k | G_0(z) \sum_{m=-\infty}^\infty [c(\omega)x]_m x |r, m\rangle \quad (4.2)$$

with x the column vector whose m th line is $\langle rm | \Psi \rangle$. Equation (4.2) defines Ψ . Once its energy is known, the column vector x is determined from the equation

$$\left[c(\omega) - \frac{1}{r_0(z) \sum_j a_j \sum_k \lambda_j^k |\xi_j^k\rangle \langle \xi_j^k|} \right] x = 0 \quad (4.3)$$

The matrix $[c(\omega)]$ in equation (4.3) is a symmetric Laurent matrix that is, it is a double infinite matrix with constant terms along the principal diagonal and the diagonals parallel to the principal diagonal. The function ω is called the symbol of the Laurent matrix. It has been established that if ω is bounded on the circle then $[c(\omega)]$ generates a bounded operator on $l^2(Z)$ and has a range ω . Details of these properties are given in [5]. Note that if the range of ω contains zero, then $[c(\omega)]$ is not invertible.

The wave function in momentum space $\langle p|\Psi\rangle$ is

$$\Psi(p) = \frac{\sum_j a_j \sum_k \lambda_j^k |\xi_j^k\rangle \langle \xi_j^k|}{E - \frac{p^2}{2M}} \sum_{m=-\infty}^{\infty} [c(\omega)x]_m (-1)^m J_m(pa) \left(\frac{\exp(im\phi_p)}{\sqrt{2\pi}} \right) \quad (4.4)$$

where p in (4.4) is real, positive or zero. Normalization of bound states is achieved using matrix multiplication.

$$\langle \Psi|\Psi\rangle = \left(\sum_j a_j \sum_k \lambda_j^k |\xi_j^k\rangle \langle \xi_j^k| \right)^2 [c(\omega)x]^\dagger \mathbb{T}(z) [c(\omega)x] \quad (4.5)$$

where \mathbb{T} is a diagonal matrix with diagonal element defined by

$$T(z)_{m,m} = \langle \xi_s | G_0(z) G_0(z) | \xi_n \rangle = - \left\langle \xi_s \left| \frac{\partial G_0(z)}{\partial z} \right| \xi_n \right\rangle \quad (4.6)$$

The matrix elements $\langle \xi_s | G_0(z) G_0(z) | \xi_n \rangle$ can also be expressed in terms of Bessel and Hankel functions [6], so that

$$\langle \Psi|\Psi\rangle = [c(\omega)x]^\dagger \left(\sum_j a_j \sum_k \lambda_j^k |\xi_j^k\rangle \langle \xi_j^k| \right)^2 + \frac{i\pi M^2 a_j \left[J_m(pa_j) (H_{m-1}^{(1)}(pa_j) - H_{m+1}^{(1)}(pa_j)) + H_m^{(1)}(pa_j) (J_{m-1}(pa_j) - J_{m+1}(pa_j)) \right]}{2p} \quad (4.7)$$

The exact normalized eigenvector corresponding to the Hamiltonian H_λ with eigenvalue z_u say has been given in [1] to be

$$|\Psi_u\rangle = \frac{G_0(z_u) \sum_n |\xi_n\rangle \langle \xi_n | \Psi_u\rangle}{\sqrt{\sum_{n,s} \langle \Psi_u | \xi_n\rangle \langle \xi_n | G_0(z_u) G_0(z_u) | \xi_s\rangle \langle \xi_s | \Psi_u\rangle}} \quad (4.8)$$

The coefficients $\langle \xi_n | \Psi_u\rangle$ are the elements of a column eigenvector associated with the zero eigenvalue of the matrix $b(z_u)$. Without loss of generality $\langle \xi_n | \Psi_u\rangle$ is taken to be real. This then gives the result

$$\langle r | G_0(z_u) | \xi_j \rangle = \langle r | \exp(-i\mathbf{a}_j \cdot \mathbf{p}) G_0(z_u) r_j^k | r_j^k, m_j^k \rangle \quad (4.9)$$

For bound state, the small z behavior of the matrix $b(z)$ gives for the diagonal elements

$$b_{n,n}(0) = 1 + \frac{M\lambda_n r_n^2}{|m_n|} \quad \text{if } m_n \neq 0 \quad (4.10)$$

$$b_{n,n}(0) \approx 1 - 2M\lambda_n r_n^2 \log(p_z r_n) \quad \text{if } m_n = 0 \quad (4.11)$$

The non-diagonal elements give for the same centre but different projectors

$$b_{s,n}(z) \approx \delta_{m_s m_n} \frac{M\lambda_s r_s r_n}{|m_n|} \left(\frac{r_s}{r_n} \right)^{|m|} \quad \text{with } m_n \neq 0 \quad (4.12)$$

With $m_n = 0$ we have

$$b_{s,n}(z) \approx -2\delta_{m_s m_n} M\lambda_s r_s r_n \log(p_z r_s) \approx -2\delta_{m_s m_n} M\lambda_s r_s r_n \log(p_z) \quad (4.13)$$

The non-diagonal elements give for different centres

$$b_{s,n}(z) \approx - \frac{2^{1-2|m_n|} M\lambda_s r_n^{1+|m_n|} r_s^{1+|m_n|}}{(m_n!)^2} p_z^{2|m_n|} \log\left(\frac{a_j - a_i}{p_z} \right), \quad m_n = m_s \quad (4.14)$$

For $m_n \neq m_s$ the non-diagonal elements give for different centres

$$b_{s,n}(z) \approx (-1)^{m_n - m_s} h(m_n - m_s) h(m_n) h(m_s) \exp(i\varphi_{a_j - a_i}(m_n - m_s)) M_0 \quad (4.15)$$

where

$$M_0 = 2^{|m_n - m_s| - |m_n| - |m_s|} M\lambda_s \frac{r_s^{1+|m_s|} r_n^{1+|m_n|}}{(a_i - a_j)^{|m_n - m_s|}} \frac{(m_n - m_s - 1)!}{|m_n|! |m_s|!} (p_z)^{|m_n| - |m_s| - |m_n - m_s|} \quad (4.16)$$

These are the conditions for bound states. These results are general but can be applied to specific cases.

5.0 On the Dimensions of the Vector Space Generated by the Bound States

For a bound state labelled by k the energy $E_k < 0$ depends on the parameter λ_j^k for a fixed mass M and radius a_j . The dimensions of the vector space generated by bound states are determined as follows; if $E_k(\lambda_j^k)$ exists for an arbitrary small $|\lambda_j^k|$ values then

$$\lim_{|\lambda_j^k| \rightarrow 0} E_k(\lambda_j^k) = 0 \tag{5.1}$$

Indeed, for a normalized eigenvector $|\psi\rangle$ of the Hamiltonian H one has

$$\langle \psi | H | \psi \rangle = E_k(\lambda_j^k) < 0 \tag{5.2}$$

Since $\langle \psi | \frac{p^2}{2M} | \psi \rangle \geq 0$, one deduces that

$$\sum_j a_j \sum_k \lambda_j^k \langle \psi | \xi_j^k \rangle \langle \xi_j^k | \psi \rangle \sum_{m_j^k=-\infty}^{\infty} \sum_{m_j^k=-\infty}^{\infty} c_q(\omega) |a_j, m_j^k\rangle \langle a_j, m_j^k| \rightarrow 0 \tag{5.3}$$

as $|\lambda_j^k| \rightarrow 0$. So, if $E_k(\lambda_j^k)$ does not exist for arbitrary small value of $|\lambda_j^k|$ then there exist values λ_{jc}^k of λ_j^k for which a bound state exist if $|\lambda_j^k| > |\lambda_{jc}^k|$ with energy tending to 0 as $|\lambda_j^k| \rightarrow |\lambda_{jc}^k|$ and transforms into a continuum state if $|\lambda_j^k| < |\lambda_{jc}^k|$. Thus, for each $E_k(\lambda_j^k)$ there is a critical value. The dimension of the vector space generated by bound states is therefore determined if these critical values are determined. Thus, counting the number of bound states amounts essentially to determining the critical points. At critical values, the energy goes to zeros and therefore we are interested at the limit where p_z tends to zero along the positive imaginary axis. In that limit we have

$$\langle a_n m_n | G_0(z) | a_n m'_n \rangle \sim \begin{cases} -\delta_{m_n m'_n} \frac{M}{|m_n|}, & |m_n| < 0 \\ 2M \left[\gamma + \log\left(\frac{a_n p_z}{2}\right) - \frac{i\pi}{2} \right] \equiv Y, & m_n = 0 \end{cases} \tag{5.4}$$

γ is the Euler constant.

6.0 Conclusion

The general theory presented in this paper is useful for studying the spectrum of finite two-dimensional complex systems involving arbitrary geometrical configurations. It is also useful in the study of collisional processes involving two-dimensional targets with complex geometrical configurations. The benefit of our model lies not only on the possibility of choosing the geometrical configuration of the system, but also on the flexibility of the choice parameters corresponding to each centred interactions. The strength parameters λ_j^k , range parameters r_j^k , angular momentum parameters m_j^k can be varied independently. In this paper, we provided, for a Riemann space, a general method for studying genuine anisotropic interactions confined in a Riemann space. To the best of our knowledge, this general theory has not been presented before in the literature. It was shown that, the dimension of the vector space generated by the bound states in the model we considered, reduces as the number of inter-particle interactions N in the surface increases. In particular, by restricting the parameter values of these model cases, the simple case where only one bound state exists could be considered. Applications to specific examples would be given in another paper.

7.0 References

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