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2004 J. Phys. A: Math. Gen. 37 5689

(http://iopscience.iop.org/0305-4470/37/21/014)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **37** (2004) 5689–5696 PII: S0305-4470(04)73940-2

Supersymmetric quantum merchanics, orthogonal states and the Pauli exclusion principle

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Received 19 December 2003, in final form 14 April 2004
Published 12 May 2004
Online at stacks.iop.org/JPhysA/37/5689
DOI: 10.1088/0305-4470/37/21/014

Abstract

Starting from the orthonormal eigenfunctions which are the solutions of the Schrödinger equation for a given potential it is shown that sets of functions orthogonal to the eigenstates inside a region of varying radius R may be constructed. These sets of functions may in turn be used to construct a new set of functions which satisfy bound-state boundary conditions and are themselves solutions of the Schrödinger equation in a new potential. The bound-state spectrum of the new potential is related to the spectrum of the original potential in a definite manner. The relationship of this construction of a new potential to the inverse scattering theory approach based on the Gelfand–Levitan equation and the potentials constructed using supersymmetric quantum mechanics (SUSYQM) is explored. The connection of this approach to other approaches based on the implementation of orthogonality and their relation to Pauli exclusion principle is examined.

PACS numbers: 02.30.Gp, 03.65.Fd, 11.30.Pb

1. Introduction

Inverse scattering theory is concerned with the question of construction of a potential from given data on bound-state parameters and scattering phaseshifts. The Gelfand–Levitan equation (Gelfand and Levitan 1951) and the Marchenko equation (Marchenko 1955) were for a long time the equations which were used to study inverse scattering probelms (Chadan and Sabatier 1977). The link between supersymmetric quantum mechanics (SUSYQM) (Witten 1981, Andrianov *et al* 1984, Sukumar 1985a) and inverse scattering theory (Sukumar 1985b) has provided new insights. It has been shown that a combination of a pair of supersymmetric (SUSY) transformations may be used to recover the results from the Gelfand–Levitan approach. An alternative pair of SUSY transformations leads to the construction of singular potentials. The construction of singular potentials using a pair of SUSY transformations has been used to

illustrate the relation between deep and shallow potentials in a variety of problems in nuclear physics (Baye 1987, 1994). Section 2 of this paper examines the question of the construction of a new potential by the elimination of a certain number of bound-states of a potential starting from a new point of view namely the orthogonal states inside a region of variable radius R.

The construction of potentials which do not possess a specified set of bound-states has a long history in the theory of the scattering of complex particles. In section 3 of the paper the relationship of the approach adopted in this paper with some of the other approaches which have been used in the past is explored. Section 4 contains the conclusions. Units in which $\hbar = 1$ and the reduced mass $\mu = 1$ are used throughout this paper so that $\hbar^2/2\mu = 1/2$.

2. Orthogonal states inside a region of size R and new potentials

Let Ψ_i be the normalized eigenstates which are solutions of the radial Schrödinger equation for a potential V in the space $[0, \infty]$

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + 2\,(V - E_i)\right)\Psi_i = 0. \tag{1}$$

A function which is orthogonal to the ground state in the interval $[0, R]$ is then given by

$$F(r, R) = \Psi_2(r) - \Psi_1(r)\frac{\int_0^R \Psi_1(y)\Psi_2(y)\,\mathrm{d}y}{\int_0^R \Psi_1^2(y)\,\mathrm{d}y}. \tag{2}$$

There is a unique linear combination of Ψ_1 and Ψ_2 for each value of the size of the box R which is orthogonal to Ψ_1 inside the box region. The function $F(r, R)$ may be used to construct a new function Φ_2 given by

$$\Phi_2(r) = F(r, r). \tag{3}$$

It is the purpose of this paper to show that functions such as Φ_2 are themselves eigenstates of the Schrödinger equation at energy E_2 for a new potential which has a spectrum identical to that of the original potential apart from missing the ground state. This procedure then corresponds to the construction of a new potential by the elimination of the ground state of a given potential but preserving the rest of the spectrum. It is easy to generalize this approach to the elimination of arbitrary number of bound-states. To eliminate the n lowest bound-states we proceed as follows. The orthonormal eigenstates of V may be used to construct a matrix M of dimension (n, n) whose elements are given by

$$M_{ij}(R) = \int_0^R \Psi_i(y)\Psi_j(y)\,\mathrm{d}y. \tag{4}$$

Next we construct a matrix N of dimension $(n + 1, n + 1)$ whose elements are given by

$$\begin{aligned} N_{ij} &= M_{ij} \qquad i, j = 1, 2, \ldots, n \\ N_{i,n+1} &= \int_\infty^R \Psi_i(y)\Psi_m(y)\,\mathrm{d}y \\ N_{n+1,i} &= \Psi_i(r) \\ N_{n+1,n+1} &= \Psi_m(r) \end{aligned} \tag{5}$$

where the index m can take any value. It must be noted that the limits on the integral defining $N_{i,n+1}$ are from ∞ to R. Using the orthonormality of the eigenstates Ψ_i we can also write this element in the form

$$N_{i,n+1} = \int_0^R \Psi_i(y)\Psi_m(y)\,\mathrm{d}y - \delta_{im}. \tag{6}$$

When $m > n$ the δ_{im} term will not contribute. However, if m lies in the range $[1, n]$ the δ_{im} term will contribute and therefore for all values m we can consider

$$F_m(r, R) = \frac{\text{Det } N}{\text{Det } M}. \tag{7}$$

It is clear that when $m > n$

$$\int_0^R F_m(r, R)\Psi_j(r)\,\mathrm{d}r = 0 \qquad \text{if} \quad j = 1, 2, \ldots, n \tag{8}$$

because two rows arising from the matrix N become identical and the determinant vanishes. We have thus established that the functions $F_m(r, R)$ with $m > n$ are orthogonal to the eigenstates $\Psi_j(r)$ in the domain $[0, R]$ when the index j lies in the range [1,n]. The functions $F_m(r, R)$ also have the property that in the limit $R \to \infty$ they tend to $\Psi_m(r)$ because all the overlap integrals except the diagonal ones in the matrices in equation (7) vanish. Therefore, if we define

$$\Phi_m(r) = F_m(r, r) \tag{9}$$

then the functions $\Phi_m(r)$ and $\Psi_m(r)$ have the same asymptotic behaviour for large r.

Expansion of the determinant in the numerator of equation (7) and the use of the definition of the inverse of a matrix leads to

$$F_m(r, R) = \Psi_m(r) - \Psi_j(r)M^{-1}_{jk}(R)\tilde{M}_{km}(R) \tag{10}$$

where the elements of the matrix $\tilde{M}$ are given by

$$\tilde{M}_{jk}(r) = \int_\infty^r \Psi_j(y)\Psi_k(y)\,\mathrm{d}y = M_{jk}(r) - \delta_{jk}. \tag{11}$$

The function Φ_m in equation (9) can then be written as

$$\Phi_m(r) = \Psi_m(r) - \Psi_j(r)M^{-1}_{jk}(r)\tilde{M}_{km}(r). \tag{12}$$

In all the above expressions the repeated indices are summed in the range $(1, n)$. When the index $m = l \leqslant n$ the use of

$$M_{kl} = \delta_{kl} + \tilde{M}_{kl} \tag{13}$$

leads to the representation

$$\Phi_l(r) = \Psi_j(r)M^{-1}_{jl}(r). \tag{14}$$

Thus in terms of the solutions to the linear equations given by

$$M_{jk}(r)\Phi_k(r) = \Psi_j(r) \qquad j, k = 1, 2, \ldots, n \tag{15}$$

for all values of m without any restriction we can write equation (11) as

$$\Phi_m(r) = \Psi_m(r) - \Phi_k(r)\tilde{M}_{km}(r) \tag{16}$$

where all of the Φ_m satisfy the same boundary conditions as Ψ_m in the limit $r \to \infty$.

We can use the simple case of $n = 1$ to illustrate the structure of the above equations. For $n = 1$

$$\begin{aligned}
M_{11} &= \int_0^r \Psi_1^2(y)\,\mathrm{d}y \\
\tilde{M}_{12} = M_{12} &= \int_0^r \Psi_1(y)\Psi_2(y)\,\mathrm{d}y \\
\tilde{M}_{11} = M_{11} - 1 &= \int_\infty^r \Psi_1^2(y)\,\mathrm{d}y \\
\Phi_1(r) &= \frac{\Psi_1(r)}{M_{11}} \\
\Phi_2(r) &= \Psi_2(r) - \Phi_1(r)M_{12}
\end{aligned} \tag{17}$$

Φ_2 satisfies bound-state boundary conditions while Φ_1 diverges when $r \to 0$ and does not satisfy bound-state boundary conditions.

We now return to the general case of arbitrary n and examine the differential equation satisfied by Φ defined by equation (16). Differentiation of this equation twice, use of the Wronskian relation

$$\Psi_j \frac{\mathrm{d}\Psi_k}{\mathrm{d}r} - \frac{\mathrm{d}\Psi_j}{\mathrm{d}r}\Psi_k = 2(E_j - E_k)\int_\infty^r \Psi_j(y)\Psi_k(y)\,\mathrm{d}y \tag{18}$$

and rearrangement of the terms lead to the expression

$$\frac{\mathrm{d}^2\Phi_m}{\mathrm{d}r^2} = \frac{\mathrm{d}^2\Psi_m}{\mathrm{d}r^2} - \frac{\mathrm{d}^2\Phi_k}{\mathrm{d}r^2}\tilde{M}_{km} - 2\Psi_m\frac{\mathrm{d}}{\mathrm{d}r}\sum_{k=1}^{n}(\Phi_k\Psi_k) + 2(E_m - E_k)\Phi_k\tilde{M}_{km}. \tag{19}$$

The Schrödinger equation satisfied by Ψ namely equations (1), and (16) may then be used to eliminate Ψ_m to obtain

$$(L + 2E_m)\Phi_m + \sum_{k=1}^{n}((L + 2E_k)\Phi_k)\tilde{M}_{km} = 0 \tag{20}$$

where the operator L is defined by

$$L = \frac{\mathrm{d}^2}{\mathrm{d}r^2} - 2\left(V - \frac{\mathrm{d}}{\mathrm{d}r}\sum_j \Phi_j\Psi_j\right). \tag{21}$$

If $m = l \leqslant n$ using equation (13) this gives

$$\sum_k ((L + 2E_k)\Phi_k)M_{kl} = 0 \qquad l = 1, 2, \ldots, n. \tag{22}$$

These linear equations imply that

$$(L + 2E_k)\Phi_k = 0 \qquad \text{if} \quad \mathrm{Det}\,M \neq 0 \quad k = 1, 2, \ldots, n. \tag{23}$$

When used in equation (20) this implies that

$$(L + 2E_m)\Phi_m = 0 \qquad m = 1, 2, \ldots, n, n+1, \ldots. \tag{24}$$

Thus we have shown that Φ_m for any value of m satisfies the Schrödinger equation given by

$$\frac{\mathrm{d}^2\Phi_m}{\mathrm{d}r^2} = 2(V_n - E_m)\Phi_m \tag{25}$$

where the new potential V_n is given by

$$V_n = V - \frac{\mathrm{d}}{\mathrm{d}r}\sum_j \Phi_j\Psi_j. \tag{26}$$

Using the property of the determinant

$$\frac{\mathrm{d}}{\mathrm{d}r}\ln\mathrm{Det}\,M = \sum_j\sum_k \Phi_j M^{-1}_{jk}\Psi_k = \sum_k \Phi_k\Psi_k \tag{27}$$

the potential $\tilde{V}$ may be written in the form

$$V_n = V - \frac{\mathrm{d}^2}{\mathrm{d}r^2}\ln\mathrm{Det}\,M. \tag{28}$$

We can also infer from equations (11) and (16) that when $m > n$ the solutions Φ_m have the same asymptotic behaviour as Ψ_m as $r \to \infty$ and also vanish as $r \to 0$ and therefore satisfy the boundary conditions appropriate for a bound-state. But when $m \leqslant n$ then it can be shown

using equation (15) that in the limit $r \to 0$ the solutions ϕ_m diverge and therefore do not satisfy the boundary conditions of a bound-state. Therefore, we can conclude that the potential V_n supports bound-states at the same energies E_m as V when $m > n$ with the eigenfunctions given by equation (15) and does not have normalizable eigenstates when $m \leqslant n$. These expressions for the potential obtained from the elimination of the first n bound-states of V are in agreement with the derivation of singular potentials by Baye (1987). However, in this paper we have derived these expressions by examining the orthogonality of states inside a region of varying radius without any reference to supersymmetry. This opens up the possibility of a better understanding of the physical content of the relation between deep and shallow potentials both of which can explain a given set of experimental data.

2.1. Orthogonal states outside a region of size R and new potentials

In the discussion presented above we considered functions $F(r, R)$ which were orthogonal to the first n bound-states of V in the domain $[0, R]$. An alternative procedure would be to consider functions $\tilde{F}(r, R)$ which are orthogonal to the first n bound-states of V in the domain $[R, \infty]$ given by

$$\tilde{F}_m(r, R) = \Psi_m(r) - \Psi_j(r)\tilde{M}^{-1}_{jk}(R)M_{km}(R). \tag{29}$$

$\tilde{F}_m$ can then be used to define a set of new functions

$$\tilde{\Phi}_m(r) = \tilde{F}_m(r, r) = \Psi_m(r) - \Psi_j(r)\tilde{M}^{-1}_{jk}(r)M_{km}(r). \tag{30}$$

Following the same kind of reasoning as in the previous calculation it can be established that for $m = l \leqslant n$

$$\tilde{\Phi}_l(r) = -\Psi_j(r)\tilde{M}^{-1}_{jl}(r) \qquad l = 1, 2, \ldots, n. \tag{31}$$

In terms of the solutions to the linear equations given by

$$\tilde{M}_{jk}(r)\tilde{\Phi}_k(r) = -\Psi_j(r) \qquad j, k = 1, 2, \ldots, n \tag{32}$$

for all values of m without any restriction we can write

$$\tilde{\Phi}_m(r) = \Psi_m(r) + \tilde{\Phi}_k(r)M_{km}(r) \tag{33}$$

all of which satisfy the same boundary conditions as Ψ_m in the limit $r \to 0$. By differentiating this equation twice and using the Wronskian and the Schrödinger equations satisfied by Ψ we can establish that

$$\frac{\mathrm{d}^2\tilde{\Phi}_m}{\mathrm{d}r^2} = 2(\tilde{V}_n - E_m)\tilde{\Phi}_m \qquad m = 1, 2, , , n, n+1, \ldots \tag{34}$$

where the new potential is given by

$$\tilde{V}_n = V - \frac{\mathrm{d}^2}{\mathrm{d}r^2}\ln \mathrm{Det}\,\tilde{M}. \tag{35}$$

Examination of equation (33) shows that for $m > n$ the functions $\tilde{\Phi}_m$ satisfy bound-state boundary conditions and therefore are eigenstates of $\tilde{V}_n$ while for $m \leqslant n$ they do not satisfy bound-state boundary conditions. Hence the potential $\tilde{V}_1$ supports bound-states at the same energies E_m as V when $m > n$ with the eigenfunctions given by equation (33) and does not have normalizable eigenstates when $m \leqslant n$. This expression for the potential obtained from the elimination of the first n bound-states of V is identical to the corresponding potential obtained using the Gelfand–Levitan equations (Abraham and Moses 1980). For scattering energies the phase shifts in $\tilde{V}_n$ are related to the phase shifts in V in a definite manner as discussed in Sukumar (1985b). Equations (28) and (35) are the main results of this section

which establish that the method used in this paper leads to the same results as those obtained using SUSYQM. In the following section the connection of the present approach to other approaches in the literature is examined.

3. Connection with other approaches and the Pauli exclusion principle

There have been many attempts over the last 65 years to study the effect of the Pauli exclusion principle in the scattering of a projectile by a target both of which may have internal structure. The first was the resonating group method (RGM) which was invented by Wheeler (1937). The basic idea was to build up a wavefunction for the whole nucleus out of cluster wavefunctions each of which takes into account the interactions within and between individual groups of nucleons. The nucleons spend a part of their time in each of several groupings and resonate between these different groupings. The linear combinations of wavefunctions describing the different groupings take into account symmetries such as the Pauli principle. A few years later Buckingham and Massey (1941) published a calculation of neutron–deuteron scattering with a resonating group wavefunction which satisfied the proper space and spin symmetries. In subsequent years many resonating group calculations for nucleon–nucleus and nucleus–nucleus scattering were made with properly antisymmetrized wavefunctions. An example is a calculation of ^{16}O + ^{16}O elastic scattering by Wada and Horiuchi (1988). The resonating group wavefunction for the elastic scattering of two nuclei is an antisymmetrized product of wavefunctions for each cluster and a wavefunction $\psi(\mathbf{r})$ where $\mathbf{r}$ is the coordinate of the centre of mass of one cluster relative to the other. The wavefunction $\psi(\mathbf{r})$ satisfies a non-local Schrödinger equation where the non-local kernel $K(\mathbf{r}, \mathbf{r}')$ incorporates the effects of the Pauli principle. Certain states of relative motion are forbidden by the Pauli principle and these are automatically excluded by the properties of the non-local kernel.

The resonating group kernel is very complicated and must be calculated accurately in order to exclude the Pauli forbidden states. In 1968 Saito proposed a simplified approach called the orthogonality condition model (OCM) (Saito (1968, 1977)). The OCM equation for the wavefunction of relative motion $\psi(\mathbf{r})$ has a similar structure to the RGM equation. The simplified non-local kernel contains projection operators designed to make $\psi(\mathbf{r})$ orthogonal to the Pauli forbidden states. The OCM has been used widely for studying bound and resonant cluster states in light nuclei. Buck *et al* (1977) proposed an even simpler approach with a deep local potential to describe the nucleus–nucleus interation. They noted that the strongly bound-states in such a potential were very similar to the Pauli excluded states in the RGM or OCM and argued that those states should be excluded as physical states. Phase shifts and resonances in alpha–alpha, ^{3}He–alpha and ^{16}O–^{16}O scattering calculated with their method gave a good representation of the available experimental data and of the results of full-scale calculations with complete antisymmetrization.

Swan (1955, 1968) investigated the possibility of using shallow local potentials for scattering problems involving complex particles. Whenever the compound state of the target and projectile involves more than a full shell of electrons, neutrons or protons then the Pauli exclusion principle forbids the formation of cluster states with certain intercluster quantum numbers. Swan (1968) argued that for n excluded compound states the phase shift/binding energy-equivalent two-body potential should have a repulsive core as $r \to 0$ of the form $2n(2n + 2l + 1)/2r^2$ in addition to the usual centrifugal barrier $l(l + 1)/2r^2$ term. Swan's work clearly established, that in contast to the usual restrictions to non-singular potentials in potential scattering theory, the scattering of composite systems permits the presence of certain singularities which have their physical origin in the Pauli exclusion principle.

Alternative projection procedures have been designed by other authors. Celenza and Shakin (1979) examined the influence of orthogonality constraints in proton induced reactions. Continuum proton wavefunctions which are solutions of an optical-model Hamiltonian are generally not orthogonal to bound proton wavefunctions having the same quantum numbers. But two different Hamiltonians are used to define the continuum and bound-states of the proton. The proton distorted wave should in principle be orthogonal to the bound-states of the proton but since two different Hamiltonians are used it is clear that they would not be orthogonal in general. Celenza and Shakin solved the problem by introducing a new optical-model Hamiltonian $\tilde{H}$ with a parameter λ present so that $\tilde{H}$ is orthogonal to the bound-states and the scattering states of $\tilde{H}$ are chosen such that λ may take values which implement the required orthogonality. Boffi *et al* (1982) studied a similar problem arising from the lack of orthogonality between continuum final states in knockout reactions and suggested the use of effective operators to correct for the orthogonality defect.

Lehman (1982) studied the representation of the Pauli exclusion effects in the spin $1/2$ state of the α–nucleon interaction. He considered both a repulsive potential and an attractive potential with excluded Pauli forbidden bound-states. Results for the nuclides He and Li of mass number $A = 6$ showed that at low energies both interactions give good fits to the phase shifts but they differ at higher energies. Lehman concluded that the results for the ground-state three-body binding energies for the $A = 6$ nuclides suggested that the attractive excluded bound-state interaction gives a better representation of the Pauli exclusion principle effects in the spin $1/2$ state than the repulsive form.

All the studies mentioned above were conducted prior to the development of supersymmetric quantum mechanics which traces its historical roots to the seminal paper by Witten (1981). All the works mentioned above employ projection operator techniques and derive effective Hamiltonians which are non-local. A connection between supersymmetric transformations and inverse scattering theory was made in 1985 (Sukumar 1985a, b). Baye (1987) showed how two SUSY transformations may be used to produce singular potentials with singularities of the form discussed in Swan's work (Swan 1968) and applied the technique to study $\alpha - \alpha$ scattering. In contrast to the methods used prior to 1982 SUSY transformations produce new potentials which are guaranteed to be local. The connection between SUSYQM, the Pauli principle and the nucleon–alpha scattering has been discussed by Amado *et al* (1990). There have been other studies of scattering with Pauli-blocked bound-states in compound systems many of which are based on imposing an orthogonality constraint (Lehman 1982, Masui *et al* 2003). In a recent study Masui *et al* (2003) have considered the implementation of the Pauli principle for nucleons between clusters by applying the orthogonality condition model which leads to non-local potentials and have applied it to the study of $O^{16} + \alpha$ single channel system and also to $Li^9 + n$ coupled-channel system. As emphasised by Amado *et al* (1990) it is clear that if inelasticity is ignored then the construction of Baye (1987) based on SUSYQM provides a unique construction of a local potential for the α–nucleon interaction that both gives the correct scattering phase shifts and also respects the Pauli principle. The method used in this paper starts from an orthogonality condition inside a region of variable radius and generates a local potential which is identical to the singular potential derived by Baye (1987, 1994) using a two-step SUSY procedure.

4. Conclusions

In this paper it has been shown that the two ways of constructing a new local potential by the elimination of the lowest n bound-states of a given potential namely the Gelfand–Levitan procedure and the 2-step SUSY procedure for singular potentials, can both be viewed as arising

from two different ways of constructing states orthogonal to the lowest n bound-states in the domain $[0, R]$ or the domain $[R, \infty]$ and satisfying the same boundary conditions as Ψ_m either as $r \to \infty$ or as $r \to 0$. The orthogonalization argument discussed in this paper provides further insights into the structure of the inverse scattering theory. All previous methods for implementing Pauli exclusion principle in the scattering of composite systems lead to effective potentials which are non-local. The construction of the potentials discussed in this paper have as their starting point considerations of orthogonality and therefore it sheds new light on how the Pauli principle may operate to produce effective local potentials.

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