Exact solution of the Schrodinger and Klein-Gordon equations for generalised Hulthen potentials

1981 J. Phys. A: Math. Gen. 14 383

(http://iopscience.iop.org/0305-4470/14/2/015)

J. Phys. A: Math. Gen. **14** (1981) 383–394. Printed in Great Britain

Exact solution of the Schrödinger and Klein–Gordon equations for generalised Hulthén potentials

M Znojil

Institute of Nuclear Physics, Czechoslovak Academy of Sciences, 250 68 Řež, Czechoslovakia

Received 17 May 1980

Abstract. For the class of generalised Hulthén s-wave potentials

$$V_{\mathrm{GH}}^{(p)}(r) = -\sum_{i=1}^{p} g_i a_i \exp(-\gamma_i r) \Big/ \Big(1 - \sum_{j=1}^{p} a_j \exp(-\gamma_j r)\Big), \quad p \geqslant 1,$$

the exact solution is presented for both the Schrödinger and Klein–Gordon equations. This simultaneous solubility represents a new non-perturbative treatment of the kinematical relativistic corrections and is based on a non-standard generalisation of the hypergeometric function.

1. Introduction

The non-relativistic Schrödinger equation is usually considered much simpler than its relativistic (Dirac or Klein–Gordon) counterparts. Hence, the approximate non-relativistic description is often used even for genuine relativistic binding or scattering (pions, quarks, etc, see Quigg and Rosner 1979 and references therein). Apart from the difficulties of interpretation connected with the existence of antiparticles etc (Bjorken and Drell 1964), the formal reason is that the exact solution is understood to be represented by the classical special functions. All Hamiltonians which do not admit such a solution are indiscriminately treated by universal perturbation and/or numerical methods. In this sense the non-relativistic Schrödinger equation is much better suited for modelling because many exactly solvable non-relativistic Hamiltonians H_0 exist (Newton 1965).

From the methodological point of view there is a broad gap between the special (exactly solvable, usually non-relativistic) and general (realistic, perturbed or relativistic) Hamiltonians. We suggest that it be bridged using the algebraic method of matrix recurrences (Znojil 1980, referred to as I hereafter. See also § 2.1). In brief, we may extend the class of H_0, especially in the relativistic domain, once we admit the use of the non-standard special functions.

For practical purposes some of the new exact solutions of the Schrödinger or relativistic equations may be made fully analogous to the old special functions, thus representing a 'minimal sophistication' of the mathematics. This is the case of the generalised s-wave exponential potentials described in I, which may contain an arbitrary number of free constants fitting almost any shape of the realistic (local) interaction $V(r)$.

0305-4470/81/020383+12$01.50

In this paper we shall extend the results of I and introduce the generalised Hulthén s-wave potential

$$V_{\mathrm{GH}}^{(p)}(r) = -\frac{\sum_{i=1}^{p} g_i a_i \exp(-\gamma_i r)}{1-\sum_{j=1}^{p} a_j \exp(-\gamma_j r)}, \qquad 0 < \gamma_1 \leqslant \gamma_2, \ \ldots, \ \gamma_{p-1} \leqslant \gamma_p. \tag{1}$$

The corresponding solution of the Schrödinger equation is described in § 2.2 and is shown to be a straightforward generalisation of the Gauss hypergeometric function ${}_2F_1(\ldots)$. The quantisation of the non-relativistic bound states is standard (zeros of the Jost function) and the numerical test (§ 2.3) confirms both the reliability of the method and the economy of the solution.

There are some descriptive features of the potential V_{GH} which are physically satisfactory.

(i) Near the origin ($r \sim 0$), the Coulomb-like behaviour may be attained in the limit $\Sigma\, a_j \to 1$.

(ii) At intermediate distances, various forms of the Coulomb screening, strong interaction potentials etc may be fitted.

(iii) In the asymptotic region ($r \gg 1$), the exponential decrease roughly simulates the one-boson exchange mechanism of interaction with the small relative error $O(\ln r/r)$ in the coordinate r.

(iv) Some of the old solvable potentials (Hulthén, Eckart, Bargmann) are contained in equation (1) as special cases (Newton 1965).

Nevertheless, the most gratifying feature of V_{GH} is its semigroup property $V_{\mathrm{GH}}^{(p)}(r)\, V_{\mathrm{GH}}^{(p')}(r) = V_{\mathrm{GH}}^{(p'')}$, $p'' = p + p'$. A consequence of this is the possibility of solving also the relativistic Klein–Gordon equation with the potentials V_{GH} in exactly the same way. This is demonstrated in § 3.1. For $p \geqslant 2$, the generalised solution ${}_2^pF_1(\ldots)$ in general cannot be expressed in terms of the special functions. It is therefore entirely new in the context of relativistic quantum mechanics. Its further aspects are discussed in §§ 3.2 and 4 and in the Appendix.

2. Schrödinger equation

2.1. *The method*

Consider an arbitrary linear homogeneous equation

$$H|y\rangle = 0. \tag{2}$$

The method of solution suggested in I is briefly as follows:

(a) We specify the initial function $|X_1^1\rangle$.

(b) We assume that the action of H on $|X_1^1\rangle$ generates the new functions $|X_2^m\rangle$, $m = 1, 2, \ldots, M_2$ such that

$$H|X_1^1\rangle = \sum_{m=1}^{M_2} B_1^{1m}|X_2^m\rangle \tag{3}$$

where B_1^{1m} are arbitrary parameters.

(c) The repeated action of H on $|X_2^m\rangle$ is assumed to lead to the other sets of functions $|X_k^n\rangle$, $n = 1, 2, \ldots, M_k$, $k = 2, 3, 4, \ldots$ which satisfy the fundamental linear

relations

$$H|X_k^n\rangle = \sum_{m=1}^{M_k} A_k^{nm}|X_k^m\rangle + \sum_{m=1}^{M_{k+1}} B_k^{nm}|X_{k+1}^m\rangle \tag{4}$$

for $n = 1, 2, \ldots M_k$, and $k = 2, 3, \ldots$.

(d) The matrices of parameters A_k^{nm}, B_k^{nm} in equation (4) must be such that the sum

$$|Y\rangle = |X_1\rangle - B_1(1/A_2)|X_2\rangle + B_1(1/A_2)B_2(1/A_3)|X_3\rangle - \ldots \tag{5}$$

is convergent.

It is a direct consequence of the assumptions (a)–(d) that the series (5) satisfies equation (2) identically. If equation (2) represents the Schrödinger equation (H = Hamiltonian minus energy) then (5) may describe the scattering or bound states provided that it satisfies the proper boundary conditions.

To illustrate the method and to show that it can lead to non-trivial results, we pick up the Hulthén potential ($V_{\mathrm{GH}}^{(p)}$ with $p = 1$, $\gamma_1 = 1$) and transform the corresponding Schrödinger equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\chi(r) + V_{\mathrm{GH}}^{(1)}(r)\chi(r) = -\kappa^2\chi(r) \tag{6}$$

into the form (2) where $\chi(r) = \langle r|y\rangle$ and

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \kappa^2 + a_1 \exp(-r)\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - g_1 - \kappa^2\right). \tag{7}$$

Further, we choose the function $\exp(H - \kappa r) = \langle r|X_1^1\rangle$ as initialisation, and infer that the action of H generates the set of exponentials

$$\langle r|X_k^1\rangle = \exp[-(\kappa + k - 1)r], \qquad M_k = 1,\ k = 1, 2, \ldots. \tag{8}$$

The fundamental relation (4) will hold with

$$A_k^{11} = -(k-1)(2\kappa + k - 1), \qquad B_k^{11} = a_1(\alpha + k - 1)(\beta + k - 1),$$

$$\alpha = \kappa + \mu, \qquad \beta = \kappa - \mu, \qquad \mu = (\kappa^2 + g_1)^{1/2}, \qquad k = 1, 2, \ldots. \tag{9}$$

It is not surprising that the sum (5) coincides with the well-known (un-normalised) solution

$$\chi(r) = \exp(-\kappa r)\ {}_2F_1(\alpha, \beta, 2\kappa + 1, a_1 \exp(-r)). \tag{10}$$

Its properties may be found in the standard textbooks (e.g. Newton 1965). We only mention here that choosing $\kappa = +\sqrt{\kappa^2}$ or $\kappa = -\sqrt{\kappa^2}$ we obtain the two independent solutions which may be used to satisfy arbitrary initial or boundary conditions. In the special case of the non-relativistic bound states ($\kappa^2 > 0$, i.e. κ = real), the choice $\kappa > 0$ guarantees the correct asymptotic behaviour and the proper quantisation follows from the boundary condition in the origin, $\langle 0|y\rangle = 0$. Thus the real roots κ of the transcendental equation

$${}_2F_1(\alpha, \beta, 2\kappa + 1, a_1) = 0 \tag{11}$$

define the bound-state energies. For $a_1 = 1$, the alternative exact formula

$$\beta = \kappa - (\kappa^2 + g_1)^{1/2} = 1 - N, \qquad 2 \leq N < 1 + \sqrt{g_1} \tag{12}$$

follows from the theory of the Gauss function ${}_2F_1(\ldots)$ (Gradshteyn and Ryzhik 1971).

2.2. Exact solution

The s-wave Schrödinger equation (6) with the generalised Hulthén potential (1) may be multiplied by the denominator $D(r)=1-\sum_{i=1}^{p} a_i \exp(-\gamma_i r)$ of the potential from the left. Of course we assume that it is a non-zero function for all r, i.e.

$$D(r)=1-\sum_{i=1}^{p} a_i \exp(-\gamma_i r)>0. \tag{13}$$

Further, we slightly simplify the form of H in equation (2) by the factorisation

$$\chi(r)=\langle r|y\rangle \exp(-\kappa r) \tag{14}$$

having in mind the asymptotic behaviour of the bound-state solutions for $\kappa^2>0$. This leads to the operator

$$H=-\Big(1-\sum_{i=1}^{p} a_i \exp(-\gamma_i r)\Big)\frac{d^2}{dr^2}$$
$$+\Big[\gamma-1-\sum_{i=1}^{p} a_i(\alpha_i+\beta_i)\exp(-\gamma_i r)\Big]\frac{d}{dr}+\sum_{i=1}^{p} a_i\alpha_1\beta_i \exp(-\gamma_i r), \tag{15}$$

$$\gamma=2\kappa+1, \qquad \alpha_i=\kappa+\mu_i, \qquad \beta_i=\kappa-\mu_i, \qquad \mu_i=(\kappa^2+g_i)^{1/2}, \qquad i=1,2,\ldots p$$

to be used in the method of § 2.1.

The groups of functions $|X_k^m\rangle$, $m=1,2,\ldots M_k$ may be composed of exponentials

$$\langle r|X_k^{i_1 i_2\cdots i_p}\rangle=\exp(-\theta_k^{i_1 i_2\cdots i_p} r), \qquad \theta_k^{i_1 i_2\cdots i_p}=\sum_{j=1}^{p}\gamma_j i_j=\theta_k^m,$$

$$M_k=M_k(p)=\binom{k+p-2}{p-1}. \tag{16}$$

They are numbered by the composite index $m\{i_1, i_2, \ldots i_p\}$ with the p non-negative integers $i_1, i_2, \ldots i_p$ subjected to the restriction $i_1+i_2+\ldots+i_p=k-1$. It is easy to show that the action of H (15) on $|X_k^m\rangle$ (16) satisfies the fundamental recurrences (4) and (3) when the diagonal matrix A has the elements

$$A_k^{mm}=-\theta_k^m(\theta_k^m+\gamma-1). \tag{17}$$

The proper B matrix connects just the two neighbouring indices $m=(i_1, i_2, \ldots i_j, \ldots i_p)$ and $m_j'=(i_1, i_2, \ldots i_j+1, \ldots i_p)$ differing in one component:

$$B_k^{mm_j'}=a_j(\theta_k^m+\alpha_j)(\theta_k^m+\beta_j). \tag{18}$$

Due to the diagonality of A, we may immediately write

$$-\Big(B_k\frac{1}{A_{k+1}}\Big)^{mm_j'}=\frac{a_j(\theta_k^m+\alpha_j)(\theta_k^m+\beta_j)}{(\theta_k^m+\gamma_j)(\theta_k^m+\gamma_j+\gamma-1)} \tag{19}$$

so that the formal solution (5) of equation (2) may be given the final form

$$\langle r|Y\rangle={}_2^gF_1(\{\alpha_i\},\{\beta_i\},\gamma,\{a_i\exp(-\gamma_i r)\})$$
$$=1+\sum_{k=2}^{\infty}\sum_{r_1=r_2=\cdots=r_{k-1}=1}^{p}\prod_{l=1}^{k-1}\frac{(\alpha_{r_l}+\sum_{i=1}^{l-1}\gamma_{r_i})(\beta_{r_l}+\sum_{j=1}^{l-1}\gamma_{r_j})a_{r_l}\exp(-\gamma_{r_l}r)}{(\sum_{n=1}^{l}\gamma_{r_n}+\gamma-1)(\sum_{m=1}^{l}\gamma_{r_m})}. \tag{20}$$

This notation is inspired by the special case of equation (20) ${}_2^1F_1(\alpha_1,\beta_1,\gamma,$

$\exp(-\gamma_1 r)) \equiv {}_2F_1(\alpha_1, \beta_1, \gamma, \exp(-\gamma_1 r))$. Some properties of the generalised hypergeometric series (20) are discussed in the Appendix.

Since we have an estimate

$$\sum_{m'=1}^{M_{k+1}} -\left(B_k \frac{1}{A_{k+1}}\right)^{mm'} \langle r|X_{k+1}^{m'}\rangle = \langle r|X_k^m\rangle \sum_{j=1}^{p} a_j \exp(-\gamma_j r) \times [1 + (\alpha_j + \beta_j + 1 - 2\gamma_j - \gamma)/\theta_k^m + O(1/k^2)] \tag{21}$$

and $(k-1)\gamma_1 \leqslant \theta_k^m \leqslant (k-1)\gamma_p$, the sufficient convergence condition for (20) reads

$$\left|\sum_{j=1}^{p} a_j \exp(-\gamma_j r)\right| < 1, \qquad r \in (0, \infty). \tag{22}$$

This is consistent with the absence (equation (13)) of poles of $V(r)$ on the real axis.

On the boundary of the convergence region, we may still prove the convergence for a broad class of potentials, although the detailed general discussion is complicated by the necessity to determine the roots r_0 of the two transcendental equations

$$\sum_{j=1}^{p} a_j \exp(-\gamma_j r_0) = \pm 1. \tag{23}$$

The Coulomb-like potential with $r_0 = 0$ deserves special attention due to its physical character. Considering only the particular case of $r_0 = 0$ with $a_j > 0$, and with the real κ, α_j and β_j, $j = 1, 2, \ldots p$, we may replace equation (22) by the more subtle (Raabe) criterion and obtain the sufficient condition for absolute convergence

$$\gamma + 2\sum_{j=1}^{p} a_j\gamma_j > \sum_{j=1}^{p} a_j(\alpha_j + \beta_j) + \gamma_1 + 1 \tag{24}$$

for the solution (20). We note that (24) with $a_j > 0$ does not admit the singularity $O(r^{-2})$ in the origin ($D'(0) > \gamma_1/2$, cf (13)).

Of course, the quantisation of the bound states follows again from the boundary condition $\langle 0|Y\rangle = 0$, i.e.

$${}_2^pF_1(\{\alpha_i\}, \{\beta_i\}, \gamma, \{a_i\}) = 0. \tag{25}$$

This merely represents the zeros of the Jost function and generalises formula (11) to cover all $p \geqslant 1$.

2.3. Numerical test

The search for the roots of the transcendental equation (25) is a numerical procedure. Its precision and computation time may significantly worsen when the convergence is not rapid enough, due to the rapid increase in the number of terms in the sum (20) for higher summation indices k.

To verify the practical applicability of our solution ${}_2F_1(\ldots)$, $p > 1$, we have chosen the Eckart potential

$$V_E(r) = -\frac{g_{1E}a_E \exp(-r)}{1 - a_E \exp(-r)} - \frac{g_{2E}a_E \exp(-r)}{(1 - a_E \exp(-r))^2}, \qquad a_E < 1, \qquad g_{2E} < \tfrac{1}{4} \tag{26}$$

which is a non-trivial special case of V_{GH} and still possesses an exact solution in terms of the hypergeometric functions. Putting $\lambda = \frac{1}{2} - (\frac{1}{4} - g_{2E})^{1/2}$ and $\xi = a_E \exp(-r)$, $\chi(r) =$

$\xi^{\kappa}(1-\xi)^{\lambda}\phi(\xi)$ in the Schrödinger equation (6), we obtain the Gauss differential equation

$$\xi(1-\xi)\frac{d^2}{d\xi^2}\phi(\xi)+[\gamma-(\alpha+\beta+1)\xi]\frac{d}{d\xi}\phi(\xi)-\alpha\beta\phi(\xi)=0,$$

$$\alpha=\kappa+\lambda+\mu, \qquad \beta=\kappa+\lambda-\mu, \qquad \gamma=2\kappa+1, \qquad \mu=(\kappa^2+g_{1E})^{1/2} \tag{27}$$

with the solution $\phi(\xi)={}_2F_1(\alpha,\beta,\gamma,\xi)$. The roots of the boundary condition in the origin

$${}_2F_1(\alpha,\beta,a_E)=0 \tag{28}$$

determine the eigenvalues.

Representing now the Eckart potential in the form $V_{GH}^{(p)}$ where we put $p=2$ and

$$\gamma_1=1, \qquad \gamma_2=2, \qquad a_1=2a_E, \qquad a_2=-a_E^2,$$
$$g_1=g_{1E}+g_{2E}, \qquad g_2=g_{1E}. \tag{29}$$

we obtain (25) as the alternative transcendental equation for the binding energies κ. Insertion of both forms of the solution $\chi(r)$ into the same root-searching subroutine leads to the same eigenvalues. Their position (e.g. table 1) was confirmed by an independent evaluation with the replacement $\lambda\to 1-\lambda$. Thus the test has demonstrated the practical applicability and reliability of the Dirichlet series representation (20) of the Schrödinger equation solution.

Table 1. Eigenvalues of the Eckart potential $V_E(r)$, obtained numerically from both forms (28) and (25) of the boundary condition $\langle 0|y\rangle=0$.

a_E	κ_1	κ_2
0·1	0·5921	
0·2	0·1099	1·3225
0·3	0·6161	1·9873

For small $a_E\leqslant 0.3$, the computer time used is comparable for both representations. The resulting precision is no worse in the ${}_2^2F_1$ case, in spite of the unfavourable properties of this particular example. The convergence is hindered since $a_1+a_2=a_E(2-a_E)\gg a_E$ and the same terms occur repeatedly due to the degeneracy $a_2\exp(-\gamma_2 r)=-[a_1\exp(-\gamma_1 r)]^2$. For higher a_E's, therefore, the use of our representation becomes lengthy and less precise. Only the old representation works on the boundary $a_E=1$ of the convergence region. The finite fourteen-digit precision of the computer arithmetic leads even then to the 5% deviation when the numerical root is compared with the exact formula

$$\kappa=\frac{g_{1E}-(N-\lambda)^2}{2(N-\lambda)}, \qquad 1\leqslant N<\lambda+(g_{1E})^{1/2} \tag{30}$$

obtainable by analytic means (cf § 3.2).

3. Klein–Gordon equation

3.1. The Schrödinger-like formulation

In the present context the most important property of the stationary Klein–Gordon equation (KGE) in the s wave

$$[E - W(r)]^2\chi(r) + \hbar^2c^2(\mathrm{d}^2/\mathrm{d}r^2)\chi(r) = m^2c^4\chi(r) \tag{31}$$

is the possibility of rewriting in the form of the Schrödinger-like equation (6). In the units $\hbar = c = 2m = 1$ we put $E = \frac{1}{2} - k^2$ where $k > 0$ for bound states. Another restriction, that is $k^2 < 1$, must be imposed to guarantee the the stability of the vacuum. For $k^2 > 1$, the many-body character of the annihilation and the mechanism of its stopping (Rafelski *et al* 1978) lie beyond the scope of the one-body relativistic equation. Thus we may also put $k^2 - k^4 = \kappa^2 > 0$ ($\kappa^2 < 1/4$) and obtain an equivalence between the Klein–Gordon and Schrödinger equations (31) and (6), respectively, with the correspondence

$$V(r) = (1 - 2k^2)W(r) - W^2(r) \tag{32}$$

between the potentials.

The use of the generalised Hulthén potentials

$$W(r) = \frac{\Sigma_{i=1}^{q} G_i A_i \exp(-\Gamma_i r)}{1 - \Sigma_{j=1}^{q} A_j \exp(-\Gamma_j r)}, \qquad A_j > 0, \qquad \sum_{j=1}^{q} A_j < 1 \tag{33}$$

in the original form (31) of KGE leads to its Schrödinger-like form (6)+(1). For $i = 1, \ldots q, q+1, \ldots 2q, 2q+1, \ldots p$, and with $p = q(q+3)/2$, the parameters γ_i, a_i and g_i in (1) are equal to

$$\begin{aligned} &\Gamma_1, \ldots \Gamma_q, 2\Gamma_1, \ldots 2\Gamma_q, \Gamma_1 + \Gamma_2, \ldots \Gamma_{q-1} + \Gamma_{qi} \\ &2A_1, \ldots 2A_q, -A_1^2, \ldots -A_q^2, -2A_1A_2, \ldots -2A_{q-1}A_q; \end{aligned} \tag{34}$$

and

$$\begin{aligned} &(\tfrac{1}{2} - k^2)G_1, \ldots (\tfrac{1}{2} - k^2)G_q, G_1(1 - 2k^2 - G_1), \ldots, G_q(1 - 2k^2 - G_q), \\ &(\tfrac{1}{2} - k^2)(G_1 + G_2) - G_1G_2, \ldots (\tfrac{1}{2} - k^2)(G_{q-1} + G_q) - G_{q-1}G_q, \end{aligned}$$

respectively. Inserting (34) into (22) we prove that the convergence criterion is satisfied. Thus the general solution of KGE may be expressed as the superposition of the two generalised hypergeometric series (20) with $\kappa = +(k^2 - k^4)^{1/2}$ and $\kappa_- = -(k^2 - k^4)^{1/2}$ respectively.

The consistent interpretation of the relativistic binding is non-trivial—compare, for instance, the detailed discussion of the Klein–Gordon equation in Bjorken and Drell (1964) or Rafelski *et al* (1978). In as far as we are interested in the solutions of the corresponding differential equation rather than in its interpretation, we shall not go into detail here and accept the quantisation rules in full analogy with the non-relativistic case: at both infinity ($r \to \infty$) and the origin ($r \to 0$) we require $\chi(r) \to 0$. In this way, the $\kappa_- < 0$ will be eliminated as before and the numerical determination of energy $E = mc^2 - k^2$ will proceed along the same lines. The possible additional energy dependence of the potential parameters will of course be irrelevant in this context.

3.2. Example: bound state in the Hulthén potential

In general the practical applications of V_{GH} in both the non-relativistic and relativistic regions is connected with the transcendental equation (25). Although the numerical test of § 2.3 has confirmed its suitability, the structure of the solution is less transparent.

The special case of V_{GH} (33) with $q=1$ and $A=1$ (Hulthén potential V_H) has provided a good picture of some general features of the non-relativistic spectrum, due to the existence of the alternative non-numerical formula (12). Fortunately, its relativistic analogue also exists. We shall describe it here in detail.

It is a consequence of the two prescriptions (29) and (34) that KGE with the potential V_H becomes formally equivalent to the Schrödinger equation with the Eckart potential (26). With the proper assignment of the potential parameters ($\gamma_{1E}=\Gamma\neq 1$)

$$a_E=A, \qquad g_{1E}=(-G^2+G(1-2k^2))/\Gamma^2, \qquad g_{2E}=G^2/\Gamma^2,$$
$$\lambda=\tfrac{1}{2}-(\tfrac{1}{4}-G^2/\Gamma^2)^{1/2}, \qquad \xi=A\exp^{-\Gamma r}, \tag{35}$$

KGE may be further transformed into the Gauss hypergeometric differential equation (27). Using the identities valid for the Gauss functions (Gradshteyn and Ryzhik 1971) we may write the general solution in the form

$$\chi(r)=C_1[Z(\kappa,\lambda,\xi)+Z(\kappa,1-\lambda,\xi)]+C_2[Z(-\kappa,\lambda,\xi)+Z(-\kappa,1-\lambda,\xi)],$$
$$Z(\varkappa,\lambda,\xi)=\frac{\Gamma(1-2\lambda)(1-\xi)^{\lambda}\xi^{\kappa}{}_2F_1(\alpha,\beta,2\lambda,1-\xi)}{\Gamma(\kappa-\lambda+1+\mu)\Gamma(\kappa-\lambda+1-\mu)}, \tag{36}$$
$$\kappa=(k^2-k^4)^{1/2}/\Gamma, \qquad \mu=(\kappa^2+g_{1E})^{1/2}, \qquad \alpha,\beta=\kappa+\lambda\pm\mu.$$

The standard boundary conditions for $r\to\infty$ imply $C_2=0$. At the point $r=0$, the standard techniques fail, due to the strong singularity of the potential with $A=1$: The classical particle would fall into the origin. A similar phenomenon exists in non-relativistic quantum theory. When we interpret (31) as the Schrödinger equation, the spectrum ceases to be bounded from below for $G>\Gamma/2$, the wavefunctions

$$\chi(r)\sim r^{1/2}\sin(\text{const}+\ln r(G^2/\Gamma^2-\tfrac{1}{4})^{1/2})+\ldots$$

oscillate rapidly near the origin. For the weaker singularity, $G<\Gamma/2$, the quantisation of the bound states may be obtained from an additional requirement $\chi(r)\sim r^{1/2+\epsilon}$, $\epsilon>0$ (from the finiteness of the kinetic energy $\langle\chi|T|\chi\rangle<\infty$). Hence we shall treat KGE in the same way, and arrive at the quantisation condition for $\chi(r)$, equation (36), in the same form as in § 2.3,

$$\kappa-\lambda+1-\mu=-m, \qquad m=0,1,\ldots \tag{37}$$

Due to the k-dependence of g_1 and μ (35), equation (37) differs from equation (30) and defines the energies $E=\frac{1}{2}-k^2$ as the roots of the sixth-order polynomial. As a consequence of the restrictions on the admissible values of G and k in the relativistic case, the parametrisation

$$G=(\Gamma/2)\sin 2\alpha, \qquad \alpha\in(0,\pi/4)$$
$$k=\sin\beta, \qquad \beta\in(0,\pi/2) \tag{38}$$

implies

$$0<\lambda=\sin^2\alpha<\tfrac{1}{2}$$
$$0<g_2=\tfrac{1}{4}\sin^2 2\alpha<\tfrac{1}{4} \tag{39}$$
$$0<\kappa^2=(1/4\Gamma^2)\sin^2 2\beta<1/4\Gamma^2.$$

Then the quantisation condition (37) acquires the trigonometric form

$$2\Gamma m+\Gamma+\Gamma\cos 2\alpha+\sin 2\beta=[1-(\cos 2\beta-\Gamma\sin 2\alpha)^2]^{1/2}. \tag{40}$$

First, we shall consider the special case $\Gamma=1$. Introducing the new angular variables

$$u=\alpha+\beta-\pi/4\in(-\pi/4,\pi/2),\qquad v=\alpha-\beta+(\pi/4)\in(-\pi/4,\pi/2), \tag{41}$$

we may simplify equation (40) into

$$2m+1+2\cos u\cos v=(1-4\sin^2 u\cos^2 v)^{1/2}. \tag{42}$$

Since $\cos u>0$ and $\cos v>0$ we obtain $m<0$. Hence the existence of the very first bound state may be possible on the boundary of the α and β domain only. Since $m=0$ is consistent with equation (42) only at $\cos v=0$, we solve KGE (31) directly for $G=\frac{1}{2}$ and $k=0$ and obtain

$$\chi(r)=(1-\exp(-r))^{1/2}(C_1+C_2\ln(\exp(r)-1)). \tag{43}$$

This 'zero-energy bound state' is not in fact the true bound state, in as far as it cannot be normalised in the standard way.

We next fix the characteristics $m=\beta=0$ of the state (43) and permit $\Gamma\neq 1$. From equation (40), we obtain $\alpha=\alpha_0$, $\alpha_0=\tan^{-1}\Gamma$ so that this state exists and is shifted towards $\alpha=\alpha_0<\pi/4$ for $\Gamma<1$. It is reasonable to assume now that for $\alpha>\alpha_0$, the $M+1>1$ states ($m=0,1,\ldots M$) may exist in general. We easily show from equation (40) with $\beta=0$ that the number $M+1$ of states may become arbitrarily large for a sufficiently broad potential, that is for

$$\Gamma<\Gamma_M=\frac{2\sin 2\alpha}{(2M+1)^2+2(2M+1)\cos 2\alpha+1}. \tag{44}$$

At the maximal strength of the potential ($\alpha=\pi/4$, $\sin 2\alpha=1$, $\cos 2\alpha=0$), formula (44) may be simply compared with its non-relativistic counterpart

$$\Gamma<\Gamma_M^0=2/[(2M+1)+1]^2. \tag{45}$$

Thus the last bound state will be lost in the non-relativistic limit whenever the value of the constant Γ lies in one of the intervals $(1/(2+4N+2N^2),\ 1/(1+2N+2N^2))$, $N=0,1,2,\ldots$. We may summarise this situation as follows:

(i) The non-relativistic equation with the Hulthén potential (33), $q=1$ and $A=1$, may possess an arbitrary number of the bound states given by equation (47) and

$$k=k_{\text{non-rel}}=\frac{G-(m+1)^2\Gamma^2}{2(m+1)\Gamma},\qquad G\geqslant\Gamma^2 \tag{46}$$

(cf equation (12)). The corresponding relativistic equation holds only for sufficiently weak coupling ($G<\Gamma/2$). For potential wells which are 'too weak' ($\Gamma\geqslant 1$), it has no bound states at all.

(ii) For the fixed potential width $\Gamma<1$ and coupling $G<\Gamma/2$, the situation is reversed and new purely relativistic bound states may appear. The magnitude of the energy

$$k=k_{\mathrm{rel}}=\tfrac{1}{2}[2-\Gamma\sin 2\alpha-(2m+1+\cos 2\alpha)Q]^{1/2},$$
$$Q^2=4[(2m+1)^2+2(2m+1)\cos 2\alpha+1]^{-1}-\Gamma^2>0 \tag{47}$$

follows from equation (40). We note that the antiparticle level band $\tilde{k}^2=1-k^2$ remains well separated even for $\alpha=\pi/4$ and $\Gamma\to 0$ since $k^2\to(2-\sqrt{2})/4<\frac{1}{2}$ for the ground state $m=0$. This means that the relativistic modification of $V(r)$ (32) and therefore also the value of the energy shift $k^2_{\text{non-rel}}-k^2_{\text{rel}}$ (cf (46)) are always negative. Further, this implies that the Hulthén potential remains subcritical (it cannot produce particle condensation) when it is kept regular at the origin ($G<\Gamma/2$).

4. Summary

We have obtained closed solutions of the Schrödinger equation for a broad class of the generalised Hulthén s wave potentials V_{GH}. They are represented analytically by the Dirichlet series (20), which generalises the Gauss hypergeometric function ${}_2F_1$ and is convergent in the large domain of parameters including all complex energies in most cases. The practical applicability of the solution is illustrated by the non-trivial numerical example.

The semigroup property of the potentials V_{GH} leads to the simultaneous solubility of the corresponding relativistic Klein–Gordon equations. This means that our $p>1$ generalisations ${}^{p}_{2}F_1$ of the hypergeometric function ${}^{1}_{2}F_1\equiv{}_2F_1$ are an important tool for the non-perturbative investigation of the relativistic corrections. Of course, the one-body character of our approach leads to the physical (many-body and radiative correction) uncertainties. Nevertheless, it may be used as a mathematical model estimating the kinematic relativistic effects or confirming the reliability of the highly popular non-relativistic descriptions of semi-relativistic systems (e.g. quarks). We have demonstrated this in detail in the case of the singular Hulthén potential. We have shown that even the Coulomb-like singularity may be strong enough to produce the significant relativistic corrections. Their non-perturbative character is proven, and shown to generate the new bound states of purely relativistic origin.

When compared with the sum of exponentials in I, the potentials under consideration, V_{GH}, comprise the physically interesting special cases of the screened Coulomb interaction $V(r)\sim 1/r$, $r\ll 1$. Moreover, they admit also a singularity of order $1/r^2$ at the origin (compare the example of §§ 2.3 and 3.2 with $A=1$). In view of the fact that this is merely the singularity of the centrifugal term $l(l+1)/r^2$ for $l>0$, we may use our exact solution for the systematic approximations even in the higher partial waves.†

† One of the possibilities is to replace the potential $V_l(r)$ in the radial Schrödinger or Klein–Gordon equation by zero or any simple (solvable) potential $V_{l0}(r)$ for all $r>R_0\gg 0$, and to fit the function $v(l,r)=V_l(r)+l(l+1)/r^2$, with an arbitrary precision ϵ_l, by $V_{\mathrm{GH}}(r)$ in the finite interval $r\in(0,R_0)$. The exact solution of the approximate equation will then be obtained by matching the logarithmic derivatives at R_0. In principle, the modification of the potentials ought to be removed by the limiting transition $R_0\to\infty$, $\varepsilon_l\to 0$. In practice, we believe that for any realistic interaction $V_l(r)$ and any partial wave $l\geq 0$, the most efficient estimates of the sufficient finite value of the cutoff $R_0<\infty$ are more likely to be based on the fit $V_{\mathrm{GH}}(r)\sim v(l,r)$ achieved with the fixed $\epsilon_l>0$ and minimal p, complemented by the first-order perturbation corrections.

Appendix: Properties of the generalised hypergeometric series

Instead of equation (14) let us write

$$\chi(r) = \exp(-\kappa r)\Big(1 - \sum_{i=1}^{p} a_i \exp(-\gamma_i r)\Big)\langle r|y\rangle \tag{A1}$$

and write the Schrödinger equation (6) with the potential (1) in the form (2). Then the operator H will be obtained in the form (15) again, with the only modification

$$\alpha_i \to \bar{\alpha}_i = \alpha_i + \gamma_i, \qquad \beta_i \to \bar{\beta}_i = \beta_i + \gamma_i, \qquad i = 1, 2, \ldots p.$$

Hence the alternative form of the solution (20) reads

$$\langle r|Y\rangle = \Big(1 - \sum_{j=1}^{p} a_j \exp(-\gamma_j r)\Big)\, {}_2^pF_1(\{\alpha_i + \gamma_i\}, \{\beta_i + \gamma_i\}, \gamma, \{a_i \exp(-\gamma_i r)\}) \tag{A2}$$

(the same normalisation $\langle\infty|Y\rangle = 1$). This is an example of the generalisation of Kumar transformation formulae, which holds for the Gauss functions ${}_2F_1 \equiv {}_2^1F_1$.

Formally, ${}_2F_1$ is a function of p variables $x_i = a_i \exp(-\gamma_i r)$. For the degenerate case $\alpha_i = \alpha, \beta_i = \beta, i \in \overline{1, p}$, it may be related to the old Gauss function by the obvious identity

$${}_2^pF_1(\{\alpha\}, \{\beta\}, \gamma, \{x_i\}) = {}_2F_1\Big(\alpha, \beta, \gamma, \sum_{j=1}^{p} x_j\Big) \tag{A3}$$

which follows directly from the definition (20). Putting $p = 2$ we see that ${}_2^2F_1$ is a non-trivial generalisation of ${}_2F_1$ to two variables and does not coincide with any of the Appell functions F_1, F_2, F_3 or F_4 (Gradshteyn and Ryzhik 1971).

Next let us consider the limiting transition $a_j \to 0$, $g_j a_j \to G_j \neq 0$ in the potential (1) for t indices $j = j_i$, $i = 1, 2, \ldots t$, $t \leqslant p$. Since the limit of equation (19) has the form

$$-\Big(B_k \frac{1}{A_{k+1}}\Big)^{mm_j} = \frac{G_j}{(\theta_k^m + \gamma_j)(\theta_k^m + \gamma_j + \gamma - 1)}, \qquad j = j_i, \tag{A4}$$

the corresponding confluent form ${}_2^pF_1^{(t)}$ of the generalised hypergeometric series is given by the series (20) with the substitution $a_{r_l} \exp(-\gamma_{r_l} r) \to -G_{r_l} \exp(-\gamma_{r_l} r)$ and $(\alpha_{r_l} + \Sigma^l)(\beta_{r_l} + \Sigma^l) \to 1$ in the numerator for all $r_l = j_i$, $i = 1, 2, \ldots t$. This substitution improves the convergence, so that the new confluent series ${}_2^pF_1^{(t)}$ will exist for any G_{ji}. It should be noted that the fully confluent form ${}_2^pF_1^{(p)}$ is closely related to the generalised Bessel function (I).

Formula (20) is very compact but the original representation (5) may sometimes be useful in the computation. We may return to the simple upper index by introducing the ordering $m = 1, 2, \ldots,$

$$\begin{aligned} m &= \binom{k+p-3-i_p}{p-1} + \binom{k+p-4-i_p-i_{p-1}}{p-2} + \ldots + \binom{i_1}{1} + 1 \\ &= m(i_1, i_2, \ldots, i_{p-1}) \leqslant M_k = M_k(p) = \binom{k+p-2}{p-1}. \end{aligned} \tag{A5}$$

The mapping $(k, m) \leftrightarrow \{i_j\}$ is one-to-one, with the recurrent inversion

$$\begin{aligned} & i_j = \max y, \qquad \binom{k_j + p_j - 3 - y}{p_j - 1} + 1 \geqslant m_j \\ & m_{j-1} = m_j - \binom{k_j + p_j - 3 - i_j}{p_j - 1} \geqslant 1 \\ & k_{j-1} = k_j - i_j \geqslant 1, \qquad p_{j-1} = p_j - 1 \geqslant 1 \end{aligned} \tag{A6}$$

for $j = p, p-1, \ldots 2$ and with the initialisation $m_p = m$, $k_p = k$, $p_p = p$. The algorithmic form of equation (A6) is also available. To perform the step $m \to m+1$ for $m < M_k$, we must

(i) put $s = i_1$ and $t = 1$,
(ii) if $s \neq 0$ then put $i_1 = 0$ and $t = 2$,
(iii) find n such that $2 \leqslant n \leqslant p$, $i_n \neq 0$ and all $i_j = 0$ for $t \leqslant j \leqslant n-1$,
(iv) put $i_n = i_n - 1$ and $i_{n-1} = s + 1$.

As a consequence of our ordering, we arrive at the matrices $-B_k(1/A_{k+1}) = L_k = L_k(p)$ with the simple block structure

$$L_k(p) = \begin{pmatrix} L_1^0(p), & L_1(p-1), & 0, & \ldots & \ldots & 0 \\ 0, & L_2^0(p), & L_2(p-1), & 0, & \ldots & 0 \\ & \ldots & & & & \\ 0 & \ldots & \ldots & 0, & L_k^0(p), & L_k(p-1) \end{pmatrix} \tag{A7}$$

where $L_k^0(p)$ is a diagonal part of $L_k(p)$ given by equation (19) with $j = p$. This may be checked by using the explicit formulae (19) and the definitions

$$\begin{aligned} & m = m(i_1, i_2, \ldots, i_j, \ldots i_{p-1}) \leqslant M_k(p) \\ & m_j' = m(i_1, i_2, \ldots, i_j + 1, \ldots, i_{p-1}) = m + \binom{k + p - 3 - i_p}{p-2} + \ldots \\ & + \binom{k + j - 2 - i_p - \ldots - i_{j+1}}{j-1} \leqslant M_{k+1}(p). \end{aligned} \tag{A8}$$

They specify the positions of the non-zero elements of the sparse matrix $L_k(p)$ so that an efficient evaluation of the sum (5) may alternatively be based on the recurrent character of equation (A7) with respect to p.

References

Bjorken J D and Drell S D 1964 *Relativistic Quantum Mechanics* (New York: McGraw-Hill)
Gradshteyn I S and Ryzhik I M 1971 *Tablicy integralov, summ i proizv* (Moscow: Nauka).
Newton R G 1965 *Scattering theory of waves and particles* (New York: McGraw Hill)
Quigg C and Rosner J L 1979 *Phys. Rep.* **56** 167–235
Rafelski J, Fulcher L P and Klein A 1978 *Phys. Rep.* **38C** 227
Znojil M 1980 *J. Math. Phys.* **21** 1629