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Properties of bound states of the Schrödinger equation with attractive Dirac delta potentials

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Abstract

We have studied bound states of the Schrödinger equation for an attractive potential with any finite number (P) of Dirac delta-functions in \mathbf{R}^n where $n = 1, 2, 3, \dots$. The potential is radially symmetric for $n \geq 2$ and is given as $V(r) = -\frac{\hbar^2}{2m} \sum_{i=1}^P \sigma_i \delta(r - r_i)$ where $\sigma_i > 0$, $r_1 < r_2 < \dots < r_P$, and $r_i \in (0, +\infty)$ for $n \geq 2$, $r_i \in (-\infty, +\infty)$ for $n = 1$. By separating angular degrees of freedom, the radial equation is obtained for $n \geq 2$ and applications of the boundary conditions lead to P transfer matrices which are used to form an equation for the eigenvalues. We have proven that, for given n and l , the bound state solutions of the radial equation are non-degenerate and there are at most P bound state solutions of the radial equation and hence P bound state energy levels for a potential with P attractive Dirac delta-functions. Given l and $n \geq 2$, for $P = 1$, we have shown that there exists one and only one solution of the radial equation if $\sigma_1 r_1 > 2l + n - 2$ and none otherwise. We have also proven that there are at most P positive roots for the equation $\mathbf{X}_{22}(k) = 0$ where $\mathbf{X} = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} = M_P M_{P-1} \dots M_1$ and $M_i \in SL(2, \mathbf{R})$ are the particular transfer matrices mentioned above.

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1. Introduction

Bound state solutions of the Schrödinger equation for a particle of mass m in a potential with one or two attractive delta-functions are commonly investigated in quantum mechanics [1–3]. However, no rigorous study of any finite number of Dirac delta-functions in \mathbf{R}^n for arbitrary n can be found in the literature. In this paper, we present rigorous analysis of bound states for a potential with any finite number of attractive Dirac delta-functions. We take the potential radially symmetric for $n \geq 2$.

Studies of Dirac delta-function potentials are also useful to get information on the solutions of the Schrödinger equation with some finite potentials which lead to Dirac delta potentials

for certain limits of their parameters. Thus, the information on the existence of a bound state for a given potential can be obtained from this limit. For example, the square well potential in one dimension becomes a Dirac delta potential when its width goes to zero and its depth goes to infinity such that their product is finite. Since the Schrödinger equation with an attractive Dirac delta potential in one dimension always has one bound state, one concludes that the square well potential has also at least one bound state. The analysis of a Kronig–Penney model with a periodic potential which has an infinite number of Dirac delta-functions is also helpful to understand the electronic band structure of crystals [4, 5].

A potential with one attractive delta-function can be solved exactly in the one-dimensional case. For potentials with attractive delta-functions in higher dimensions and with more than one delta-function in one dimension can be solved numerically since one should find roots of a transcendental equation to obtain eigenvalues. In this paper, we show a way to find this equation for the eigenvalues of bound states by using transfer matrices. We also prove some theorems on the properties of the eigenfunctions for the bound states. Finally, by using these theorems, we present a general theorem for some particular matrices which are elements of $SL(2, \mathbf{R})$.

Although delta-functions do not exactly represent realistic potentials, very short-ranged interactions may be investigated by using these functions. For example, the attractive interaction experienced by a neutron when it approaches a nucleus of radius r_1 can be modelled by using one delta potential $U(r) = -g_1\delta(r - r_1)$ [2]. This crude model can be improved by using several delta potentials with different g_i and r_i values, depicting the shell structure of the nucleus. Thus, our bound states calculations for a single particle can be utilized for the mean-field approximation of complicated many-body interactions of the nucleus. Similarly, new materials such as concentric ring shape polymeric molecules might be designed and synthesized, such that certain particles will experience short-ranged interactions on concentric spherical or cylindrical surfaces. Carbon nanotubes are possible candidates for such structures. Furthermore, the analysis below may shed light on surface physics problems such as impurities deposited with concentric ring structures or circular molecules directly attached on a substrate.

2. Results and discussion

We first obtain bound state eigenfunctions of the Schrödinger equation for a potential with P attractive Dirac delta-functions in n dimensions. The potential is given as

$$V(r) = -\frac{\hbar^2}{2m} \sum_{i=1}^P \sigma_i \delta(r - r_i) \quad (1)$$

where the strengths of the delta-functions are $\sigma_i > 0$, $r_1 < r_2 < \dots < r_P$ with $r_i \in (0, +\infty)$ for $n \geq 2$ and $r_i \in (-\infty, +\infty)$ for $n = 1$. The factor $\frac{\hbar^2}{2m}$ is for calculational convenience. Throughout this work, σ_i are always positive numbers and r_i are ordered as defined above. Then, the time-independent Schrödinger equation in \mathbf{R}^n becomes

$$H\Psi = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right) \Psi(x_1, \dots, x_n) = E\Psi(x_1, \dots, x_n) \quad (2)$$

where $\nabla^2 = \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2}$. Since the potential depends only on r for $n \geq 2$, we write the wavefunction in terms of spherical coordinates as $\Psi = f_{n,l}(r)Y_{l,n}(\omega)$ where $Y_{l,n}(\omega)$ is an n -dimensional spherical harmonic of degree l and $\omega = (\theta_1, \dots, \theta_{n-1})$, angular coordinates which we define below [6, 7]. When $n = 1$, we take $l = 0$ and $Y_{0,1} = 1$ leading to $\Psi = f_{1,0}$. Thus, we can use $\Psi = f_{n,l}(r)Y_{l,n}(\omega)$ for $n = 1, 2, 3, \dots$

Since the bound states have negative energies, we define $k^2 = -\frac{2m}{\hbar^2} E > 0$ with $k > 0$. For $n = 1$, we get the equation

$$\frac{d^2 f_{1,0}(r)}{dr^2} + \left\{ \sum_{i=1}^P \sigma_i \delta(r - r_i) \right\} f_{1,0}(r) - k^2 f_{1,0}(r) = 0. \tag{3}$$

By using the dimensionless parameter $v = kr$, we obtain

$$\frac{d^2 f_{1,0}(v)}{dv^2} + \left\{ \sum_{i=1}^P \frac{\sigma_i}{k} \delta(v - v_i) \right\} f_{1,0}(v) - f_{1,0}(v) = 0 \tag{4}$$

where $v_i = kr_i$ for $i = 1, 2, \dots, P$. When $v \neq v_i$, equation (4) reduces to

$$\frac{d^2 f_{1,0}(v)}{dv^2} - f_{1,0}(v) = 0. \tag{5}$$

Equation (5) has two linearly-independent solutions, e^v and e^{-v} . By taking $v_0 = -\infty$ and $v_{P+1} = +\infty$, we define i th interval as $[v_{i-1}, v_i]$, for $i = 1, 2, \dots, P + 1$. Then, the general solution of equation (4) is

$$f_{1,0}(v) = a_i e^{-v} + b_i e^v \quad \text{when } v \in [v_{i-1}, v_i] \quad \text{and} \quad i = 1, 2, \dots, P + 1. \tag{6}$$

Since $e^v \rightarrow +\infty$ as $v \rightarrow +\infty$ and $e^{-v} \rightarrow +\infty$ as $v \rightarrow -\infty$, we have to take $a_1 = 0$ and $b_{P+1} = 0$ which leads to $b_1 e^v$ for the first interval and $a_{P+1} e^{-v}$ for the $(P + 1)$ th interval as the regular solutions of equation (4).

For an arbitrary $n \geq 2$, the Cartesian coordinates of $\vec{r} = (x_1, \dots, x_n)$ are given in terms of the spherical coordinates:

$$\begin{aligned} x_1 &= r \cos \theta_1 \\ x_2 &= r \sin \theta_1 \cos \theta_2 \\ &\dots \\ x_{n-1} &= r \sin \theta_1 \sin \theta_2 \dots \sin \theta_{n-2} \cos \theta_{n-1} \\ x_n &= r \sin \theta_1 \sin \theta_2 \dots \sin \theta_{n-2} \sin \theta_{n-1} \end{aligned} \tag{7}$$

where $0 \leq r < \infty, 0 \leq \theta_j \leq \pi$ for $j \leq n - 2$ and $0 \leq \theta_{n-1} \leq 2\pi$. Then, the Laplacian in spherical coordinates becomes

$$\nabla^2 = \frac{1}{r^{n-1}} \frac{d}{dr} \left(r^{n-1} \frac{d(\cdot)}{dr} \right) + \frac{\Omega_{LB}}{r^2} \tag{8}$$

where the Laplace–Beltrami operator, Ω_{LB} , on the sphere S^{n-1} , satisfies

$$\Omega_{LB} Y_{l,n}(\omega) = -l(l + n - 2) Y_{l,n}(\omega) \tag{9}$$

and $Y_{l,n}(\omega)$ is an n -dimensional spherical harmonics of degree l for $l = 0, 1, 2, \dots$ and $\omega = (\theta_1, \dots, \theta_{n-1})$. The degeneracy of the eigenvalue $-\alpha_l = -l(l + n - 2)$ is $m_{l,n} = \frac{(2l+n-2)(l+n-3)!}{l!(n-2)!}$ for $n \geq 2$ and $l \geq 0$ [6, 7].³

By writing $\Psi = f_{n,l}(r) Y_{l,n}(\omega)$ and using equation (7), we have the radial equation,

$$\frac{1}{r^{n-1}} \frac{d}{dr} \left(r^{n-1} \frac{df_{n,l}(r)}{dr} \right) + \left\{ \sum_{i=1}^P \sigma_i \delta(r - r_i) \right\} f_{n,l}(r) - \left(k^2 + \frac{\alpha_l}{r^2} \right) f_{n,l}(r) = 0 \tag{10}$$

for $l = 0, 1, 2, \dots$

³ $m_{0,2} = 1$. This can also be obtained from the general formula by first inserting $l = 0$, doing cancellations and then inserting n .

Inserting $v = kr$, $v_i = kr_i$, one obtains

$$\frac{1}{v^{n-1}} \frac{d}{dv} \left(v^{n-1} \frac{df_{n,l}(v)}{dv} \right) + \left\{ \sum_{i=1}^P \frac{\sigma_i}{k} \delta(v - v_i) \right\} f_{n,l}(v) - \left(1 + \frac{\alpha_l}{v^2} \right) f_{n,l}(v) = 0. \quad (11)$$

Defining $g_{n,l} = v^{\frac{n-2}{2}} f_{n,l}$, we get

$$\frac{1}{v} \frac{d}{dv} \left(v \frac{dg_{n,l}(v)}{dv} \right) + \left(\sum_{i=1}^P \frac{\sigma_i}{k} \delta(v - v_i) \right) g_{n,l}(v) - \left(1 + \frac{\left(l + \frac{n-2}{2} \right)^2}{v^2} \right) g_{n,l}(v) = 0. \quad (12)$$

When $v \neq v_i$, equation (12) reduces to

$$\frac{1}{v} \frac{d}{dv} \left(v \frac{dg_{n,l}(v)}{dv} \right) - \left(1 + \frac{\left(l + \frac{n-2}{2} \right)^2}{v^2} \right) g_{n,l}(v) = 0. \quad (13)$$

This is Bessel's equation which has two linearly-independent solutions that are the modified Bessel functions of the first kind $I_{\left(l + \frac{n-2}{2} \right)}(v)$ and the third kind $K_{\left(l + \frac{n-2}{2} \right)}(v)$.

By taking $v_0 = 0$ and $v_{P+1} = +\infty$, we define the i th interval as $[v_{i-1}, v_i]$ for $i = 1, 2, \dots, P+1$. Then, for $\mu = l + \frac{n-2}{2}$, the general solution of equation (12) is

$$g_{n,l}(v) = a_i K_\mu(v) + b_i I_\mu(v) \quad \text{when } v \in [v_{i-1}, v_i] \quad \text{and } i = 1, 2, \dots, P+1. \quad (14)$$

Since $K_\mu(v) \rightarrow +\infty$ as $v \rightarrow 0$ and $I_\mu(v) \rightarrow +\infty$ as $v \rightarrow +\infty$, we have to take $a_1 = 0$ and $b_{P+1} = 0$ which leads to $b_1 I_\mu(v)$ in the first interval and $a_{P+1} K_\mu(v)$ in the $(P+1)$ th interval as the regular solutions of equation (12).

For a point $y \in (-\infty, +\infty)$ for $n = 1$ and $z \in (0, +\infty)$ for $n \geq 2$, we define the region A as $[y, +\infty)$ for $n = 1$ and $[z, +\infty)$ for $n \geq 2$ and the region B as $(-\infty, y]$ for $n = 1$ and $[0, z]$ for $n \geq 2$. Thus, the solutions $\phi_A \in \{e^{-v}, K_\mu(v)\}$ are regular in region A and $\phi_B \in \{e^v, I_\mu(v)\}$ are regular in region B, where the first functions in the brackets are for $n = 1$ and the second ones for $n \geq 2$. Then, the bound state solutions of equation (4) or (12) are

$$g_{n,l}(v) = a_i \phi_A(v) + b_i \phi_B(v) \quad \text{when } v \in [v_{i-1}, v_i] \quad \text{and } i = 1, 2, \dots, P+1. \quad (15)$$

The continuity of the wavefunction at the boundary of i th and $(i+1)$ th intervals leads to

$$a_i \phi_A(v_i) + b_i \phi_B(v_i) = a_{i+1} \phi_A(v_i) + b_{i+1} \phi_B(v_i). \quad (16)$$

By multiplying equation (4) with dv and equation (12) with $v dv$, we integrate these equations between $v_i - \epsilon$ and $v_i + \epsilon$. Letting $\epsilon \rightarrow 0^+$ and using the continuity of the wavefunctions, we get

$$(a_{i+1} \phi'_A(v_i) + b_{i+1} \phi'_B(v_i)) - (a_i \phi'_A(v_i) + b_i \phi'_B(v_i)) + \frac{\sigma_i}{k} (a_i \phi_A(v_i) + b_i \phi_B(v_i)) = 0 \quad (17)$$

where $'$ denotes differentiation with respect to v . By solving linear equations (16) and (17) for a_{i+1} and b_{i+1} in terms of a_i and b_i , we obtain the recursion relations

$$\begin{aligned} a_{i+1} &= \left(1 + \frac{\sigma_i \phi_A(v_i) \phi_B(v_i)}{k W_i} \right) a_i + \left(\frac{\sigma_i (\phi_B(v_i))^2}{k W_i} \right) b_i \\ b_{i+1} &= \left(-\frac{\sigma_i (\phi_A(v_i))^2}{k W_i} \right) a_i + \left(1 - \frac{\sigma_i \phi_A(v_i) \phi_B(v_i)}{k W_i} \right) b_i \end{aligned} \quad (18)$$

where $W_i = W_i[\phi_A, \phi_B] = \phi_A(v_i) \phi'_B(v_i) - \phi_B(v_i) \phi'_A(v_i)$ is the Wronskian.

We define the transfer matrix M_i and write equation (18) in terms of M_i :

$$\begin{pmatrix} a_{i+1} \\ b_{i+1} \end{pmatrix} = M_i \begin{pmatrix} a_i \\ b_i \end{pmatrix} = \begin{pmatrix} 1 + \frac{\sigma_i \phi_A(v_i) \phi_B(v_i)}{k W_i} & \frac{\sigma_i (\phi_B(v_i))^2}{k W_i} \\ -\frac{\sigma_i (\phi_A(v_i))^2}{k W_i} & 1 - \frac{\sigma_i \phi_A(v_i) \phi_B(v_i)}{k W_i} \end{pmatrix} \begin{pmatrix} a_i \\ b_i \end{pmatrix}. \quad (19)$$

Thus,

$$\begin{pmatrix} a_{P+1} \\ b_{P+1} \end{pmatrix} = M_P M_{P-1} \cdots M_1 \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \mathbf{X} \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \tag{20}$$

where the matrix $\mathbf{X} = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} = M_P M_{P-1} \cdots M_1$ is a function of k for given σ_i and r_i values. Since we demand $a_1 = 0$ and $b_{P+1} = 0$ for regular solutions, then we obtain $\mathbf{X}_{22}(k) = 0$ which is a transcendental equation in general. The positive real roots of the equation $\mathbf{X}_{22}(k) = 0$ will be used to find the energy levels, $E = -\frac{\hbar^2}{2m} k^2$.

Since $W(e^{-v}, e^v) = 2$ and $W(K_\mu(v), I_\mu(v)) = \frac{1}{v}$, we have

$$M_i = \begin{pmatrix} 1 + \frac{\sigma_i}{2k} & \frac{\sigma_i e^{2kx_i}}{2k} \\ -\frac{\sigma_i e^{-2kx_i}}{2k} & 1 - \frac{\sigma_i}{2k} \end{pmatrix} \tag{21}$$

for $n = 1$ and

$$\begin{aligned} M_i &= \begin{pmatrix} 1 + \frac{\sigma_i v_i I_\mu(v_i) K_\mu(v_i)}{k} & \frac{\sigma_i v_i (I_\mu(v_i))^2}{k} \\ -\frac{\sigma_i v_i (K_\mu(v_i))^2}{k} & 1 - \frac{\sigma_i v_i I_\mu(v_i) K_\mu(v_i)}{k} \end{pmatrix} \\ &= \begin{pmatrix} 1 + \gamma_i I_\mu(kr_i) K_\mu(kr_i) & \gamma_i (I_\mu(kr_i))^2 \\ -\gamma_i (K_\mu(kr_i))^2 & 1 - \gamma_i I_\mu(kr_i) K_\mu(kr_i) \end{pmatrix} \end{aligned} \tag{22}$$

for $n \geq 2$ with $\gamma_i = \sigma_i r_i$ and $v_i = kr_i$ for $i = 1, 2, \dots, P$. Thus, by solving $\mathbf{X}_{22}(k) = 0$, we obtain k and hence M_i which in turn determine $g_{n,l}$ exactly.

Before we prove some results on the bound states, we prove a property of $F_\mu(v) = I_\mu(v)K_\mu(v)$.

Lemma 1. $F_\mu(v) = I_\mu(v)K_\mu(v)$ is a monotonically decreasing function of v for $v > 0$ and $\mu > -1$.

Proof. We use the following representation of $F_\mu(v) = I_\mu(v)K_\mu(v)$ (6.535 entry of Gradshteyn and Ryzhik [8]),

$$F_\mu(v) = I_\mu(v)K_\mu(v) = \int_0^\infty \frac{x}{x^2 + v^2} [J_\mu(x)]^2 dx \tag{23}$$

where $\text{Re}(v) > 0$ and $\text{Re}(\mu) > -1$. By taking the derivative respect to v , we obtain

$$\frac{dF_\mu(v)}{dv} = -2v \int_0^\infty \frac{x}{(x^2 + v^2)^2} [J_\mu(x)]^2 dx. \tag{24}$$

For real $v > 0$ and $\mu > -1$, the integrand and hence the integral are positive. Thus, $\frac{dF_\mu}{dv} < 0$ and the lemma is proven. \square

The asymptotic behaviour of $I_\mu(v)$ and $K_\mu(v)$ is [9]

$$I_\mu(v) \approx \frac{v^\mu}{2^\mu \Gamma(1 + \mu)} \quad K_\mu(v) \approx \frac{2^{\mu-1} \Gamma(\mu)}{v^\mu} \quad \text{as } v \rightarrow 0 \tag{25}$$

for $\mu > 0$ and

$$I_0(0) = 1 \quad K_0(v) \approx \log\left(\frac{2}{v}\right) \quad \text{as } v \rightarrow 0 \tag{26}$$

and

$$I_\mu(v) \approx \frac{e^v}{\sqrt{2\pi v}} \quad K_\mu(v) \approx \sqrt{\frac{\pi}{2v}} e^{-v} \quad \text{as } v \rightarrow \infty. \tag{27}$$

Therefore, the maximum value of $F_\mu(v) = I_\mu(v)K_\mu(v)$ is equal to $\frac{1}{2\mu}$ for $\mu > 0$ and ∞ for $\mu = 0$ while $F_\mu(v) \rightarrow 0$ as $v \rightarrow \infty$.

Theorem 1. For the potential $V(r) = -\frac{\hbar^2}{2m}\sigma_1\delta(r - r_1)$:

- (a) there always exists one and only one bound state energy level E for $n = 1$ or $n = 2$ with $l = 0$,
 (b) for given l and $n \geq 2$, there always exists one and only one bound state energy level E if $\sigma_1 r_1 > 2l + n - 2$ and none otherwise.

Proof.

- (a) We have shown that $k = \sqrt{-\frac{2m}{\hbar^2}E} > 0$ values for bound state are obtained from the equation $(M_1)_{22} = 0$. For $n = 1$, $(M_1)_{22} = 1 - \frac{\sigma_1}{2k} = 0$ will always have a solution $k = \frac{\sigma_1}{2} > 0$ for any $\sigma_1 > 0$. For $n = 2$ with $l = 0$, we have $(M_1)_{22} = 1 - \gamma_1 F_0(v) = 0$. By lemma 1, for $\mu = l + \frac{n-2}{2}$, $F_\mu(v)$ decreases monotonically and $F_0(v) \rightarrow \infty$ as $v \rightarrow 0$ and $F_0(v) \rightarrow 0$ as $v \rightarrow \infty$. Hence, there exists one and only one value of $v_B > 0$ such that $F_0(v_B) = \frac{1}{\gamma_1}$ and $k = \frac{v_B}{r_1} > 0$.
 (b) For $\mu > 0$, $F_\mu(v) \leq \frac{1}{2\mu}$ and $F_\mu(v)$ decreases to zero monotonically, then $(M_1)_{22}$ increases monotonically from $(1 - \frac{\gamma_1}{2\mu})$ to 1. Therefore, for a given l , there exists one and only one bound state solution of equation (12) if $1 - \frac{\gamma_1}{2\mu} < 0$ or $\sigma_1 r_1 > 2\mu = 2l + n - 2$ and none otherwise. The theorem is proven. \square

By writing the bound state wavefunction in terms of the original variables, we have

$$\Psi = \begin{cases} f_{1,0}(kr) = g_{1,0}(kr) & \text{for } n = 1 \text{ and } r \in (-\infty, \infty) \\ f_{n,l}(kr)Y_{l,n}(\omega) = (kr)^{\frac{2-n}{2}}g_{n,l}(kr)Y_{l,n}(\omega) & \text{for } n \geq 2 \text{ and } r \in [0, \infty). \end{cases} \quad (\dagger)$$

We note that since $g_{n,l} \propto r^{(l+\frac{n-2}{2})}$, then $\Psi \propto r^l$ as $r \rightarrow 0$ for $n \geq 2$.

For $g_{n,l}(v)$ part of the bound states Ψ , we define equation (¶) by combining equations (4) and (12) as

$$\begin{aligned} \frac{d^2 g_{1,0}(v)}{dv^2} + \left\{ \sum_{i=1}^P \frac{\sigma_i}{k} \delta(v - v_i) \right\} g_{1,0}(v) - g_{1,0}(v) &= 0 & \text{for } n = 1 \\ \frac{1}{v} \frac{d(v \frac{dg_{n,l}(v)}{dv})}{dv} + \left\{ \sum_{i=1}^P \frac{\sigma_i}{k} \delta(v - v_i) \right\} g_{n,l}(v) - \left(1 + \frac{(l + \frac{n-2}{2})^2}{v^2} \right) g_{n,l}(v) &= 0 & \text{for } n \geq 2. \end{aligned} \quad (\P)$$

We will prove the following theorems for the bound state solutions of equation (¶).

Theorem 2. Given n and l , the bound state solutions $g_{n,l}(kr)$ of equation (¶) are non-degenerate.

Proof. The bound state solutions of equation (¶) are given as $g_{n,l}(v) = a_i \phi_A(v) + b_i \phi_B(v)$ when $v \in [v_{i-1}, v_i]$ for $i = 1, 2, \dots, P+1$. If they are degenerate, for given n and l , there are $g_{n,l}$ functions with different a_i and b_i for the same k value. Equation (19) shows that all the a_i and b_i for $i \geq 1$ are found by

$$M_i \cdots M_1 \begin{pmatrix} 0 \\ b_1 \end{pmatrix}$$

where the M_i are given by equation (21) or (22). For given parameters σ_i , and r_i , since all M_i are functions of k , then all M_i are the same for degenerate $g_{n,l}$ functions. Thus, a_i and b_i are uniquely determined by b_1 which is fixed by the normalization of $g_{n,l}$. Therefore, a_i and b_i

are unique for given σ_i, r_i and k . Hence, for given n and l , the bound state solutions $g_{n,l}(kr)$ of equation (¶) are non-degenerate and the theorem is proven. \square

Theorem 3. *If $g_{n,l}(v)$ is a bound state solution of equation (¶), then both $g_{n,l}(v)$ and $\frac{dg_{n,l}(v)}{dv}$ cannot be zero at two points in the same interval $[v_{i-1}, v_i]$ for $i = 2, \dots, P$ and they are non-zero in the first and $(P + 1)$ th intervals.*

Proof. $g_{n,l}(v) = b_1\phi_B(v)$ in the first interval and $g_{n,l}(v) = a_{P+1}\phi_A(v)$ in the $(P + 1)$ th interval. $g_{n,l}$ and $\frac{dg_{n,l}(v)}{dv}$ cannot vanish at all for $i = 1$ and $i = P + 1$ since $\phi_A \in \{e^{-v}, K_\mu(v)\}$ and $\phi_B \in \{e^v, I_\mu(v)\}$, $\phi_A(v) > 0, \phi_B(v) > 0, \phi'_A(v) < 0$ and $\phi'_B(v) > 0$ for v values which are defined for $\phi_A(v), \phi_B(v)$.

For $i = 2, \dots, P$, assume that both $g_{n,l}(v)$ and $\frac{dg_{n,l}(v)}{dv}$ are zero at two points u_1 and u_2 in the i th interval. Then,

$$a_i\phi_A(u_1) + b_i\phi_B(u_1) = 0 \tag{28}$$

and

$$a_i\phi'_A(u_2) + b_i\phi'_B(u_2) = 0. \tag{29}$$

By solving these linear equations for a_i and b_i , we obtain

$$a_i[\phi_A(u_1)\phi'_B(u_2) - \phi_B(u_1)\phi'_A(u_2)] = 0 \tag{30}$$

and

$$b_i[\phi_B(u_1)\phi'_A(u_2) - \phi_A(u_1)\phi'_B(u_2)] = 0. \tag{31}$$

Thus, the brackets of equations (30) and (31) do not vanish due to the properties of ϕ_A, ϕ_B and their derivatives which we show above. Hence, we get $a_i = 0$ and $b_i = 0$. Then, by using transfer matrices and their inverses (which exist since $\det(M_i) = 1$ for all i), we get $a_j = 0$ and $b_j = 0$ for all $j = 1, \dots, P + 1$. This leads to the wavefunction which is identically zero and cannot be a bound state. The theorem is proven. \square

Theorem 4. *For given n and l , a bound state solution $g_{n,l}(v)$ cannot be zero at two points in the same interval $[v_{i-1}, v_i]$ for $i = 2, \dots, P$.*

Proof. Assume that $g_{n,l}(u_1) = 0$ and $g_{n,l}(u_2) = 0$ at two points u_1 and u_2 in an interval $[v_i, v_{i+1}]$. Then, by Rolle's theorem, there exists a point u between u_1 and u_2 such that $g'_{n,l}(u) = 0$. This contradicts theorem 3, hence $g_{n,l}(v)$ cannot be zero at two points u_1 and u_2 in the same interval and the theorem is proven. \square

Theorem 5. *If there exists a bound state solution $g_{n,l}(kr)$ of equation (¶) for the potential $V_1(r) = -\frac{\hbar^2}{2m}\sigma_1\delta(r - r_1)$, then there exists at least one bound state solution $g_{n,l}(kr)$ of equation (¶) with the potential $V(r) = V_1(r) - \frac{\hbar^2}{2m}\sum_{i=2}^P\sigma_i\delta(r - r_i)$ for $i = 2, \dots, P$.*

Proof. If there exists a bound state solution $g_{n,l}(kr)$ of equation (¶) with the potential $V(r) = -\frac{\hbar^2}{2m}\sigma_1\delta(r - r_1)$, we have

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_1(r) \right] \Psi = E\Psi \tag{32}$$

where Ψ is defined in terms of $g_{n,l}(kr)$ in equation (†). Then, by using the 'volume element' $d\tau$ in \mathbf{R}^n , we get

$$\int_{\mathbf{R}^n} \Psi^* \left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) \right] \Psi d\tau < \int_{\mathbf{R}^n} \Psi^* \left[-\frac{\hbar^2}{2m}\nabla^2 + V_1(r) \right] \Psi d\tau \tag{33}$$

since $\int_{\mathbf{R}^n} \Psi^*[V(r) - V_1(r)]\Psi d\tau < 0$. The theorem is proven. \square

Corollary 1. For the potential $V(r) = -\frac{\hbar^2}{2m} \sum_{i=1}^P \sigma_i \delta(r - r_i)$, there always exists at least one bound state solution $g_{n,l}(kr)$ of equation (9) for $n = 1$ or $n = 2$ with $l = 0$.

Proof. By theorems 1 and 5, the corollary is proven. \square

We will prove theorem 6 about the number of bound state solutions, $g_{n,l}(kr)$, of equation (9) with $V(r) = -\frac{\hbar^2}{2m} \sum_{i=1}^P \sigma_i \delta(r - r_i)$ for given n and l values. The first part of the proof is a modification of the proof given on page 455 of Hilbert–Courant, vol 1 [10]. This proof states that for the Sturm–Liouville problem, the eigenvalue of a state with a larger number of zeros is larger than the eigenvalue of a state with fewer zeros.

First we prove a lemma for self-adjoint operators which have delta-functions.

Lemma 2. Let L be a self-adjoint operator and h_1 and h_2 be the continuous solutions of the following equation in the interval $[u_1, u_2] \subset \mathbf{R}$,

$$L[h_i] = \frac{d}{dv} \left(Q \frac{dh_i}{dv} \right) + Jh_i = \lambda_i Sh_i \quad (34)$$

where $J(v) = \sigma_1 \delta(v - v_1) + G(v)$ with arbitrary real σ_1 , $u_1 < v_1 < u_2$ and λ_i is the eigenvalue with the weight function S . Let $Q(v)$, $G(v)$ and $S(v)$ be continuous in the interval $[u_1, u_2]$ and the derivatives of h_i be continuous in $[u_1, v_1]$ and $(v_1, u_2]$ and the left and right derivatives of h_i about $v = v_i$, $\lim_{\epsilon \rightarrow 0^+} \frac{dh_i(v)}{dv} \Big|_{v=v_1-\epsilon} = h'_i(v_1^-)$ and $\lim_{\epsilon \rightarrow 0^+} \frac{dh_i(v)}{dv} \Big|_{v=v_1+\epsilon} = h'_i(v_1^+)$, exist for $i = 1, 2$. Then,

$$\int_{u_1}^{u_2} (h_1 L[h_2] - h_2 L[h_1]) dv = (QW[h_1, h_2]) \Big|_{v=u_1}^{v=u_2} \quad (35)$$

where $W[h_1, h_2]$ is the Wronskian of two different eigenfunctions of equation (34).

Proof. For a given L and continuous h_i , we have

$$\lim_{\epsilon \rightarrow 0^+} \int_{v_1-\epsilon}^{v_1+\epsilon} L[h_i] dv = Q(v_1)[h'_i(v_1^+) - h'_i(v_1^-)] + \sigma_1 h_i(v_1) = 0 \quad (36)$$

where $h'_i(v_1^+)$ and $h'_i(v_1^-)$ are right and left derivatives, respectively. Thus,

$$Q(v_1)[h'_i(v_1^+) - h'_i(v_1^-)] = -\sigma_1 h_i(v_1). \quad (37)$$

By using equation (34), we get

$$h_1 L[h_2] - h_2 L[h_1] = \frac{d(QW[h_1, h_2])}{dv} = (\lambda_2 - \lambda_1) Sh_1 h_2. \quad (38)$$

Since h'_i is continuous in $[u_1, v_1 - \epsilon]$ and $(v_1 + \epsilon, u_2]$, we have

$$\begin{aligned} \lim_{\epsilon \rightarrow 0^+} \int_{u_1}^{v_1-\epsilon} (h_1 L[h_2] - h_2 L[h_1]) dv &= \lim_{\epsilon \rightarrow 0^+} (QW[h_1, h_2]) \Big|_{v=u_1}^{v=v_1-\epsilon} \\ &= Q(v_1)[h_1(v_1)h'_2(v_1^-) - h_2(v_1)h'_1(v_1^-)] \\ &\quad - Q(u_1)[h_1(u_1)h'_2(u_1) - h_2(u_1)h'_1(u_1)] \end{aligned} \quad (39)$$

and

$$\begin{aligned} \lim_{\epsilon \rightarrow 0^+} \int_{v_1+\epsilon}^{u_2} (h_1 L[h_2] - h_2 L[h_1]) dv &= \lim_{\epsilon \rightarrow 0^+} (QW[h_1, h_2]) \Big|_{v=v_1+\epsilon}^{v=u_2} \\ &= Q(u_2)[h_1(u_2)h'_2(u_2) - h_2(u_2)h'_1(u_2)] \\ &\quad - Q(v_1)[h_1(v_1)h'_2(v_1^+) - h_2(v_1)h'_1(v_1^+)]. \end{aligned} \quad (40)$$

Thus,

$$\begin{aligned}
 \int_{u_1}^{u_2} (h_1 L[h_2] - h_2 L[h_1]) \, dv &= \lim_{\epsilon \rightarrow 0^+} \int_{u_1}^{v_1 - \epsilon} (h_1 L[h_2] - h_2 L[h_1]) \, dv \\
 &\quad + \lim_{\epsilon \rightarrow 0^+} \int_{v_1 + \epsilon}^{u_2} (h_1 L[h_2] - h_2 L[h_1]) \, dv \\
 &= Q(v_1)[h_1(v_1)h_2'(v_1^-) - h_2(v_1)h_1'(v_1^-)] - Q(u_1)[h_1(u_1)h_2'(u_1) \\
 &\quad - h_2(u_1)h_1'(u_1)] + Q(u_2)[h_1(u_2)h_2'(u_2) - h_2(u_2)h_1'(u_2)] \\
 &\quad - Q(v_1)[h_1(v_1)h_2'(v_1^+) - h_2(v_1)h_1'(v_1^+)] \\
 &= (QW[h_1, h_2])|_{v=u_1}^{v=u_2} + Q(v_1)h_2(v_1)[h_1'(v_1^+) - h_1'(v_1^-)] \\
 &\quad - Q(v_1)h_1(v_1)[h_2'(v_1^+) - h_2'(v_1^-)] \\
 &= (QW[h_1, h_2])|_{v=u_1}^{v=u_2} + Q(v_1)h_2(v_1)(-\sigma_1 h_1(v_1)) - Q(v_1)h_1(v_1)(-\sigma_1 h_2(v_1)) \\
 &= (QW[h_1, h_2])|_{v=u_1}^{v=u_2}. \tag{41}
 \end{aligned}$$

The lemma is proven. □

Theorem 6. *Given n and l , there exist at most P bound state solutions $g_{n,l}(kr)$ of equation (¶) with the potential $V(r) = -\frac{\hbar^2}{2m} \sum_{i=1}^P \sigma_i \delta(r - r_i)$.*

Proof. We define self-adjoint operators

$$L_{n,l}[h] = \frac{d}{dr} \left(Q_n \frac{dh}{dr} \right) + J_{n,l}h \tag{42}$$

where $Q_1 = 1$ and $J_{1,0} = \sum_{i=1}^P \sigma_i \delta(r - r_i)$ where $r \in (-\infty, +\infty)$ for $n = 1$ and $Q_n = r^{n-1}$ and $J_{n,l} = r^{n-1} \sum_{i=1}^P \sigma_i \delta(r - r_i) - r^{n-3}l(l + n - 2)$ where $r \in [0 + \infty)$ for $n \geq 2$. Then

$$L_{n,l}[f_{n,l}] = -\lambda_i S_n f_{n,l} \tag{43}$$

represents equations (3) and (10) with the vanishing boundary conditions for $f_{n,l}^4$ and $S_1 = 1, S_n = r^{n-1}$ where $r \in [0 + \infty)$ for $n \geq 2$. Here we take $-\lambda_i$ since larger $k^2 = -\lambda_i$ values correspond to smaller bound state energy levels, $E = \frac{\hbar^2}{2m} \lambda_i$. For given n and l , we consider two eigenvalues of this equation such that $-\lambda_1 > -\lambda_2$ or $\lambda_2 > \lambda_1$. Then,

$$L_{n,l}[h_1] = -\lambda_1 S_n h_1 \tag{44}$$

and

$$L_{n,l}[h_2] = -\lambda_2 S_n h_2. \tag{45}$$

Using equations (44) and (45), we obtain

$$h_2 L_{n,l}[h_1] - h_1 L_{n,l}[h_2] = \frac{d(Q_n W[h_2, h_1])}{dr} = (\lambda_2 - \lambda_1) S_n h_1 h_2. \tag{46}$$

Assume that h_2 does not change sign between the two zeros u_1 and u_2 of h_1 . Without loss of generality, we take h_1 and h_2 positive between u_1 and u_2 . By integrating equation (46) over r between u_1 and u_2 and using lemma 2, we get

$$(Q_n W[h_2, h_1])|_{r=u_1}^{r=u_2} = Q_n \left(h_2 \frac{dh_1}{dr} - h_1 \frac{dh_2}{dr} \right) \Big|_{r=u_1}^{r=u_2} = (\lambda_2 - \lambda_1) \int_{u_1}^{u_2} S_n h_1 h_2 \, dr. \tag{47}$$

By inserting $h_1(u_1) = 0, h_1(u_2) = 0$, we obtain

$$Q_n(u_2)h_2(u_2)h_1'(u_2) - Q_n(u_1)h_2(u_1)h_1'(u_1) = (\lambda_2 - \lambda_1) \int_{u_1}^{u_2} S_n h_1 h_2 \, dr. \tag{48}$$

⁴ For $n = 2, l = 0, I'_0(0) = 0$ and the value of $f_{n,l}$ vanishes at the boundaries for other cases.

The right-hand side of equation (48) is positive, but the left-hand side is negative since Q_n and h_2 are positive in the interval $[u_1, u_2]$ and $h'_1(u_1) > 0$ and $h'_1(u_2) < 0$. Thus, the contradiction shows that h_2 should change sign in this interval. The first eigenfunction has no zeros in the interior and the m th eigenfunction will have $m - 1$ zeros [10]. From equation (†), we find that the zeros of $f_{n,l}$ and $g_{n,l}$ are the same for $v = kr \in (0, \infty)$ and $k > 0$. Since ϕ_A and ϕ_B of equation (15) are positive, $g_{n,l}$ cannot have zeros in the interior of the first and $(P + 1)$ th intervals⁵ and by theorem 4, there can be at most one zero in each interval $[v_{i-1}, v_i]$ for $i = 2, \dots, P$. Thus, there can be at most $P - 1$ zeros and at most P bound state solutions $g_{n,l}(kr)$ of which the first eigenfunction has no zeros. The theorem is proven. \square

Theorem 7. *There exist at most P bound state energy levels of the Schrödinger equation for the potential $V(r) = -\frac{\hbar^2}{2m} \sum_{i=1}^P \sigma_i \delta(r - r_i)$.*

Proof. By theorem 2, $g_{n,l}$ are non-degenerate and theorem 6 states that there are at most P bound state solutions for $g_{n,l}$. Thus, the transcendental equation $\mathbf{X}_{22}(k) = 0$ for the matrix $\mathbf{X} = M_P M_{P-1} \cdots M_1$ has at most P positive real roots where M_i s are defined in (21) or (22). The theorem is proven. \square

We note that the matrices M_i can be written as $M_i = I + N_i$ where I is the identity matrix and N_i is a nilpotent matrix such that $N_i^2 = \mathbf{0}$. All entries of M_i matrices are real, $\text{tr}(M_i) = 2$ and $\det(M_i) = 1$. Thus, $M_i \in SL(2, \mathbf{R})$. By using theorem 6, we present a generalized version of the equation $\mathbf{X}_{22}(k) = 0$ for some generalizations of M_i matrices and prove theorem 8 for these particular matrices.

Theorem 8. *Let the matrices $U_i \in SL(2, \mathbf{R})$ and $Z_i \in SL(2, \mathbf{R})$ be defined as*

$$U_i = \begin{pmatrix} 1 + \frac{a_i}{f(\zeta)} & \frac{a_i}{f(\zeta)} e^{b_i f(\zeta)} \\ -\frac{a_i}{f(\zeta)} e^{-b_i f(\zeta)} & 1 - \frac{a_i}{f(\zeta)} \end{pmatrix} \quad (49)$$

where a_i are arbitrary positive real numbers for $i = 1, 2, \dots, P$ and b_i are real numbers such that $b_1 < b_2 < \dots < b_P$ and

$$Z_i = \begin{pmatrix} 1 + c_i I_\mu(d_i f(\zeta)) K_\mu(d_i f(\zeta)) & c_i [I_\mu(d_i f(\zeta))]^2 \\ -c_i [K_\mu(d_i f(\zeta))]^2 & 1 - c_i I_\mu(d_i f(\zeta)) K_\mu(d_i f(\zeta)) \end{pmatrix} \quad (50)$$

where c_i are arbitrary positive real numbers for $i = 1, 2, \dots, P$ and d_i are positive real numbers such that $d_1 < d_2 < \dots < d_P$ and $f(\zeta)$ is any real, positive definite, one-to-one and onto function for $\zeta \in (0, \infty)$. Then, for the matrix $\mathcal{U} = \begin{pmatrix} \mathcal{U}_{11} & \mathcal{U}_{12} \\ \mathcal{U}_{21} & \mathcal{U}_{22} \end{pmatrix} = U_P U_{P-1} \cdots U_1$ ($\mathcal{Z} = \begin{pmatrix} \mathcal{Z}_{11} & \mathcal{Z}_{12} \\ \mathcal{Z}_{21} & \mathcal{Z}_{22} \end{pmatrix} = Z_P Z_{P-1} \cdots Z_1$), equation $\mathcal{U}_{22}(\zeta) = 0$ ($\mathcal{Z}_{22}(\zeta) = 0$) has at most P positive real roots.

Proof. We take $y = f(\zeta) > 0$. Then, U_i and Z_i matrices reduce to M_i matrices which are defined in (21) and (22), respectively. By theorem 7, there are at most P positive y values which satisfy $\mathcal{U}_{22}(y) = 0$ ($\mathcal{Z}_{22}(y) = 0$). Since $f(\zeta)$ is a one-to-one and onto function for $\zeta \in (0, \infty)$, its inverse exists and $\zeta = f^{-1}(y)$. Thus, there are at most P positive real ζ values which satisfy $\mathcal{U}_{22}(\zeta) = 0$ ($\mathcal{Z}_{22}(\zeta) = 0$). The theorem is proven. \square

⁵ Here we consider only the zeros in the interior and exclude the zero value at the boundary $r = 0$ for $n \geq 2$.

3. Conclusions

In this paper, we have analyzed the bound state properties of the Schrödinger equation for a particle of mass m in a potential with P attractive Dirac delta-functions in n dimensions. The potential is radially symmetric for $n \geq 2$. We have obtained transfer matrices to determine the bound state eigenfunctions and a transcendental equation for the corresponding eigenvalues. We have proven that, for given n and l , the bound state solutions of the radial equation are non-degenerate and there are at most P bound state energy levels for a potential with P attractive Dirac delta-functions. We have shown that for the potential $V(r) = -\frac{\hbar^2}{2m}\sigma_1\delta(r-r_1)$, there exists one and only one bound state energy level E if $\sigma_1 r_1 > 2l + n - 2$ and none otherwise for $n \geq 2$. We have also proven that there always exists at least one bound state for a potential with any number of attractive Dirac delta-functions for $n = 1$ or $n = 2$ with $l = 0$. For the bound state solutions of the radial equation, we have demonstrated that $g_{n,l}$ cannot have two zeros and both $g_{n,l}$ and $\frac{dg_{n,l}}{dw}$ cannot be zero at two points in an interval between the locations of consecutive delta-functions. Finally, we have proven that there are at most P positive roots of equation $\mathcal{U}_{22}(\zeta) = 0$ ($\mathcal{Z}_{22}(\zeta) = 0$) where $\mathcal{U} = \begin{pmatrix} \mathcal{U}_{11} & \mathcal{U}_{12} \\ \mathcal{U}_{21} & \mathcal{U}_{22} \end{pmatrix} = U_P U_{P-1} \cdots U_1$ ($\mathcal{Z} = \begin{pmatrix} \mathcal{Z}_{11} & \mathcal{Z}_{12} \\ \mathcal{Z}_{21} & \mathcal{Z}_{22} \end{pmatrix} = Z_P Z_{P-1} \cdots Z_1$) and $U_i, Z_i \in SL(2, \mathbf{R})$ are some particular matrices which are introduced in theorem 8.

These results may be useful for the study of the attraction of a neutron by a nucleus. By considering the shell structure of the nucleus and taking attractive delta potentials at some r_i locations, the bound state spectrum of the neutron may be obtained by inserting empirical values for σ_i and r_i . Our results may also be applied to the bound state spectrum of certain particles in some novel materials which could be designed with some concentric spherical or cylindrical strata.

In this paper, we have not considered the properties of more general potentials with Dirac delta-functions which are not radially symmetric. This is a much more difficult problem which we would like to examine in the future.

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