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Sum rules and the domain after the last node of an eigenstate

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Abstract

It is shown that it is possible to establish sum rules that must be satisfied at the nodes and extrema of the eigenstates of confining potentials which are functions of a single variable. At any boundstate energy the Schrödinger equation has two linearly independent solutions one of which is normalizable while the other is not. In the domain after the last node of a boundstate eigenfunction the unnormalizable linearly independent solution has a simple form which enables the construction of functions analogous to Green's functions that lead to certain sum rules. One set of sum rules gives conditions that must be satisfied at the nodes and extrema of the boundstate eigenfunctions of confining potentials. Another sum rule establishes a relation between an integral involving an eigenfunction in the domain after the last node and a sum involving all the eigenvalues and eigenstates. Such sum rules may be useful in the study of properties of confining potentials. The exactly solvable cases of the particle in a box and the simple harmonic oscillator are used to illustrate the procedure. The relations between one of the sum rules and two-particle densities and a construction based on supersymmetric quantum mechanics are discussed.

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1. Introduction

There is a well-defined procedure for constructing Green's functions for describing solutions to linear second-order differential equations with inhomogeneous terms [1]. This procedure may be employed to study solutions to the Schrödinger equation in one dimension. For problems with spherical symmetry partial wave decomposition effectively reduces the three-dimensional Schroedinger equation to a radial equation in r-space and hence the techniques for constructing Green's functions in one dimension are applicable. Green's functions may be used to establish trace formulae in which the integrals over Green's function may be related to sums involving the eigenvalues of the homogeneous differential equation [2–4]. Such trace formulae are very

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useful in checking the accuracy of the numerically computed eigenvalues. The recent interest in the real spectra of non-Hermitian Hamiltonians exhibiting PT symmetry [5–7] has initiated accurate numerical computation of eigenvalues of PT symmetric Hamiltonians and the trace formulae have proved to be useful.

In this work we consider the two linearly independent solutions to the Schroedinger equation at an eigenenergy and show that it is possible to construct functions which are suitable for studying various sums over eigenstates in the domain outside the last node of a chosen eigenfunction. In section 2 it is shown that it is possible to construct new sum rules involving all the eigenstates and eigenvalues. In section 3 the examples of a particle in a box and the simple harmonic oscillator are used to illustrate the sum rules. The relations between the sum rules, two particle densities and super symmetric quantum mechanics are discussed in section 4. Units in which $\hbar = 1$ and the mass $\mu = \frac{1}{2}$ are used throughout the paper so that $\frac{\hbar^2}{2\mu} = 1$.

2. Nodes, extrema and sumrules

We develop a formalism in this section which would be suitable for applications to either the radial Schrödinger equation for a specific partial wave in the domain $[0, \infty]$ or the full line $[-\infty, +\infty]$. We consider the solutions to

$$\frac{d^2}{dr^2}\Psi_j = (V - E_j)\Psi_j \tag{1}$$

satisfying the boundary conditions at the lower and upper end points of the domain at x_0 and x_1,

$$\mathrm{Lt}_{r\to x_0}\Psi_j \to 0, \qquad \mathrm{Lt}_{r\to x_1}\Psi_j \to 0 \tag{2}$$

for the normalized eigenstates Ψ_j corresponding to the eigenvalues E_j. The state with $j = 1$ corresponds to the groundstate with no nodes and the state Ψ_j has $(j - 1)$ nodes. Let the nodes of the eigenstate Ψ_n be at $r = R_0$ and let the outermost node be at $r = \tilde{R}_0$. Then Ψ_n has no nodes in the domain $\tilde{R}_0 < r < x_1$. The second linearly independent solution at E_n is then given by

$$\tilde{\Psi}_n(r) = \Psi_n(r)\int_R^r \frac{1}{\Psi_n^2(y)}\,dy, \tag{3}$$

where R is a constant which may be chosen according to some appropriate requirement. If we choose $R > \tilde{R}_0$ then in the domain $R < r < x_1$ there can be no infinities arising from the denominator inside the integral and $\tilde{\Psi}_n$ is well defined in this domain. The Wronskian relation

$$\Psi_n\frac{d}{dr}\tilde{\Psi}_n - \tilde{\Psi}_n\frac{d}{dr}\Psi_n = 1 \tag{4}$$

shows that $\mathrm{Lt}_{r\to R_0}\tilde{\Psi}_n \neq 0$ but has a finite value determined by the derivative of Ψ_n at $r = R_0$.

The differential equation satisfied by the eigenstates may be used to represent the Wronskian between the states j and k $(j \neq k)$ in terms of the overlap integrals between the different orthonormal eigenstates in the form

$$\int_{x_0}^r \Psi_k(y)\Psi_j(y)\,dy = \int_{x_1}^r \Psi_k(y)\Psi_j(y)\,dy = \frac{(\Psi_k\dot{\Psi}_j - \dot{\Psi}_k\Psi_j)}{(E_k - E_j)}, \tag{5}$$

where the dot denotes a derivative with respect to r. If we now define

$$G(r,\tilde{r}) = \sum_{j\neq n}\frac{\Psi_j(r)\Psi_j(\tilde{r})}{(E_n - E_j)}, \tag{6}$$

where the sum is over a complete set of eigenstates excluding the state n, then using the equality in equation (5) it can be established that

$$\left(\Psi_n(r)\frac{\partial}{\partial r} - \dot{\Psi}_n(r)\right) G(r,\tilde{r}) = \sum_{j\neq n} \Psi_j(\tilde{r}) \int_{x_1}^{r} \Psi_n(y)\Psi_j(y)\,\mathrm{d}y. \tag{7}$$

Green's functions $G(r,\tilde{r};E)$ considered in the usual textbooks (see [1], for example) are constructed at energies E which are not one of the eigenenergies E_n. In contrast, the function G considered here is constructed with $E = E_n$. Using the completeness relation satisfied by the eigenstates

$$\sum_{j\neq n} \Psi_j(\tilde{r})\Psi_j(y) = \delta(\tilde{r}-y) - \Psi_n(\tilde{r})\Psi_n(y) \tag{8}$$

it can be shown that

$$\left(\Psi_n(r)\frac{\partial}{\partial r} - \dot{\Psi}_n(r)\right) G(r,\tilde{r}) = -\Psi_n(\tilde{r}) \left(\theta(r-\tilde{r})\int_{x_1}^{r} + \theta(\tilde{r}-r)\int_{x_0}^{r}\right) \Psi_n^2\,\mathrm{d}y, \tag{9}$$

where $\theta(z)$ is the unit step function which vanishes when $z < 0$ and has value 1 when $z > 0$.

2.1. Sum rules at nodes of Ψ_n

Various interesting relations follow from the differential equation (9). If we choose $r = R_0$, where R_0 is a node of the state Ψ_n at which $\Psi_n(R_0) = 0$ then we get the relation

$$\sum_{j\neq n} \frac{\Psi_j(R_0)\Psi_j(\tilde{r})}{(E_n - E_j)} = \frac{\Psi_n(\tilde{r})}{\dot{\Psi}_n(R_0)} \left(\theta\,(R_0-\tilde{r})\int_{x_1}^{R_0} + \theta(\tilde{r}-R_0)\int_{x_0}^{R_0}\right) \Psi_n^2\,\mathrm{d}y. \tag{10}$$

In particular, setting $\tilde{r} = R_0$ in equation (10) leads to

$$\sum_{j\neq n} \frac{\Psi_j^2(R_0)}{(E_n - E_j)} = 0. \tag{11}$$

Squaring both sides of equation (10), integrating over the variable $\tilde{r}$ in the full range $[x_0, x_1]$ and using the orthonormality of the states Ψ_j it may be shown that

$$\sum_{j\neq n} \frac{\Psi_j^2(R_0)}{(E_n - E_j)^2} = \frac{1}{\dot{\Psi}_n^2(R_0)} \int_{x_0}^{R_0} \Psi_n^2\,\mathrm{d}y \int_{R_0}^{x_1} \Psi_n^2\,\mathrm{d}z. \tag{12}$$

At any node of any eigenstate the rest of the eigenstates must fulfil the conditions implied by equations (11) and (12).

2.2. Sum rules at extrema of Ψ_n

Another special case of equation (9) arises when $r = R_1$, where R_1 is an extremum of Ψ_n which satisfies $\dot{\Psi}_n(R_1) = 0$. Equation (9) simplifies to

$$\sum_{j\neq n} \frac{\dot{\Psi}_j(R_1)\Psi_j(\tilde{r})}{(E_n - E_j)} = \frac{\Psi_n(\tilde{r})}{\Psi_n(R_1)} \left(\theta(R_1-\tilde{r})\int_{R_1}^{x_1} - \theta(\tilde{r}-R_1)\int_{x_0}^{R_1}\right) \Psi_n^2\,\mathrm{d}y \tag{13}$$

which when differentiated with respect to $\tilde{r}$ and evaluated at $\tilde{r} = R_1$ leads to the identity

$$\sum_{j\neq n} \frac{\dot{\Psi}_j^2(R_1)}{(E_n - E_j)} = -\delta(\tilde{r} - R_1)|_{\tilde{r}=R_1}. \tag{14}$$

Using the completeness relation of the eigenstates the above relation may also be given in the form

$$\sum_{j\neq n}\left(\frac{\dot{\Psi}_j^2(R_1)}{(E_n-E_j)}+\Psi_j^2(R_1)\right)=-\Psi_n^2(R_1). \tag{15}$$

Squaring both sides of equation (13), integrating over the variable $\tilde{r}$ in the full range $[x_0, x_1]$ and using the orthonormality of the states Ψ_j it can be shown that

$$\sum_{j\neq n}\frac{\dot{\Psi}_j^2\,(R_1)}{(E_n-E_j)^2}=\frac{1}{\Psi_n^2(R_1)}\int_{x_0}^{R_1}\Psi_n^2\,\mathrm{d}y\int_{R_1}^{x_1}\Psi_n^2\,\mathrm{d}z. \tag{16}$$

At any extremum of any eigenstate the derivative of all other eigenstates must satisfy the conditions implied by equations (15) and (16).

2.3. *Integral relations valid outside the last node of Ψ_n*

The differential equation (9) satisfied by the function G defined by equation (6) is a first-order differential equation which can be brought to the form

$$\frac{\partial}{\partial r}\frac{G\,(r,\tilde{r})}{\Psi_n(r)}=\frac{\Psi_n(\tilde{r})}{\Psi_n^2(r)}\left(\theta\,(r-\tilde{r})\int_r^{x_1}\Psi_n^2\,\mathrm{d}z-\theta\,(\tilde{r}-r)\int_{x_0}^{r}\Psi_n^2\,\mathrm{d}z\right) \tag{17}$$

and can be integrated from an arbitrary point r_2 to get the relation

$$\frac{G(r,\tilde{r})}{\Psi_n(r)}-\frac{G\,(r_2,\tilde{r})}{\Psi_n\,(r_2)}=\Psi_n(\tilde{r})\int_{r_2}^{r}\frac{\mathrm{d}y}{\Psi_n^2}\left(\theta\,(y-\tilde{r})\int_y^{x_1}-\theta\,(\tilde{r}-y)\int_{x_0}^{y}\right)\Psi_n^2\,\mathrm{d}z. \tag{18}$$

It is also possible to establish a differential equation for $G(r,r)$. Using equations (5) and (6) and the limiting value $\mathrm{Lt}_{z\to 0}\,\theta(z)=1/2$ it can be established that

$$S(r)\equiv G(r,r)=\sum_{j\neq n}\frac{\Psi_j^2(r)}{(E_n-E_j)} \tag{19}$$

satisfies

$$\Psi_n^2\frac{\mathrm{d}}{\mathrm{d}r}\frac{S}{\Psi_n^2}=\left(\int_r^{x_1}\Psi_n^2\,\mathrm{d}y-\int_{x_0}^{r}\Psi_n^2\,\mathrm{d}y\right). \tag{20}$$

This equation can be integrated from any point r_2 to give

$$S(r)=\frac{\Psi_n^2(r)}{\Psi_n^2\,(r_2)}S\,(r_2)+\Psi_n^2(r)\left(\int_{r_2}^{r}\frac{\mathrm{d}y}{\Psi_n^2}\left(\int_y^{x_1}\Psi_n^2\,\mathrm{d}z-\int_{x_0}^{y}\Psi_n^2\,\mathrm{d}z\right)\right). \tag{21}$$

Different choices of $\tilde{r}$ and r_2 in equation (18) lead to different integral relations. If we set $\tilde{r}=r_2$ in equation (18) then the resulting expression can be rearranged to give

$$\frac{G\,(r,r_2)}{\Psi_n(r)\Psi_n\,(r_2)}-\frac{G\,(r_2,r_2)}{\Psi_n^2\,(r_2)}=\int_{r_2}^{r}\frac{\mathrm{d}y}{\Psi_n^2(y)}\left(\theta\,(y-r_2)\int_y^{x_1}-\theta\,(r_2-y)\int_{x_0}^{y}\right)\Psi_n^2(z)\,\mathrm{d}z. \tag{22}$$

By interchanging the labels r and r_2 another relation like that given above may be derived and by addition of the two relations we can show that

$$\sum_{j\neq n}\frac{1}{E_n-E_j}\left(\frac{\Psi_j(r)}{\Psi_n(r)}-\frac{\Psi_j\,(r_2)}{\Psi_n\,(r_2)}\right)^2=-\int_{r_<}^{r_>}\frac{\mathrm{d}y}{\Psi_n^2(y)}, \tag{23}$$

where $r_<$ ($r_>$) is the smaller (larger) of (r, r_2). The integrand in equation (23) is free of singularities in the domain of integration if both r and r_2 are greater than the last node $\tilde{R}_0$ of Ψ_n.

Various integral relations follow from equation (23). For example multiplying equation (23) by $\Psi_n^2(r)\Psi_n^2(r_2)$, integrating over both the variables from $\tilde{R}_0$ to x_1 and using the notation

$$A_{jk} = \int_{\tilde{R}_0}^{x_1} \Psi_j(y)\Psi_k(y)\,\mathrm{d}y \tag{24}$$

and noting that when $r = R_0$ is a node of Ψ_n equation (5) gives

$$A_{nj} = \frac{\dot{\Psi}_n(R_0)\Psi_j(R_0)}{(E_n - E_j)}, \qquad j \neq n, \tag{25}$$

we can establish that

$$A_{nn}\sum_{j\neq n}\frac{A_{jj}}{(E_n - E_j)} - \dot{\Psi}_n^2(\tilde{R}_0)\sum_{j\neq n}\frac{\Psi_j^2(\tilde{R}_0)}{(E_n - E_j)^3} = -\int_{\tilde{R}_0}^{x_1}\Psi_n^2(r)\,\mathrm{d}r\int_r^{x_1}\frac{\mathrm{d}y}{\Psi_n^2(y)}\int_y^{x_1}\Psi_n^2(z)\,\mathrm{d}z$$
$$= -\int_{\tilde{R}_0}^{x_1}\frac{\mathrm{d}r}{\Psi_n^2(r)}\int_{\tilde{R}_0}^{r}\Psi_n^2(y)\,\mathrm{d}y\int_r^{x_1}\Psi_n^2(z)\,\mathrm{d}z. \tag{26}$$

A special case of the above relation arises if we consider the groundstate with $n = 1$ for which $\tilde{R}_0 = x_0$ and for all the eigenstates $\Psi_j(\tilde{R}_0) = 0$. We thus get the sum rule

$$\sum_{j=2}^{\infty}\frac{1}{(E_1 - E_j)} = -\int_{x_0}^{x_1}\Psi_1^2(r)\,\mathrm{d}r\int_r^{x_1}\frac{\mathrm{d}y}{\Psi_1^2(y)}\int_y^{x_1}\Psi_1^2(z)\,\mathrm{d}z \tag{27}$$

which expresses the inverses of the separation of the eigenvalues of a confining potential from the groundstate eigenvalue in terms of an integral over the nodeless groundstate eigenfunction.

The main results derived in this paper are the relations expressed in equations (9), (11), (12), (15), (16), (23), (26) and (27). In the following sections exactly solvable examples will be used to illustrate the sum rules derived in this section.

3. Examples of sum rules at nodes and extrema

3.1. Particle in a box

In this section we consider the example of a free particle confined in a box with infinite walls at $x_0 = 0$ and $x_1 = \pi$. The normalized eigenfunctions and eigenenergies are given by

$$\Psi_j(r) = \sqrt{\frac{2}{\pi}}\sin jr, \qquad E_j = j^2, \qquad j = 1, 2 \ldots. \tag{28}$$

There is a node of the eigenfunction Ψ_n at $R_0 = \pi(n-1)/n$. We first examine the sum

$$G(r,\tilde{r}) = \frac{2}{\pi}\sum_{j\neq n}\frac{\sin jr\sin j\tilde{r}}{(n^2 - j^2)} \tag{29}$$

which can be simplified using partial fractions, addition formulae for trigonometric functions and standard sums over sine functions [8] to the form

$$G(r,\tilde{r}) = \frac{\sin nr\sin n\tilde{r}}{\pi n}\left(-\frac{1}{2n} + r\cot nr + \tilde{r}\cot n\tilde{r} - \pi\cot nr_>\right), \tag{30}$$

where $r_>$ is the larger of $(r, \tilde{r})$. Using

$$\int_0^{R_0}\Psi_n^2(q)\,\mathrm{d}q = \frac{R_0}{\pi} = \frac{n-1}{n} \tag{31}$$

and

$$\dot{\Psi}_n(R_0) = \sqrt{\frac{2}{\pi}} n \cos(n-1)\pi = (-1)^{n-1} n \sqrt{\frac{2}{\pi}} \tag{32}$$

it is simple to show that for $r = R_0$ equation (30) becomes

$$G(R_0, \tilde{r}) = \frac{\Psi_n(\tilde{r})}{\dot{\Psi}_n(R_0)} \left(\theta(\tilde{r} - R_0) \frac{n-1}{n} - \theta(R_0 - \tilde{r}) \frac{1}{n} \right) \tag{33}$$

thereby verifying equation (10). For the choice $\tilde{r} = R_0 = \pi - \pi/n$ equations (29) and (33) can be used to give

$$\sum_{j \neq n} \frac{\sin^2 jR_0}{(n^2 - j^2)} = 0 \tag{34}$$

verifying equation (11). Equation (33) can be squared and integrated over $\tilde{r}$ to show that

$$\sum_{j \neq n} \frac{\sin^2 jR_0}{(n^2 - j^2)^2} = \frac{\pi^2}{4} \frac{n-1}{n^4} \tag{35}$$

which is the sum rule arising from equation (12) in this case.

We next examine

$$\dot{G}(r, \tilde{r}) = \frac{2}{\pi} \sum_{j \neq n} j \frac{\cos jr \sin j\tilde{r}}{n^2 - j^2} \tag{36}$$

which can be evaluated by taking the derivative of the relation in equation (30) with respect to r. There is an extremum of Ψ_n at $R_1 = \pi - \pi/(2n)$. Hence

$$\dot{G}(R_1, \tilde{r}) = \frac{\sin n\tilde{r}}{\pi} (-R_1 \csc nR_1 + \pi \csc nR_1 \theta(R_1 - \tilde{r})). \tag{37}$$

Using

$$\int_0^{R_1} \Psi_n^2 \, dy = \frac{R_1}{\pi} \tag{38}$$

it can be shown that

$$-\theta(\tilde{r} - R_1) \int_0^{R_1} \Psi_n^2 \, dy + \theta(R_1 - \tilde{r}) \int_{R_1}^{\pi} \Psi_n^2 \, dy = \left(-\frac{R_1}{\pi} + \theta(R_1 - \tilde{r}) \right) \tag{39}$$

which together with equation (37) verifies equation (13) at the last extremum of Ψ_n at R_1. Differentiation of equation (37) with respect to $\tilde{r}$, evaluation at the point $\tilde{r} = R_1$ and use of the completeness relation leads to

$$\frac{2}{\pi} \sum_{j \neq n} j^2 \frac{\cos^2 jR_1}{(n^2 - j^2)} = -\frac{2}{\pi} \sum_j \sin^2 jR_1. \tag{40}$$

It is possible to prove this directly by starting from the equality in equation (30) for $r = \tilde{r}$ and show that for $R_1 = \pi - \pi/(2n)$,

$$\begin{aligned} \frac{\pi}{2} G(R_1, R_1) &= \sum_{j \neq n} \frac{\sin^2 jR_1}{n^2 - j^2} = -\frac{1}{4n^2}, \\ \frac{\pi}{4} \left(\frac{\partial^2}{\partial r^2} G(r, r) \right) \Bigg|_{r=R_1} &= \sum_{j \neq n} \frac{j^2 \cos 2jR_1}{n^2 - j^2} = -\frac{3}{4} \end{aligned} \tag{41}$$

which leads to the relation

$$\sum_{j\neq n}\left(\frac{j^2\cos^2 jR_1}{(n^2-j^2)}+\sin^2 jR_1\right)=-1=-\sin^2 nR_1 \tag{42}$$

thereby verifying equation (15). By squaring equation (37) and integrating over $\tilde{r}$ it can also be shown that

$$\sum_{j\neq n}\frac{j^2\cos^2 jR_1}{(n^2-j^2)^2}=\frac{\pi^2}{16}\frac{2n-1}{n^2} \tag{43}$$

which is the sum rule arising from equation (16) in the present case.

We next examine equation (21) which in this example becomes

$$\Delta=\frac{G(r,r)}{\Psi_n^2(r)}-\frac{G(r_2,r_2)}{\Psi_n^2(r_2)}=\int_{r_2}^{r}\frac{\mathrm{d}y}{\sin^2 y}\left(\int_y^{\pi}\sin^2 nz\,\mathrm{d}z-\int_0^y\sin^2 nz\,\mathrm{d}z\right). \tag{44}$$

Using equation (30) it can be shown that

$$\Delta=\frac{2r-\pi}{2n}\cot nr-\frac{2r_2-\pi}{2n}\cot nr_2 \tag{45}$$

in agreement with the direct evaluation of the integral on the right-hand side of equation (44).

We next examine equation (23) which in this example gives the relation

$$\frac{G(r,r)}{\Psi_n^2(r)}+\frac{G(r_2,r_2)}{\Psi_n^2(r_2)}-2\frac{G(r,r_2)}{\Psi_n(r)\Psi_n(r_2)}=-\frac{\pi}{2}\int_{r_<}^{r_>}\frac{\mathrm{d}y}{\sin^2 y}=\frac{\pi}{2n}(\cot nr_>-\cot nr_<). \tag{46}$$

Using equation (30) to express the various terms on the left-hand side of equation (46) it is easy to check that the sum of the terms on the left-hand side yields the expression on the right-hand side of the equation.

The triple integral on the right-hand side of equation (27) for this example can be evaluated to give

$$\frac{2}{\pi}\int_0^{\pi}\sin^2 x\,\mathrm{d}x\int_x^{\pi}\frac{\mathrm{d}y}{\sin^2 y}\int_y^{\pi}\sin^2 z\,\mathrm{d}z=\frac{3}{4} \tag{47}$$

and using partial fractions it may be shown that

$$\sum_{j=2}^{\infty}\frac{1}{(1-j^2)}=-\frac{3}{4} \tag{48}$$

thus verifying equation (27).

3.2. Simple harmonic oscillator

We consider an oscillator potential $V=x^2$ in the range $[-\infty,\infty]$ corresponding to a frequency $\omega=2$. The oscillator length parameter equals 1 in the units we have used in this paper. The energy levels and the eigenfunctions are given by

$$E_{j+1}=(2j+1),\qquad \Psi_{j+1}=\left(\frac{1}{\pi}\right)^{1/4}\sqrt{\frac{1}{2^j j!}}\exp(-x^2/2)H_j(x),\qquad j=0,1,2,\ldots, \tag{49}$$

where $H_j(x)$ are Hermite polynomials which satisfy

$$\frac{\mathrm{d}H_j}{\mathrm{d}x}=2jH_{j-1}(x),\qquad H_{2j}(0)=(-)^j\frac{(2j)!}{j!},\qquad H_{2j+1}(0)=0. \tag{50}$$

We examine the sum rules arising from the choice $n = 2$ which corresponds to the first excited state which has a single node at $x = 0$. All the antisymmetric states with even values of j vanish at $x = 0$ and the symmetric states corresponding to odd values of j have limiting values at $x = 0$ given by

$$\Psi_{2j+1}^2(0) = \sqrt{\frac{1}{\pi}}\left(\frac{1}{2^{2j}(2j)!}\right)\left(\frac{(2j)!}{j!}\right)^2, \qquad j = 0, 1, \ldots, \tag{51}$$

where the first two factors on the right-hand side arise from the normalization integrals of the harmonic oscillator eigenfunctions [9] and the last factor arises from the values of the even order Hermite polynomials at $x = 0$ [10]. Hence

$$\sum_{j\neq 2}^{\infty} \frac{\Psi_j^2(0)}{E_2 - E_j} = \sqrt{\frac{1}{4\pi}}\left(-\sum_{k=0}^{\infty}\frac{(2k)!}{(2^k k!)^2}\frac{1}{2k-1}\right)$$
$$= \sqrt{\frac{1}{4\pi}}\,\mathrm{Lt}_{z\to 1}\,(1-z)^{1/2} = 0 \tag{52}$$

which verifies equation (11) for $n = 2$.

We next examine

$$\sum_{j\neq 2}^{\infty} \frac{\Psi_j^2(0)}{(E_2 - E_j)^2} = \sqrt{\frac{1}{16\pi}}\sum_{k=0}^{\infty}\frac{(2k)!}{(2^k k!)^2}\frac{1}{(2k-1)^2}$$
$$= \sqrt{\frac{1}{16\pi}}\,\mathrm{Lt}_{z\to 1}(z\arcsin z + (1-z^2)^{1/2}) = \frac{\sqrt{\pi}}{8}. \tag{53}$$

The normalized eigenfunction for $n = 2$ given by

$$\Psi_2(x) = \left(\frac{4}{\pi}\right)^{1/4} x\exp(-x^2/2) \tag{54}$$

can be used to show that

$$\frac{1}{\dot{\Psi}_2^2(0)}\int_{-\infty}^{0}\Psi_2^2\,\mathrm{d}y\int_0^{\infty}\Psi_2^2\,\mathrm{d}z = \frac{\sqrt{\pi}}{8} \tag{55}$$

which when considered together with equation (53) verifies equation (12) for the $n = 2$ first excited state of the simple harmonic oscillator.

To examine the sum rule arising from extrema of eigenfunctions we consider the groundstate $n = 1$ which has an extremum at $x = 0$. For all the symmetric states corresponding to all odd values of j the derivative of the eigenfunction at $x = 0$ vanishes and for the antisymmetric states corresponding to even values of j the derivative at $x = 0$ is given by

$$\dot{\Psi}_{2j}^2(0) = \sqrt{\frac{1}{\pi}}\frac{1}{2^{2j-1}}\frac{1}{(2j-1)!}\left(\frac{(2j)!}{j!}\right)^2, \qquad j = 1, 2, \ldots. \tag{56}$$

Using the values of the eigenfunctions and their derivatives at $x = 0$ given by equations (51) and (56) we can show that

$$\sum_{j\neq 1}\left(\frac{\dot{\Psi}_j^2(0)}{E_1 - E_j} + \Psi_j^2(0)\right) = -\sqrt{\frac{1}{\pi}}\left(\sum_{k=0}^{\infty} - \sum_{k=1}^{\infty}\right)\frac{(2k)!}{(2^k k!)^2}$$
$$= -\sqrt{\frac{1}{\pi}} = -\Psi_1^2(0) \tag{57}$$

thereby verifying equation (15) for the groundstate of the oscillator.

We next consider

$$\sum_{j=2}^{\infty} \frac{\dot{\Psi}_j^2(0)}{(E_1 - E_j)^2} = \sqrt{\frac{1}{4\pi}} \sum_{k=0}^{\infty} \frac{1}{(2^k k!)^2} \frac{(2k)!}{(2k+1)}$$
$$= \sqrt{\frac{1}{4\pi}} \, \mathrm{Lt}_{z\to 1}(\arcsin z) = \sqrt{\frac{\pi}{16}}. \tag{58}$$

It can be shown that for the normalized groundstate eigenfunction

$$\Psi_1(x) = \left(\frac{1}{\pi}\right)^{1/4} \exp(-x^2/2), \qquad \frac{1}{\Psi_1^2(0)} \int_{-\infty}^{0} \Psi_1^2 \, \mathrm{d}y \int_0^{\infty} \Psi_1^2 \, \mathrm{d}z = \frac{1}{4}\sqrt{\pi} \tag{59}$$

which when taken together with equation (58) verifies the sum rule given by equation (16) for the $n = 1$ groundstate of the oscillator.

4. Discussion

In this paper sum rules which must be satisfied at the nodes and extrema of boundstate eigenfunctions of confining potentials have been established. The sum rules in equations (11), (12), (15) and (16) have been verified for the case of a particle confined in a box and also explicitly for the case of a simple harmonic oscillator in the ground or first excited states. However the sum rules are valid for all states of the oscillator and for all confining potentials. When scattering states are present the expressions have to be modified by the addition of an integral to take account of the contribution from the scattering states to the sum over the contribution from the discrete states.

We have shown that in the domain after the last node of an eigenfunction the feature that the inverse of the eigenfunction is singularity free may be used to establish a variety of relations between the values of all the other eigenfunctions in this region and integrals involving the nodeless eigenfunction. We have illustrated the sum rules in equations (23) and (27) for the case of a particle in a box for which the sums and integrals converge and can be carried out analytically. For the harmonic oscillator the sum and integral in equation (27) do not converge.

The antisymmetric wavefunction for two non-interacting identical fermions moving in the same single particle potential V such that one of them is in the state Ψ_n and the other in Ψ_j is given by

$$\Phi_{nj}(r_1, r_2) = \sqrt{\tfrac{1}{2}}(\Psi_n(r_1)\Psi_j(r_2) - \Psi_n(r_2)\Psi_j(r_1)). \tag{60}$$

The relationship in equation (23) may also be given in terms of Φ_{nj} in the form

$$\sum_{j\neq n} \frac{\Phi_{nj}^2(r_1, r_2)}{E_n - E_j} = -\frac{1}{2}\Psi_n^2(r_1)\Psi_n^2(r_2) \int_{r_<}^{r_>} \frac{\mathrm{d}y}{\Psi_n^2} \tag{61}$$

which sheds an interesting light on the sum rule in terms of joint probability density of two-particle states.

Supersymmetric quantum mechanics may be used to interpret the integral on the right-hand side of equation (26). If we consider a potential $\tilde{V}$ which is identical to V in the region outside the last node of Ψ_n at $\tilde{R}_0$ but has an infinite wall at the last node, then the boundstate solutions in $\tilde{V}$ must vanish at $r = \tilde{R}_0$ and as $r \to x_1$. The groundstate energy of $\tilde{V}$ must be $\tilde{E}_1 = E_n$ because Ψ_n goes to zero at $r = \tilde{R}_0$ and as $r \to x_1$ but has no nodes inbetween. Ψ_n is the groundstate eigenfunction of $\tilde{V}$ but has to be renormalized to 1 in the region $[\tilde{R}_0, x_1]$. Let the other boundstate eigenvalues of $\tilde{V}$ satisfying boundstate boundary conditions at $\tilde{R}_0$

and x_1 be $\tilde{E}_j$, $j = 2, 3, \ldots$. A supersymmetric partner to the potential $\tilde{V}$ constructed by the elimination of its groundstate at $\tilde{E}_1 = E_n$ is

$$\tilde{V}_1 = \tilde{V} - \frac{d^2}{dr^2} \ln \Psi_n(r), \qquad r > \tilde{R}_0, \tag{62}$$

which is free of singularities for $r > \tilde{R}_0$. This construction which is based on the methods of supersymmetric quantum mechanics [11] guarantees that the boundstate spectrum of $\tilde{V}_1$ is identical to that of $\tilde{V}$ except for missing the groundstate of $\tilde{V}$ at $\tilde{E}_1$ (i.e.) $\tilde{V}_1$ has spectrum $\tilde{E}_j$, $j = 2, 3, \ldots$. It may be shown that a solution at the energy E_n in $\tilde{V}_1$ is $\tilde{\Phi} = 1/\Psi_n$. From this solution two other solutions which satisfy boundary conditions at $\tilde{R}_0$ and x_1 can be constructed in the form

$$\begin{aligned} \tilde{\Phi}_1 &= \frac{1}{\Psi_n(r)} \int_{\tilde{R}_0}^{r} \Psi_n^2(y)\, dy, \qquad \mathrm{Lt}_{r\to\tilde{R}_0} \tilde{\Phi}_1(r) \to 0, \\ \tilde{\Phi}_2 &= \frac{1}{\Psi_n(r)} \int_{x_1}^{r} \Psi_n^2(y)\, dy, \qquad \mathrm{Lt}_{r\to x_1} \tilde{\Phi}_2(r) \to 0 \end{aligned} \tag{63}$$

with the Wronskian

$$W = \tilde{\Phi}_1 \frac{d}{dr}\tilde{\Phi}_2 - \tilde{\Phi}_2 \frac{d}{dr}\tilde{\Phi}_1 = \int_{\tilde{R}_0}^{x_1} \Psi_n^2(y)\, dy. \tag{64}$$

These solutions may be used to construct a Green's function for the potential $\tilde{V}$ given by

$$\tilde{G}_1(r, \tilde{r} > r) = \frac{\tilde{\Phi}_1(r)\tilde{\Phi}_2(\tilde{r})}{W}, \qquad \mathrm{Lt}_{r\to\tilde{R}_0} \tilde{G} \to 0, \qquad \mathrm{Lt}_{\tilde{r}\to x_1} \tilde{G} \to 0 \tag{65}$$

and $\tilde{G}_1(r, \tilde{r}) = \tilde{G}_1(\tilde{r}, r)$. The trace of this Green's function [3] is related to the spectrum of $\tilde{V}_1$ by

$$\int_{\tilde{R}_0}^{x_1} \tilde{G}_1(r, r)\, dr = \frac{1}{W} \int_{\tilde{R}_0}^{x_1} \frac{dr}{\Psi_n^2} \int_{\tilde{R}_0}^{r} \Psi_n^2\, dy \int_{x_1}^{r} \Psi_n^2\, dz = \sum_{j\neq 1} \frac{1}{E_n - \tilde{E}_j}. \tag{66}$$

Using equations (60), (61), (64) and (66) it may be shown that

$$\begin{aligned} \sum_{j\neq n} \frac{1}{E_n - E_j} \int_{\tilde{R}_0}^{x_1} \int_{\tilde{R}_0}^{x_1} \Phi_{nj}^2(r_1, r_2)\, dr_1\, dr_2 &= W \int_{\tilde{R}_0}^{x_1} \tilde{G}_1(r, r)\, dr \\ &= \left(\int_{\tilde{R}_0}^{x_1} \Psi_n^2(y)\, dy \right) \sum_{j\neq 1} \frac{1}{E_n - \tilde{E}_j} \end{aligned} \tag{67}$$

expressing the trace of Green's function for the supersymmetric partner potential $\tilde{V}_1$ with the energy spectrum ($\tilde{E}_j$, $j = 2, 3, \ldots$) in terms of two-particle densities in the potential V with the energy spectrum (E_j, $j = 1, 2, \ldots, n, \ldots$).

We conclude by reiterating that the sum rules expressed in equations (11), (12), (15) and (16) must be satisfied at all the nodes and extrema of the boundstate eigenfunctions of confining potentials in one dimension. Also the sum rule in equation (23) for confining potentials is a key result derived in this paper. As noted before it is possible to extend the sum rule to potentials which have scattering states by the addition of an additional integral to include the contribution from the scattering states in addition to the contribution from the discrete states which are included in equation (23). We have focused attention on confining potentials because of the existence of exactly solvable problems for which the sum rules can be explicitly verified. We have verified the sum rules for two exactly solvable confining potentials. We have interpreted one of the sum rules using the notion of two particle densities and established a connection with the trace of Green's function of a supersymmetric partner in supersymmetric quantum mechanics.

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