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Sum rules for zeros and intersections of Bessel functions from quantum mechanical perturbation theory

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ABSTRACT

Bessel functions play an important role for quantum states in spherical and cylindrical geometries. In cases of perfect confinement, the energy of Schrödinger and massless Dirac fermions is determined by the zeros and intersections of Bessel functions, respectively. In an external electric field, standard perturbation theory therefore expresses the polarizability as a sum over these zeros or intersections. Both non-relativistic and relativistic polarizabilities can be calculated analytically, however. Hence, by equating analytical expressions to perturbation expansions, several sum rules for the zeros and intersections of Bessel functions emerge.

1. Introduction

Bessel functions are ubiquitous in mathematical physics [1,2]. In particular, they arise as solutions to wave equations in cylindrical and spherical geometries. In non-relativistic quantum mechanics, the solutions to the Schrödinger equation in cylinders and spheres are ordinary $J_p(x)$ and spherical $j_p(x)$ Bessel functions, respectively. Moreover, in the case of perfect (infinite barrier) confinement, the eigenvalues are squares of zeros λ of Bessel functions, i.e. arguments for which $J_p(\lambda)=0$, see e.g. [3,4]. In relativistic quantum mechanics, a related situation arises. Here, spinor eigenfunctions are expressed in terms of Bessel functions. In the general case, the boundary condition is quite complicated [5]. For massless Dirac fermions, however, perfect confinement leads to a boundary condition in terms of intersections κ [6–8], i.e. arguments for which $J_p(\kappa)=\pm J_{p+1}(\kappa)$.

In many quantum mechanical problems, an approximate solution can be found using perturbation theory, which typically results in a sum-over-states expression for the desired quantity. Thus, in problems defined by a total Hamiltonian $H=H_0+H_1$, where H_1 is a "small" perturbation, an approximate solution is found by expanding the full wave function in the set formed by the unperturbed eigenstates $\psi_n^{(0)}$ given by $H_0\psi_n^{(0)}=E_n^{(0)}\psi_n^{(0)}$. In certain cases, however, an exact solution to low order in H_1 can be found using e.g. Dalgarno–Lewis [9] or logarithmic [10] perturbation theory. For instance, consider an inversion-symmetric system subjected to an odd-parity perturbation. The prototypical example of this would be an atom in the presence of a constant electric field oriented along the x-axis $\vec{F}=F\hat{x}$ leading to a perturbation $H_1=Fx$. By symmetry then, non-degenerate unperturbed states have definite parity and the first order correction to the eigenvalue vanishes. A first-order correction $\psi_n^{(1)}$ to the wave function exists, however, and is governed by the inhomogeneous equation $(H_0-E_n^{(0)})\psi_n^{(1)}=-H_1\psi_n^{(0)}$ obtained by collecting first order terms. For static perturbations, the first order wave function provides exact second order energies $E_n^{(2)}=\langle\psi_n^{(1)}|H_1|\psi_n^{(0)}\rangle$. Similarly, perturbation by a time-harmonic electric field yields the frequency dependent polarizability of the system. The "exact" Dalgarno–Lewis and logarithmic perturbation theories [9,10] are based on finding exact solutions to the first order problem and, in turn, deriving exact second order quantities from such solutions.

The present work explores the possibility of finding new sum rules for Bessel function zeros λ and intersections κ by applying quantum mechanical perturbation theory. Several sum rules for the zeros are already known [4,11–16] but, to the knowledge of the present author, none exist for the intersections. We consider problems, in which energies and matrix elements of unperturbed states are expressible in terms of Bessel zeros or intersections in non-relativistic and relativistic theories, respectively. For problems that are, in fact, exactly

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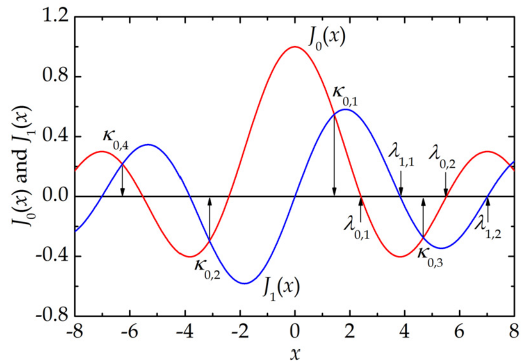

Fig. 1. Zeros of $J_0(x)$ and $J_1(x)$ as well as intersections, for which $J_0(x) = J_1(x)$.

solvable, equating sum-over-states and exact solutions leads to new mathematical identities for λ and κ. Specifically, in the non-relativistic case, we consider the response of an electron in a D dimensional quantum well to a time-harmonic electric field. Here, the exact frequency (ω) dependent solution for the first order wave function and polarizability $\alpha(\omega)$ is known [17]. By Taylor expanding $\alpha(\omega)$ and examining the coefficients of different powers of ω, an infinite set of sum rules for the Bessel zeros are derived. In the relativistic case, we consider massless Dirac fermions confined to a two-dimensional disk. Here, perturbation by a static electric field leads to an exactly solvable problem for arbitrary angular momentum [18]. Hence, sum rules for intersections between consecutive Bessel function J_p and J_{p+1} are found.

Below, we take $\lambda_{p,n}$ to be the n-th positive zero of $J_p(x)$ with p real but not necessarily integer. Also, $\kappa_{p,n}$ is the n-th intersection between $J_p(x)$ and $J_{p+1}(x)$ such that $J_p(\kappa_{p,n}) = J_{p+1}(\kappa_{p,n})$ for p integer. Both positive and negative intersections exist and we order them by the index n according to increasing absolute value. As an example, the cases $p = 0, 1$ are illustrated in Fig. 1.

2. Massive Schrödinger fermions

We start by considering the non-relativistic Schrödinger scenario for a D-dimensional sphere with perfect confinement. Physically, the Bessel function index p is related to the space dimension D by $p = D/2 - 1$. In the present section, we restrict attention to states with vanishing angular momentum. Using a radial coordinate r normalized by the particle radius a, the functions $r^{-p} J_p(\lambda_{p,n} r)$ are then the (un-normalized) radial eigenfunctions of a D-dimensional quantum well [17]. In addition, the eigenvalues are $E^{(0)}_{p,n} = \lambda^2_{p,n}$.

A number of sum rules for $\lambda_{p,n}$ involving only a single value of p are known including the result by Calogero [11]

$$\sum_{\substack{m=1 \\ m\neq n}}^{\infty} \frac{\lambda^2_{p,n}}{\lambda^2_{p,m} - \lambda^2_{p,n}} = \frac{p+1}{2}, \tag{1}$$

as well as sums with higher inverse powers $(\lambda^2_{p,m} - \lambda^2_{p,n})^{-2}$ and $(\lambda^2_{p,m} - \lambda^2_{p,n})^{-3}$ derived by Ahmed and Calogero [12]. These sum rules all concern the (difference between) squares of zeros $\lambda^2_{p,n}$. Explicit expressions for sums of inverse even powers $\lambda^{-2s}_{p,m}$ with s integer are given by Elizalde et al. [4] and the relation to the zeta function was discussed by Actor and Bender [13]. In addition, a result by Baricz et al. [14] involves the fourth power

$$\sum_{\substack{m=1 \\ m\neq n}}^{\infty} \frac{\lambda^4_{p,n}}{\lambda^4_{p,m} - \lambda^4_{p,n}} + \frac{1}{2}\sum_{m=1}^{\infty} \frac{\lambda^2_{p,n}}{\lambda^2_{p,m} + \lambda^2_{p,n}} = \frac{p+2}{4}. \tag{2}$$

All of these results are restricted to relations between zeros of a single Bessel function $J_p(\lambda_{p,n} r)$. In contrast, the results of the present work all involve zeros and intersections of two consecutive orders i.e. J_p and J_{p+1}. Afanasiev [15] derived a number of results for zeros in this case including the analogy of the Calogero sum rule

$$\sum_{m=1}^{\infty} \frac{\lambda^2_{p,n}}{\lambda^2_{p+1,m} - \lambda^2_{p,n}} = p+1. \tag{3}$$

While validity was claimed only for integer and half-integer p, this result as well as others in Ref. [15] appears to be valid for general p. We will comment on the relation between the results of the present work and those of Ref. [15] below. Sums of the type $\sum_m (\lambda^s_{p,m} J_{p+1}(\lambda_{p,m}))^{-1}$ considered in Ref. [16] also relate J_p and J_{p+1}. Finally, we note that analytic sum rules for Bessel *functions* exist [19] but these appear to be of little use for zeros and intersections of these functions.

Perturbation by a time dependent electric field $F\cos(\omega t)$ induces new frequency components in the wave function [17]. The induced dipole moment is calculated from the perturbed wave function and, in turn, the exact frequency dependent polarizability of the state (p, n) is given by [17]

$$\alpha_{p,n}(\omega) = -\frac{4\alpha_0}{\omega^2}\left\{1 + \frac{2\lambda^2_{p,n}}{(p+1)\omega^2}\left(\frac{\sqrt{\lambda^2_{p,n}+\omega}\, J_p(\sqrt{\lambda^2_{p,n}+\omega})}{J_{p+1}(\sqrt{\lambda^2_{p,n}+\omega})} + \frac{\sqrt{\lambda^2_{p,n}-\omega}\, J_p(\sqrt{\lambda^2_{p,n}-\omega})}{J_{p+1}(\sqrt{\lambda^2_{p,n}-\omega})}\right)\right\}. \tag{4}$$

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