SOME USEFUL TECHNIQUES IN BOUND STATE THEORY AND QUANTUM DISCONTINUITY PHENOMENON

by

TESFAYE KOROTO

A THESIS SUBMITTED IN PARTIAL FULFILLMENT FOR THE DEGREE OF MASTER OF SCIENCE IN PHYSICS IN THE ADDIS ABABA UNIVERSITY

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ABSTRACT

This study is broadly divided into two parts.

The first deals with a set of useful results in non-relativistic quantum mechanics that prove to be useful in a variety of contexts. Although elementary, they have remained obscure for a long time. The advent of quarkonium spectroscopy has basically revealed their importance.

The second part considers the quantum discontinuity phenomenon. Its origin is carefully traced. Two original partially exactly solvable models are proposed that exhibit such a phenomenon.

CONTENTS

PROLOGUE

Non-relativistic quantum mechanics has been the basis of our understanding of physics at the micro level. In a wide variety of situations, such as in atomic and condensed matter physics it, indeed, provides the correct description of physical reality. More often than not problems can not be solved exactly. Frequently, we do not quite know what are the precise interactions involved in various situations. In such cases, coupled with rich mathematical techniques and theorems plus semi-classical and intutive reasoning one can still recover a working description of the problem in hand. Although our comprehension of relativistic system is not equally advanced, Schrodinger theory, in the form of the binding limiting situation, provides a valuable guide towards further progress. In field theory, scattering theory, nuclear and sub-nuclear physics where exact forces are hard to pin point this limiting knowledge comes in very handy.

The developments in particle physics that began in the seventies has left non-relativistic quantum mechanics with an enhanced role. We now believe that hadrons are bound states of quarks. Mesons are bound states of a $q\bar{q}$ type where q could be one of the six possible varieties of quarks. It seems that the new mesons can be thought of as such bound states with the quarks moving non-relativistically. Much as we approach the positronium problem, we can approach the $q\bar{q}$ problem. However, the relevant potential function is not clear. But based on the data on masses, life times, decay modes, etc. one can often try to establish classes of potentials that can be relevant. The outcome has been a reapraisal of established techniques and an effort towards finding new applications of such techniques. Thus, one now finds that elementary quantum mechanical results like the Feynmann-Hellmann theorem and the Virial theorem can have very powerful consequences. A major aim of this work is to present a study of such techniques and combine them with the notion of scaling, sum rules, general normalization techniques and the intimate relationships between seemingly unrelated binding potentials. The first four chapters are devoted to techniques of such a general nature in non-relativistic quantum mechanics.

As mentioned earlier, approximation techniques occupy a very central place in quantum mechanics. A very important and valuable such technique is bound state perturbation theory. Basic to it is the assumption of the existence of a suitable small parameter expansion. The vital and natural inquiry relates to the validity of such expansions. Such studies have led to the realization that sometimes energy can be a discontinuous function of such parameters. If that happens, the system can display what is known as quantum discontinuity. Quantum discontinuity models have been studied to a limited extent analytically and more readily via numerical means. The second major aim of this work is to propose some original and analytically solvable models of such a phenomenon. Chapter 5 is devoted to such a study.

CHAPTER 1

THE FEYNMANN-HELLMANN AND VIRIAL THEOREMS AND THEIR APPLICATIONS[1]

In this chapter we discuss theFeynmann-Hellmann theorem, the Virial theorem and related theorems which have recently gained a wide-ranging application particularly in the field of quarkonium physics[1]. Additional applications of these theorems will be indicated.

2.1 The Feynmann-Hellmann Theorem[2]

The variation of an energy eigenvalue with respect to a prameter is equal to the expectation value of the variation of the Hamiltonian with respect to that parameter in the corresponding state.

i.e.,

$$\frac{\partial E}{\partial \lambda} = \langle i | \frac{\partial H}{\partial \lambda} | i \rangle \tag{1.1}$$

where λ is any parameter upon which the Hamiltonian depends.

<u>Proof</u>: The time-independent Schrodinger equation is given by

$$H(\lambda) \; | i \rangle = E_i(\lambda) \; | i \rangle \tag{1.2}$$

let

$$\langle i | i \rangle = 1 \tag{1.3}$$

pre-multiplying (1-2) by $\langle i |$ we get

$$\langle i | \; H(\lambda) \; | i \rangle = E_i(\lambda) \tag{1.4}$$

differentiating this with respect to λ yields:

$$\langle \frac{\partial i}{\partial \lambda} | H(\lambda) \; | i \rangle + \langle i | \frac{\partial H}{\partial \lambda} | i \rangle + \langle i | H | \frac{\partial i}{\partial \lambda} \rangle = \frac{\partial E_i}{\partial \lambda} \tag{1.5}$$

Using (1-2) this reduces to

$$E_i \{ \langle \frac{\partial i}{\partial \lambda} | i \rangle + \langle i | \frac{\partial i}{\partial \lambda} \rangle \} + \langle i | \frac{\partial H}{\partial \lambda} | i \rangle = \frac{\partial E_i}{\partial \lambda} \qquad (1.6)$$

or

$$E_i \frac{\partial}{\partial \lambda} \langle i | i \rangle + \langle i | \frac{\partial H}{\partial \lambda} | i \rangle = \frac{\partial E_i}{\partial \lambda}$$

Using (1-3) this reduces to

$$\frac{\partial E_i}{\partial \lambda} = \langle \frac{\partial H}{\partial \lambda} \rangle_i \qquad (1.1).$$

This proves the theorem.

Applications:

(a) Consider a two body interaction in which the potential energy is central and is independent of the reduced mass(μ).

i.e.,
$$H(\mu) = T(\mu) + V(r) \qquad (1.7)$$
$$= - \frac{\hbar^2}{2\mu} \nabla^2 + V(r)$$

differentiating this with respect to μ we get

$$\frac{\partial H}{\partial \mu} = - \frac{1}{\mu}(- \frac{\hbar^2}{2\mu} \nabla^2) = - \frac{1}{\mu} [H(\mu) - V(r)] \qquad (1.8)$$

using (1-1) this yields

$$\frac{\partial E_i}{\partial \mu} = - \frac{1}{\mu}(E_i - \langle V(r) \rangle_i) = - \frac{\langle T \rangle_i}{\mu} < 0 \qquad (1.9)$$

This is a result which could have been anticipated. It shows that an energy level decreases as the reduced mass increases.

(b) Consider a monotonically increasing potential

$$V'(r) \geq 0, \quad r \geq 0 \qquad (1.10)$$

The classical turning point is given by

$$V(r_c) = E \tag{1.11}$$

therefore,

$$\frac{\partial E}{\partial \mu} < 0 \implies \frac{dV(r_c)}{dr_c} \frac{\partial r_c}{\partial \mu} < 0$$

in reference to (1.9) this yields:

$$\frac{\partial r_c}{\partial \mu} < 0 \tag{1.12}$$

which is an obvious result that reveals that the classical turning point decreases as the reduced mass increases.

(c) Killingbeck[3] uses the Feynmann-Hellmann theorem to calculate some useful expectation values. He considers a one dimensional anharmonic oscillator problem.

i.e.,

$$-D^2\psi + \mu x^2\psi + \lambda x^{2m}\psi = E\psi \tag{1.13}$$

where m is a positive integer

using (1.1) this gives

$$\langle\psi_n | x^2 | \psi_n\rangle = \frac{\partial E_n}{\partial \mu} \tag{1.14}$$

He argues that the use of this theorem for numerical calculations of such expectation values has advantage over methods used prior to this. (Earlier methods connect different energy levels). Varying the reduced mass by a small amount Δ, i.e., $\mu \pm \Delta$, $\mu \pm 2\Delta$, etc. a good estimate to the variation of an energy eigenvalue with respect to the reduced mass could be obtained, giving rise to a good estimate of the expectation value of (1.14). He employs a general eigenvalue equation of the form

$$F(E,\mu,\lambda) = 0 \tag{1.15}$$

with which

$$\langle x^2 \rangle = - \frac{(\partial F/\partial \mu)_E}{(\partial F/\partial E)_\mu} \tag{1.16}$$

Further applications of this theorem will be indicated in the sequel.

2.2 The Virial Theorem and Related Theorems[1,4]

In classical mechanics, for motion in a bounded region of space, if the potential energy is a homogeneous function (of degree k) of the coordinates, and if the kinetic energy is a quadratic function of velocities, a simple relation holds between the time averages of these quantities.

i.e.,

$$2\bar{T} = k\bar{V} \tag{1.17}$$

In this section we derive a general relation from which a quantum analogue of the classical virial theorem and some other theorems will be deduced.

Consider the reduced radial Shrodinger equation

$$\frac{\hbar^2}{2\mu} u''(r) + \{E-V(r) - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\}u(r) = 0 \tag{1.18}$$

where u(r) satisfies

$$\int_0^\infty [u(r)]^2 dr = 1,\ u(r) = rR(r),\ \psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_\ell^m(\theta,\phi)$$

Equation (1.18) could be conviniently rewritten as:

$$-u''(r) = L(r)\ u(r) \tag{1.19}$$

where

$$L(r) = \frac{2\mu}{\hbar^2}\{E - V(r) - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\} \tag{1.20}$$

Multiplying (1.19) by $r^q u'(r)$ and integrating from o to ∞ (where q is to be chosen as is required), we get:

$$-\int_0^\infty r^q u'(r)u''(r)dr = \int_0^\infty r^q u'(r)L(r)u(r)dr \tag{1.21}$$

using $u''(r)u'(r) = \frac{1}{2}\frac{d}{dr}[u'(r)]^2$ and $u(r)u'(r) = \frac{1}{2}\frac{d}{dr}[u(r)]^2$ in this, we obtain:

$$- r^q[u'(r)]^2 \Big|_0^\infty + q\int_0^\infty r^{q-1}[u'(r)]^2 dr =$$

$$= r^q L(r)[u(r)]^2 \Big|_0^\infty - q\int_0^\infty r^{q-1}[u(r)]^2 - \int_0^\infty r^q\, L'(r)[u(r)]^2 dr \tag{1.22}$$

Partially integrating the left-hand side of (1.22) using $d[u(r)u'(r)] = \{[u'(r)]^2 + u(r)u''(r)\}dr$ and omitting the upper limit contributions of the integrated terms, which vanishes for bound state problems, we obtain

$$r^q[u'(r)]^2 \Big|_0 - qr^{q-1}u(r)u'(r)\Big|_0 + q\int_0^\infty r^{q-1}\, L(r)[u(r)]^2 dr$$

$$- q(q-1)\int_0^\infty r^{q-2}u(r)u'(r)dr =$$

$$= r^q u(r)u''(r)\Big|_0 - \langle q\, r^{q-1}\, L(r) + r^q\, L'(r)\rangle \tag{1.23}$$

Integrating the last term of the left-hand-side of this by parts, we obtain:

$$\{r^q[u'(r)]^2 - qr^{q-1}u(r)u'(r) - \frac{q(q-1)}{2}r^{q-2}[u(r)]^2 - r^q u(r)u''(r)\}\Big|_{r=o}$$

$$= -\langle 2qr^{q-1}\, L(r) + r^q L'(r) + \frac{q(q-1)(q-2)}{2}r^{q-3}\rangle \tag{1.24}$$

To evaluate the left-hand-side of this we use

$$u_\ell(r) \xrightarrow[r \to 0]{} a_\ell r^{\ell+1} \tag{1.25}$$

and (1.24) takes the form

$$(2\ell+1)a_\ell^2\ \delta_{q;2\ell} = -\ \langle 2qr^{q-1}L(r)+r^q\ L'(r) + \frac{q(q-1)(q-2)}{2}\ r^{q-3}\rangle \qquad (1.26)$$

This is the required generalized virial theorem. It holds for $q \geq -2\ell$, because for $q < -2\ell$ the integrated terms diverge at the origin.

In what follows, we shall see some important relations derivable from (1.26) and some applications of these relations would be indicated.

(a) If we set $q = \ell = o$ in (1.26) we obtain

$$a_o^2 = -\ \langle L'(r)\rangle = \frac{2\mu}{\hbar^2}\langle\frac{dV}{dr}\rangle \qquad (1.27)$$

making use of $u'(o) = R(o)$, $u_\ell(r) \to (\ell+1)a_\ell r^\ell$ for $r \to o$ and $R(o) = \sqrt{4\pi}\ \psi_{100}\ (o)$, the following expression for the ground state wave-function at the origin is obtained from (1.27).

$$|\ \psi_{100}\ (o)|^2 = \frac{\mu}{2\pi\hbar^2}\langle\frac{dV}{dr}\rangle \qquad (1.28)$$

(b) Choosing $q = 1$, $\ell \neq q$ Eq.(1.26) yields

$$2\langle L(r)\rangle = -\ \langle r\,L'(r)\rangle \qquad (1.29)$$

using (1.20) this reduces to

$$E - \langle V(r)\rangle = \langle T\rangle = \frac{1}{2}\langle r\ \frac{dV}{dr}\rangle \qquad (1.30)$$

This is the quantum mechanical analogue of the classical virial theorem. We now come to mention some of its applications.

For power-law potentials, i.e.,

$$V(r) = \lambda r^{\nu} \tag{1.31}$$

equation (1.30) gives

$$\langle V(r) \rangle = \frac{2E}{\nu+2}$$

or,

$$\langle T \rangle = \frac{\nu E}{\nu+2} \tag{1.32}$$

For a linear potential this yields:

$$\langle r \rangle = \frac{1}{\lambda} \langle v \rangle = \frac{2}{3\lambda} E \tag{1.33}$$

Choosing $q = 2$, $\ell \neq q$ in Eq.(1.26) the following relation for Coulomb potentials is obtained

$$\langle r \rangle = \frac{3\lambda}{4E} + \frac{\ell(\ell+1)\hbar^2}{4\mu E} \langle \frac{1}{r} \rangle \tag{1.34}$$

using (1.30) this reduces to:

$$\langle r \rangle = \frac{3}{2\langle r^{-1} \rangle} + \frac{\ell(\ell+1)\hbar^2}{2\mu\lambda} \tag{1.35}$$

For other choices of q spatial moments of higher order could be obtained in terms of those already found, and it is possible to find the coefficients a_ℓ for linear potential and Coulomb potential using (1.26).

In some recent papers of A.K. Common[5] and A. Khare[6] theorems of this section are used to prove theorems giving bounds to the kinetic energy of a quarkonium system and mass dependence of the Hamiltonian of a quarkonium system respectively.

(a) If m is the common mass of quark-antiquark and if T(m) is the kinetic energy of the quarkonium system with suffixes corresponding to the particular state the system is in, the following theorems give bounds to the kinetic energy of any state of a quarkonium system.

Theorem[5a]

i) $T(m) \leq \frac{1}{2} \langle \frac{dV}{dr} \rangle \langle r \rangle$, if $\frac{d^2V}{dr^2} \leq 0$, $r > 0$

$$\text{ii)}\quad T(m) \leq \frac{1}{2} \langle \frac{dV}{dr} \rangle \frac{\langle r^2 \rangle}{\langle r \rangle}, \quad \text{if } \frac{d}{dr}\left(r\frac{dV}{dr}\right) \leq 0,\ r > 0 \tag{1.36}$$

iii) $T(m) \geq \frac{1}{2} \langle \frac{dV}{dr} \rangle \frac{\langle 1/r \rangle}{\langle 1/r^2 \rangle}$, if $\frac{d}{dr}\left(r^2\frac{dV}{dr}\right) \geq 0$, $r > 0$

Proof: Using the virial theorem:

$$T(m) = \frac{1}{2} \int_0^\infty r\, u^2(r)\, \frac{dV}{dr}\, dr \tag{1.37}$$

we have:

$$\langle r \rangle \langle \frac{dV}{dr} \rangle - 2T(m) = \int_0^\infty [\langle r \rangle - r] u^2(r) \frac{dV}{dr}\, dr \tag{1.38}$$

partially integrating this, using $\psi = \frac{dV}{dr}$,

$d\phi = [\langle r \rangle - r]u^2(r)dr$, we obtain:

$$\langle r \rangle \langle \frac{dV}{dr} \rangle - 2T(m) = - \int_0^\infty \int_0^r [\langle r \rangle - r'] u^2(r')dr' \frac{d^2V}{dr^2}\, dr \tag{1.39}$$

We know that $\int_0^r [\langle r \rangle - r']u^2(r')dr' \xrightarrow[r \to \infty]{} 0$ and is non-negative for small r. Therefore (1.36)(i) is proved.

Similarly,

$$\langle r^2\rangle\langle\frac{dV}{dr}\rangle - 2T(m)\langle r\rangle = \int_0^\infty [r\langle r^2\rangle - \langle r\rangle r]u^2(r)\left(\frac{1}{r}\frac{dV}{dr}\right)dr$$

$$= \int_0^\infty\int_0^r [r'\langle r^2\rangle - \langle r\rangle r']u^2(r')dr'\frac{d}{dr}\left(\frac{1}{r}\frac{dV}{dr}\right)dr \qquad (1.40)$$

and with a similar argument (1.36)(ii) could be easily proved. To prove (1.36)(iii), we use:

$$\langle\frac{1}{r}\rangle\langle\frac{dV}{dr}\rangle - 2T(m)\langle\frac{1}{r^2}\rangle = \int_0^\infty \left[\frac{1}{r^2}\langle\frac{1}{r}\rangle - \frac{1}{r}\langle\frac{1}{r^2}\rangle\right]u^2(r)\left(r^2\frac{dV}{dr}\right)dr$$

partially integrating this reduces to

$$\langle\frac{1}{r}\rangle\langle\frac{dV}{dr}\rangle - 2T(m)\langle\frac{1}{r^2}\rangle = \int_0^\infty\int_0^r \left[\frac{1}{r'}\langle\frac{1}{r^2}\rangle - \frac{1}{r'^2}\langle\frac{1}{r}\rangle\right]u^2(r')dr'\frac{d}{dr}\left(r^2\frac{dV}{dr}\right)dr \qquad (1.41)$$

It could be verified that the integration over r' yields a negative value for small r. With this the proof of (1.36)(iii) follows easily.

(b) In [5b], simple bounds relating T_{1s} and $|u_{1s}(o)|$ are derived, where $u_{1s}(r)$ satisfies $|u_{1s}'(r)| \leq |u_{1s}'(o)|$ for $\frac{dV}{dr} \geq o$. If $u_{1s}^2(r)$ has a unique maximum at $r = r_3$, then $u_{1s}'(r) > o$ for $r < r_3$ and $u_{1s}'(r) < o$ for $r > r_3$. Hence,

$$\int_{r_3}^\infty u_{1s}'^2(r)dr \leq u_{1s}'(o)\int_{r_3}^\infty u_{1s}'(r)\,dr = -u_{1s}'(o)\int_{r_3}^\infty u_{1s}'(r)dr \qquad (1.42)$$

The final result follows from $u_{1s}(o) = o$, $u_{1s}(r) \xrightarrow[r\to\infty]{} o$ and $u_{1s}(r)$ is positive in the range of integration. Using $\frac{d}{dr}u_{1s}(r)\,dr =$ $= \frac{d}{dr}\{[u_{1s}^2(r)]^{\frac{1}{2}}\}\,dr = \{\frac{d}{dr}u_{1s}^2(r)\}^{\frac{1}{2}}\,dr$, we get:

$$\int_{r_3}^{\infty} u_{1s}'^2(r)dr \le u_{1s}'(o) \{-2\int_{r_3}^{\infty} u_{1s}'(r)u_{1s}(r)dr\}^{\frac{1}{2}}$$

$$\le 2^{\frac{1}{2}} u_{1s}'(o)[\int_{r_3}^{\infty} dr\, u_{1s}'^2(r)]^{1/4} [\int_{r_3}^{\infty} dr\, u_{1s}^2(r)]^{1/4}$$

Let $\int_o^{r_3} u_{1s}^2(r)\, dr = \beta$, $\int_{r_3}^{\infty} u_{1s}^2(r)dr = 1-\beta$ and follow the same line of argument and we will obtain:

$$T_{1s} = \frac{1}{m}\int_o^{\infty} u_{1s}'^2(r)dr \le \frac{2^{2/3}}{m}[u_{1s}'(o)]^{4/3} (\beta^{1/3} + (1-\beta)^{1/3})$$

or,

$$T_{1s} \le \frac{2^{4/3}}{m} [u_{1s}'(o)]^{4/3} \quad \text{for } \frac{dV}{dr} \ge o \tag{1.43}$$

Similar simpler bounds can be derived in the same way.

(c) A. Khare[6] proves the following theorem for mass independent potential using both the virial theorem and the Feynmann-Hellmann theorem:

<u>Theorem</u>: If $\frac{d^2V}{dr^2} \gtrless 0$, $\frac{dV}{dr} \ge 0$, then

$$\frac{\partial}{\partial m} \{m^{1/3} < T_{1\ell} >\} \lessgtr 0 \tag{1.44}$$

where T is the kinetic energy and 1ℓ is to refer to a state of angular momentum ℓ and with one node in its reduced radial wavefunction $u_\ell(m,r)$ including the origin.

<u>Proof</u>: Using the virial theorem:

i.e.,

$$E(m) = \frac{1}{2}\int_o^{\infty} u^2(mr)[2V(r) + r\frac{dV}{dr}]\, dr \tag{1.45}$$

and the Feynmann-Hellmann theorem

$$\frac{\partial E(m)}{\partial m} = -\frac{1}{2m}\int_0^\infty u^2(m,r)\, r\,\frac{dV}{dr} = -\frac{\langle T\rangle}{m} \tag{1.46}$$

adding these two we get:

$$E + 3m\frac{\partial E}{\partial m} = \frac{1}{2}\int_0^\infty u^2(r)[2V - 2r\frac{dV}{dr}]\, dr \tag{1.47}$$

As we shall see in chapter 3 (sec.3.2), for all nodeless wavefunctions $u_\ell(m,r)$, the function

$$G(r) = \frac{\partial}{\partial m}\int_0^r dr'\, u_{1\ell}^{\,2}(r',m) \tag{1.48}$$

satisfies $\quad G(r) \geq 0$ provided $\frac{dV}{dr} \geq 0$. Hence,

$$\frac{\partial}{\partial m}[E+3m\frac{\partial E}{\partial m}] = -2\frac{\partial}{\partial m}\langle T\rangle_{1\ell} = -3m^{-1/3}\frac{\partial}{\partial m}(m^{1/3}\langle T\rangle_{1\ell})$$

$$= \int_0^\infty G(r)[\frac{d}{dr}(\frac{dV}{dr}) - \frac{dV}{dr}]dr$$

$$= \int_0^\infty G(r)r\frac{d^2V}{dr^2}\, dr$$

$$\lessgtr 0\ , \quad \text{if } \frac{d^2V}{dr^2} \gtrless 0; \quad \frac{dV}{dr} \geq 0 \tag{1.49}$$

which proves the theorem.

The foregoing examples coroborate our emphasis on the application of the theorems of this chapter in recent studies peculiar to quarkonium physics.

CHAPTER 2

QUANTUM MECHANICAL SUM RULES AND BOUND STATE NORMALIZATION[1]

Sum rules and normalization techniques are widely applied in quantum physics. All the associated techniques can not be exhausted in such a study. Therefore, we restrict ourselves to some general remarks on quantum mechanical sum rules and exhibit the derivation of certain classes of sum rules. In this chapter, we also develop an elegant technique of normalizing bound state wavefunctions.

2.1 Quantum Mechanical Sum Rules[1,7]

We make a general remark on the sum of squares of the transition matrix elements of an operator and derivations of sum rules weighted by energy and squares of the transition energy are shown. Moreover, we give a few illustrations of the very powerful and unexpected results of quantum mechanical sum rules.

Given an operator O we easily see that

$$\langle i|OO^{+}|i\rangle = \sum_{\text{all states } n} \langle i|O|n\rangle\langle n|O^{+}|i\rangle = \sum|\langle i|O|n\rangle|^{2} = |\langle i|O|i\rangle|^{2} + \sum_{n\neq i}|\langle i|O|n\rangle|^{2} \tag{2.1}$$

We use (2.1) to derive the following sum rules.

a) Energy weighted sum rules are generated by the double commutator $[[H,O],O^{+}]$, where H is the Hamiltonian. The expectation value of this double commutator in a state $|i\rangle$ is:

$$\langle i|[[H,O],O^+]|i\rangle = \sum_n \{\langle i|[H,O]|n\rangle \langle n|O^+|i\rangle - \langle i|O^+|n\rangle \langle n|[H,O]|i\rangle$$

$$= 2\sum_n (E_i - E_n)\ |\langle i|O|n\rangle|^2\} \tag{2.2}$$

Consider a one-dimensional problem:

$$H = \frac{p^2}{2\mu} + V(x),\ O = O(x) \tag{2.3}$$

the commutator

$$[H,O] = -\frac{i\hbar}{2\mu}\{p\frac{dO}{dx} + \frac{dO}{dx}p\} \tag{2.4}$$

and the double commutator is given by:

$$[[H,O],O^+] = -\frac{\hbar^2}{\mu}\ \frac{dO}{dx} \tag{2.5}$$

Therefore, (2-2) takes the form

$$\langle i||\frac{dO}{dx}|^2|i\rangle = \frac{2\mu}{\hbar^2}\sum (E_n - E_i)\ |\langle i\ |O|n\rangle|^2 \tag{2.6}$$

For $O(x) = x$ (2-6) gives the famous Thomas-Rieche-Khun[8] sum rule which Heisenberg[9] used in developing his commutation relations.

i.e.,

$$\frac{2\mu}{\hbar^2}\ \sum_n\ (E_n - E_i)|\langle i|X|n\rangle|^2 = 1 \tag{2.7}$$

b) Sum rules weighted by the square of the transition energy are generated by $|[H,O]|^2$.

Consider

$$\langle i||[H,O]|^2|i\rangle = \sum_n \langle i|[H,O]|n\rangle\langle n|[H,O]^+|i\rangle = \sum_n (E_i - E_n)^2|\langle i|O|n\rangle|^2 \tag{2.8}$$

For $$0 = x, \quad [H,0]^{2} = \frac{2\hbar^2}{\mu} \, (H-V(x)) \tag{2.9}$$

Therefore, (2.8) reduces to:

$$E_i - \langle V \rangle_i = \frac{\mu}{2\hbar^2} \, \Sigma \, (E_i - E_n)^2 \, |\langle i \mid x \mid n \rangle|^2 \tag{2.10}$$

The right hand side of (2.10) is positive. According to the Feynmann-Hellmann theorem, the left hand side is $-\mu \frac{\partial E_i}{\partial \mu}$. Therefore, $\frac{\partial E_i}{\partial \mu} < 0$, in agreement with (1.9).

Invoking the virial theorem (1-30), (2.10) reduces to:

$$\frac{\mu}{\hbar^2} \sum_n (E_i - E_n)^2 |\langle i|x|n\rangle|^2 = \langle i|xV'|i\rangle \tag{2.11}$$

These examples illusrate some of the interesting consequences of sum rules.

2.2 Bound State Normalization

Quantum mechanical states of a system are vectors in the Hilbert space which are normalizable either to unity or to Dirac's delta function. Therefore, the need of normalizing a state function is obvious. In this section, we develop a technique via which normalization of bound states of a system is easily attained. An illustrative example will also be discussed.

Keeping $2\mu = \hbar^2$, the Schrodinger equation for a symmetric potential in one-dimension could be written as:

$$\phi''(x) + [E-V(x)] \, \phi(x) = 0 \tag{2.12}$$

where $\phi(x)$ is subject to either of the two boundary conditions:

$$\phi(0) = 0, \ \phi'(0) = 1 \quad \text{(odd)} \tag{2.13a}$$

or

$$\phi(0) = 1, \ \phi'(0) = 0 \quad \text{(even)} \tag{2.13b}$$

and

$$\phi(x) \xrightarrow[|x| \to \infty]{} 0.$$ If we write:

$$I = \int_0^\infty [\phi(x)]^2 dx \tag{2.14}$$

the normalized eigenfunction $\psi(x) = a\phi(x)$ could be expressed as:

$$\psi(x) = \frac{1}{2I} \phi(x) \tag{2.15}$$

The foregoing argument on one dimensional symmetric potential problem could be extended to three dimensional central potential problems. The reduced radial wavefunction in three dimensions satisfies boundary condition (2.13a) and its normalization condition is:

$$U(r) = \phi(r)/\sqrt{I} \tag{2.16}$$

According to (1.28) the Schrodinger wavefunction at the origin is given by

$$\psi(0) = u'(o)/\sqrt{4\pi}$$

or

$$|\psi(0)|^2 = \frac{1}{4\pi I} \tag{2.17}$$

The left-hand side of (2.17) is associated with decay width in particle physics. Therefore, (2.17) displays an important application of evaluation of the normalization integral.

To develop our technique, let:

$$\dot{\phi} = \frac{\partial\phi}{\partial E} \tag{2.18}$$

differentiating (2.12) with respect to E yields

$$\dot{\phi}'' + \phi + (E-V)\,\dot{\phi} = 0 \tag{2.19}$$

multiplying (2.12) by $\dot{\phi}$ and (2.19) by ϕ and taking their difference we obtain

$$\phi^2 = \phi''\,\dot{\phi} - \dot{\phi}''\phi = [\dot{\phi}\,\phi' - \dot{\phi}'\,\phi]' \tag{2.20}$$

Therefore, $$I = [\dot{\phi}\,\phi' - \dot{\phi}'\,\phi]\Big|_0^\infty \tag{2.21}$$

With either of the two boundry conditions the contribution at the lower limit is zero. To compute the contribution at infinity let:

$$\phi(x,E) = C_1 f_1(x,E) + c_2 f_2(x,E) \tag{2.22}$$

where $$\lim_{x\to\infty} f_1(x,E) = 0 \tag{2.23}$$

and $$\lim_{x\to\infty} f_2(x,E) = \pm\infty \tag{2.24}$$

The constants C_1 and C_2 depend on energy. For an energy eigenvalue E_n

$$C_2(E_n) = 0 \tag{2.25}$$

and

$$\phi(x,E_n) = C_1(E_n) f_1(x,E_n) \tag{2.26}$$

for large values of x,

$$\bar{\phi}(X,E_n) = \frac{\partial}{\partial E} \{C_2(E)\, f_2(X,E)\}_{E=E_n} \text{ . Thus, } \bar{\phi}(X,E_n) = f_2(X,E_n) \left.\frac{dC_2(E)}{dE}\right|_{E=E_n} \tag{2.27}$$

and

$$I_n = C_1(E_n) \left.\frac{dC_2(E)}{dE}\right|_{E=E_n} W(f_2,f_1) \tag{2.28}$$

where

$$W(f_2,f_1) = f_2 f_1' - f_1 f_2' \tag{2.29}$$

Since the Schrodinger equation does not involve first derivative, the Wronskian is independent of x. This enables us to evaluate the Wronskian in (2.28) for any value of x. We will come shortly to its evaluation. One thing to note is that the product of a diverging function f_2 and f_1, which dies out for large x, gives finite result.

Now, we want to have alternate expressions of (2.28) for even-parity and odd-parity solutions. For even-parity solutions:

$$\phi(0,E) = C_{1e} f_1(0,E) + C_{2e} f_2(0,E) = 1 \tag{2.30}$$

and

$$\phi'(0,E) = C_{1e} f_1'(0,E) + C_{2e} f_2'(0,E) = 0 \tag{2.31}$$

From which

$$C_{1e} = - f_2'(0,E)/W(f_2, f_1) \tag{2.32}$$

and

$$C_{2e} = f_1'(0,E) / W(f_2,f_1) \tag{2.33}$$

Therefore,

$$\frac{dC_{2e}}{dE} = \frac{\partial f_1'(0,E)}{\partial E} \Big/ W(f_2,f_1) - \frac{f_1'(0,E)\frac{\partial W}{\partial E}}{W^2} \qquad (2.34)$$

From (2.33), the vanishing of C_{2e} at an even eigenvalue E_e implies that

$$f_1'(0,E_e) = 0 \qquad (2.35)$$

Therefore,

$$\left.\frac{dC_{2e}}{dE}\right|_{E=E_e} = \left.\frac{\partial f_1'(0,E)}{\partial E}\right|_{E=E_e} \Big/ W(f_2,f_1) \qquad (2.36$$

If we evaluate the Wronskian at the origin for even parity eigenvalues we obtain:

$$W(f_2,f_1) = - f_1(0,E_e)f_1'(0,E_e) \qquad (2.37)$$

Therefore, combining (2.28), (2.32), (2.36) and (2.37) we get:

$$I_e = \left.\frac{\partial f_1'(0,E)}{\partial E}\right|_{E=E_e} \Big/ f_1(0,E_e) \qquad (2.38)$$

which is the normalization integral for even-parity bound state.

Similarly, for odd-parity bound states

$$\phi(0,E) = C_{10}f_1(0,E) + C_{20}f_2(0,E) = 0 \qquad (2.39a)$$

and

$$\phi'(0,E) = C_{10}f_1'(0,E) + C_{20}f_2'(0,E) = 0 \qquad (2.39b)$$

i.e.,
$$C_{10}(E) = f_2(0,E) / W(f_2,f_1) \tag{2.40}$$

$$C_{20}(E) = - f_1(0,E) / W(f_2,f_1) \tag{2.41}$$

and

$$\frac{dC_{20}(E)}{dE} = - \frac{\partial f_1(0,E)}{\partial E} / W + f_1(0,E) \frac{\partial W}{\partial E} / W^2 \tag{2.42}$$

The vanishing of C_{20} at an odd-parity eigenvalue E_o implies that:

$$f_1(0,E_o) = 0 \tag{2.43}$$

and

$$\left.\frac{dC_2(E)}{dE}\right|_{E=E_o} = - \left.\frac{\partial f_1(0,E)}{\partial E}\right|_{E=E_o} / W(f_2,f_1) \tag{2.44}$$

Evaluation of the Wronskian at the origin gives:

$$W(f_2,f_1) = f_2(0,E_o) f_1'(0,E_o) \tag{2.45}$$

Therefore,

$$I_o = - \left.\frac{\partial f_1(0,E)}{\partial E}\right|_{E=E_o} / f_1'(0,E_o) \tag{2.46}$$

As an illustration of the use of the technique we have developed, consider a linear potential

$$V(x) = |x| \tag{2.47}$$

To solve for the Schrodinger equation in the region $(0, \infty)$ it is suitable to cast the equation to a complex plane. The solution to a general second order differential equation

$$w''(z) + p(z)\, w'(z) + q(z)\, w(z) = 0 \qquad (2.48)$$

could be obtained using power series method provided the functions W(z), p(z) and q(z) are regular at a point z_o. The recursion relation one will obtain is:

$$W_{n+2} = - \frac{\{ \sum_{k=o}^{n} p_{n-k}\, w_{k+1}\, (k+1) + \sum_{k=o}^{n} q_{n-k}\, w_k \}}{(n+1)\,(n+2)} \qquad (2.49)$$

where p_i, q_i, w_i are the i^{th} coefficients of the expansion.

The Schrodinger equation corresponding to (3.48), for $2\mu = \hbar^2$ is:

$$\psi''(x) - (x-E)\,\psi(x) = 0 \qquad (2.50)$$

which has the form of Airy's equation

$$w''(z) - zw(z) = 0 \qquad (2.51)$$

Comparing this with (2.48) and (2.49), two independent solutions $w_1(z)$ and $w_2(z)$ could be obtained, where

$$w_1(o) = 1 \;,\; w_1'(o) = 0 \qquad (2.52)$$

$$w_2(o) = 0 \;,\; w_2'(o) = 1 \qquad (2.53)$$

The general solution of this equation is the Airy's function

$$A_i(z) = A_i(o)w_1(z) - A_i'(o)w_2(z) \qquad (2.54)$$

where

$$A_i(o) = 1/3^{2/3}\ \Gamma(\tfrac{2}{3}) \text{ and } A_i'(o) = 1/3^{\frac{1}{3}}\ \Gamma(\tfrac{1}{3}) \qquad (2.55)$$

and it converges for $|z| \to \infty$

Therefore, the damped solution of (2.50) is:

$$f_1(x,E) = A_i(x-E) \qquad (2.56)$$

Referring to (2.35) and (2.43) the energy eigenvalues are specified by the zeros of Airy's function. Namely,

$$A_i'(-E_e) = 0 \quad \text{(for even-parity solutions)} \qquad (2.57)$$

and

$$A_i(-E_o) = 0 \quad \text{(for odd-parity solutions)} \qquad (2.58)$$

Thence, the normalization integral for even parity solutions is:

$$I_e = -\frac{A_i''(-E_e)}{A_i(-E_e)} \qquad (2.59)$$

But

$$A_i''(x-E) - (x-E)\ A_i(x-E) = 0 \qquad (2.60)$$

Therefore,

$$I_e = E_e \qquad (2.61)$$

Similarly,

$$I_o = \frac{A_i'(-E_o)}{A_i'(-E_o)} = 1 \qquad (2.62)$$

From which the probability density at the origin for this potential in three dimensions yields

$$|\psi(o)|^2 = 1/4\pi \tag{2.63}$$

Further applications of this normalization technique will be indicated in Chapter 4.

CHAPTER 3

SCALING PROPERTIES OF THE SCHRÖDINGER EQUATION AND MASS DEPENDENCE OF THE SCHRÖDINGER WAVEFUNCTIONS[1]

A suitable scale of measuring a quantity depends on the system for which that quantity is to be measured. Each problem in quantum mechanics has a scale appropriate to it. For instance, the oscillator length and the Bohr radius are length scales corresponding to the harmonic oscillator and the hydrogen atom problems respectively. While rescaling the Schrodinger equation according to a specific problem the scales of all dynamic variables associated with the problem will change accordingly. Moreover, the wavefunction itself depends on the parameters (such as mass, coupling constant, etc.) involved in the scale of the problem. This chapter is devoted to the scaling properties of the Schrodinger equation, in particular, for power-law potentials and to mass dependence of the Schrodinger wavefunctions.

3.1 Scaling Properties of the Schrodinger Equation

For power-law potentials, the mass dependence of energy levels, distance scales and wavefunctions follow from elementary rescaling operations. In this section, we discuss the scaling properties of such potentials. The logarithmic potential falls into this category because it is a suitably chosen limit of a power-law potential. In addition, the kinetic energy, potential energy and total bound state energy are related in a simple fashion for such potentials.

Consider $$V(r) = \lambda r^{\nu} \quad (-2 < \nu < \infty) \quad \text{(power-law)} \tag{3.1}$$

and $$V(r) = C\ln(r/r_o) \quad \text{(logarithmic)} \tag{3.2}$$

It follows that

$$\frac{\partial}{\partial r'}\Big[\lim_{\substack{\lambda\to\infty \\ \nu\to o}} \lambda r'^{\nu}\Big] = \lim_{\substack{\lambda\to\infty \\ \nu\to o}} \frac{\nu\lambda r'^{\nu}}{r'} \xrightarrow[\nu\lambda = C]{} \frac{C}{r'} \tag{3.3}$$

Integrating this from $r' = r_o$ to $r' = r$ yields:

$$\lim_{\substack{\nu\to o \\ \lambda\to\infty}} [\lambda r^{\nu}]\Big|_{r_o}^{r} = C\ln(r/r_o) \quad (C = \nu\lambda), \tag{3.4}$$

which shows that the logarithmic potential is a limiting case of power-law potential.

From (1.30), the kinetic energy, potential energy and total bound state energy are related as

$$\langle T \rangle = E - \langle V \rangle = \tfrac{1}{2}\langle r\frac{dV}{dr}\rangle = \tfrac{1}{2}\nu\langle V \rangle \tag{3.5}$$

which yields $$\langle T \rangle = \frac{E}{2+\nu} \quad \text{(for power-law)} \tag{3.6}$$

and $$\langle T \rangle = \frac{C}{2} \quad \text{(for logarithmic)} \tag{3.7}$$

To see the mass and coupling strength dependence it is suitable to cast the reduced radial Schrodinger equation:

$$\frac{\hbar^2}{2\mu}u''(r) + [E - \lambda r^{\nu} - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}]u(r) = 0 \tag{3.8}$$

in a dimensionless form. In a dimensional system where C = 1 ([L]=[T], where C is the velocity of light),

$$[\lambda] = [\hbar]^{-\nu} \; [\lambda]^{1+\nu} \tag{3.9}$$

Using a scale transformation

$$\left(\frac{\hbar^2}{2\mu|\lambda|}\right)^{-\frac{1}{2+\nu}} r = \rho \tag{3.10}$$

(such scaling arguments appear in [10-15])

and with
$$u(r) \equiv w(\rho) \tag{3.11}$$

where ρ is a dimensionless variable, Eq.(3.8) takes on the following dimensionless form

$$w''(\rho) + [E - \mathrm{sgn}(\lambda)\,\rho^{\nu} - \frac{\ell(\ell+1)}{\rho^2}]w(\rho) = 0 \tag{3.12}$$

where
$$E = \left(\frac{\hbar^2}{2\mu|\lambda|}\right)^{-2/2+\nu} \left(\frac{\hbar^2}{2\mu}\right) \varepsilon \tag{3.13}$$

$\mathrm{sgn}(\lambda) = \lambda/|\lambda|$, and ε and ρ are dimensionless.

Consequent to (3.10) and (3.13) the dependence of level spacings and quantities involving dimensions of length could be related to the parameters in these equations. From (3.13), level spacings are scaled as:

$$\Delta E \propto \left(\frac{h^2}{2\mu}\right)^{\nu/2+\nu} \; |\lambda|^{2/2+\nu}$$

which indicates that $\Delta E \propto (\frac{\lambda}{\mu})^{\frac{1}{2}}$ for harmonic oscillator and $\Delta E \propto |\lambda|^2 \mu$ - (for Coulomb potential). These results are readily confirmed since the exact solutions to these problems are well known. Similarly, $\Delta E \propto (\lambda^2/\mu)^{1/3}$ for linear potential.

Equation (3.14) indicates that ΔE increases as μ increases, for singular potential and that it decreases as μ increases for non-singular potentials, For pure power-law potential, which is not shifted by coordinate translation, the foregoing results hold for the eigenvalues themselves.

According to (3.10) lengths are scaled as

$$L \propto [\mu |\lambda|]^{-\frac{1}{2+\nu}} \tag{3.15}$$

The probability density at the origin, a quantity of paramount significance in particle physics phenomenology, has dimensions of inverse volume. Its scale is

$$|\psi(o)|^2 \propto (\mu|\lambda|)^{3/2+\nu} \tag{3.16}$$

For a linear potential this yields $|\psi(o)|^2 \propto \mu|\lambda|$, which agrees with Eq.(1.28).

Our scaling argument ensures that the form of (3.16) will not change for any fixed ρ away from the origin. i.e.,

$$|\psi[(\frac{\hbar^2}{2\mu|\lambda|})^{\frac{1}{2}+\nu}\rho]|^2 \propto (\mu|\lambda|)^{3/2+\nu} \tag{3.17}$$

We will come to additional applications of the scaling arguments of this section in Chapter 4.

3.2 Mass dependence of the Schrodinger wavefunctions

An important class of applications concerns the dependence of observables on mass[23]. In this section we shall show that for any potential which is monotonically increasing for $x > o$, the probability that a bound particle lies within a fixed distance from the origin is an increasing function of μ. Or, the probability flows inward across any arbitrarily chosen boundary when μ is increased. Probability also flows inward when the potential strength is increased. We start with one dimensional symmetric potential and make the usual extension to the three dimensional central potential. In terms of the wavefunction u(x), normalized according to:

$$\int_o^\infty [u(x)]^2 dx = 1 \tag{3.18}$$

We have
$$P(R) = \int_o^R dx\,[u(x)]^2 \tag{3.19}$$

So that
$$0 \leq P(R) \leq 1 \quad \text{and} \quad P'(R) \geq 0 \tag{3.20}$$

We want to demonstrate that for symmetric potentials satisfying

$$V'(x) \geq 0, \quad x > 0 \tag{3.21}$$

the function
$$G(R) = \frac{1}{2}\frac{\partial P(R)}{\partial \mu} = \int_o^R dx\; u(x)\frac{\partial u(x)}{\partial \mu} \tag{3.22}$$

Satisfies $$G(R) \geq 0, \quad 0 \leq R \leq \infty \tag{3.23}$$

For both even-parity and odd-parity ground states. Consider the Schrodinger equation in the form

$$u''(x) = -\frac{2\mu}{\hbar^2}[E - V(x)]u(x) \tag{3.24}$$

and apply $u(x)\frac{\partial}{\partial\mu}$ to obtain:

$$u(x)\frac{\partial u''(x)}{\partial\mu} = -\frac{2\mu}{\hbar^2}[E - V(x) + \mu\frac{\partial E}{\partial\mu}][u(x)]^2 \tag{3.25}$$

This is further simplified using Eq.(1.9) as:

$$u(x)\frac{\partial u''(x)}{\partial\mu} = \frac{2}{\hbar^2}[V(x)-\langle V\rangle][u(x)]^2 + \frac{2\mu}{\hbar^2}[V(x)-E]u(x)\frac{\partial u(x)}{\partial\mu} \tag{3.26}$$

Subtracting $\frac{\partial u}{\partial\mu}$ x (3.24) from this and integrating from 0 to R we get:

$$\int_0^R dx[u\frac{\partial u}{\partial\mu} - u''\frac{\partial u}{\partial\mu}] = \frac{2}{\hbar^2}\int_0^R dx[V-\langle V\rangle][u(x)]^2 \tag{3.27}$$

For both even - and odd-parity solutions partial integration of the left-hand-side yields:

$$u(R)\frac{\partial u'(R)}{\partial\mu} - u'(R)\frac{\partial u(R)}{\partial\mu} = \frac{2}{\hbar^2}\int_0^R dx[V - \langle V\rangle][u(x)]^2 \leq 0 \tag{3.28}$$

where the inequality is a consequence of (3.21).

The function

$$G'(R) = u(R)\frac{\partial u(R)}{\partial\mu} \tag{3.29}$$

Vanishes only for $u(R) = 0$ or $\frac{\partial u(R)}{\partial \mu} = 0$. To check whether an extremum of G is a minimum or a maximum, we evaluate G"(R) and using (3.28) it could be inferred that

$$G''(R) > 0 \quad \text{if} \quad u(R) = 0 \text{ (minimum)} \tag{3.30}$$

and

$$G''(R) < 0 \quad \text{if} \quad \frac{\partial u(R)}{\partial \mu} = 0 \text{ (maximum)} \tag{3.31}$$

From its definition, G(R) vanishes for both $R = 0$ and $R = \infty$. Since the ground state wavefunctions (u(r)) are nodeless, (3.23) is established because a minimum of G(R) occurs at nodes of u(R) and G(R) can become negative in $(0 < R < \infty)$ only if it has a minimum.

The proof just concluded for odd-parity case directly establishes (3.23) in three dimension for the S-wave ground state. Applying the same arithmetic to the Schrodinger equation of the form (1.18) for the three dimensional arbitrary values of angular momentum ℓ. We shall see in Chapter 4 that the inward flow of probability could be established for excited states as well, for specific potentials.

In a precisely parallel argument a similar result for the variation of P(R) with the potential strength could be attained. To this end, let $V(x) \to k\,V(x)$ in the Schrodinger Eq.(3.24) and substitute $\frac{\partial}{\partial k}$ for $\frac{\partial}{\partial \mu}$ in subsequent steps. Analogous to (3.28) you will obtain

$$u(R)\,\frac{\partial u'(R)}{\partial \mu} - u'(R)\,\frac{\partial u(R)}{\partial \mu} = \frac{2\mu}{\hbar^2}\int_0^R dx[V - \langle V\rangle][u(x)]^2 \leq 0 \tag{3.32}$$

The discussion following (3.28) applies, mutatis mutandis, to the present case and shows that $\frac{\partial p(R)}{\partial k} \geq 0$, under the same conditions for which $\frac{\partial p(R)}{\partial \mu} \geq 0$.

Specific applications of the results of this chapter will be elaborated in the next chapter.

CHAPTER 4

RELATIONS AMONG POWER-LAW POTENTIALS AND APPLICATIONS[1,16]

In our previous discussions we have encountered two types of power-law potentials. One class contains potentials of the type $\lambda r^{\nu}(-2 < \nu < o)$ that are singular at the origin. The other class contains potentials with $\nu > o$. They are well behaved at the origin but rise infinitely as $r \to \infty$. Pairwise relations exist between these two classes of potentials. The best known example is the duality noticed between the Coulomb and oscillator problems a long time ago by Shwinger[17]. We would explore this type of connection or duality in detail in this chapter. Other applications of the procedures developed in the preceding will also be pointed out.

4.1 Relations Among Power-Law Potentials

The Schrödinger equation

$$\frac{\hbar^2}{2\mu} u''(r) + [E - \lambda r^{\nu} - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}]u(r) = 0 \qquad (3.8)$$

is related to another equation which is similar in form. To find out the related Schrodinger-like equation we introduce a new length variable:

$$z = r^{-\nu/\bar{\nu}} \qquad (4.1)$$

where $\bar{\nu}$ is a power to be determined, and use the transformation

$$u(r) = z^{-[1+\bar{\nu}/\nu]/2} \, v(z) \qquad (4.2)$$

With this (3.8) takes the form

$$\frac{\hbar^2}{2\mu}\left(\frac{\hat{\nu}}{\nu}\right)^{-2}\{z^{2[\hat{\nu}/\nu+1]}\,v''(z)+\frac{1}{4z^2}\,[1-(\hat{\nu}/\nu)^2]z^{2[(\hat{\nu}/\nu)+1]}\,v(z)\}$$

$$+\{E-\lambda z^{-\hat{\nu}}-\frac{\ell(\ell+1)}{2\mu z^2}\,z^{2[\hat{\nu}/\nu+1]}\}\,v(z)=0 \qquad (4.3)$$

Multiplying this by $\left(\frac{\hat{\nu}}{\nu}\right)^2 z^{\hat{\nu}}$ we find:

$$\frac{\hbar^2}{2\mu}\,z^{2[\hat{\nu}/\nu+1]+\nu}\,v''(z)+\{-\lambda\left(\frac{\hat{\nu}}{\nu}\right)^2+E\left(\frac{\hat{\nu}}{\nu}\right)^2 z$$

$$-\frac{\hbar^2}{2\mu z^2}\,[\ell(\ell+1)\left(\frac{\hat{\nu}}{\nu}\right)^2-\frac{1}{4}\,(1-\left(\frac{\hat{\nu}}{\nu}\right)^2]z^{2[\hat{\nu}/\nu+1]+\hat{\nu}}\}\,v(z)=0 \qquad (4.4)$$

The choice (4.2) has ensured that this last equation contains no first derivative. The freedom of choice we have over $\hat{\nu}$ enables us to require

$$2\left[\frac{\hat{\nu}}{\nu}+1\right]+\hat{\nu}=0 \qquad (4.5)$$

with which we recover a Schrödinger-like equation,

$$\frac{\hbar^2}{2\mu}\,v''(z)+[\bar{E}-\hat{\lambda}\,z^{\hat{\nu}}-\frac{\hat{\ell}(\hat{\ell}+1)\hbar^2}{2\mu z^2}]\,v(z)=0 \qquad (4.6)$$

where

$$\bar{E}=-\lambda\,(\hat{\nu}/\nu)^2\;,\quad \hat{\lambda}=-E\left(\frac{\hat{\nu}}{\nu}\right)^2 \qquad (4.7)$$

and

$$\hat{\ell}(\hat{\ell}+1)=\ell(\ell+1)(\hat{\nu}/\nu)^2-\frac{1}{4}\,(1-(\hat{\nu}/\nu)^2) \qquad (4.8)$$

Completing the square on both sides of (4.8) we solve for $\tilde{\ell}$ in terms of ℓ. For u regular at the origin we have

$$u_\ell(r) \sim r^{\ell+1}, \quad r \to o \qquad (1.25)$$

and the choice

$$\tilde{\ell} + \tfrac{1}{2} = -(\tilde{\nu}/\nu)(\ell + \tfrac{1}{2}) \qquad (4.9)$$

ensures that

$$v_{\tilde{\ell}}(z) \sim z^{\ell+1} \qquad (4.10)$$

is also a solution regular at the origin. From (4.1) & (4.5) we have:

$$z = r^{1/(1+\tilde{\nu}/2)} = r^{1+\nu/2} \qquad (4.11)$$

This indicates that for $-2 < \nu < \infty$ the point $r = o$ maps into $z = o$ and the point $r = \infty$ maps into $z = \infty$.

The relation between the equations (3.8) and (4.6) is of a special interest. As it is transparent from (4.5) this relation connects the bound-state spectrum of an infinitely rising potential ($\nu > o$) with that of a singular potential ($-2 < \tilde{\nu} < o$).

4.2 Applications

But for a few exceptions, we focus almost entirely on power-law potentials.

The Infinite Square Well: An infinite square well of width R corresponds to the $\nu \to \infty$ limit of a power-law potential provided the coupling strength is given by $R^{-\nu}$.

$$V(r) = \lim_{\nu \to \infty} (r/R)^{\nu} = \begin{cases} 0 , & r < R \\ \infty , & r > R \end{cases} \tag{4.12}$$

According to (3.13) the dependence of its eigenvalues on mass and well width is given by

$$E = \frac{\hbar^2}{2\mu R^2} \tag{4.13}$$

Which behaves as the kinetic energy of a particle of mass μ in a box of length R. This result was to be expected as this is the only energy scale one can construct for this problem.

The following two examples are additional applications of the scaling arguments of Chapter 4. The probability density $|\psi(o)|^2$ is of interest in leptonic decays of massive neutral vector mesons v° which are $^3S_1$ bound states of a quark and an antiquark. The decay width is given by:

$$\Gamma(v^{\circ} \to \ell^{+} \ell^{-}) = 16 \pi \hbar^3 \alpha^2 e_Q^2 |\psi(o)|^2 / M_v^2 \tag{4.14}$$

where α is the fine structure constant, e_Q is the quark charge in units of the proton charge and M_v is the vector meson mass. Using (3.16) we have

$$\Gamma(v \to \ell^{+} \ell^{-}) \propto e_Q^2 (\mu|\lambda|)^{3/2+\nu} / M_v^2 \tag{4.15a}$$

$$\propto e_Q^2 \mu^{-(1+2\nu)/2+\nu} |\lambda|^{3/2+\nu}, \nu \geq -1 \tag{4.15b}$$

In the second expression binding energies are neglected. For $\nu > -1$, the scale of M_v will be set by μ for the low-lying levels because $\frac{\Delta E}{\mu}$ does not grow with increasing μ according to (3.14), we therefore assume $M_v \approx 2(2\mu)$ + small binding corrections for constituents of mass 2μ.

The second example to which the scaling law (3.15) may be applied is the transition matrix elements of electric and magnetic multipole operators and sizes of bound states with given quantum numbers. The electric multipole matrix elements scale as

$$\langle n' | E_j | n \rangle \propto L^j \tag{4.16}$$

while magnetic multipole matrix elements behave as:

$$\langle n' | M_j | n \rangle \propto L^{j-1}/\mu \tag{4.17}$$

Since radiative widths are given by

$$\Gamma (E_j \text{ or } M_j) \propto p_\gamma^{2j+1} | \langle n' | E_j \text{ or } M_j | n \rangle |^2 \tag{4.18}$$

with $p_\gamma \approx \Delta E$, we find:

$$\Gamma (E_j) \propto \mu^{-[2j(1+\nu)+\nu]/(2+\nu)} \quad |\lambda|^{2(j+1)/(2+\nu)} \tag{4.19}$$

and

$$\Gamma (M_j) \propto \mu^{-[2j(1+\nu)+3\nu+2]/(2+\nu)} \quad |\lambda|^{2(j+2)/2+\nu)} \tag{4.20}$$

For potentials less singular than the Coulomb potential near $r = o$ (i.e., for $\nu > -1$), the relative importance of higher multipoles decreases with increasing μ. It is amusing that for $-2 < \nu < -1$ the rapid growth of $p_Y \simeq \Delta E$ with μ can lead to an increasing prominence of high multipole transitions in the limit of large μ. For any power ν in the interval $-2 < \nu < \infty$, an increase in the coupling constant increases the importance of high multipole transitions.

The Logarithmic Potential: Rewriting $|\lambda|$ in terms of the potential energy (3.14) we arrive at:

$$\Delta E \propto \{[\frac{|v(r)|^{1/\nu}}{r}]^2/(2\mu/\hbar^2)\}^{1/1+2/\nu} \quad (4.21)$$

Which shows that the energy levels vary more slowly than any power of μ for a potential varying more slowly than any power of r. Clearly, such a potential is the logarithmic potential and we want to verify that it supports energy levels which are mass independent. In Chapter 3, we have shown that the logarithmic potential is the $\nu \to o$ limit of a power-law potential. In fact, $\nu = o$ supports no bound state. However, if one rescales the Schrodinger equation by the transformation (3.10) while keeping $\nu = o$, it is possible to determine the form of the potential supporting such a transformation.

Let
$$V(r) = \lambda U(r) \quad (4.22)$$

where U is dimensionless. The rescaled Schrodinger equation reads:

$$w''(\rho) + [(E/\lambda) - U([\frac{\hbar^2}{2\mu|\lambda|}]^{\frac{1}{2}}\rho) - \frac{\ell(\ell+1)}{\rho^2}]\, w(\rho) = 0 \quad (4.23)$$

The dimensionless energy eigenvalue is simply:

$$\varepsilon = E/\lambda \tag{4.24}$$

The eigenvalue differences are independent of μ, if and only if under a scale transformation $\mu \to \sigma\mu$

$$U(\rho[\frac{\hbar^2}{2\sigma\mu|\lambda|}]^{\frac{1}{2}}) = U(\rho[\frac{\hbar^2}{2\mu|\lambda|}]^{\frac{1}{2}})+f(\sigma) \tag{4.25}$$

Differentiating this with respect to σ and μ and separating variables, we find

$$U(r) = \ell n(r/r_o), \; f(\sigma) = -\tfrac{1}{2}\ell n\sigma \tag{4.26}$$

Thus, for logarithmic potential the level spacings are independent of μ[18]. It is only the parameter λ that sets the scale of the spacings as shown by (4.24).

To establish the uniqueness of the logarithmic potential in generating such a mass independent level spacing we will show in a different way that the Schrodinger equation can be scaled only for power-law and logarithmic potentials. Writing the Schrödinger Hamiltonian as:

$$\mathbf{H} = (p^2/2\mu) + V(r) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \tag{4.27}$$

Consider the effect of a scale change for which

$$r \to kr \quad \text{and} \quad p \to p/k \tag{4.28}$$

The rescaled Hamiltonian is:

$$\mathbf{H}(k) = (p^2/2\mu k^2) + V(kr) + \frac{\ell(\ell+1)\,\hbar^2}{2\mu k^2 r^2} \tag{4.29}$$

The most general condition upon which the eigenvalues of $\mathbf{H}$ and that of $\mathbf{H}(k)$ are identical except for possible change in scale and shifts in the zero of energy suggests that $\mathbf{H}(k)$ be a linear function of $\mathbf{H}$ so as to preserve the quadratic dependence on momentum, and hence V(r) must be a linear function of V(kr)

$$V(r) = AV(kr) + B \tag{4.30}$$

This is the condition upon the scaling behaviour of the potential that ensures the desired scaling properties of the Schrödinger equation.

Consider an infinitesimal scale transformation and Taylor expand (4.30) about $k = 1$. We thereby obtain:

$$V(r) = A[V(r) + (k-1)\, r\, V'(r)]+B \tag{4.31}$$

Rewriting this as

$$\frac{dV}{V(1-A)-B} = \frac{1}{(k-1)}\ \frac{dr}{r} \tag{4.32}$$

We see that it admits two possible solutions. For $A \neq 1$, integration of (4.32) yields:

$$\frac{\ln[V(1-A)-B]}{1-A} = \frac{1}{k-1}\ \ell nr \quad + \quad \text{const.} \tag{4.33}$$

Which is a power-law potential, and for A - 1 integration of (4.32) yields

$$V(r) = -\frac{B}{(k-1)}\,\ell n(r/r_\circ) \tag{4.34}$$

which is a logarithmic potential. This shows that the logarithmic potential is unique in generating level spacings that are independent of mass because the Schrödinger equation exhibits the desired scaling behaviour only for power-law and logarithmic potentials.

In Ref.[18] the dimensionless levels ε have been calculated numerically in the logarithmic potential (for $\sqrt{r_0 \; 2\mu\lambda/\hbar^2} = 1$) and a comparison between three potentials ($V = -1/\sqrt{r}$, $V = \ell n\, r$ and $V = r$) is made where for all the three, the comformity of the Feynman-Hellmann theorem (1.9) is verified and that the levels spread apart as μ is increased, for the singular potential. For the linear potential, on the other hand, the levels are packed together as μ is increased. The logarithmic potential represents an intermediate situation where the level spacing is mass-independent.

Bound-State Normalization: We apply normalization techniques of Chapter 2 to specific cases of interest.

Harmonic Oscillator: Consider the radial Schrödinger equation of the harmonic oscillator problem (with $2\mu = h^2$)

$$\text{i.e.,}\quad \phi''(r) - (r^2 - E)\,\phi(r) = 0 \tag{4.35}$$

Which has the form of the Weber parabolic cylinder equation:

$$\frac{d^2w(x)}{dx^2} - \left(\frac{x^2}{4} + a\right)w(x) = 0 \tag{4.36}$$

Whose asymptotic solution is the parabolic cylinderical function[19]:

$$U(a,x) = \cos \pi(\frac{1}{4} + \frac{a}{2})Y_1 - \sin\pi(\frac{1}{4} + \frac{a}{2})Y_2 \tag{4.37}$$

where

$$Y_1 = \frac{\sqrt{\pi}\ \sec \pi(\frac{1}{4} + \frac{a}{2})}{2^{a/2+\frac{1}{4}}\ \Gamma(\frac{3}{4} + \frac{a}{2})} y_1 \quad Y_2 = \frac{\sqrt{\pi}\ \cos \pi(\frac{1}{4} + \frac{a}{2})}{2^{a/2-\frac{1}{4}}\ \Gamma(\frac{1}{4} + \frac{a}{2})} y_2$$

$$y_1 = e^{x^2/4}\ \{1+(a - \tfrac{1}{2}) \frac{x^2}{2!} + (a - \tfrac{1}{2})(a - \tfrac{3}{2})\frac{x^4}{4!} + \ldots\}$$

$$y_2 = e^{x^2/4}\ \{x+(a - \tfrac{3}{2}) \frac{x^3}{3!} + (a - \tfrac{3}{2})(a - \tfrac{7}{2})\frac{x^5}{5!} + \ldots\}$$

Using the WKB approximation,[24] the solution of (4.36) is:

$$w(x) \sim x^{-a-\frac{1}{2}} \quad e^{-x^2/4} \tag{4.38}$$

$$\text{i.e.,} \quad u(a,x) \sim x^{-a-\frac{1}{2}} \quad e^{-x^2/4}$$

Comparison of (4.1) and (4.2) shows that the solutions of (4.1) which are damped at infinity are:

$$f_1(r,E) = U(-E/2,\ r\sqrt{2})$$

$$\sim r^{E/2 - \frac{1}{2}}\ e^{-r^2/2} \tag{4.39}$$

the eigenvalue condition is

$$f_1(0,E_n) = 0 \tag{2.44}$$

which according to (5.40) yields:

$$E_n = 4n-1, \qquad n = 1,2,... \tag{4.40}$$

and the normalization integral (3.47) gives:

$$I_n = \frac{\Pi}{8} \frac{\Gamma(n)}{\Gamma(n+\frac{1}{2})} \tag{4.41}$$

A similar result can of course be obtained using the properties of Hermite polynomials[20].

<u>Coulomb Potential</u>: Consider the reduced radial Schrödinger equation of the hydrogen atom

$$\{\frac{-\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} - \frac{Ze^2}{r} + E_H\}\phi(r) = 0 \tag{4.42}$$

Upon choosing $\hbar^2 = 2\mu$, $Ze^2 = 1$ and $K^2 = - E = E_H$, this could be simplified as:

$$\phi''(r) + (-K^2 + \frac{1}{r} + \frac{\ell(\ell+1)}{r^2})\,\phi(r) = 0 \tag{4.43}$$

using a scale transformation

$$r = k\rho \quad , \quad \phi(r) \equiv \phi(\rho) \tag{4.44}$$

this could be changed to the Whittaker equation

$$\phi''(\rho) - \{\frac{1}{4} - \frac{k}{\rho} - \frac{1-4m^2}{4\rho^2}\}\,\phi(\rho) = 0 \tag{4.45}$$

where

$$k = \frac{1}{2K}, \quad \ell = m - \tfrac{1}{2} \qquad (4.46)$$

Using the transformation

$$w(\rho) = \rho^{-c/2} e^{\rho/2} \quad \phi(\rho) \qquad (4.47)$$

and further substituting

$$2k = c - 2a, \quad 2m = c - 1 \qquad (4.48)$$

this could be related to the confluent hypergeometric equation

$$\rho w''(\rho) + (c - \rho) w'(\rho) - aw(\rho) = 0 \qquad (4.49)$$

and the solutions are related as[21],

$$\phi_{k,m}(\rho) = \frac{\rho^{m+\frac{1}{2}}}{\Gamma(m-k+\frac{1}{2})} \quad e^{-\rho/2} \; {}_1F_1(m-k+\tfrac{1}{2};\; 2m+1;\; \rho) \qquad (4.50)$$

where ${}_1F_1(a;b;\rho)$ is the confluent hypergeometric function

for $\ell = o$ we have:

$$\phi_{k,m}(r) \sim r\, e^{-kr} \; {}_1F_1(1 - \frac{1}{2k};\; 2, 2kr) \qquad (4.51)$$

This representation in terms of Whittaker functions eases the evaluation of asymptotic solutions. The decomposition of the asymptotic solution into damped and unbounded parts, according to (1.23) - (1.25) yields coefficients

$$C_1(E) = \frac{1}{2k}\,\Gamma(1+\frac{1}{2k}) = -\frac{i\,e^{-i\pi/2(\frac{1}{2k})}}{2k\Gamma(1+\frac{1}{2}k)} \tag{4.52}$$

$$C_2(E) = -\frac{i\,e^{-i\pi/2(\frac{1}{2k})}}{2k\Gamma(1-\frac{1}{2}k)} \tag{4.53}$$

with [19]

$$f_1(r,E) \sim (2kr)^{\frac{1}{2k}}\,e^{-kr} \tag{4.54}$$

$$f_2(r,E) \sim (2kr)^{-\frac{1}{2k}}e^{kr} \tag{4.55}$$

using the relation

$$\Gamma(1-\frac{1}{2k}) = \frac{\Pi}{\Gamma(\frac{1}{2k})\,\sin\,(\frac{\Pi}{2k})} \tag{4.56}$$

the vanishing of $C_2(E)$ at energy eigenvalues yields

$$\frac{1}{2k} = n \quad , \quad n = 1,2,\ldots \tag{4.57}$$

So that

$$E_n = -\frac{1}{4n^2} \tag{4.58}$$

A brief calculation of the normalization integral using (1.29) and dropping a phase factor $e^{i\pi}$, which the normalization of the wavefunction will take care of, yields:

$$I_n = 2n^3 \tag{4.59}$$

which could also be obtained by elementary means[22].

Mass Dependence of the Schrödinger Wavefunctions: As an application of the result of Chapter 3 to power-law and logarithmic potentials we prove the following theorem:

Theorem: For power-law or logarithmic potential, the function

$$G(R) = \frac{1}{2}\frac{\partial}{\partial\mu}\int_0^R dr[u(r)]^2 = \int_0^R dr\, u(r)\,\frac{\partial u(r)}{\partial\mu} \qquad (3.22)$$

i) is non-negative for $0 < R < \infty$

ii) vanishes only at radial nodes of the wavefunction for any bound state.

We use equations (3.10), (3.11) and (3.18) and we further define a Scaled transformation

$$\tilde{w}(\rho) = \left(\frac{\hbar^2}{2\mu|\lambda|}\right)^{\frac{1}{2(2+\nu)}} w(\rho) \qquad (4.60)$$

Which is independent of μ and λ and which satisfies

$$\int_0^\infty [\tilde{w}(\rho)]^2 d\rho = 1 \qquad (4.61)$$

With this one obtains:

$$\frac{\partial u(r)}{\partial\mu} = \frac{1}{2\mu(2+\nu)u(r)}\frac{d}{dr}(r[u(r)]^2) \qquad (4.62)$$

and

$$G(R) = \frac{1}{2\mu(2+\nu)} R[u(R)]^2 \qquad (4.63)$$

This proves the theorem, since $\nu > -2$.

The $\nu \to o$ limit and the $\nu \to \infty$ limit of (4.63) give results corresponding to logarithmic potential and an infinitely deep well respectively as was explained in Chapter 3.

Thus, the probability that a particle lies within a spherical shell of radius R can not decrease as the mass μ is increased. The result (4.63) shows that probability does not flow past nodes in the reduced radial wavefunction. A similar statement holds for variations of the coupling strength λ. Using (4.60) we can show that:

$$G(R) = \frac{1}{2} \frac{\partial}{\partial|\lambda|} \int_o^\infty [u(r)]^2 dr = \frac{R[u(r)]^2}{2|\lambda|(2+\nu)} \geq 0 \qquad (4.64)$$

For S-wave square well potential G(R) is non-negative but it does not vanish at the nodes of the wavefunction[23]. However, as is required by (4.30) it has minima at these points. To derive a result analogous to (4.63), for within the well, with:

$$V(r) = \begin{cases} -V_o , & o \leq r < a \\ 0 , & a \leq r < \infty \end{cases} \qquad (4.65)$$

We use

$$u(r) = A \sin kr, \quad o \leq r \leq a, k = 2\mu(E+V_o) \qquad (4.66)$$

Where the dependence of A on k is obtained using boundry conditons and

$$u(r) = Be^{-kr}, \quad a \leq r < \infty \qquad (4.67)$$

Where $$- K = k \cot ka \tag{4.68}$$

and $$A^2 = 2K/1 + aK \tag{4.69}$$

Within the well, we find

$$\frac{\partial u}{\partial \mu} = \{ \frac{u(r)}{A} \frac{dA}{dk} + \frac{r\, u'(r)}{k} \} \frac{dk}{d\mu} \tag{4.70}$$

Thus,

$$G(R) = \int_o^R [r \frac{u'(r)}{k} + \frac{u(r)}{A} \frac{dA}{dk}] \frac{dk}{d\mu} dr\, u(r) \tag{4.71}$$

Integrating the first term by parts, using $\frac{1}{2} \frac{d}{dk}[\ln(\frac{A^2}{k})] = \frac{1}{A} \frac{dA}{dk} - \frac{1}{2k}$ we find that:

$$G(R) = \alpha R[u(r)]^2 + \beta \int_o^R dr[u(r)]^2 \tag{4.72}$$

Where $$\alpha = \frac{1}{2k} \frac{dk}{d\mu} , \quad \beta = \frac{1}{2} \frac{d}{dk} [\ln(\frac{A^2}{k})] \tag{4.73}$$

Using the expressions for A and K it could be verified that

$$\alpha , \beta > 0 \tag{4.74}$$

for $o \leq r \leq a$. Hence,

$$G(R) \geq 0 \quad \text{for} \quad R \leq a \tag{4.75}$$

It could be shown, using results of Chapter 3, that $G(R) \geq 0$ for $R \geq a$ as well. Equation (4.72) shows that G(R) doesn't vanish at the nodes of the reduced radial wavefunction.

The most general class of potentials for which $G(R) \geq 0$ for all bound states, or for all s-waves has not yet been characterized, but it is expected that such potentials be monotonically increasing functions of coordinates and have some degree of smoothness. For example, it is shown in [23] that for a finite square well nested within an infinite sqaure well $G(R)$ could become negative for an s-wave level.

These are only some of the applications of the techniques developed in the preceeding chapters. These techniques have proved to be extremely important in describing bound states of quarkonium.

CHAPTER 5

QUANTUM DISCONTINUITY

A quantum discontinuity may occur when the energy of a quantum particle is not a continuous function of some relevant coupling parameter. This phenomenon is intimately linked to the behaviour of the Rayleigh Schrodinger perturbation expansion as a function of such a coupling constant. We therefore, begin by reviewing some basic features of Rayleigh Schrodinger perturbation theory (RSPT).

Suppose the total Hamiltonian H of a single bounded particle can be decomposed as

$$H = H_0 + V \tag{5.1}$$

For book keeping purposes let us rewrite (5.1) as

$$H = H_0 + \lambda V \tag{5.2}$$

where the continuous parameter λ will finally be set equal to unity. Here H_0 is the part whose eigenvalue problem is assumed to be exactly solvable $|n^\circ\rangle$ being its eigenkets and ε_n° the corresponding eigenvalues. It is next assumed that to each such pair $|n^\circ\rangle$ and ε_n° there is an eigenket $|n\rangle$ and eigenvalue ε_n of H that may be expanded in a perturbation series

$$|n\rangle = |n^\circ\rangle + \lambda|n^{(1)}\rangle + \ldots + \lambda^k|n^{(k)}\rangle + \ldots \tag{5.3}$$

$$\varepsilon_n = \varepsilon_n^\circ + \lambda\,\varepsilon_n^{(1)} + \ldots + \lambda^k\,\varepsilon_n^{(k)} + \ldots \tag{5.4}$$

As λ grows from zero to one, one then assumes that $|n^{\circ}\rangle$ develops smoothly into $|n\rangle$ and ε_n^{o} into ε_n. In the same manner we expect that if λ is reduced from one to zero one smoothly recovers the set $\varepsilon_n^{o}, |n^{(o)}\rangle$ from the corresponding set ε^{n}, $|n\rangle$. The superscript on each term gives the power of (the matrix element) V that it is expected to come out proportional to. A term with superscript k is called the k^{th} order term or the k^{th} order correction. The power of the book keeping index λ does the same job. One hopes that as k increases the corrections get smaller. RSPT provides a systematic means of computing successive corrections. Its details which we skip here[17,25] reveal that for it to work, a necessary condition is

$$A \equiv \left| \frac{\langle m^{\circ} | V | n^{\circ} \rangle}{\varepsilon_n^{o} - \varepsilon_m^{o}} \right| << 1.$$

Moreover, one also hopes that small perturbations (A << 1) lead to small modifications in the unperturbed function and energy. It is also generally expected that as $\lambda \to o$, $|n\rangle \to |n^{\circ}\rangle$ and $\varepsilon_n \to \varepsilon_n^{o}$ smoothly. The most crucial assumption RSPT makes is the validity of the expansions like (5.3), (5.4) themselves. For example, $\varepsilon_n(\lambda)$ should be an analytic function of λ in a non-zero domain surrounding $\lambda = o$ in the complex λ-plane. In some cases such an expansion may not exist even. The bound states of a very weak attractive potential do not come out of doing perturbations on free particle states. They simply can't. A power series expansion obviously implies that physics with $V \to 0^{+}$ and $V \to 0^{-}$ could at most be marginally different. We shall dwell further upon this point in detail in the sequel. For the moment let us point out an elementary example. A weak attractive potential in 1-d necessarily supports at least one bound state but a weak repulsive potential simply can't. The bound state of a shallow square well is $\epsilon = - mV^2a^2/2h^2$. This is certainly not the first (or second) term in a power series in V. Were this the case this formula would have to give us the correct result for either sign of V, but a state with $\epsilon < o$ for a repulsive potential is clearly impossible.

Many many interesting questions thus arise, concerning, for example, the energy expansion (5.4). Let us note some of these. Firstly, does such an expansion converge? If it does, then does it always converge to the correct eigenvalue? More explicitly, can it ever converge to a wrong eigenvalue? Is such an expansion merely asymptotic so that upto a certain order it converges to the desired result but then deviates away from it. Then can it converge or diverge but be not asymptotic to the correct eigenvalue? Can it diverge and yet be uniquely summable to the correct result via some known mathematical theorems?

Such questions have been frequently asked in the last 15 years or so and using specific models many authors have searched for the answers. A possibility like convergence to a wrong limit is certainly extremely disturbing particularly in the context of quantum field theory where perturbation theory is perhaps the only known way of making systematic calculations. Hence, it becomes a matter of supreme importance to know what kind of theories can be expected to possess such undesirable features. A further discussion of such theories is certainly beyond our scope[29,30].

We now come to a brief resumé of various studies alluded to in the last paragraph.

also independent of g just as $\varepsilon_+(g)$ is but it does not vanish.

$$\varepsilon_-(g) = -2, \quad g \neq o \tag{5.7}$$

Hence,
$$\lim_{g\to o} \varepsilon_-(g) = -2 \neq \varepsilon_-(o) = \varepsilon(o) = o \tag{5.8}$$

the limit being taken for real values of g. Note that for all such values of g, $\varepsilon_-(g)$ is well defined since $H_-(g)$ is bounded below and has a well defined purely discrete spectrum. This implies that the Rayleigh Schrödinger perturbation series is not asymptotic (but is term by term well defined and non-vanishing). Thus, the question whether it converges or not is really irrelevant.

Calogero also provides an extremely simple recipe to manufacture other models that display the same phenomenon that $H_\pm(g)$ do. He introduces a real function $\phi(x)$, regular for all real values of x and divergent (say proportionally to a power) as $x \to \pm\infty$. Define a Hamiltonian

$$H = p^2 + \frac{d\phi}{dx} + \phi^2(x) \tag{5.9}$$

For any $\phi(x)$, so defined, this Hamiltonian is clearly bounded below and has a purely discrete spectrum. One then sees that the ground state energy ε vanishes provided $\phi(\pm\infty) = \mp\infty$ with

$$\psi(x) = \exp \int \phi(x)dx \tag{5.10}$$

as the admissible ground state function. Simple examples arising out of such a construction are disucssed in his work. Further examples arising

The system is said to display quantum discontinuities.

In his models the occurence of discontinuities is accompanied by a loss of normalizability by the associated wavefunctions.

Moreover, in all his models the limiting process forces the subsidiary wells to grow infinitely wide. Their minima recede to infinity and their depths remain fixed or diverge. Hence, prior to the discontinuous jump, there appears a tendency amongst a group of levels to accumulate near the minimum of the relevant subsidiary well.

In short, under the limiting process one witnesses a discontinuous behaviour of the energies, a loss of normalizability by the wavefunctions and a marked convergence of levels near a suitable minimum. Analytically, usually the discontinuity of only a single level per potential is deducible in the examples of Calogero.

Recently, a solvable and a very instructive model that illustrates the discontinuity phenomenon has been proposed[31]. In it the discontinuous behavior of any finite set of lowest lying levels can be deduced analytically. The associated wavefunctions tend to disappear entirely in the limiting process and no accumulation a la Calogero materializes.

The Calogero models essentially deal with the perturbations of an oscillator. Varma and co-workers[32] focussed attention on a class of problems that represent polynomial perturbations of a Coulomb problem. Such problems were first introduced by Killingbeck[33] and are relevant to atomic physics and quark confinement theories. Killingbeck's motivation was agin to explain the failure of RSPT under suitable conditions. To be more precise Saxena, Srivastava and Varma, utilizing the numerical Hill determinant technique considered the Hamiltonian

$$H = \frac{p^2}{2} - \frac{1}{r} + 2\lambda r + 2\lambda^2 r^2 , \quad o \leq r \leq \infty$$

and established the discontinuous behaviour of the $\ell = o$ levels in the $\lambda \to o$ limit. Their studies were extended by Pandey and Varma[34] to Hamiltonians involving two coupling constnats with

$$H = \frac{p^2}{2} - \frac{1}{r} + 2\mu r + 2\lambda^2 r^2$$

They again found discontinuities when μ and λ were made to vanish suitably. Specifically, the eigenvalue spectra were shown to possess discontinuities whenever the associated potential functions possess different number of minima in the two limits $\lambda \to o$, $\mu \to o^+$ and $\lambda \to o$, $\mu \to o^-$.

Our aim is now to propose a model of the above class where the discontinuities can be deduced analytically and be rationalized in terms of the normalization characterstics of the associated functions. Specifically, we consider a slight variation of the generalized Killingbeck potential deployed by Pandey and Varma[34] in which the Coulomb term is made repulsive. We write the relevant radial equation as

$$R'' + \frac{2}{\rho} R' + [\varepsilon - \frac{2}{\rho} - \mu\rho - \alpha^2\rho^2 - \frac{\ell(\ell+1)}{\rho^2}]R = 0 \tag{5.11}$$

Here we have used Coulombic units and a dimensionless radial variable ρ such that

$$r = \gamma\rho, \quad \gamma = \frac{\hbar^2}{m_e e^2}, \quad \varepsilon = \frac{E}{R_y}, \quad R = \frac{m\, e^4}{2\hbar^2} \tag{5.12}$$

and the associated Killingbeck potential is

$$V(\rho) = \frac{2}{\rho} + \mu\rho + \alpha^2\rho^2 \tag{5.13}$$

It is readily seen that as $\rho \to o$,

$$R \sim \rho^{\ell} \tag{5.14}$$

and as $\rho \to \infty$, the dominant assymptotic behaviour is

$$R \sim e^{-\alpha\rho^2/2} \tag{5.15}$$

We therefore try a solution of the form

$$R(\rho) = \rho^{\ell} \; v(\rho) \exp[\beta\rho - \frac{\alpha\rho^2}{2}] \tag{5.16}$$

Substituting (5.16) in (5.11) we find for v, the equation

$$v''(\rho)+[p/\rho + 2\beta - 2\alpha\rho]v'(\rho)+[\varepsilon + \beta^2 - \alpha(p+1) + \frac{p\beta-2}{\rho} - (\mu + 2\alpha\beta)\rho]v(\rho) = 0 \tag{5.17}$$

Where

$$p = 2\ell + 2 \tag{5.18}$$

The yet unspecified parameter β can now be chosen to eliminate the linear term in the square bracket multiplying v. Thus, we set

$$\mu = -2\alpha\beta \tag{5.19}$$

For $V(\rho)$ we try the power series solution

$$v(\rho) = \sum_{n=o}^{\infty} a_n \rho^n \tag{5.20}$$

With $a_o \neq o$ so as to guarantee the correct limiting behaviour of $R(\rho)$ near the origin. Substituting (5.20) in (5.17) we now have the three-term relation with successive co-efficients

$$n(n+p-1)a_n + [\beta(p+2n-2)-2]a_{n-1} + [\varepsilon+\beta^2-\alpha(p+2n-3)]a_{n-2} = 0 \tag{5.21}$$

It immediately follows that v will be a polynomial of degree k provided

$$a_k \neq 0 \ (5.22), \quad a_{k+1} = 0 \ (5.23) \quad \text{and} \quad a_{k+2} = 0 \ (5.24)$$

where $\quad k = o, 1, 2, \ldots.$

Conditions (5.22) - (5.24) readily imply that for such solutions

$$\varepsilon = -\beta^2 + \alpha(p+2k+1) \tag{5.25}$$

But, for such solutions to materialize the linear and quadratic couplings have to be constrained by the condition $a_{k+1} = o$ (5.23). Through a repeated use of the recursion relation (5.17) and remembering that the overall scale of v is immaterial (i.e., a_o can be set equal to one) we arrive, instead of (5.23), at the determinantal condition

$$\begin{vmatrix} \beta p-2 & 1.p & 0 & & & & \\ 2k\alpha & \beta(p+2)-2 & 2.(p+1) & 0 & & & \\ 0 & 2(k-1)\alpha & \beta(p+4)-2 & 3(p+2) & 0 & & \\ \cdot & 0 & & & & & \\ \cdot & \cdot & & & & & \\ \cdot & \cdot & & & & & \\ & & & & & & k(p+k-1) \\ & & & 2\alpha & & & \beta(p+2k)-2 \end{vmatrix} = 0 \qquad (5.26)$$

The structure of this determinant is such that there always appear (k+1) real roots β_o , β_1 ..., β_k corresponding to polynomial solutions $v_k^{(i)}$ of degree k with energies

$$\varepsilon_i^{(k)} = -\left(\beta_i^{(k)}\right)^2 + \alpha\,(p+2k+1) \qquad (5.27)$$

With $i = 0, 1, 2, \ldots, k$. Each solution corresponds to a suitable value of the ratio μ/α.

In the following we will be interested in the limits $\mu \to o$, $\alpha \to o$. We learn that such a limit can be approached in a manner that allows β to be held at any fixed value that can be arbitrarily chosen. In this limit we also see that geometrically we have a potential well with a far off minimum located at $\rho_{min} \approx \left|\frac{\mu}{\alpha^2}\right|$ and where the well depth is

$V_{min} \simeq -\beta^2 = -\frac{\mu^2}{4\alpha^2}$. Under the limit of interest to us the depth remains fixed and the minimum recedes to infinity.

It is now expedient to turn to some simple illustrative cases.

i) k = o: Here we have the results

$$\beta^{(o)} = \frac{2}{p} \quad \text{or} \quad \frac{\mu}{\alpha} = -\frac{4}{p} \tag{5.28}$$

$$\varepsilon^{(o)} = -[\beta^{(o)}]^2 + \alpha(p+1) \tag{5.29}$$

$$v(\rho) = 1 \tag{5.30}$$

We have zero radial node solution ($n_r = o$). The depth of the well (as $\alpha \to o$) is very nearly $-[\beta^{(o)}]^2$ and the above level is situated almost at the bottom of the well. The exact value of $\beta^{(o)}$, i.e., the ratio $\frac{\mu}{\alpha}$ is for us to choose and thereby one specifies the precise manner in which $\alpha, \mu \to o$. As α and μ are switched off from their infinitesimal values in the stipulated manner, the state must change abruptly and the associated energy with it, to conform to the dictums of the residual repulsive Coulomb potential that has no negative levels. A controllable discontinuous energy jump is in clear evidence. Were one to consider the state of angular momentum ℓ_o (say $\ell_o >> 1$) and $n_r = o$ then this state's energy would be heading for the bottom of the well as $\alpha \to o+$ and $\mu \to o^-$. It follows that the levels with $n_r = o$ and $\ell < \ell_o$ would lie still lower than the level we are focusing on. Thus, prior to the discontinuous jump an accummulation of levels near the minimum of the well a la Calogero is also in clear evidence.

Upon first glance a rather disturbing feature seems to emerge. As $\alpha,\ \mu \to o$ and $\beta^{(o)}$ remains fixed the radial function

$$R(\rho) \quad \to \quad \rho^{\ell}\ e^{+\beta^{(o)}\rho} \tag{5.31}$$

seems to be non-normalizable. But it is readily seen that a repulsive Coulomb potential does indeed have such a non-normalizable formally exact negative energy solution. Clearly it does not belong to the physical Hilbert space. Now turning the argument around it seems rather natural to argue that upon the switching on of the infinitesimal couplings α, μ a particle in the Hilbert space of a repulsive Coulomb potential looses all memory of this state and begins to behave as if it started out in a state outside this space. This situation is obviously untenable. Hence, the above line of reasoning must be erroneous. Indeed it is!

We have paid no attention to the normalizability of the state function. In a traditional quantum situation the overall scale of a wavefunction is not important. But here, it is. For simplicity consider the $n_r = o$, $\ell = o$ case. The function in hand is

$$R(\rho) = N\ e^{2\rho - \alpha\rho^2/2} = N\ e^{-\alpha/2\,(\rho^2 - \frac{4}{\alpha}\rho)} = N\ e^{2/\alpha}\ e^{-\frac{\alpha}{2}(\rho - 2/\alpha)^2}$$

Hence, the normalization integral is

$$I = N^2\ e^{4/\alpha} \int \rho^2\ e^{-\alpha(\rho-2/\alpha)^2}\ d\rho$$

Clearly, in the limit $\alpha \to o$, the dominant behaviour of N will be dictated by the factor $e^{-2/\alpha}$. Hence, as $\alpha \to o$, $N \to o$. The normalized function simply disappears everywhere!

Thus, the quantum discontinuity in hand can be understood in terms of the disappearance of the state itself as α is switched off. As long as $\alpha \neq o$, the system stays in this state. At $\alpha = o$ such a state is no more available. At $\alpha = o$ we must go back to the Schrödinger equation and solve the problem of the repulsive Coulomb potential. Clearly therefore at $\alpha = o$, the system does not have a dual choice of states. In the same manner when an infinitesimal α is switched on the system would jump into the entirely new configuration that emerges naturally via the Schrödinger equation of the full problem.

It is also possible to understand the entire situation geometrically. As soon as α is switched on, a new potential well emerges whose depth and location of the minimum is specified above. If $\alpha \to o$ in the manner specified, the minimum recedes to infinity while the depth remains fixed. The probability function recedes towards infinity accordingly. When α is zero the far away well abruptly disappears and with it the state. Although the picture is intutively clear, it is indeed gratifying that we have been able to verify the fact in a quantitative manner. This is one important advantage our procedure has over the exhaustive numerical studies of Pandey and Varma[34]. Besides, we have demonstrably learnt that the scale of a wavefunction that can normally be ignored can indeed play a fundamentally important role. Had this role been not available we would have been forced into the awkward explanation that we attempted in the begining.

Eq.(5.29) seems to suggest that the energy $\varepsilon^{(o)}(\alpha)$ could be formally thought of to have an expansion in powers of α with the first term as the zeroth order term and the second as a first order term, the other terms being identically zero. In view of our explanations above it should be evident that such is certainly not the case. The first term does not have the status of a zero order term and is not recovered in the limit $\alpha = o$. The same holds for the wavefunction of (5.31) which has a term by term finite and a convergent expansion in α. Such term by term finite and convergent expansions have thus nothing to do with Rayleigh Schrödinger perturbation theory.

We have for clarity envisaged a limit $\alpha \to o^+$, $\mu \to o^-$ such that the well depth remains fixed as the well recedes to infinity. This restriction can be removed without affecting the conclusions at all. For example, we could allow β to grow indefinitely (see Eq.(5.19)) in the process. The discontinuous jumps would grow larger accordingly. On the other hand we could let $\alpha \to o^+$, $\mu \to o^-$ such that $\beta \to o^+$. Repeating the analysis we again find that although there is no jump in energy, the limiting wavefunction has nothing to do with the corresponding wavefunction of a repulsive Coulomb problem. The reader can easily convince himself that this includes the interesting possibilities of the well depth going to zero with the location remaining fixed or moving inwards towards $\rho = o$. In all cases the normalized wavefunction always disappears. We see here the interesting possibility of no discontinuity in the energy function still accompanied by an abrupt change in the wave function. As far as we know such a scenario has not been reported before.

So far we have considered the $k = o$ case which led to only $n_r = o$ solutions with ℓ unrestricted. This has enabled us to exhibit most of the principal features of our results that we wish to discuss. Some correspond to just one set of couplings but different node numbers. Again we shall not furnish the straight forward but lengthy details here.

Next, we would like to point out another related model of the discontinuity phenomenon. It involves a potential of the type

$$V(\rho) = \frac{2}{\rho} + \mu\rho + \gamma\rho^2 + \lambda^2\rho^4 \tag{5.50}$$

Setting $$R(\rho) = \rho^{\ell} \exp[\beta\rho - \lambda\rho^3/3]v(\rho) \tag{5.51}$$

we find that the function v satisfies the equation

$$v'' + [\frac{p}{\rho} + 2\beta - 2\lambda\rho^2]v' + [\varepsilon + \beta^2 + \frac{p\beta-2}{\rho} - (\mu + \lambda(p+2))\rho - (\gamma + 2\beta\lambda)\rho^2]v = 0$$

Selecting $\gamma = -2\beta\lambda$ and by setting $v = \sum_{n=o}^{\infty} a_n \rho^n$ we obtain the following four term recursion relation

$$n(n+p-1)a_n + [\beta(p+2n-2)-2]a_{n-1} + [\varepsilon+\beta^2]a_{n-2} - [\mu+\lambda(p+2n-4)]a_{n-3} = 0 \tag{5.53}$$

clearly v will be a polynomial of degree k provided

$$a_k \neq o, \quad a_{k+1} = a_{k+2} = a_{k+3} = o \tag{5.54}$$

Using (5.54) in (5.53) we immediately find that for v to be a polynomial of degree k we must have

$$\mu = -\lambda(p + 2k + 2) \tag{5.55}$$

Thus, for k = o the requirements turn out to be

$$\mu = -\lambda(p+2) \quad \ldots (5.56) \qquad \beta = \frac{2}{p} \tag{5.57}$$

$$\varepsilon = -\beta^2 \quad \ldots (5.58) \qquad \text{and} \qquad V(\rho) = 1 \qquad (5.59)$$

The required quadratic coupling is $\gamma = -\frac{4}{p}\lambda$. Thus, as $\lambda \to o$, $V(\rho) \to 2/\rho$ and $\varepsilon \approx -\beta^2$. A discontinuous jump must obtain as λ is switched off.

Similarly in the limit $\lambda \to o$, we obtain for the k = 1 case, the following set of results

a)

$$\beta_1^{(1)} \approx \frac{2}{p} + \sqrt{\frac{p\lambda}{2}} + \sqrt{\frac{2}{p}}\,(p+1)\,\lambda \qquad (5.60)$$

$$\varepsilon_1^{(1)} \approx -\frac{4}{p^2} + (p+1)\left[\frac{p}{2} - 4\sqrt{\frac{2}{p}}\right]\lambda \qquad (5.61)$$

$$V_1^{(1)}(\rho) = 1 - \sqrt{\frac{p\lambda}{2}}\,\rho \quad (\text{so that } n_r = 1) \qquad (5.62)$$

b)

$$\beta_o^{(1)'} \approx \frac{2}{p} - \sqrt{\frac{p\lambda}{2}} - \sqrt{\frac{2}{p}}\,(p+1)\,\lambda \qquad (5.63)$$

$$\varepsilon_o^{(1)'} \approx -\frac{4}{p^2} + (p+1)\left[\frac{p}{2} + 4\sqrt{\frac{2}{p}}\right]\lambda \qquad (5.64)$$

$$V_1^{(o)'}(\rho) = 1 + \sqrt{\frac{\lambda p}{2}}\,\rho \qquad (n_r = o) \qquad (5.65)$$

c)

$$\beta_o^{(1)} = \frac{2}{p+2} + \frac{p^2(p+2)\lambda}{8} \qquad (5.66)$$

$$\varepsilon_o^{(1)} = -\frac{4}{(p+2)^2} - p(p+1)\,\lambda \qquad (5.67)$$

$$V_1^{(o)}(\rho) = 1 + \frac{4}{p(p+2)}\,\rho \qquad (n_r = o) \qquad (5.68)$$

For higher k the algebra becomes increasingly tedious. Moreover, one cannot determine beforehand as to how many exact solutions will obtain at a given k value.

EPILOGUE

The foregoing exposition has considered some elementary techniques in bound state theory. The results discussed are elementary. Their implications have been seen to be powerful and illuminating. It can be hoped that as the field of quarkonium spectroscopy develops, the general approach based on Feynmann-Hellmann theorem, virial theorem, etc., would find more and more applications. The relationship amongst power-law potentials also continues to find new and powerful applications (see, e.g., [35]). Another useful technique that we could not consider due to lack of space and time is that of semiclassical reasoning. The interested reader is referred to [1].

Our work shows the importance of worrying about the normalization factors. As we have seen in the last Chapter, in it, lies the key to the understanding of the quantum discontinuity phenomenon. An important challenge in this field is to propose a realizable model of such a phenomenon. We believe that the variation of the Killingbeck model that we have considered, allows us to achieve such a goal. A Wigner crystal provides the basic two-dimensional repulsive Coulomb interaction. A magnetic field perpendicular to the plane can generate an r^2 potential. An electric field in the plane generates a linear r term with an angular dependence. Thus, the whole potential is not separable as such. But if we focus attention in a narrow angular range in a suitable direction we may find "pockets" where the electrons may be trapped and display the desired phenomenon upon a suitable tuning and variation of the applied fields. This deserves to be tested by experimentalists.

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