CERN TH.4056/84

BOUNDS TO GREEN FUNCTIONS AND LOWER BOUNDS
TO THE SPECTRUM OF A POSITIVE HAMILTONIAN

A Recollection of Discussions with V.J. Glaser

R.A. Bertlmann^{*)}

CERN - Geneva

^{*)} Permanent address: Institute of Theoretical
Physics, University of Vienna, Boltzmanngasse,
A-1090 Vienna.

CERN TH.4056/84
November 1984

Vladimir Jurko Glaser left us in January of this year, and I feel sad and deeply sorry. I always will remember him teaching me physics, speaking in a very nice "alt-österreichisch" manner and producing formulae on the blackboard in his office at CERN for hours.

André Martin is organizing a collection of works to honour the memory of V.J. Glaser and I am very happy to contribute to it since I feel these discussions should not be lost.

The "sessions" on quantum mechanics I remember most; this is the part I want to recollect. Glaser has developed energy bounds - lower bounds to the spectrum of a positive Hamiltonian: first the "simple semi-classical" bound and second the "oscillator" bound. My little contribution to that consisted of a collaboration to improve these bounds. We obtained the "improved semi-classical" bound and the "improved oscillator" bound (or "perturbation" bound). For the latter, in spring 1983 there already existed a common manuscript which we intended to publish.

In summarizing these bounds, I will explain in Chapter 1 the "simple semi-classical" bound and in Chapter 2 the "improved semi-classical" bound. Chapter 3 contains the "oscillator" bound and Chapter 4 the "improved oscillator" bound for which I use the joint manuscript. Finally in Chapter 5 I also want to present Glaser's investigations of powerlike moments.

ENERGY BOUNDS

An upper bound to the energy of a Hamiltonian can easily be obtained from a variational principle¹⁾ or by use of so-called moments²⁾. A lower bound, however, is more difficult to obtain and will be of interest in this presentation.

1. "Simple semi-classical" bound

In order to study the spectrum of the Hamiltonian

$$H = \frac{P^2}{m} + V, \quad V \geq 0 \quad (1.1)$$

let us begin to study the exponential Green function - the partition function.

Then the following inequality is true³⁾:

$$Z(t) = \text{tr} e^{-(\frac{p^2}{m} + V)t} \leq \text{tr} e^{-\frac{p^2}{m}t} e^{-Vt} = Z_{\text{class}}(t), \quad t > 0. \quad (1.2)$$

This corresponds to the classical case where the commutator $[p^2, V(x)] = 0$ vanishes.

Evaluating now the classical Green function in (d-dimensional) x-space

$$Z_{\text{class}}(t) = \int d^d x \langle x | e^{-\frac{p^2}{m}t} | x \rangle e^{-V(x)t} \quad (1.3)$$

$$= \left(\frac{m}{4\pi t}\right)^{\frac{d}{2}} \int d^d x e^{-V(x)t}, \quad (1.4)$$

and assuming V to be homogenous of degree s $[V(t^{1/s}x) = t(V(x))]$, then the t-dependence of Z_{class} is explicitly given by:

$$Z_{\text{class}}(t) = m^{\frac{d}{2}} t^{-f} K_d \quad (1.5)$$

where

$$K_d = \int \frac{d^d y}{(4\pi)^{d/2}} e^{-V(y)} \quad (1.6)$$

and

$$f = d \frac{s+2}{2s}. \quad (1.7)$$

For a power law potential, our special case of interest

$$V = \lambda |x|^s \quad (1.8)$$

the result for (1.6), is especially simple:

$$K_d = \frac{\Omega_d}{(4\pi)^{d/2}} \lambda^{-\frac{d}{s}} \frac{1}{d} \Gamma\left(\frac{d}{s} + 1\right) \quad (1.9)$$

and Ω_d denotes the d-dimensional angular space (e.g., $\Omega_1=2$, $\Omega_2=2\pi$, $\Omega_3=4\pi, \dots$).

Now the question is how to get a lower bound on the spectrum of H. Let us again start with the inequality

$$Z_{\text{class}}(t) \geq \text{tr} e^{-Ht} = \sum_{k=1}^{\infty} e^{-E_k t} \geq n e^{-E_n t} \quad (1.10)$$

(Recall that all eigenvalues are assumed to be ordered and $V \geq 0$). Then lower bounds to the energy of H are

$$\frac{1}{t} \ln \frac{n}{Z_{\text{class}}(t)} \leq E_n \quad (1.11)$$

for all $t > 0$. The best bound is given by the supremum over t

$$E_n^{\text{simple class}} = \sup_t \left[\frac{1}{t} \ln \frac{n}{Z_{\text{class}}(t)} \right] \leq E_n \quad (1.12)$$

Let us calculate Eq. (1.12). By defining a variable τ

$$\tau = t \left(\frac{n}{m^{d/2} K_d} \right)^{1/f} \quad (1.13)$$

the supremum occurs at $\tau = e$ and finally yields the result for the "simple semi-classical" bound

$$E_n^{\text{simple class}} = m^{-\frac{s}{2+s}} \frac{f}{e} \left(\frac{n}{K_d} \right)^{1/f} \leq E_n \quad (1.14)$$

with γ and K_d given by Eqs. (1.7) and (1.6) (recall that n labels here all ordered levels including angular momentum).

For the example of a power law potential, Eq. (1.8), we insert (1.9) and the bound has the form

$$E_n^{\text{simple class}} = \lambda^{\frac{2}{2+s}} m^{-\frac{s}{2+s}} \frac{d}{e} \frac{2+s}{2s} \left[\frac{(4\pi)^{d/2}}{\Omega_d} \frac{d}{\Gamma(\frac{d}{2}+1)} n \right]^{\frac{2s}{2+s} \frac{1}{d}} \leq E_n \quad (1.15)$$

This bound has the right scaling properties for λ and m of a power law potential.

For the one-dimensional case we just put $d=1$ in formula (1.15). But for s -waves ($\ell=0$) in three dimensions which we are more interested in, we take as a rule $d=1$ in the Green function and $d=3$ in phase space

$$E_{n,\ell=0}^{\text{simple class}} = \lambda^{\frac{2}{2+s}} m^{-\frac{s}{2+s}} \frac{1}{e} \frac{2+s}{2s} \left(\frac{2\sqrt{\pi}}{\Gamma(\frac{1}{s}+1)} n_{\ell=0} \right)^{\frac{2s}{2+s}} \leq E_{n,\ell=0}. \quad (1.16)$$

Bound (1.16) has the same n -dependence (for large n) in terms of s as the WKB formula of Quigg and Rosner⁴⁾ [see Eq. (2.19)].

The numerical values of the ground states we have listed for several power law potentials on Table 1. However, these results are rather far from their exact values; the "simple classical approximation" was just too crude. But as we demonstrate in the next chapter, this bound can be improved considerably, thus becoming meaningful.

2. "Improved semi-classical" bound

Here we begin with a Hamiltonian (in three dimensions) having definite angular momentum ℓ

$$H_{\ell} = -\frac{1}{m} \frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{mr^2} + V(r) = \frac{p_{\ell}^2}{m} + V(r), \quad V \geq 0 \quad (2.1)$$

and we consider the inequality for Green functions for the ℓ -th wave

$$Z_{\ell}(t) = \text{tr} e^{-H_{\ell}t} Q_{\ell} \leq \text{tr} e^{-\frac{p_{\ell}^2}{m}t} e^{-Vt} Q_{\ell} = Z_{\ell}^{\text{class}}(t). \quad (2.2)$$

Q_{ℓ} is the projection operator onto a state with angular momentum ℓ .

Calculating the "classical" trace, we get

$$Z_{\ell}^{\text{class}}(t) = (2\ell+1) \cdot \int_0^{\infty} dr r^2 G_{\ell}^{(0)}(r, r) e^{-V(r)t}, \quad (2.3)$$

where $G_{\ell}^{(0)}$ is the free Green function for the ℓ -th wave

$$G_{\ell}^{(0)}(r, r') = \langle r | e^{-\frac{p_{\ell}^2}{m}t} | r' \rangle \quad (2.4)$$

$$= \left(\frac{m}{4\pi t} \right)^{\frac{3}{2}} e^{-\frac{m}{4t}(r^2 + r'^2)} a_{\ell}(s), \quad (2.5)$$

$$a_\ell(s) = 4\pi s^\ell \left(\frac{1}{s} \frac{d}{ds} \right)^\ell \frac{\hbar s}{s}, \quad (2.6)$$

$$s = \frac{m r r'}{2t}. \quad (2.7)$$

For s-waves ($\ell=0$) the "classical" Green function simplifies to

$$Z_{\ell=0}^{\text{class}}(t) = \left(\frac{m}{4\pi t} \right)^{\frac{1}{2}} \left[\int_0^\infty dr e^{-V(r)t} - \int_0^\infty dr e^{-\frac{m}{t}r^2} e^{-V(r)t} \right]. \quad (2.8)$$

Neglecting the second integral, we recover the "simple classical" result from Chapter 1; including it [which diminishes $Z_{\ell=0}^{\text{class}}(t)$] we certainly improve all bounds.

Now we want to calculate improved energy bounds for the example of power law potentials, Eq. (1.8). Then Eq. (2.8) turns into

$$Z_{\ell=0}^{\text{class}}(t) = m^{\frac{1}{2}} t^{-\delta} K - J_s(t) \quad (2.9)$$

where

$$\delta = \frac{2+s}{2s} \quad (2.10)$$

$$K = \frac{1}{2\sqrt{\pi}} \lambda^{-\frac{1}{s}} \Gamma\left(\frac{1}{s}+1\right) \quad (2.11)$$

(recall the rule of the preceding chapter: $d=1$ in the Green function and $d=3$ in phase space)

and
$$J_s(t) = \left(\frac{m}{4\pi t} \right)^{\frac{1}{2}} \int_0^\infty dr e^{-t\lambda r^s - \frac{m}{t}r^2}. \quad (2.12)$$

For the energy bound we have to calculate supremum (1.12) together with the "improved classical" Green function (2.9). But instead of maximizing numerically over all t , we calculate a "best" bound with that t which maximizes the "simple classical" result. A quick investigation of integral (2.12) shows that this choice is already nearly best.

The supremum of (1.12) occurs at ($\tau=e$)

$$t_m = e \left(\frac{n_{\ell=0}}{m^{1/2} K} \right)^{-\frac{1}{f}} \quad (2.13)$$

so that the correction, the second integral, then is

$$J_s(t_m) = \frac{1}{2\sqrt{\pi} a} \int_0^{\infty} dx e^{-x^s - \frac{x^2}{a^2}}, \quad (2.14)$$

with

$$a = \frac{e^{\delta} \Gamma(\frac{1}{s} + 1)}{2\sqrt{\pi} n_{\ell=0}} \quad (2.15)$$

For a "best" energy bound we calculate bound (1.11) at t_m by inserting $Z_{\lambda=0}^{\text{class}}(t_m)$. Finally we want to present this "improved semi-classical" bound in the following way:

$$E_{n,\ell=0}^{\text{improved class}} = E_{n,\ell=0}^{\text{simple class}} \cdot k_s \leq E_{n,\ell=0} \quad (2.16)$$

where $E_{n,\ell=0}^{\text{simple class}}$ is given by Eq. (1.16) and the correction factor k_s turns out to be

$$k_s = 1 - \ln \left(1 - \frac{e^{\delta}}{n_{\ell=0}} J_s(t_m) \right)^{\frac{1}{f}} \quad (2.17)$$

We have now computed the correction factor k_s for several potentials and have listed the results for ground states in Table 1. The improvement is quite large: k_s is approximately a factor 2.

In summary, bound (2.16), which corresponds to a "semi-classical" approximation, lies always below the exact quantum result. It is easy to obtain and turns out numerically quite well for "moderate" potentials. However, bound (2.16) is not as good as the bound for ground states of Barnes, Brascamp and Lieb⁵⁾ who work with a more sophisticated method (optimizing Young's inequality). For comparison we recall their formula

$$E^{BBL} = \lambda^{\frac{2}{2+s}} m^{-\frac{s}{2+s}} d^{\frac{2+s}{2s}} \left(\frac{\Gamma(\frac{d}{2} + 1)}{\Gamma(\frac{d}{s} + 1)} \right)^{\frac{2s}{2+s} \cdot \frac{1}{d}} e^{\frac{s-2}{s+2}} \leq E_1 \quad (2.18)$$

(d=3 in three dimensions) and list their results in Table 1.

Finally, we also want to compare the "semi-classical" result with a WKB formula derived by Quigg and Rosner⁴⁾:

$$E_{n, \ell=0}^{WKB} = \lambda^{\frac{2}{2+s}} m^{-\frac{s}{2+s}} \left[\frac{(2+s)\sqrt{\pi} \Gamma(\frac{2+s}{2s})}{\Gamma(\frac{1}{s})} \cdot (n_{\ell=0} - \frac{1}{4}) \right]^{\frac{2s}{2+s}}. \quad (2.19)$$

Formula (2.19) appears as a lower bound at least empirically, and as shown in Table 1 it is closest to the exact result.

3. "Oscillator" bound

The idea is the following: one starts with a positive Hamiltonian (1.1) and splits it into a comparison Hamiltonian H_0 and a positive potential V_1

$$H = H_0 + V_1, \quad V_1 \geq 0. \quad (3.1)$$

Applying to the operator inequality

$$H_0 \subseteq H \quad (3.2)$$

the minimax principle¹⁾, one quickly obtains lower bounds to the spectrum of H

$$E_n^0 \leq E_n \quad (3.3)$$

[E_n^0 (E_n^0) are the ordered eigenvalues of $H(H_0)$]. Of course H_0 should be chosen such that the energies E_n^0 are known. A quick and simple choice is the harmonic oscillator

$$H_0 = \frac{p^2}{m} + \frac{m\omega^2}{4} x^2 - C_\omega \quad (3.4)$$

Let us calculate the bounds for the example of power law potentials, Eq. (1.8). Then the constant C_ω in (3.4) is determined by the positivity condition

$$V_1 = \lambda |x|^s - \frac{m\omega^2}{4} x^2 + C_\omega \geq 0 \quad (3.5)$$

Taking the minimal shift yields

$$C_\omega = \frac{s-2}{2s} \left(\frac{1}{s\lambda} \right)^{\frac{2}{s-2}} \left(\frac{m}{2} \right)^{\frac{s}{s-2}} \omega^{\frac{2s}{s-2}} \quad (3.6)$$

Now the minimal principle, Eq. (3.3), imposes the lower bound [in three dimensions, s-waves ($\ell=0$)]

$$E_{n,\ell=0}^0 = \omega \left(2(n_{\ell=0} - 1) + \frac{3}{2} \right) - C_\omega \leq E_{n,\ell=0} \quad ; \quad n=1,2,\dots \quad (3.7)$$

where ω is still free to be chosen. For a best bound one chooses the supremum over ω which results in the following "oscillator" bound

$$E_{n,\ell=0}^{osc} = \lambda^{\frac{2}{2+s}} m^{-\frac{s}{2+s}} 2^{\frac{2s}{2+s}} \left(\frac{s}{2} + 1 \right) \left(\frac{2}{s} \right)^{\frac{s}{2+s}} \left(n_{\ell=0} - \frac{1}{4} \right)^{\frac{2s}{2+s}} \leq E_{n,\ell=0} \quad (3.8)$$

That is a simple lower bound for $s > 2$. For $s < 2$, however, the inequalities (3.2), (3.3) and (3.5) change and formula (3.8) becomes an upper bound to E_n . Note that bound (3.8) has the correct scaling law in λ and m for power law potentials and it has exactly the same n -dependence as the WKB-formula of Quigg and Rosner⁴⁾, Eq. (2.19). Furthermore, it coincides for the ground state with a bound of Baumgartner⁶⁾ derived on different grounds [see Eq. (24) in Ref. 6)].

We have listed the numerical results of "oscillator" bound (3.8) for several potentials in Table 1. For moderate potentials they are approximately within 20% of the exact result and lie below the "improved semi-classical" result (the region around the oscillator $s=2-3$ excluded). But we can also improve the "oscillator" bound. This can be achieved by a perturbation approach and will be discussed in the next chapter.

4. "Improved oscillator" bound or "perturbation" bound

In the following we will construct a perturbation procedure - inequalities - for the exponential Green function from which we derive energy bounds.

The Hamiltonian we write as

$$H_\lambda = H_0 + \lambda V, \quad V \geq 0 \quad (4.1)$$

where λ is some coupling constant.

The exponential Green function

$$Z_\lambda(t) = \langle x | e^{-H_\lambda t} | y \rangle, \quad t > 0 \quad (4.2)$$

can be written as the Laplace transform of a positive measure⁷⁾

$$Z_\lambda(t) = \int_0^\infty e^{-\lambda s} d\mu_t(s), \quad d\mu_t(s) \geq 0. \quad (4.3)$$

Then for any real polynomial

$$P(s) = \sum_{\mu=0}^n a_\mu s^\mu, \quad a_\mu \text{ real} \quad (4.4)$$

the moments are positive

$$P^2\left(-\frac{\partial}{\partial \lambda}\right) Z_\lambda = \int_0^\infty P^2(s) e^{-\lambda s} d\mu_t(s) \geq 0 \quad (4.5)$$

producing such a system of positive inequalities

$$\sum_{\mu, \nu} a_\mu a_\nu Z_\lambda^{(\mu+\nu)} \geq 0 \quad (4.6)$$

where

$$Z_\lambda^{(\mu)} = \left(-\frac{\partial}{\partial \lambda}\right)^\mu Z_\lambda.$$

This implies that all principal determinants are positive; let us choose two systems.

First system:

$$D_n(z_\lambda) = \begin{vmatrix} z_\lambda^{(0)} & z_\lambda^{(1)} & \dots & z_\lambda^{(n)} \\ z_\lambda^{(1)} & \dots & & \\ \vdots & & & \\ z_\lambda^{(n)} & \dots & & z_\lambda^{(2n)} \end{vmatrix} \geq 0 \quad (4.7)$$

Second system:

$$\tilde{D}_{n+1}(z_\lambda) = \begin{vmatrix} z_\lambda^{(1)} & z_\lambda^{(2)} & \dots & z_\lambda^{(n+1)} \\ z_\lambda^{(2)} & \dots & & \\ \vdots & & & \\ z_\lambda^{(n+1)} & \dots & & z_\lambda^{(2n+1)} \end{vmatrix} \geq 0 \quad (4.8)$$

Calculating now these systems to a given order, we derive "perturbation" bounds to the Green function $Z_\lambda(t)$, Eq. (4.2).

$D_1(z_\lambda) \geq 0$ leads to a lower bound

$$Z_\lambda^{\text{low}}(t) = Z_0(t) e^{-\frac{|\dot{Z}_0|}{Z_0} \lambda} \leq Z_\lambda(t), \quad (4.9)$$

with

$$\dot{Z}_\lambda = -Z_\lambda^{(1)} < 0;$$

whereas $\tilde{D}_2(z_\lambda) \geq 0$ gives the upper bound which we are finally interested in:

$$Z_\lambda(t) \leq Z_0(t) [1 - K_\lambda(t)] = Z_\lambda^{\text{up}}(t), \quad (4.10)$$

where the correction term has the form

$$K_\lambda(t) = \frac{\dot{Z}_0^2}{Z_0 \ddot{Z}_0} \left[1 - e^{-\frac{\ddot{Z}_0}{|\dot{Z}_0|} \lambda} \right] \quad (4.11)$$

and

$$\ddot{Z}_0 = Z_0^{(2)}.$$

The Green functions can now be calculated in terms of unperturbed H_0 and potential V :

$$Z_0(t) = \langle x | e^{-H_0 t} | y \rangle \quad (4.12)$$

$$\dot{Z}_0(t) = - \int_0^t d\tau \langle x | e^{-H_0(t-\tau)} V e^{-H_0 \tau} | y \rangle \quad (4.13)$$

$$\ddot{Z}_0(t) = 2 \int_0^t \int_0^t d\tau_1 d\tau_2 \theta(\tau_1 - \tau_2) \langle x | e^{-H_0(t-\tau_1)} V e^{-H_0(\tau_1-\tau_2)} V e^{-H_0 \tau_2} | y \rangle. \quad (4.14)$$

For bounds of higher orders one just goes on in the algorithm.

Besides the more general interest of inequalities (4.9) and (4.10), they are useful for deriving bounds to the energy spectrum of Hamiltonian (4.1), especially to improve the simple "oscillator" bound from before.

To obtain a lower bound on the energy, we proceed very much as in Chapter 1 and recall Eq. (1.10). Inequalities (4.9) and (4.10) are valid for any Z_λ and therefore also for the trace and for $\lambda=1$. Therefore we obtain the inequality:

$$n e^{-E_n t} \leq Z_1(t) \leq Z_1^{up}(t) \quad (4.15)$$

which leads to the lower "perturbation" bound

$$E_n^{low} = \sup_t \left[\frac{1}{t} \ln \frac{n}{Z_1^{up}(t)} \right] \leq E_n, \quad (4.16)$$

where Z_1^{up} is given by Eqs. (4.10) and (4.11).

As an illustrative example we have calculated the bound (4.16) for the quartic potential in one dimension

$$v(x) = x^4. \quad (4.17)$$

Instead of perturbing the free motion $p^2/2$ by potential (4.17), we prefer to perturb a harmonic oscillator by the corresponding double well and improve in this way the simple "oscillator" bound (for one dimension) of Chapter 3.

We define a harmonic oscillator ($m = 2$)

$$H_0 = \frac{p^2}{2} + \frac{\omega^2}{2} x^2 - \frac{\omega^4}{16} \quad (4.18)$$

and a double well

$$V = \left(x^2 - \frac{\omega^2}{4} \right)^2, \quad (4.19)$$

where ω is still free at our disposal.

For the Green functions Z_0 , $\dot{Z}_0$ and $\ddot{Z}_0$, we have to evaluate the corresponding traces. For this, one can choose either the Fock-space by introducing Heisenberg operators or the x -space by working explicitly with the oscillator Green function. Now we follow the first method and demonstrate briefly the second in the appendix.

Introducing the creation and annihilation operator, the oscillator (4.18) can be written in the familiar form

$$H_0 = \omega N + g(\omega), \quad (4.20)$$

where $N = a^+ a$ is the particle number operator and $g(\omega)$ is a function

$$g(\omega) = \frac{\omega}{2} - \frac{\omega^4}{16}. \quad (4.21)$$

Expressing next the (imaginary) time evolution of the operator

$$x_\tau = e^{H_0 \tau} x e^{-H_0 \tau} \quad (4.22)$$

in terms of the creation operator a^+ and the annihilation operator a

$$x_\tau = \frac{1}{\sqrt{2\omega}} \left(a e^{-\omega \tau} + a^+ e^{\omega \tau} \right) \quad (4.23)$$

we are prepared to calculate all traces.

Z_0 is trivial

$$Z_0 = \text{tr} e^{-H_0 t} = e^{-g t} \text{tr} e^{-\omega N t} \quad (4.24)$$

$$= \frac{e^{-\frac{2}{\omega} \bar{x}}}{1-z}, \quad (4.25)$$

where $\bar{x} = \omega t$ and $z = e^{-\bar{x}}$.

For the first order perturbation

$$\dot{Z}_0 = -t \cdot \text{tr} e^{-H_0 t} \dot{V}(x) \quad (4.26)$$

we insert the double well (4.19) together with (4.23) (with $\tau=0$), then we have to evaluate a sum of terms like

$$\sum_{\nu} c_{\nu} \text{tr} e^{-\omega N t} N^{\nu} = \sum_{\nu} c_{\nu} \left(-\frac{\partial}{\partial \omega t}\right)^{\nu} \text{tr} e^{-\omega N t} \quad (4.27)$$

where c_{ν} are some constants. The result is

$$\dot{Z}_0(\omega, \bar{x}) = -Z_0(\omega, \bar{x}) \frac{\bar{x}}{4\omega^3(1-z)^2} \left[3(1+z)^2 - \omega^3(1-z^2) + \frac{\omega^6}{4}(1-z)^2 \right]. \quad (4.28)$$

The second order perturbation

$$\ddot{Z}_0 = 2 \int_0^t d\tau (t-\tau) \text{tr} e^{-H_0 t} V(x_{\tau}) V(x) \quad (4.29)$$

contains, besides (4.27), only simple integrals

$$\sum_{\nu} c_{\nu} \text{tr} e^{-\omega N t} N^{\nu} \int_0^t d\tau (t-\tau) e^{-\mu_{\nu} \omega t} \quad (4.30)$$

with μ_{ν} some constants and we would like to express the result in the following way:

$$\ddot{Z}_0(\omega, \bar{x}) = Z(\omega, \bar{x}) \frac{1}{128} \sum_{i=0}^4 I_i(\omega, \bar{x}), \quad (4.31)$$

$$\begin{aligned}
 \text{where} \\
 I_0 &= \frac{1}{2} \omega^6 \bar{x}^2 \\
 I_1 &= -4 \omega^3 \bar{x}^2 \frac{1+z}{1-z} \\
 I_2 &= \frac{4\bar{x}}{(1-z)^2} \left[\bar{x}(5 + 18z + 5z^2) + 4(1-z^2) \right] \\
 I_3 &= -\frac{48\bar{x}}{\omega^3(1-z)^3} \left[\bar{x}(1 + 11z + 11z^2 + z^3) + 4(1+z-z^2-z^3) \right] \\
 I_4 &= \frac{24\bar{x}}{\omega^6(1-z)^4} \left[3\bar{x}(1 + 20z + 54z^2 + 20z^3 + z^4) + \right. \\
 &\quad \left. + 4(7 + 20z - 20z^3 - 7z^4) \right] .
 \end{aligned} \tag{4.32}$$

Now we know Z_0 , $\dot{Z}_0$ and $\ddot{Z}_0$ explicitly and we calculate $Z_1^{\text{up}}(\omega, \bar{x})$ via (4.10) and (4.11) which we insert into (4.16) to obtain the lower energy bound. For the ground state we have

$$E_1^{\text{low}}(\omega, \bar{x}) = g(\omega) + \frac{\omega}{\bar{x}} \left[\ln(1 - e^{-\bar{x}}) - \ln(1 - K_1(\omega, \bar{x})) \right] \leq E_1 . \tag{4.33}$$

Instead of taking now in Eq. (4.33) the supremum over all ω and $\bar{x}$, we come rather close to it by choosing that $\omega(\omega_m = 2^{1/3})$ which maximizes the oscillator energy

$$E_1^{\text{osc}} = g(\omega_m) = 2^{1/3} \frac{3}{8} = 0.47247 . \tag{4.34}$$

This simple oscillator bound being the "oscillator" bound (for one dimension and $s=4$) of the preceding chapter, it can be improved now by the "perturbative" correction term. This term appears meaningful only for some "intermediate" $\bar{x}$ values. Let us choose $\bar{x} = 5.3$ so that we can safely neglect terms like $e^{-\bar{x}}$. This drastically simplifies the formula for K_1

$$K_1(\omega, \bar{x}) = \frac{C_1^2(\omega)}{C_2(\omega, \bar{x})} , \tag{4.35}$$

where

$$\begin{aligned} C_1(\omega) &= \frac{1}{4} \left(1 - \frac{\omega^3}{4} - \frac{3}{\omega^3} \right) \\ C_2(\omega, \bar{x}) &= \frac{1}{128} \left[\frac{\omega^6}{2} - 4\omega^3 + 20 \left(1 + \frac{4}{5\bar{x}} \right) - \frac{48}{\omega^3} \left(1 + \frac{4}{\bar{x}} \right) + \frac{72}{\omega^6} \left(1 + \frac{28}{3\bar{x}} \right) \right] \end{aligned} \quad (4.36)$$

In this approximation the lower bound turns out as

$$E_1^{\text{low, approx}}(\omega, \bar{x}) \Big|_{\substack{\omega = \omega_m \\ \bar{x} = 5.3}} = 2^{\frac{1}{3}} \frac{3}{8} (1 + 0.19535) = 0.56477 \quad (4.37)$$

and varies only little from the exact lower bound

$$E_1^{\text{low}}(\omega, \bar{x}) \Big|_{\substack{\omega = \omega_m \\ \bar{x} = 5.3}} = 2^{\frac{1}{3}} \frac{3}{8} (1 + 0.18520) = 0.55997 \quad (4.38)$$

We observe that the "perturbation" correction improves the simple "oscillator" result by 19% which is quite appreciable and even more than we could expect from such a perturbation procedure. However, bound (4.38) [or (4.37)] is still not excellent and about 16% below the exact value

$$E_1 = 0.66799 \quad (4.39)$$

obtained by numerical integration of the Schrödinger equation, the reason being that our reference energy, the oscillator energy (4.34) was still too small [29% below (4.39)].

Like in the "semi-classical" case we cannot compete with the bound of Barnes, Brascamp and Lieb⁵⁾ [see Eq. (2.18)] who get for our example

$$E^{\text{BBL}} = 0.63989 \quad (4.40)$$

and are only 4% below the exact value.

5. Perturbation inequalities to Green functions and convergence of power moments

During the last years, several authors²⁾ investigated quantities like

$$\langle x | (H+E)^{-N} | x \rangle \Big|_{x=0} = \sum_{n=1}^{\infty} (E_n + E)^{-N} |\psi_n(0)|^2 \quad (5.1)$$

which have an important analogue in relativistic field theory commonly known as QCD sum rules⁸⁾. Naturally the question arises under which conditions the power moments (5.1) converge. Some time ago, Grosse and Martin⁹⁾ proved that moments (5.1) converge for $N > 3/2$ but for potentials which can be integrated locally down to $|x| = 0$. This unfortunately excludes the important Coulomb potential. But within a WKB approximation the author¹⁰⁾ could include the Coulomb potential for $N > 3/2$. The final answer was given by Glaser who proved that moments (5.1) indeed converge for any potential where H is defined (no rotational symmetry necessary) and for $N > 3/2$ - the convergence condition of the free moment.

The proof is as follows. Let us study the exponential Green function

$$\langle x | e^{-Ht} | y \rangle = G_t(x, y) , \quad t > 0 \quad (5.2)$$

and consider two separate cases:

Case A where the potential is bounded from below

$$H = \frac{p^2}{2} + v(x) \quad (5.3)$$

and

$$v \geq \min v = v_0 . \quad (5.4)$$

Next v is split into two parts:

$$v = V_0 + V \quad (5.5)$$

with

$$V_0 < 0 , \quad V \geq 0 \quad (5.6)$$

and

$$H_0 = \frac{p^2}{2} + V_0 \quad (5.7)$$

will be regarded as the unperturbed part of the total Hamiltonian

$$H = H_0 + V . \quad (5.8)$$

Then operator H satisfies the well-known integral equation

$$e^{-Ht} = e^{-H_0 t} - \int_0^t e^{-H_0(t-\tau)} V e^{-H\tau} d\tau, \quad t > 0 \quad (5.9)$$

which can be iterated several times, producing such upper and lower bounds to the Green function (5.2) in terms of even and odd perturbations (recall that all factors are positivity preserving, $V \geq 0$)

$$\langle x | \sum_{m=0}^{2n+1} I_m(t) | y \rangle \leq \langle x | e^{-Ht} | y \rangle \leq \langle x | \sum_{m=0}^{2n} I_m(t) | y \rangle, \quad (5.10)$$

where

$$I_m(t) = (-1)^m \int_0^t d\tau_1 d\tau_2 \dots d\tau_m \theta(\tau_1 \geq \tau_2 \geq \dots \geq \tau_m) \times \\ \times e^{-H_0(t-\tau_1)} V e^{-H_0(\tau_1-\tau_2)} V \dots e^{-H_0(\tau_{m-1}-\tau_m)} V e^{-H_0\tau_m} \quad (5.11)$$

Inequalities (5.10) are of more general interest. We concentrate, however, on Green functions with power N . A multiplication of (5.10) by $e^{-Et} t^{N-1}$ generates the following lower and upper bounds

$$\frac{1}{\Gamma(N)} \int_0^\infty dt e^{-Et} t^{N-1} \sum_{m=0}^{2n+1} \langle x | I_m(t) | y \rangle \leq \langle x | (H+E)^{-N} | y \rangle \quad (5.12)$$

and

$$\langle x | (H+E)^{-N} | y \rangle \leq \frac{1}{\Gamma(N)} \int_0^\infty dt e^{-Et} t^{N-1} \sum_{m=0}^{2n} \langle x | I_m(t) | y \rangle. \quad (5.13)$$

To investigate the convergence condition for moments (5.1), it is enough to choose $n=0$ in (5.13)

$$\langle x | (H+E)^{-N} | x \rangle \leq \frac{1}{(2\pi)^{\frac{d}{2}} (E+v_0)^{N-\frac{d}{2}}} \frac{\Gamma(N-\frac{d}{2})}{\Gamma(N)} < \infty. \quad (5.14)$$

The power moments converge if

$$N > \frac{d}{2} \quad (5.15)$$

(d is dimension of x -space) and

$$E > -v_0 = -\min v. \quad (5.16)$$

Case B where the potential is unbounded (v contains a negative singular part for $x \rightarrow 0$). Then the potential is split into

$$v = V_0 - V_- \quad (5.17)$$

with

$$V_0 \geq 0, \quad V_- \geq 0 \quad (5.18)$$

and as before

$$H_0 = \frac{p^2}{2} + V_0 \quad (5.19)$$

will be the unperturbed part of

$$H = H_0 - V_- \quad (5.20)$$

Iterating now the integral Eq. (5.9) n times (replacing V by $-V_-$) generates a lower bound

$$\sum_{m=0}^n \langle x | I_m(t) | y \rangle \leq \langle x | e^{-Ht} | y \rangle = G_t(x, y) \quad (5.21)$$

One can prove that this perturbation series converges to the exact answer if $V_- \in L_p(\mathbb{R}^n)$ for some suitable $p \geq 1$.

For an upper bound to $G_t(x, y)$, we recall that $\langle x | e^{-H_0 t} | y \rangle$ is now bounded from above by the free Green function or some suitably chosen harmonic oscillator Green function, and that one may consider the integral equation

$$G_t(x, y) = F_t(x, y) + \int_0^t d\tau \int dz F_{t-\tau}(x, z) G_\tau(z, y) V_-(z), \quad t > 0. \quad (5.22)$$

where $F_t(x, y)$ is the harmonic oscillator Green function given explicitly in the Appendix [see Eqs. (A.1) to (A.4)].

Introducing the (positive) supremum

$$s(t) = \sup_{x, y} \frac{G_t(x, y)}{F_t(x, y)} \quad (5.23)$$

Eq. (5.22) turns into an inequality

$$G_t(x, y) \leq F_t(x, y) + \int_0^t s(\tau) \int dz F_{t-\tau}(x, z) F_\tau(z, y) V_-(z) \quad (5.24)$$

and applying the Hölder inequality to the z -integration

$$G_t(x, y) \leq F_t(x, y) + \|V_-\|_p \int_0^t s(\tau) \|F_{t-\tau}(x, \cdot) F_\tau(\cdot, y)\|_q \quad (5.25)$$

with $p^{-1} + q^{-1} = 1$.

Calculating now the oscillator norm on the r.h.s. yields

$$G_t(x, y) \leq F_t(x, y) + \|V_-\|_p \int_0^t s(\tau) q^{-\frac{d}{2\tau}} N^{\frac{1}{p}}(t) N^{-\frac{1}{p}}(t-\tau) N^{-\frac{1}{p}}(\tau) F_t(x, y) \quad (5.26)$$

[$N^{-1}(t)$ is defined in the appendix, Eq. (A.3).]

Dividing the inequality (5.26) by $F_t(x, y)$, one obtains an integral inequality for $s(t)$ which only makes sense for $p > d/2$. Without trying to solve it explicitly $G_t(x, y)$ will have a bound of the form

$$G_t(x, y) \leq c e^{\kappa t} F_t(x, y) \quad , \quad (5.27)$$

where c and κ are positive constants.

Then for a Green function of power N the bound is of the form

$$\langle x | (H + E)^{-N} | y \rangle \leq \frac{c}{\Gamma(N)} \int_0^\infty dt e^{-(E - \kappa)t} t^{N-1} F_t(x, y) \quad (5.28)$$

so that the moment ($y=x$) is again finite, provided

$$N > \frac{d}{2} \quad , \quad E > \kappa \quad (5.29)$$

and

$$\|V_-\|_{\frac{d}{2} + \epsilon} < \infty \quad . \quad (5.30)$$

Condition (5.30) also includes potentials singular like

$$V \sim -\frac{\alpha}{r^\beta} \quad , \quad \beta < 2 \quad . \quad (5.31)$$

APPENDIX

Here we briefly demonstrate the calculation of Z_0 , $\dot{Z}_0$ and $\ddot{Z}_0$ in x-space with the help of the oscillator Green function

$$F_t(x, y) = \langle x | e^{-\left(\frac{p^2}{2} + \frac{\omega^2}{2} x^2 - \frac{d}{2} \omega\right) t} | y \rangle \quad (A.1)$$

$$= N^{-1}(t) e^{-\left\{\frac{\omega}{4} a(t) (x-y)^2 + \frac{\omega}{4} a^{-1}(t) (x+y)^2\right\}} \quad (A.2)$$

where

$$N^{-1}(t) = \left[\frac{\pi}{\omega} (1 - e^{-2\omega t}) \right]^{\frac{d}{2}} \quad (A.3)$$

and

$$a(t) = (1 + e^{-\omega t}) / (1 - e^{-\omega t}) \quad (A.4)$$

(d is the dimension).

Z_0 and $\dot{Z}_0$, Eqs. (4.24) and (4.26), are quickly calculated since the traces contain only simple Gaussian integrals like

$$\int_0^\infty e^{-cx^2} x^{2n} dx \quad ; \quad n = 0, 1, 2, \dots \quad (A.5)$$

The second order perturbation $\ddot{Z}_0$, Eq. (4.29), now contains two oscillator Green functions

$$\ddot{Z}_0 = 2 e^{-g(\omega)t} \int_0^t d\tau (t-\tau) \iint_{-\infty}^{\infty} dx dy F_{t-\tau}(x, y) F_{\tau}(y, x) V(x) V(y) \quad (A.6)$$

which involve double Gaussian integrals like

$$\iint_{-\infty}^{\infty} dx dy e^{-bx^2} e^{-cy^2} x^{2m} y^{2n} \quad ; \quad \begin{matrix} m = 0, 1, 2, \dots \\ n = 0, 1, 2, \dots \end{matrix} \quad (A.7)$$

and are also easy to compute. b and c are functions in $e^{-\omega t}$ so that the remaining τ integration is trivial and leads to results (4.31) and (4.32).

TABLE

s	exact C ₁ (s)	osc C ₁ (s)	simple class C ₁ (s)	k _s	improved class C ₁ (s)	WKB C ₁ (s)	BBL C ₁ (s)
0.5	1.8334	1.9398*	1.1563	1.4310	1.6547	1.8117	1.7782
1	2.3381	2.4764*	1.2829	1.6458	2.1114	2.3203	2.3067
2	3.0000	3.0000	1.4715	1.8257	2.6865	3.0000	3.0000
3	3.4506	3.1886	1.6034	1.8966	3.0410	3.4412	3.4218
4	3.7997	3.2451	1.7001	1.9327	3.2859	3.7519	3.6999
5	4.0892	3.2463	1.7739	1.9545	3.4670	3.9828	3.8950
6	4.3386	3.2237	1.8319	1.9692	3.6073	4.1612	4.0385
7	4.5587	3.1913	1.8787	1.9798	3.7195	4.3032	4.1482
14	5.6362	2.9634	2.0546	2.0145	4.1390	4.8237	4.5141
∞	9.8696	2.2500	2.3115	2.0585	4.7581	5.5517	4.9296

We have compared the several bounds with the exact ground state energies of power law potentials (1.8). We have listed in the first column the exact energies which are obtained by numerical integration of the Schrödinger equation, in the second the "oscillator" bounds (3.8), in the third the "simple semi-classical" bounds (1.16), in the fourth the correction factor (2.17), in the fifth the "improved semi-classical" bounds (2.16), in the sixth the WKB formula of Quigg and Rosner⁴⁾, Eq. (2.19), and in the seventh the bounds of Barnes, Brascamp and Lieb⁵⁾, Eq. (2.18). We have always plotted the scaled energies

$$C_1(s) = E_1 \cdot \lambda^{-\frac{2}{2+s}} m^{\frac{s}{2+s}}.$$

The stars * mean upper bounds.

REFERENCES

- 1) W. Thirring, A Course in Mathematical Physics, Vol. 3, Springer Verlag.
- 2a) J.S. Bell and R.A. Bertlmann, Nucl. Phys. B177 (1981) 218.
- 2b) R.A. Bertlmann, Phys. Lett. 122B (1983) 417.
- 2c) B. Durand, L. Durand and J.B. Whitenton, Phys. Lett. 124B (1983) 410; Phys. Rev. D28 (1983) 597 and 607.
- 2d) P. Pascual, E. de Rafael and R.A. Bertlmann, "QCD-like sum rules in quantum mechanics", to be published.
- 3a) S. Golden, Phys. Rev. 137 (1965) B1127.
- 3b) K. Symanzik, J. Math. Phys. 6 (1965) 1155.
- 3c) C.J. Thompson, J. Math. Phys. 6 (1965) 1812.
- 3d) M. Breiteneker and H.R. Grümmer, Comm. Math. Phys. 26 (1972) 276.
- 3e) M.B. Ruskai, Comm. Math. Phys. 26 (1972) 280.
- 4) C. Quigg and J.L. Rosner, Phys. Rep. 56 (1979) 167.
- 5) J.F. Barnes, H.J. Brascamp and E.H. Lieb, Studies in Mathematical Physics, eds. E.H. Lieb, B. Simon and A.S. Wightman, Princeton University Press 1976, p. 83.
- 6) B. Baumgartner, J. Phys. A: Math. Gen. 12 (1979) 459.
- 7) D. Bessis, P. Moussa and M. Villani, J. Math. Phys. 16 (1975) 2318.
- 8) M.A. Shifman, A.I. Vainshtein and V.I. Zakharov, Nucl. Phys. B147 (1979) 385, 448, 519.
- 9) H. Grosse and A. Martin, Nucl. Phys. B148 (1979) 413.
- 10) R.A. Bertlmann, Acta Phys. Austriaca 53 (1981) 305.