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THEORY OF THE INVERSE PROBLEM FOR CONFINING POTENTIALS

I. -- ZERO ANGULAR MOMENTUM

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A B S T R A C T

We prove that if the sequence of $\ell = 0$ energy levels of a particle in a spherically symmetric confining potential is known, together with the magnitudes of the corresponding wave functions at the origin, the potential is uniquely determined.

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1. INTRODUCTION

The description of the recently discovered particles J/ψ and T as quark-antiquark bound states interacting by a static potential has met considerable success¹⁾. The explanation and the prediction of the various energy levels is very impressive, and even though we should have had faith to believe in quarks before that discovery, we are now like Thomas and we have no choice but to believe! The potentials used by phenomenologists do not allow the quarks to escape, they contain an ad hoc "confining" force²⁾. Fortunately, one can convince oneself that the qualitative features of the model are not too sensitive to the details of the potential³⁾. This is nice for the model, but at a later stage one would like to work backwards and try to get the potential from the energy levels of the J/ψ , for instance, and, possibly, the wave functions at the origin, which are, in principle, known, because they appear in the expression of the leptonic width by Van Royen and Weisskopf⁴⁾ (notice, however, that the charge of the quarks and the colour properties must be known in advance!).

This program has been already undertaken in a practical way by Quigg, Rosner and Thacker⁵⁾ (QRT). Maybe it is worth summarizing their work right now. First they consider one-dimensional confining potentials symmetric with respect to the origin and they solve an approximate inverse problem: they give themselves the first n levels, choose a zero of energy somewhere between the n^{th} level and the $(n+1)^{\text{th}}$ level, and solve the inverse problem as if the potential was vanishing at infinity. The reflection coefficient at positive energies, which is needed to solve the classical one-dimensional inverse scattering problem, is set equal to zero and this makes the solution of the problem remarkably simple, because the potential then originates from a pure superposition of solitons. The hope is, that by increasing n one will get a potential closer and closer to the true one, and, although this is not yet demonstrated [neither in Ref. 5), nor here!] mathematically, QRT have made very impressive numerical experiments with known potentials, such as the harmonic oscillator, the linear potential, etc., in which one sees a very rapid convergence with n . In the second part of their work they deal with radial potentials $V(r)$, noticing that if one uses the reduced wave function $u = r\psi$, the energy levels coincide with the odd parity levels inside a symmetric one-dimensional potential $V(|x|)$. The even levels are missing, but there is extra information because, from the leptonic widths, $|u_1'(0)|$, the derivative of u at the origin is known. For small n , the algebraic equations relating the missing energies and $|u_1'(0)|$ can be solved numerically.

The problems of principle remain, however, and they are:

- 1) Does the knowledge of the infinite sequence of $\ell = 0$ energy levels E_i and $|u_i'(0)|^2$ fix uniquely the potential?
- 2) Can one prove, in the one-dimensional case, that the QRT procedure does converge?
- 3) Is there a systematic procedure to obtain the even parity energy levels in a symmetric potential from the knowledge of E_i and $|u_i'(0)|$, associated to the odd levels, which are the physical ones.

We have been able to answer positively 1) and 3) with, however, the unpleasant assumption that $V(r)$ is integrable at $r = 0$. This assumption which unfortunately excludes the Coulomb case as well as the behaviour $(r|\ln r|)^{-1}$, preferred by QCD adepts, is also hidden in QRT, 2) has not been answered yet. It is a perfect problem for a mathematical physicist.

To solve the problem we have two possibilities. The first one is to use as much as possible previous work on the subject which is well summarized in the review paper of Levitan and Gasymov⁶⁾. In this work the inverse problem is solved for confining potentials with the "wrong" boundary condition, i.e., imposing to $u(r)$ the condition

$$u'(r=0) = h u(r=0), \quad h \text{ finite} \quad (1)$$

and in particular $h = 0$, while we are interested in the case $u(r=0) = 0$. We shall show, however, that by giving a positive answer to question No. 3), it is possible to go from one problem to the other.

We have, however, also tried to avoid completely the use of the standard artillery of the inverse scattering problem, and succeeded at the price of an extra, hopefully "technical" assumption, that the zeros of the difference between two acceptable potentials have no accumulation points at finite r .

There are other inverse problems connected with confining potentials. For instance, what happens if one knows all ground state energies for increasing angular momentum. Such a problem will be considered in a forthcoming paper. Next comes the question of compatibility when the whole spectrum for all angular momenta is known.

2. SOME INFORMATION FROM THE LEVITAN-GASYMOV (LG) REVIEW

LG study the inverse problem for the spectrum of the differential operator on $0 \leq r < \infty$

$$-u'' + (V-E)u = 0 \quad (2)$$

with the boundary condition (1); but it will be sufficient to restrict ourselves to the case $h = 0$ or

$$u'(r=0, E) = 0. \quad (3)$$

The solution normalized to unity at the origin will be called $\varphi(r, E)$:

$$\varphi(r=0, E) = 1. \quad (4)$$

To Eq. (2) with boundary condition (3) is associated a spectral function $\rho(E)$, which plays a role in completeness properties, if $V(r)$ is locally integrable. Given $f(r)$ real square integrable, one can define

$$F(E) = \lim_{N \rightarrow \infty} \int_0^N dr f(r) \varphi(r, E), \quad (5)$$

then

$$\int_{-\infty}^{+\infty} d\rho(E) (F(E))^2 = \int_0^{\infty} dr (f(r))^2. \quad (6)$$

If $V(r)$ in addition goes to ∞ for $r \rightarrow \infty$, the spectrum is purely discrete and we have

$$d\rho(E) = dE \sum_{i=1}^{\infty} \gamma_i' \delta(E - E_i') \quad (7)$$

where the E_i' are the eigenvalues of (2) with condition (3). The normalizing constants γ_i' are given by

$$(\gamma_i')^{-1} = \int_0^{\infty} dr \varphi^2(r, E_i') \quad (8)$$

In the next section we shall give another interpretation of the spectral function (7). Next LG define

$$\sigma(E) = \begin{cases} \rho(E) & \text{for } E < 0 \\ \rho(E) - \frac{2}{\pi} \sqrt{E} & \text{for } E \geq 0 \end{cases} \quad (9)$$

Then if $V(r)$ has m derivatives

$$\int_{-\infty}^N d\sigma(E) \cos(\sqrt{E}r) \quad (10)$$

converges boundedly to a function $\phi(r)$ for $N \rightarrow \infty$, which has $(m+1)$ derivatives. Furthermore, with boundary condition (3), $\phi(r=0) = 0$.

Now, forgetting about the differential equation, LG show that if one has a spectral function ρ fulfilling the above properties one can indeed reconstruct a potential by the following procedure:

i) Using σ defined by (9), construct the kernel

$$F(r, t) = \lim_{N \rightarrow \infty} \int_{-\infty}^N d\sigma(E) \cos(\sqrt{E}r) \cos(\sqrt{E}t). \quad (11)$$

ii) Solve the Gelfand-Levitan (GL) integral equation

$$F(r, t) + K(r, t) + \int_0^r ds K(r, s) F(s, t) = 0 \quad (12)$$

for every fixed r . This equation has a unique solution.

iii) Obtain the potential by

$$V(r) = 2 \frac{d}{dr} K(r, r) \quad (13)$$

In short, the problem is completely solved except for the fact that we do not like the boundary conditions (1) or (3).

3. SOME PROPERTIES OF THE LOGARITHMIC DERIVATIVE AT THE ORIGIN OF EQUATION (2) DECREASING AT INFINITY

Under rather weak conditions on $V(r)$ one can show that for any E there exists a solution of the Schrödinger equation (2) vanishing at infinity. The logarithmic derivative of that solution

$$R(E) = \left. \frac{\frac{d}{dr} u(r, E)}{u(r, E)} \right|_{r=0} \quad (14)$$

is intimately connected with the spectrum. The zeros of (14) are the eigenvalues E'_1 defined by condition (3). On the other hand, the poles of (14) are the eigenvalues E_1 which constitute the physical spectrum. Furthermore, we shall see that there is a direct link between the inverse of (14) and the spectral function defined in the previous section.

i) Existence of solutions vanishing at infinity

One tries to prove that there is a solution of (2) which behaves asymptotically, like the WKB approximation

$$u(r, E) \underset{r \rightarrow \infty}{\sim} (V-E)^{-1/4} \exp - \int_R^r dr' \sqrt{V(r')-E} = u_0(r, E) \quad (15)$$

We shall assume that V is monotonous increasing for r big enough ($r \geq R$), and we choose the real part of the square root positive. $u_0(r, E)$ defined in (15) satisfies an equation like (2) with an energy dependent potential W

$$W = V + \frac{5}{16} \frac{V'^2}{(V-E)^2} - \frac{V''}{4(V-E)} = V + \Delta V \quad (16)$$

The second solution, linear independent to u_0 , is given by

$$v_0 = \frac{1}{2} (V-E)^{-1/4} \exp \int_R^r dr' \sqrt{V(r')-E} \quad (17)$$

According to a standard technique⁷⁾ one can transform (2) to an integral equation incorporating the boundary condition:

$$\rho(r, E) = 1 + \int_r^\infty dr' K(r, r', E) \Delta V(r') \rho(r', E) \quad , \rho = u/u_0. \quad (18)$$

It is easy to see that the kernel is bounded by

$$|K(r, r', E)| \leq \frac{1}{2 |V(r')-E|^{1/2}} \quad (19)$$

and one easily gets

$$\left| \frac{\rho(r, E)}{\rho(\infty, E)} \right| \leq \exp \frac{1}{2} \int_r^\infty dr' \left| \frac{\Delta V(r', E)}{(V(r')-E)^{1/2}} \right| \quad (20)$$

Therefore if the integrals

$$\int \frac{(V')^2}{V^{5/2}} \quad \int \frac{V''}{V^{3/2}} \quad (21)$$

converge, the existence of a solution such that $u/u_0 \rightarrow 1$ for $r \rightarrow \infty$ is established.

Furthermore, for r large enough, $|E| < M$, M arbitrary, one proves that the iterative solution of (18) converges uniformly and that $u(r, E)$ as well as $d/dr u(r, E)$ possess the analyticity properties of the individual terms of the series with respect to E . Therefore both are analytic functions of E in a cut plane with the cut beginning at $E = V(R)$. For smaller values of r , the Poincaré theorem applied directly to (2) ensures that $u(r, E)$ possesses the same analyticity properties. Therefore, for fixed r_1 and r_2

$$u(r_1, E)/u(r_2, E) \quad (22)$$

is a meromorphic function of E inside this cut plane. However, (22) is independent of the normalization; R can be chosen as large as one wishes and therefore the cut can be pushed far away since $V(r) \rightarrow \infty$ for $r \rightarrow \infty$. Therefore, (22) is meromorphic in the entire E plane. It is tempting to anticipate that by a special choice of the normalization one can make $u(r, E)$ an entire function of E . This seems to us a non-trivial step, rather delicate for very slowly rising potentials such as $V(r) = \lambda \ln r$, and we do not need this for the time being.

ii) The structure of $R(E)$

If the Schrödinger equation can be integrated down to $r = 0$, which is the case if $\int dr |V(r)|$ exists locally, one can conclude from i) that $R(E)$ is a meromorphic function of E . Notice that the familiar Coulomb potential does not satisfy the requirement of integrability and is unfortunately excluded from this study. In fact, by combining (2) with the complex conjugate we get

$$\frac{\Im R(E)}{\Im E} = \frac{\int_0^\infty |u|^2 dr}{|u(0)|^2} > 0, \quad (23)$$

that means $R(E)$ is a Herglotz function. A priori such a function grows at most like $|E|$ and decreases at most like $1/|E|$ at ∞ . It has only poles and zeros, interlaced, on the real axis. The zeros give the unphysical spectrum E'_1 ; the poles E_i the physical one. To calculate the residues at the poles it is sufficient to construct the Wronskian of the solutions at two energies:

$$u'(0, E+\Delta E)u(0, E) - u'(0, E)u(0, E+\Delta E) = -\Delta E \int_0^\infty dr u(r, E)u(r, E+\Delta E) \quad (24)$$

For $E = E_i$ we get

$$\left. \frac{d}{dE} R^{-1}(E) \right|_{E=E_i} = \frac{\int_0^\infty dr u^2(r, E_i)}{|u'(0, E_i)|^2} \quad (25)$$

and similarly for $E = E_i^!$

$$\left. \frac{d}{dE} R(E) \right|_{E=E_i^!} = - \frac{\int_0^a dr u^2(r, E_i)}{(u(0, E_i))^2} \quad (26)$$

Anticipating subsection iii) let us indicate that for $|E| \rightarrow \infty$ in complex directions as well as for $E \rightarrow -\infty$, $R(E)$ behaves like $1/\sqrt{-E}$. Therefore one can write an unsubtracted representation for $-1/R(E)$:

$$-\frac{1}{R(E)} = \sum_{i=0}^{\infty} \frac{|u(0, E_i)|^2}{E_i^! - E}, \quad \int dr u^2(r, E_i) = 1, \quad (27)$$

and a once subtracted representation for $R(E)$

$$R(E) = C + E \sum_{i=1}^{\infty} \frac{|u'(0, E_i)|^2}{E_i(E_i - E)}, \quad \int dr u^2(r, E_i) = 1. \quad (28)$$

One can make several interesting observations on (27). If we write this as a Stieljes integral, the measure is exactly the spectral measure introduced in (7). The fact that u/u' is entirely and directly fixed from the $E_i^!$ and the $|u_i(0)|^2$ without subtraction explains why this case was treated first. The second remark is that there is a very close analogy between the quantity and the R matrix of Wigner, which is $u(R)/u'(R)$ obtained by integrating from $r = 0$ till the boundary of the nucleus while we integrate the Schrödinger equation from ∞ down to zero.

We see now that if we give ourselves the $\ell = 0$ bound state energies E_i of a confined $q\bar{q}$ system, as well as the $|u'(0, E_i)|^2$, i.e., the values of $|\psi(0, E_i)|^2$, which come from the leptonic width $R(E)$ is fixed except for the subtraction constant C . We shall see that C is, in fact, not free. Then one can take the inverse of $R(E)$ and get from (27) the spectral measure which is needed to solve the inverse problem according to LG.

iii) The asymptotic behaviour of $R(E)$ for $E \rightarrow \infty$.

First we shall consider the case of potentials which have a lower bound B . In that case we shall prove in Appendix A under rather weak conditions that the WKB approximation (15) is valid for $E \rightarrow -\infty$ down to $r = 0$, so that

$$\frac{u'(0, E)}{u(0, E)} + \sqrt{-E} = O\left(\frac{1}{\sqrt{-E}}\right) \quad (29)$$

The conclusion is that the subtraction constant C in (28) is fixed, for two different constants C_1 and C_2 would give $R_1(E) - R_2(E) = C_1 - C_2$, while this difference should go to zero for $E \rightarrow -\infty$.

Next, let us generalize this to potentials which are singular but integrable at the origin. Define

$$V_0(r) = \begin{cases} V(r) & \text{for } r > r_0 \\ V(r_0) & \text{for } r < r_0 \end{cases}.$$

Combining the equations

$$u_0'' = (V_0 - E)u_0 \quad u'' = (V - E)u \quad (30)$$

for E below the ground state of V (which is supposed to exist) we get (since u and u_0 are decreasing functions of r)

$$\left| \frac{u'}{u}(0, E) - \frac{u_0'}{u_0}(0, E) \right| < \int_0^{r_0} dr' |V(r_0) - V(r')| \quad (31)$$

If V is integrable the right-hand side of (31) can be made arbitrarily small by taking r_0 small enough and one gets

$$\left| \frac{u'}{u}(0, E) + \sqrt{-E} \right| \rightarrow 0 \quad \text{for } E \rightarrow -\infty \quad (32)$$

So, again, the subtraction constant is fixed and the inverse problem is solved, in principle at least.

4. CONSTRUCTION OF THE SUBTRACTION CONSTANT

We want to go beyond merely proving that C is fixed and propose a constructive procedure to get it. We shall illustrate this by an example.

From (28) it is seen that $C = R(0)$. We can always assume that $E = 0$ is below the lowest eigenvalue for simplicity. We try to compute $R(0)$ by computing a contour integral of $R(E)/E$ along a circle Γ of radius $|E'_{N+1}|$ centred at the origin, containing the poles $E_1, E_2, \dots, E_N$. Therefore, we get

$$\frac{1}{2\pi i} \int_{\Gamma} \frac{dE R(E)}{E} = C - \sum_{i=1}^N \frac{|u'(0, E_i)|^2}{E_i} \quad (33)$$

If $R(E)$ is well approximated by $-\sqrt{-E}$ for $|\text{Arg}(-E)| < \pi - \epsilon$, ϵ small enough, the integral on the left-hand side should be close to $2\sqrt{E_{N+1}}/\pi$. To establish this a careful study of $R(E)$ in complex directions will be made in Appendix B. There we restrict ourselves to $V(r)$ lower bounded and assume

$$\begin{aligned} \alpha) & V(r) > 0 \\ \beta) & dV/dr > 0 \quad \text{for } r > r_0 \\ \gamma) & V \rightarrow \infty \quad \text{for } r \rightarrow \infty \\ \delta) & r^{-m} V(r) \searrow \quad \text{for } r > r_0, m > 0 \\ \epsilon) & r^{-\epsilon} V(r) \nearrow \quad \text{for } r > r_0, \epsilon > 0. \end{aligned} \quad (34)$$

For potentials satisfying (34) i.e., which are lower bounded, monotonous for large r , and go to infinity less faster than r^m , but faster than r^ϵ we conclude that C is given by

$$C = \lim_{N \rightarrow \infty} C_N, \quad C_N = \sum_{i=1}^N \frac{|u'_i(0, E_i)|^2}{E_i} - \frac{2}{\pi} \sqrt{E_{N+1}}. \quad (35)$$

Naturally, conditions (34) are only sufficient. We believe that (35) holds for a broader class of potentials including, for instance, one increasing like $\ln r$. Let us remark that using the semiclassical approximation for the wave functions and the energy levels [as it has been done in Ref. 8)] would immediately give (35). Notice also that if V remains finite for finite r and tends monotonically to ∞ as $r \rightarrow \infty$ the number of levels increases faster with energy than that of a square well, as can be seen by a "minimax" argument, if one replaces V by $V(R)$ for $r \leq R$ and ∞ for $r > R$. Therefore, at least in the average $\sqrt{E_{N+1}} - \sqrt{E_N} \rightarrow 0$ and we can replace $\sqrt{E_{N+1}}$ by any quantity between $\sqrt{E_{N+1}}$ and $\sqrt{E_N}$, the most practical form might be the arithmetic mean of both:

$$C = \lim_{N \rightarrow \infty} \left[\sum_{i=1}^N \frac{|u'_i(0)|^2}{E_i} - \frac{2}{\pi} \sqrt{\frac{E_N + E_{N+1}}{2}} \right] \quad (36)$$

We have tested (35) for two potentials. For the infinite square well (35) is exact (already for any finite N) if the zero of energy is taken at the bottom of the well. For the three-dimensional oscillator (35) and (36) are equivalent and we find that the corrective term is very small even for small N . We get $C_1 = -0.47466$, $C_2 = -0.47660$ and $C_3 = -0.47718$ while $C = -0.47798$.

This completes the proof that via (28) and (36) we can construct $R(E)$ and hence $1/R(E)$ and the spectral density $\rho(E)$ necessary to get the kernel in the Gelfand-Levitan equation (12). Since (28) is an absolute convergent series one obtains perhaps a more operational form for $R(E)$ putting in C:

$$R(E) = \lim_{N \rightarrow \infty} \left\{ \sum_{i=1}^N \frac{|u'(0, E_i)|^2}{E_i - E} - \frac{2}{\pi} \sqrt{\frac{E_N + E_{N+1}}{2}} \right\}. \quad (37)$$

This expression shows that it is possible to get a reasonable approximation of $R(E)$ for finite N : (37) has one zero below E_1 , exactly one zero between E_i and E_{i+1} and these zeros approach necessarily the E_i' 's as $n \rightarrow \infty$. We believe that this procedure, which has the advantage of being systematic replaces advantageously the procedure used by QRT in the case $N = 1$ and $N = 2$. We have illustrated our method for the harmonic oscillator for some N

N	E_1'	E_2'	E_3'	E_4'
2	0.643	2.880		
3	0.615	2.791	4.943	
10	0.561	2.648	4.704	6.750
50	0.526	2.565	4.587	6.605
Exact	0.500	2.500	4.500	6.500

The convergence is very slow, but this was to be expected.

5. A DIRECT UNIQUENESS PROOF

First of all we know from Section 4 that the knowledge of E_1 and $|u_1'(0)|^2$ fix also the E_1' . This means that in the associated one-dimensional problem in which $V(x)$ is symmetric with respect to the origin we know the even and odd levels. So, if someone succeeds in proving the convergence of the QRT procedure in one-dimension to a unique potential, the radial problem is solved at the same time.

Here we shall use the results of the previous section. Let $u(r, E)$ and $v(r, E)$ be the decreasing solutions of the Schrödinger equation for the potential $V(r)$ and $V(r) + \delta V(r)$. We assume that to both u and v is associated the same function $R(E)$:

$$R(E) = \frac{u'(0, E)}{u(0, E)} = \frac{v'(0, E)}{v(0, E)}. \quad (38)$$

We make now the following "technical" assumption: $V(r)$ is a continuous function, the zeros of which have no accumulation points for finite r . Let r_1 be the first zero; combining the Wronskian for u and v with (38) gives

$$-u'(r_1)v(r_1) + r_1'(r_1)u(r_1) = \int_0^{r_1} dr \delta V(r) u(r, E) v(r, E) \quad (39)$$

For E large negative we have according to the results of Section 3, iii),

$$\frac{u(r, E)}{u(0, E)} = \exp(-\sqrt{-E} r) \left[1 + O\left(\frac{1}{\sqrt{-E}}\right) \right] \quad (40)$$

and a similar equation for v , as well as

$$\frac{u'(0, E)}{u(0, E)} \simeq -\sqrt{-E} + O\left(\frac{1}{\sqrt{-E}}\right) \quad (41)$$

So we get from (39)

$$\int_0^{r_1} dr \delta V(r) \frac{u(r, E) v(r, E)}{u(0, E) v(0, E)} = O\left(\sqrt{-E} \exp(-2\sqrt{-E} r_1)\right) \quad (42)$$

However, since δV , u and v have a constant sign, the left-hand side of (42) is certainly larger than

$$\int_0^{\alpha r_1} dr \delta V(r) \simeq \exp(-2\sqrt{-E} \alpha r_1)$$

for any $0 < \alpha < 1$. Letting E go to $-\infty$ we get a contradiction unless

$$\int_0^{\alpha r_1} dr \delta V(r) = 0 \rightarrow \delta V = 0 \quad \forall 0 < r < r_1$$

We conclude

$$u'(r_1, E) v(r_1, E) - v'(r_1, E) u(r_1, E) = 0$$

and can repeat the argument and prove that δV vanishes in $r_1 < r < r_2$, and so on.

One can slightly weaken the assumption about δV . For instance, if $\int \delta V(r) dr$ has no accumulation points of zeros, the argument goes through because the estimates on u and v are also valid for higher derivatives.

Perhaps it is worth noticing that if two potentials, finite for finite r , going to infinity like r^n and having an infinite set of levels E_m in common, such that

$$\sqrt{E_{m+1}} - \sqrt{E_m} \rightarrow 0,$$

their difference δV cannot be of compact support.

Assume that δV has a compact support R . Integrate the Schrödinger equation from the origin, imposing $u(0, E) = v(0, E) = 0$ and $u'(0, E) = v'(0, E) = 1$. We get

$$u'(R, E)v(R, E) - v'(R, E)u(R, E) = - \int_0^R dr \delta V(r) u(r, E) v(r, E) = \phi(E) \quad (43)$$

and $\phi(E)$ is an entire function of order 1 of $k = \sqrt{E}$ and exponential type $2R$. It vanishes according to the assumption for $k = \pm i \sqrt{E_m}$, i.e., on a set of infinite asymptotic density on the imaginary axis. According to a known theorem (9) it is identically zero. The product $u(r, E)v(r, E)$ according to the Paley-Wiener theorem⁹⁾ can be written as

$$\int_{-2r}^{+2r} dx e^{ikx} w(r, x)$$

and from the vanishing of $\phi(E = k^2)$ we deduce

$$\int_0^R dr \delta V(r) w(r, x) = 0$$

but because of the support properties of w this can be regarded as a Volterra equation for δV and hence $\delta V = 0$.

A consequence of this result is that if one takes a confining potential and changes one or a finite number of levels, the difference between the new and the old potential extends to infinity. This will be investigated in the next section.

6. STABILITY OF THE POTENTIAL WITH RESPECT TO CHANGES OF LEVELS AND NORMALIZATION

Though the solution of the full inverse problem even with a complete set of data is technically difficult, the effect of the change of one or two levels on the potential is easily calculated, because the Gelfand-Levitan equation has a degenerate kernel in this case¹⁰⁾.

We would like to discuss the following problem: given a confining problem $v_1(r)$ with energy levels $E_n^{(1)}$ and slopes $\gamma_n^{(1)}$ determine a new potential $v_2(r)$ having a finite number of levels or/and constants changed. Since that is a standard problem let us give only a short review.

From the Wiener-Boas theorem one deduces the "Povzner-Levitan" representation for the regular wave functions u_1 and u_2 , respectively

$$u_i(k, r) = \frac{\sin kr}{k} + \int_0^r dr' K_i(r, r') \frac{\sin kr'}{k} \quad (44)$$

Solving one equation for $\sin kr/k$ and introducing it into the other equation, one obtains

$$u_2(E, r) = u_1(E, r) + \int_0^r dr' K(r, r') u_1(E, r'), \quad k^2 = E \quad (45)$$

where the kernel K is a function of K_1 and K_2 ; similarly one gets a reciprocal relation

$$u_1(E, r) = u_2(E, r) + \int_0^r dr' \tilde{K}(r, r') u_2(E, r') \quad (46)$$

Multiplying first (46) by $u_1(E, t)$, integrating with the spectral measure $d\rho_2(E)$ for the potential v_2 and using the completeness property gives

$$\int_{-\infty}^{+\infty} d\rho_2(E) u_2(E, t) u_1(E, r) = 0 \quad \text{for } t > r. \quad (47)$$

Let us remark that the spectral measure $\rho_2(E)$ used here corresponds to the "right" boundary conditions at the origin $u_2(E, 0) = 0$, and is therefore different from that defined in Eq. (7). Next multiplying (45) by $u_1(E, t)$, integrating with $d\rho_2(E)$ again, and using (47), gives

$$\int_{-\infty}^{+\infty} d\rho_2(E) u_1(E, t) u_1(E, r) + \int_0^r dr' K(r, r') \int_{-\infty}^{+\infty} d\rho_2(E) u_1(E, t) u_1(E, r') = 0, \quad (48)$$

$t < r$

Adding the obvious identity

$$K(r,t) = \int_{-\infty}^{+\infty} d\rho_1(E) \int_0^r ds K(r,s) u_1(E,s) u_1(E,t) , \quad r > t \quad (49)$$

to (48) one obtains the GL equation for the kernel K :

$$K(r,t) + F(r,t) + \int_0^r dr' K(r,r') F(r',t) = 0 \quad r > t \quad (50)$$

The input $F(r,t)$ is now given in terms of the spectral measures by

$$F(r,t) = \int_0^\infty d\sigma(E) u_1(E,r) u_1(E,t) , \quad \sigma(E) = \rho_2(E) - \rho_1(E). \quad (51)$$

Since by assumption we intend to change only a finite number of constants, σ is given by a finite sum:

$$\frac{d\sigma(E)}{dE} = \sum_{i=1}^M \gamma_i^{(2)} \delta(E - \epsilon_i^{(2)}) - \sum_{j=1}^N \gamma_j^{(1)} \delta(E - \epsilon_j^{(1)}) \quad (52)$$

It is well known that the GL equation admits a solution in closed form for a degenerate kernel like (51). The result for the potential [see Eq. (13)] is given by

$$\delta V = V_2 - V_1 = -2 \frac{d^2}{dr^2} \ln \text{Det}[1+A] . \quad (53)$$

Here A denotes a $(N+M) \times (N+M)$ dimensional matrix with entries

$$\begin{aligned} A_{ij} &= c_i \int_0^r dr' u_1(k_i, r') u_1(k_j, r') \\ c_i &= \begin{cases} -\gamma_i^{(1)} & i = 1 \dots N \\ \gamma_i^{(2)} & i = N+1 \dots N+M \end{cases} \\ k_i^2 &= \begin{cases} \epsilon_i^{(1)} & i = 1 \dots N \\ \epsilon_i^{(2)} & i = N+1 \dots N+M \end{cases} \end{aligned} \quad (54)$$

To illustrate this procedure, we have calculated δV starting with the linear potential and changing one (Fig. 1) and two bound state levels (Fig. 2).

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APPENDIX A

Here we would like to prove (29), which means that WKB is valid for $E \rightarrow -\infty$, if V is lower bounded and if:

a) V is monotonous increasing; then we use

$$u'^2(r) - (V(r) - E) u^2(r) = \int_r^\infty dr' u^2 \frac{dV}{dr'} \geq 0 \quad (A1)$$

If $E < V(0) < V(r)$, $u(r, E)$ is convex and a monotonous decreasing function of r . Hence

$$\frac{u'(r, E)}{u(r, E)} \leq -\sqrt{V(r) - E} \quad (A2)$$

so we get

$$\frac{u(R, E)}{u(r, E)} \leq \exp \left\{ - \int_r^R dr' \sqrt{V(r') - E} \right\}, \quad R > r. \quad (A3)$$

and by direct integration of the Schrödinger equation one obtains

$$\begin{aligned} - \frac{u'(0, E)}{u(0, E)} &\leq \int_0^\infty dr (V(r) - E) \exp \left\{ - \int_0^r dr' \sqrt{V(r') - E} \right\} \\ &\leq (V(0) - E) \int_0^\infty dr \exp \left\{ - r \sqrt{V(0) - E} \right\} + \int_0^\infty dr (V(r) - V(0)) \exp \left\{ - r \sqrt{V(0) - E} \right\}. \end{aligned} \quad (A4)$$

Now if

$$|V(r) - V(0)| < r^\gamma \exp(\alpha r) \quad \gamma > 0, \alpha > 0, \quad (A5)$$

we get from (A4)

$$- \frac{u'(0, E)}{u(0, E)} \leq \sqrt{V(0) - E} + C \left(\sqrt{V(0) - E} - \alpha \right)^{-(\gamma+1)} \quad (A6)$$

Combining (A6) and (A2) for $r = 0$ one obtains

$$\left| \frac{u'(0, E)}{u(0, E)} + \sqrt{V(0) - E} \right| = O\left(\frac{1}{\sqrt{|E|}}\right). \quad (A7)$$

b) Next let us remove the restriction of monotony. Assume

$$U(r) < V(r) < W(r) \quad (A8)$$

where $U(r)$ and $W(r)$ are monotonous increasing. Then it is easy, using Wronskian techniques to get

$$\sqrt{U(0) - E} + O\left(\frac{1}{\sqrt{-E}}\right) < -\frac{u'(0, E)}{u(0, E)} < \sqrt{W(0) - E} + O\left(\frac{1}{\sqrt{-E}}\right) \quad (A9)$$

if E is below the lowest bound state of U . Hence if (A8) holds with U and W obeying (A5)

$$\frac{u'(0, E)}{u(0, E)} + \sqrt{-E} = O\left(\frac{1}{\sqrt{|E|}}\right) \quad (A10)$$

which proves Eq. (29).

APPENDIX B

Here we intend to show that the subtraction constant C defined in (28) is given by

$$C = \sum_{i=1}^n \frac{|u'(0, E_i)|^2}{E_i} - \frac{2}{\pi} \sqrt{E_{n+1}'} + O(E_{n+1}'^{-\delta}) \quad \delta > 0 \quad (B1)$$

for potentials satisfying conditions (34). From (34)- δ), we deduce bounds like

$$0 < \frac{dV}{dr} < m \frac{V(r)}{r} < \frac{m}{R} (V(R))^{1/m} (V(r))^{1-\frac{1}{m}} \quad , r > R. \quad (B2)$$

We choose $R > r_0$ and intend to use

$$(u'(0, E))^2 + E (u(0, E))^2 = -2 \int_0^\infty dr V u u'. \quad (B3)$$

That means a bound on the right-hand side is needed. We divide the integral into parts

$$\int_0^\infty V u u' dr = \int_0^R V u u' dr + \int_R^\infty (V(r) - V(R)) u u' dr + \int_R^\infty V(R) u u' dr \quad (B4)$$

use partial integration, Schwarz and Minkowski inequalities and (B2) to get for $m > 1$

$$\left| 2 \int V u u' \right| < 2 V(R) \left[\int |u|^2 \int |u'|^2 \right]^{1/2} + \left[\int |u|^2 \right]^{1/m} \frac{V(R)}{R} \left[\int V |u|^2 \right]^{1-\frac{1}{m}}. \quad (B5)$$

If $m < 1$ we use instead of (B2)

$$\frac{dV}{dr} < m \frac{V(r)}{r} < m \frac{V(R)}{R} \quad \text{for } r > R \quad (B6)$$

so that (B5) is replaced by

$$\left| 2 \int V u u' \right| \leq 2 V(R) \left[\int |u|^2 \int |u'|^2 \right]^{1/2} + m \frac{V(R)}{R} \int |u|^2 \quad (B7)$$

On the other hand, combining the Schrödinger equation with the complex conjugate gives

$$\text{Im } u^* u' = \text{Im } E \int |u|^2, \quad \text{Re } u^* u' = \int |u'|^2 + \int (V - \text{Re } E) |u|^2 \quad (\text{B8})$$

from which we get the inequalities

$$\begin{aligned} |uu'| &> \text{Im } E \int |u|^2 \\ |uu'| &> \frac{\text{Im } E}{|\text{Im } E|} \int (|u'|^2 + V |u|^2) \end{aligned} \quad (\text{B9})$$

and in the special case $\text{Re } E < 0$

$$|uu'| > \int |u'|^2 + \int V |u|^2 - \text{Re } E \int |u|^2 \quad (\text{B10})$$

Inserting inequalities (B9) into (B5) and (B7) allows us to bind the left-hand side of (B5)

$$\begin{aligned} \left| 2 \int V uu' \right| &\leq \frac{|uu'(0)|}{\text{Im } E} \left\{ 2V(R) \sqrt{|E|} + m \frac{(V(R))^\sigma}{R} |E|^{1-\sigma} \right\} \\ \sigma &= \begin{cases} 1/m & \text{for } m > 1 \\ 1 & \text{for } m \leq 1 \end{cases} \end{aligned} \quad (\text{B11})$$

For $\text{Re } E < 0$, we get also

$$\left| 2 \int V uu' \right| < |uu'(0)| \left\{ \frac{2V(R)}{\sqrt{-\text{Re } E}} + m \frac{(V(R))^\sigma}{R} (-\text{Re } E)^{-\sigma} \right\} \quad (\text{B12})$$

Using these bounds in (B3) gives inequalities of the type

$$\left| R(E) + \frac{E}{R(E)} \right| < B(E) \quad (\text{B13})$$

with $R = u'/u$ and B being (except for constants) of the form

$$\begin{aligned}
 m < 2 & \left\{ \begin{array}{l} B = \frac{\sqrt{|E|}}{\gamma_m E} \\ \operatorname{Re} E < 0 \quad B = (-\operatorname{Re} E)^{-1/2} \end{array} \right. \\
 m > 2 & \left\{ \begin{array}{l} B = \frac{|E|^{1-\frac{1}{m}}}{\gamma_m E} \\ \operatorname{Re} E < 0 \quad B = (-\operatorname{Re} E)^{-1/m} \end{array} \right.
 \end{aligned} \tag{B14}$$

(B13) implies one of the inequalities

$$|\operatorname{Re} E + \sqrt{-E}| < B(E) \tag{B15a}$$

$$|\operatorname{Re} E - \sqrt{-E}| < B(E) \tag{B15b}$$

To resolve the alternative one can use the fact that $R(E)$ is analytic outside the positive real axis. Hence if any point in the complex plane is connected by a continuous path to $-\infty$ such that all points $\hat{E}$ along the path satisfy $B(\hat{E}) < \sqrt{|\hat{E}|}$ we necessarily have (B15a) with the real part of the square root positive. We can now use these bounds to estimate accurately the integral of Eq. (33), but close to E'_{N+1} we shall need a better estimate: since $R(E'_{N+1}) = 0$ we may write

$$R(E) = (E - E'_{N+1}) \sum_{i=1}^{\infty} \frac{|U'_i(0)|^2}{(E_i - E)(E_i - E'_{N+1})} \tag{B16}$$

It is easy to show that

$$\left\{ \begin{array}{l} E_N < \operatorname{Re} E < E_{N+1} \\ |\gamma_m E| \geq E_{N+1} - E_N \end{array} \right. \quad \text{or} \quad |E| = E'_{N+1} \rightarrow |E_i - E| > \frac{1}{\sqrt{2}} |E'_{N+1} - E_i| \tag{B17}$$

Hence

$$|R(E)| < \sqrt{2} |E - E'_{N+1}| \frac{d}{dE} R(E = E'_{N+1}) = \sqrt{2} |E - E'_{N+1}| \frac{\int u^2(r, E'_{N+1}) dr}{u^2(0, E'_{N+1})} \tag{B18}$$

The last expression could be evaluated semi-classically following Quigg-Rosner⁸⁾. Then we would get

$$|R(E)| < \text{const} \times |E - E'_{N+1}| \times \sqrt{E'_{N+1}} \int \frac{dr \theta(E'_{N+1} - V)}{\sqrt{E'_{N+1} - V}} \sim \text{const} \sqrt{|E|} \quad (\text{B19})$$

for $\text{Im} E = \pm |E_{N+1} - E_N| \quad E_N < \text{Re} E < E_{N+1}$

However, the validity of the semi-classical estimate, which involves details of the wave function is not completely obvious. It is probably legitimate in the case of sufficiently smooth potentials. It would simplify life enormously for, by using the maximum modulus principle for the function $R(E) E^{-\frac{1}{2}}$, it would give a bound of the form

$$|R(E)| < \text{const} \sqrt{|E|} \quad \forall E: |\text{Im} E| > \Delta E \quad (\text{B20})$$

where ΔE is the level spacing for real E .

However, here, we shall content ourselves with much cruder but strict bounds. If, for simplicity, one assumes that $V(r)$ is monotonously increasing, then $u'^2 + (E - V)u^2$ is decreasing and positive, so $|u'(r)| < \sqrt{E} |u(0)|$ if $u'(0) = 0$, and hence

$$|u(r)| < u(0) [1 + r\sqrt{E}] \quad \text{for } E = E'_{N+1} \quad (\text{B21})$$

Next, let R_c denote the classical size of the wave function, $V(R_c) = E$ and $r > R_c$, then

$$|u(r)| < u(R_c) \exp - \int_{R_c}^r dr' \sqrt{V(r') - E} \quad (\text{B22})$$

If one assumes in addition that $V(r)$ increases for $r > R_c$ faster than a power ε , which implies $R_c < cE^{1/\varepsilon}$ one can get a bound of the following form

$$\int_0^\infty |u(r, E'_{N+1})|^2 dr < (u(0, E'_{N+1}))^2 (E'_{N+1})^\delta \quad (\text{B23})$$

where $\gamma \rightarrow \infty$ for $\varepsilon \rightarrow 0$. After inserting (B23) into (B18) we are now in a position to evaluate the contour integral (33), which we split in three pieces

$$\begin{aligned}
 a) \quad & |A_g - E| < \pi - \frac{1}{(E'_{N+1})^{1/2+\varepsilon}} \\
 b) \quad & \pi - \frac{1}{(E'_{N+1})^{1/2+\varepsilon}} < \pm (A_g - E) < \pi - \frac{1}{(E'_{N+1})^\alpha} \\
 c) \quad & \pi - \frac{1}{(E'_{N+1})^\alpha} < \pm (A_g - E) < \pi
 \end{aligned} \tag{B24}$$

with α big enough. The contribution from a) is, using (B13), (B14), (B15)

$$\frac{2}{\pi} \sqrt{E'_{N+1}} \sin\left(\frac{\pi}{2} - \frac{1}{2(E'_{N+1})^{1/2+\varepsilon}}\right) + O\left(\frac{\log E'_{N+1}}{(E'_{N+1})^\tau}\right), \quad \tau = \min\left(\frac{1}{2}, \frac{1}{m}\right) \tag{B25}$$

that from b) gives

$$O\left((E'_{N+1})^{-\tau} \log E'_{N+1}\right) \tag{B26}$$

and the last contribution is $O((E'_{n+1})^\beta)$ with $\beta > 0$. The conclusion is that the subtraction constant is indeed given by (B1).

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FIGURE CAPTIONS

Figure 1 Shows the change in the potential, if one starts from the linear potential and changes one level from 2.338 to 1.5.

Figure 2 Shows the variation in the potential by changing two levels.

- Figure 1 -

- Figure 2 -