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SELF-ADJOIN EXTENSION PROBLEMS FOR SINGULAR POTENTIALS

I.Statment of problem in the Scrhrodinger equation. (Discrete spectrum).

From the demand, that Hamiltonian and $p_r = -i\left(\frac{\partial}{\partial r}+\frac{1}{\partial r}\right)$ operators are Hermitian it follows, that [1.D.Blockincev, 2.V.Pauli, 3.A.Messia]

$$\lim_{r\to 0} rR = u(0) = 0 \tag{1.1}$$

Usually are considered regular potentials in the Schrodinger equation

$$\lim_{r\to 0} r^2 V = 0 \tag{1.2}$$

$$R_{r\to 0} = C_1 r^l + C_2 r^{-(l+1)} \tag{1.3}$$

Second term in (1.3) doesn't obey (1.1) condition and is neglected usually

Singular potentials

$$\lim_{r\to 0} r^2 V \to \pm\infty \tag{1.4}$$

Transition potentials

$$\lim_{r\to 0} r^2 V \to \pm V_0 \qquad (V_0 > 0) \tag{1.5}$$

Theorem. For transition potentials (with – sign in front of V_0) Schrodinger equation except standard solutions, also have additional solutions.

Proof:

$$u'' + 2m[E - V(r)]u - \frac{l(l+1)}{r^2}u = 0; \quad u = Rr \tag{1.6}$$

At $r \to 0$ from (1.6) we obtain

$$\underset{r\to 0}{u} = a_{st} r^{\frac{1}{2}+P} + a_{add} r^{\frac{1}{2}-P} = u_{st} + u_{add} \qquad (1.7)$$

Where

$$P = \sqrt{\left(l+\frac{1}{2}\right)^2 - 2mV_0} \qquad (1.8)$$

In the region

$$0<P<1/2 \qquad (1.9)$$

Both standard and additional solutions satisfy (1.1) condition (when P>1/2 only standard solutions stay!)

From (1.8) and (1.9) we obtain condition of exsitence of additional states

$$l(l+1) < 2mV_0 \qquad (1.10)$$

In [4-H.Bethe; R. Jackiw."Intermediate quantum mechanics"] is formulated very strong requirement- Kinetic Energy matrix elements should be finite! We show, that if we take "whole" wave function additional states sustain mentioned strong requirement!

Additional solutions satisfy also requirement, that [5.-L.Schiff.Quantum mechanics.] integral from particle coordinate probability density is finite!

Remark:

We think, that isn't correct paragraph 35- "Falling on the center"in [6-L.Landau, E.Lifchitz. Quantum mechanics].where is considered behavior of $R=\frac{u}{r}$ at small r

$$\underset{r\to 0}{R} = Ar^{\frac{1}{2}+P} + Br^{\frac{1}{2}-P} \qquad (1.11)$$

In (1.11) both terms are singular (second term is more singular!) and in [7- R. Newton monograph] author notice: "If P<1/2, then the second solution is irregular in sense, that it is dominant above first solution". So R.Newton come very close to additional state problem, but don't mentioned tat they exist! In [6] potential is made regular by cutting off it at some small r_0 and the limit $r_0 \to 0$ is taken, which selects less singular solution at $r_0 \to 0$ and so additional solutions are neglected! But if we multiple (1.11) relation on r we get (7) relation, where we have, no singularity in the 0<P<1/2 region and as mentioned above u_{st} and u_{adc} are "equal in rights" members of (7) relation!

I I. Introduction of self-adjoint extension τ parameter

It is well known, that for (1.4) and (1.5) type attractive potentials [8-K.Case.Phys.Rev.80,797(1950); 9-K.Meetz.Nuovo Cimento 34, 690(1964); 10- A.Perelomov, V.Popov.TMF.vol 4 (1970)] in the Schrodinger equation is shown, that it isn't enough to know potential and is necessary to introduce one arbitrary constant, which is equivalent to give boundary condition at the origin. Indeed, when

$$2mV_0 > (l+1/2)^2 \tag{2.1}$$

As one can see from (1.8) P is complex, both u_{st} and u_{adc} solutions have same behavior at the origin and for example for $V=-\frac{g}{r^2}$ at small distances one have [7, 8]

$$u \approx A\sqrt{r}\cos\left(\sqrt{2mV_0-(l+1/2)^2}\,\ln r + B\right) \tag{2.2}$$

Once B is arbitrary constant. On the Mathematical language it means, that H is symmetric (Hermitian), but isn't Self-adjoint operator and it is necessary to introduce 1 parameter for self-adjont extension(to make H Self-adjoint !)[11-M.Reed,B.Simon:vol 2]. As was shown in [8] if B is fixed constant, then all eigensolutions form a complete orthonormal set, and E-eigenvalues are real! (Once such a properties have a Self-adjoint H operator). But in this case we have "falling" on the center and energy isn't bounded from below!

In the region

$$2mV_0 < (l+1/2)^2 \tag{2.3}$$

based on the above mentioned paragraph of [6] , is neglected u_{adc} solutions. We notice above, that u_{adc} solutions in the 0<P<1/2 region satisfy all u_{st} requirements. So is necessary to preserve it! Then for arbitrary E_1 and E_2 levels ortogonality condition is

$$m\left(E_2^2-E_1^2\right)\int_0^\infty u_2u_1 = 2P\left\{a_1^{st}a_2^{add}-a_2^{st}a_1^{add}\right\} \tag{2.4}$$

And for ortogonality right side of (14) is zero

$$\frac{a_1^{st}}{a_1^{add}}=\frac{a_2^{st}}{a_2^{add}} \qquad (2.5)$$

So, we get, that for ortogonality it is necessary to introduce self-adjoint extension τ parameter

$$\tau=\frac{a_{add}}{a_{st}} \qquad (2.6)$$

All levels have same τ parameter. From (1.7) and (2.4) we have:

a). $a_{add}=0$; $(\tau=0)$ We keep only standard levels and they are orthogonal!

b). $a_{st}=0$; $(\tau=\pm\infty)$ We keep only additional levels and they are orthogonal!

c) When $\tau\neq-\infty,0$ then both levels exist at the same time!

For some unknown reasons the Nature choose only standard levels yet!
We think, that other cases are also possible!

I I.I Scatering Problems (Continuous Spectrum).

$$V=\frac{V_0}{r^2};V_0>0 \qquad (3.1)$$

This interaction is realized in nature- physical applications: .

1).Gharge interacting with a point dipole [11-H.Camblong...Phys.Rev.Lett.87,220402 (2001)]

2).Interaction of a neutral, but polarizable atom with a charged wire [12-J.Denschlag; Phys.Rev.Lett.81.737. (1998)

3)Aaronov-Bom effect [13 –J.Audretsh…J.Phys.A28,2359 (1995)].

4).Black holes [Gupta,Shabad…]

$$U_k(r)=\sqrt{kr}\left\{A(k)J_p(kr)+B(k)J_{-p}(kr)\right\};k^2=2mE;E>0 \qquad (3.2)$$

(3.2)For 0<P<1/2 $\sqrt{r}J_{-P}(kr)$ is regular at the origin and we keep it!

a).Introduction of SAE parameter

$$I=\int_0^\infty r^2R_{k'}^*(r)R_k(r)dr=2\pi\delta(k'-k) \qquad (3.3)$$

We use integrals from [14-J.Audretsch.J.Phys.A34,235 (2001)] for Bessels functions and get

$$I=\left\{AA^*+BB^*+(B^*A+A^*B)\cos\pi p\right\}\delta(k'-k)+\frac{2\sin\pi p}{\pi(k^2-k'^2)}\left\{\left(\frac{k}{k'}\right)^p B^*(k')A(k)-\left(\frac{k}{k'}\right)^{-p} A^*(k')B(k)\right\}$$

$$\frac{B^*(k')}{A^*(k')}(k')^{-2p}=\frac{B(k)}{A(k)}k^{-2p}=\tau_p \qquad (3.5)$$

From (3.5)

$$B=\tau_p A k^{2P};k^2=2mE \qquad (3.6)$$

(3.5) is analog of (2.5) for continuous spectrum

$$AA^*\left[\tau_p^2 k^{4p}+2\tau_p k^{2p}\cos\pi p+1\right]=2\pi \qquad (3.7)$$

Based on the methodology of [14] and [15-S.Alliluev.JETP.Vol 61,p15 (1970)] articles,where is considered

$$I=\lim_{R\to\infty}\int_0^R u_{k'}^*(r)u_k(r)dr=\frac{1}{k'^2-k^2}\left[u_{k'}^*\frac{du_k}{dr}-u_k^*\frac{du_{k'}}{dr}\right]_0^R \qquad (3.8)$$

one can show, that τ parameter is introduced from the lower limit of the (3.8) integral as it was for the bound states and (3.8) is introduced from the upper limit of this integral (For bound states wave function decrease at large distances and we no analog of (3.7) relation).

b).Phase Shifts Calculation.

$$U_k(r)=\sqrt{kr}\left\{A(k)J_p(kr)+B(k)N_p(kr)\right\}; \qquad (3.9)$$

Second term is regular at the origin for 0<P<1/2 and we keep it!

$$\lim_{r\to\infty}R=\frac{u}{r}=\frac{C}{r}\sin(kr-\frac{l\pi}{2}+\delta_l) \qquad (3.10)$$

$$\delta_p=\left[l+1/2-P\right]\pi/2-arctgB/A \qquad (3.11)$$

or using (3.5) definition of SA parameter we obtain:

$$\delta_p=\left[l+1/2-p\right]\pi/2-arctg(\tau_p k^{2p}) \qquad (3.12)$$

In the literature is known only first term [16-A.M.Perelomov;V.S.Popov.TMF.Vol 4.No1(1970)]

a).B=0; $\tau_p=0$; $$\delta_p^{st}=\left[l+1/2-p\right]\pi/2 \qquad (3.13)$$

b).A=0 $\tau_p = \pm\infty$, $\delta_p^{add} = \delta_l^{st} \pm \pi/2$ (3.14)

+ sign in (3.14) is excluded, comparing it with asymptotic expression

$$N_p(kr) \approx \sqrt{2/\pi kr}\,\sin\left(kr - p\pi/2 - \pi/4\right)$$

Remarks: 1. From (3.12) we see that δ_p is depended on the energy $(k^2 = 2mE)$ for $\tau_p \neq 0, \infty$,so scale invariance is violated!

2. We considered $V = -V/r^2$ attractive potential, for which $\delta_p > 0$. As one see from (3.12) may be $\delta_p < 0$ or we get repulsive potential! So we see, that τ_p parameter may change the NATURE of potential!

We have two possibilities:

a).From the Physical motivation restrict τ_p parameter (Don't change attractive potential by repulsive!) or as one see from (3.12) demand

$$\left[l + 1/2 - p\right]\pi/2 - arctg(\tau_p k^{2p}) > 0$$

b).Agree, that τ_p can change potential nature!

$$d\sigma/d\Omega = \left|f(\theta)\right|^2;\ f(\theta) = 1/2ik\sum_{l=0}^{\infty}(2l+1)(S_l - 1)P_l(\cos\theta) \tag{3.15}$$

$$S_l = e^{2i\delta_l} \tag{3.16}$$

$$\sigma = 4\pi/k^2\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \tag{3.17}$$

$$f(\theta) = 1/2ik\sum_{l=0}^{\infty}(2l+1)f_l P_l(\cos\theta) \tag{3.18}$$

$$f_l = \frac{1}{2ik}(S_l - 1) = \frac{1}{2ik}(e^{2i\delta_l} - 1) \tag{3.19}$$

$$\sigma_l = 4\pi(2l+1)\left|f_l\right|^2 \tag{3.20}$$

Remarks:

1. $l(l+1)<2mV_0$ (1.10).So in (3.15-3.20) one need SAE for l ,which satisfy (1.10).(l=0 always satisfy it!)

2. Total cross section σ is infinite for $V=-V_0/r^2$ in usual quantum mechanics ($\tau = 0$).We show, that for A=0 ($\tau=+\infty$) and small k σ is again infinite, but in general case, when $\delta_p=[l+1/2-p]\pi/2-arctg(\tau_p k^{2p})$ σ can become finite! This problem need more careful investigation!

3. From (3.12) and (3.16) we have

$$S_p=e^{2i[l+1/2-P]\pi/2}e^{-2iarctg\tau_p k^{2p}}$$

Or

$$S_p = S_P^{st}\frac{1-i\tau_p k^{2P}}{1+i\tau_p k^{2P}} \tag{3.21}$$

For τ_p=0 or $\tau_p=\infty$ $S_p$have no poles, so $V=-V_0/r^2$ have no bound states as in usual quantum mechanics! But in the point $i\tau_p k^{2p}=-1$, S have false pole!

$$E=-\frac{i^{\frac{1}{p}-1}}{2m(\tau_p)^{\frac{1}{p}}} \tag{3.22}$$

But τ parameter in general may be complex

$$\tau=\tau_1+i\tau_2 \tag{3.23}$$

where τ_2 describes absorption processes [16].For $\tau=i\tau_2$ (full absorption) we obtain from (3.22) quasidiscret level

$$E=-\frac{i}{2m(\tau_2)^{\frac{1}{p}}} \tag{3.24}$$

IV.Scattering length a

In [16] is calculated scattering length a for the following potential in the l=0 state

$$V(r) = -\frac{V_0}{r^2}\theta(R-r) \tag{4.1}$$

We now obtain more general formula using SAE.When r<R wave function is

$$\chi_0 = \begin{cases} Ar^{1/2+P} + Br^{1/2-P}; 2mV_0 < 1/4; P = \sqrt{1/4 - 2mV_0} \\ r^{1/2}\sin(\nu \ln r + \gamma_0); 2mV_0 > 1/4; \nu = \sqrt{2mV_0 - 1/4} \end{cases} \tag{4.2}$$

γ_0 is SAE parameter, when one have "falling" on the center and is known in the literature [6,15,16]

For r>R

$$\chi_0 = C(r-a) \tag{4.3}$$

"Sewing" condition at r=R gives

$$a = -R\frac{(1-2P)AR^P + BR^{-P}(1+2P)}{(1+2P)AR^P + BR^{-P}(1-2P)}; \qquad 2mV_0 < 1/4 \tag{4.4}$$

$$a = -R\frac{1-2\nu ctg(\nu \ln R - \gamma_0)}{1+2\nu ctg(\gamma \ln R - \gamma_0)}; \qquad 2mV_0 > 1/4 \tag{4.5}$$

When B=0 we get [16] article formula

$$a = -R\frac{(1-2P)}{(1+2P)};$$

(4.6)

As P<1/2, a<0 and it corresponds to attractive potential, but from (4.4) a have no definite sign- we can't say one have attractive or repulsive interaction!

SAE now we define

$$\tau = -A/B \tag{4.7}$$

$$a = \frac{a_1\tau + b_1}{a_2\tau + b_2} \tag{4.8}$$

$$a_1 = -(1-2P)R^{1+P}; b_1 = (1+2P)R^{1-P}$$
$$a_2 = (1+2P)R^{P}; b_2 = -(1-2P)R^{-P} \qquad (4.9)$$

In the region

$$\tau_\infty < \tau < \tau_0 \qquad (4.10)$$

a>0 and we have repulsive interaction! $V(r) = -\frac{V_0}{r^2}\theta(R-r)$ is attractive potential and τ parameter from (4.10) region can change it NATURE!

Again one have two alternatives :

a). From the physical motivation exclude (4.10) region.

b). Agree that τ can change interaction nature!

Remarks:

1). We expand (4.4) and (4.5) near $2mV_0 = 1/4$ and get relation between τ and γ_0

$$2ctg\gamma_0 = \frac{\tau+1}{\tau-1} \qquad (4.11)$$

2). $\sigma_{tot} = 4\pi a^2(\tau) = \sigma(\tau)$ depends on τ! $\sigma > 0$ demand restrict τ!

V.Scattering effective radios ($2mV_0 < 1/4$)

$$r_0 = 2\int_0^\infty \left[u_0^2(r) - \chi_0^2(r)\right]dr \qquad (5.1)$$

where $$u_0 = C(r-a) \qquad (5.2)$$

$$\chi_0 = \begin{cases} Ar^{1/2+P} + Br^{1/2+P}; r < R \\ C(r-a); r > R \end{cases} \qquad (5.3)$$

$$r_0 = 2/3C^2\left\{(R-a)^3 + a^3\right\} - B^2\left\{\frac{\tau^2}{2(P+1)}R^{2P+2} - \frac{R^{2(1-P)}}{2(1-P)} + \tau R^2\right\} \qquad (5.4)$$

$$B = \frac{C(R-a)}{R^{1/2-P} - \tau R^{1/2+P}} \qquad (5.5)$$

$r_0 = r_0(\tau)$ is more complicated function, when $a = a(\tau)$.

$r_0 > 0$ demand restrict τ!

$$\sigma=\frac{4\pi a^2(\tau)}{1+a(\tau)\left[a(\tau)-r_0(\tau)\right]k^2+1/4a^2r_0^2(\tau)k^4};k^2=2mE \qquad (5.6)$$

VI.Model of Valence electron

$$V=-\frac{V_0}{r^2}-\frac{\alpha}{r};\qquad V_0,\alpha>0 \qquad (6.1)$$

Notice that,this potential "naturally" appears for coulomb potential in the Klein-Gordon equation. Following [17-W.Krolikowski; Bulletin De L' academics polonaise.Vol XVII.83(1979);18-A.A.Khelashvili,T.P.Nadareishvili, Bulletin of Georgian Acad.Sci:Vol 164.no1(2001)] we obtain general solution of Schrodinger equation for (6.1) potential

$$\begin{aligned}u=&C_1\rho^{1/2+P}e^{-\rho/2}F\left(1/2+P-\lambda,1+2P;\rho\right)+\\&+C_2\rho^{1/2-P}e^{-\rho/2}F(1/2-P-\lambda,1-2P;\rho)\end{aligned} \qquad (6.2)$$

Where P is given again by (1.8) and

$$\rho=2ik\cdot r;\quad \lambda=-i\frac{m\alpha}{k}=-i\eta;\ \mathrm{E>0};\quad k=\sqrt{2mE};\ \eta=m\alpha/k \qquad (6.3)$$

SAE

$$\tau=\frac{B}{A}(2ik)^{-2P} \qquad (6.4)$$

$$\lim_{r\to\infty}u\approx\sin\left[kr+\eta\ln 2kr-(p-1/2)\pi/2-\delta_{coul}^{st}+\delta_p\right] \qquad (6.5)$$

where

$$\delta_{coul}^{st}=\arg\Gamma\left(1/2+P-\lambda\right) \qquad (6.6)$$

$$\delta_p=arctgQ;\qquad Q=\tau_p(2k)^{2P}\frac{\Gamma(1-2P)\left|\Gamma\left(1/2+P-\lambda\right)\right|}{\Gamma(1+2P)\left|\Gamma\left(1/2-P-\lambda\right)\right|} \qquad (6.7)$$

$$\delta=\delta_p-\delta_{coul}^{st}+\pi/2\left[l+1/2-P\right] \qquad (6.8)$$

$$S_p=e^{i\pi\left[l+1/2-P\right]}\frac{\Gamma\left(1/2+P+\lambda\right)}{\Gamma\left(1/2-P-\lambda\right)}e^{2iarctgQ} \qquad (6.9)$$

$$S_P=S_P^{st}\frac{1+iQ}{1-iQ} \qquad (6.10)$$

iQ =1 is pole!

$$\frac{\Gamma(1/2-\lambda-P)}{\Gamma(1/2-\lambda+P)}=-\frac{\tau_p}{(2mk)^{2p}}\frac{\Gamma(1-2P)}{\Gamma(1+2P)}; \quad k=\sqrt{2mE}; E<0 \qquad (6.11)$$

From (6.11) we get pure $E_{st}(\tau=0)$ and $E_{add}(\tau=\pm\infty)$ eigenvalues

$$E_{st,add}=-\frac{m\alpha^2}{2\left[1/2+n_r\pm P\right]^2}=-\frac{m\alpha^2}{2\left[1/2+n_r\pm\sqrt{(l+1/2)^2-2mV_0}\right]} \qquad (6.12)$$

$$l(l+1)<2mV_0$$

$$f(\theta)=\frac{1}{2ik}\left\{\sum_{l=0}^{\left[-1/2+\sqrt{1/4+2mV_0}\right]}(2l+1)P_l(\cos\theta)\left[S_l^{st}\frac{1+i\theta}{1-i\theta}-1\right]+\sum_{\left[-1/2+\sqrt{1/4+2mV_0}\right]}^{\infty}(2l+1)P_l(\cos\theta)\left[S_l^{st}-1\right]\right\}$$

$$f(\theta)=f_{VE}+f_{SAE} \qquad (6.13)$$

When $V_0\to\infty$,in the (6.13) leading term is f_{SE} and for small V_0 is f_{SAE}

$$\frac{d\sigma}{d\Omega}=|f(\theta)|^2=|f_{VE}|^2+|f_{SAE}|^2+2\operatorname{Re}f_{VE}^*f_{SAE} \qquad (6.14)$$

$$P=\sqrt{(l+1/2)^2-2mV_0}\approx(l+1/2)-\frac{2mV_0}{2l+1} \qquad (6.15)$$

We keep in this case in f_{SAE} only l=0 term and get

$$\frac{d\sigma}{d\Omega}=\frac{1}{\eta^2 4k^2\sin^4\frac{\theta}{2}}\left[1+\frac{2(\pi V_0)^2m^3}{E}\sin^2\theta-2\pi mV_0\sqrt{\frac{2m}{E}}\cos2(\sigma_{-\frac{1}{2}}-\sigma_0)\right]+\frac{\sin^2\delta_{SAE}^0}{k^2}-\eta\frac{2\sin\delta_{SAE}^0}{k^3\sin^2\theta}\times$$

$$\times\left[\cos(\eta\ln\sin^2\frac{\theta}{2}-2\sigma_0-2mV_0\pi-\delta_{SAE}^0)-\pi mV_0\sqrt{\frac{2m}{E}}\sin\theta\cos\left(\eta\ln\sin^2\frac{\theta}{2}-2mV_0\pi-\delta_{SAE}^0-2\sigma_{-\frac{1}{2}}\right)\right]$$

where the first term is usual Reserford formula modified for VE model last two terms are caused by SAE procedure and are similar to the short range interactions. So SAE can again play a role in potential nature!This formalism can be used also for π^+,π^- scattering, where is used Klein-Gordon equation.

VIII. Concluding remarks. Summary

1. Our main result: We show, that for $\lim_{r\to 0} r^2 V \to -V_0 \;;(V_0>0)$ potentials in the region $(l+1/2)^2 > 2mV_0$ (no "falling onto center!) it is necessary to keep second additional solution in the 0<P<1/2 interval (We have our variant of Landau mentioned paragraph!) and it is also necessary to introduce self-adjoint extension τ parameter. in both bound states and scattering problems.
2. Physical quantities E, a, r_0, σ depend on τ parameter and by this reason physical picture is different then in usual quantum mechanics! (As was mentioned above SAE can change nature of potential, δ_p became energy dependent for $V=-V_0/r^2$, this potential have quasidiscret level and so on.

We have three possibilities:

1).It should be found another strong requirement in the quantum mechanic mathematical formalism, which "destroys" additional states!
2) If it isn't possible, try to ''struggle' against τ parameter by physical demands: $r_0>0, \sigma>0,$ don't change physical nature of interaction and so on.
3).Admit SAE existence and find new levels, r_0, a, σ and so on. And now it stay open the following question: Why the NATURE "select" only standard states $(\tau=0)$ yet?!

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