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NORMALIZATION OF SCATTERING STATES, SCATTERING PHASE SHIFTS AND LEVINSON'S THEOREM

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Abstract We show that the normalization integral for the Schrödinger and Dirac scattering wave functions contains, besides the usual delta-function, a term proportional to the derivative of the phase shift. This term is of zero measure with respect to the integration over momentum variables and can be discarded in most cases. Yet it carries the full information on phase shifts and can be used for computation and manipulation of quantities which depend on phase shifts. In this paper we prove Levinson's theorem in a most general way which assumes only the completeness of states. In the case of a Dirac particle we obtain a new result valid for positive and negative energies separately. We also make a generalization of known results, for the phase shifts in the asymptotic limit of high energies, to the case of singular potentials. As an application we consider certain equations, which arise in a generalized interaction picture of quantum electrodynamics. Using the above mentioned results for the phase shifts we prove that any solution of these equations, which has a finite number of bound states, has a total charge zero. Furthermore, we show that in these equations the coupling constant is not a free parameter, but rather should be treated as an eigenvalue and hence must have a definite numerical value.

1. INTRODUCTION AND RESULTS

It is a well known fact that the normalization integral of reduced radial Schrödinger wave functions contains a delta-function. A less well known fact is, that besides the delta-function, there are other terms. In this paper we shall show that the precise expression is

$$\int_0^\infty \mathrm{d}r\, u_{kl}(r)\, u_{k'l}(r) = 2\pi\delta(k-k') + \Delta(k,k') - (-1)^l\left\{2\pi\delta(k+k')\cos\left[\eta_l(k)+\eta_l(k')\right] + \Delta(k,-k')\right\}, \tag{1}$$

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where

$$\Delta\left(k,k'\right)=\begin{cases}2\eta_l'(k)\,, & k=k'\\ 0\,, & k\neq k'\end{cases}\,, \tag{2}$$

$\eta_l'(k)=\partial_k\eta_l(k)$ and $\eta_l(k)$ is a phase shift corresponding to the angular momentum l and linear momentum k. The corresponding result for the case of Dirac equation is

$$\int_0^\infty \mathrm{d}r\,\left[u_{1\epsilon\kappa}(r)\,u_{1\epsilon'\kappa}(r)+u_{2\epsilon\kappa}(r)\,u_{2\epsilon'\kappa}(r)\right]=\begin{cases}2\pi\delta\left(k-k'\right)+\Delta\left(k,k'\right)\\ \quad-(-1)^l\left\{2\pi\delta\left(k+k'\right)\cos\left[\eta_{\epsilon\kappa}(k)+\eta_{\epsilon\kappa}(k')\right]\right.\\ \qquad\left.+\Delta\left(k,-k'\right)\right\}\,, \quad \epsilon=\epsilon'\\ 0\,, \quad \epsilon\neq\epsilon'\end{cases} \tag{3}$$

where $\Delta(k,k')$ is the same function as in (2), except that the Schrödinger phase shift η_l is replaced by its relativistic counterpart $\eta_{\epsilon\kappa}$. In most physical applications (for instance the elastic scattering cross section) the normalization integrals (1) or (3) appear under the integral over k or k', and hence the terms additional to the delta-function $\delta(k-k')$ do not contribute. Yet these terms contain valuable information and can be used for the calculation of phase shifts or for the manipulation of quantities depending on them. In this paper we will use (1) and (3) to prove Levinson's theorem [1] in a most direct and general way.

This theorem is one of the most interesting nonperturbative results in quantum theory. It has many potential applications and has been applied recently in atomic physics [2],[3], in quantum field theories [4],[5], and in solid state physics (where it is known in a modified form under the name Friedel's sum rule [6]). In its original form the theorem says that

$$\eta_l(0)=n_l\pi\,, \tag{4}$$

which relates the scattering phase shift $\eta_l(0)$ at threshold (zero momentum) and for a given angular momentum l to the number of bound states n_l of the Schrödinger equation with a spherically symmetric potential. If the Schrödinger equation has a zero-energy solution which vanishes at the origin and is finite at infinity and yet not normalizable (it is called a half-bound state or zero-energy resonance and is possible only if $l=0$) then, as was first shown by R. Newton [7], Levinson's theorem is modified to read

$$\eta_0(0)=\left(n_0+\frac{1}{2}\right)\pi\,. \tag{5}$$

This result is subject to some restrictions on the potential. The most general proof of Levinson's theorem was carried out by Ni [9] and Ma [8] using the Sturm-Liouville theorem.

Their result for higher angular momenta $l \geq 1$ is (4), but for the S-state, where a zero-energy resonance is possible, they obtained

$$\eta_0(0) = n_0\pi + \frac{\pi}{2}\sin^2\eta_0(0)\,. \tag{6}$$

The authors did not try to solve this equation for $\eta_0(0)$. However, we point out that this equation is easily solved and there are only three solutions:

$$\eta_0(0) = \begin{cases} n_0\pi \\ \left(n_0 + \frac{1}{4}\right)\pi \\ \left(n_0 + \frac{1}{2}\right)\pi\,. \end{cases} \tag{7}$$

The first solution is valid for the case without a zero-energy resonance, the other two if such a resonance exists. No examples are known for the second solution. In this paper we will give yet a more general derivation of the above results, which at the same time is considerably simpler.

The first correct statement of Levinson's theorem for Dirac particles was given by Ma and Ni [10]

$$\eta_{m\kappa}(0) + \eta_{-m\kappa}(0) = \left(N_\kappa^+ + N_\kappa^-\right)\pi\,, \tag{8}$$

which is valid whenever there is no threshold resonance and

$$\eta_{m\kappa}(0) + \eta_{-m\kappa}(0) = \left(N_\kappa^+ + N_\kappa^-\right)\pi + (-1)^l\,\frac{\pi}{2}\left[\sin^2\eta_{m\kappa}(0) + \sin^2\eta_{-m\kappa}(0)\right]\,, \tag{9}$$

which is valid for the case with a threshold resonance (which can appear only in the case $\kappa = \pm 1$). Here $\pm m$ is the threshold energy of the Dirac particle, $l = |\kappa| - 1$ for $\kappa = -1, -2, \ldots$ and $l = \kappa$ for $\kappa = 1, 2, \ldots$ is the orbital angular momentum, N_κ^+ is the number of positive and N_κ^- the number of negative energy bound states of the Dirac equation and $\eta_{\pm m\kappa}(0)$ are the phase shifts at threshold. Prior to the work of Ma and Ni claims were published stating that Levinson's theorem is valid for positive and negative energies separately and in the same sense as in the nonrelativistic case, i.e. $\eta_{\pm m\kappa}(0) = N_\kappa^\pm\pi$, but later such claims were found incorrect [10]. However, we shall prove in this paper that in a modified sense these claims are correct and that

$$\eta_{m\kappa}(0) = \begin{cases} n_l^+\pi & l = 0, 1, \ldots \\ \left(n_0^+ + \frac{1}{4}\right)\pi & l = 0 \\ \left(n_0^+ + \frac{1}{2}\right)\pi & l = 0\,, \end{cases} \tag{10}$$

$$\eta_{-m\kappa}(0) = \begin{cases} n_{\bar{l}}^{-}\pi & \bar{l} = 0, 1, \ldots \\ \left(n_0^- + \frac{1}{4}\right)\pi & \bar{l} = 0 \\ \left(n_0^- + \frac{1}{2}\right)\pi & \bar{l} = 0 , \end{cases} \tag{11}$$

where n_l^+ and $n_{\bar{l}}^-$ are the numbers of bound state solutions of certain Schrödinger equations which are given in the text and $\bar{l} = l - \kappa/|\kappa|$. In (10) and (11) the first case refers to a situation without a threshold resonance and the other two cases to a situation with a threshold resonance. Equations (10) and (11) constitute the stronger statement of Levinson's theorem for Dirac particles. As a consequence of (8) and (10), (11) it follows that

$$N_\kappa^+ + N_\kappa^- = n_l^+ + n_{\bar{l}}^- , \tag{12}$$

whereas in general $N_\kappa^+ \neq n_l^+$ and $N_\kappa^- \neq n_{\bar{l}}^-$.

Besides the phase shifts at threshold one can also obtain nonperturbatively the phase shifts in the asymptotic limit of high energies. A well known result is (see ref. [11] p. 352)

$$\eta_l(k) \xrightarrow[k\to\infty]{} -\frac{m}{k}\int_0^\infty \mathrm{d}r\, V(r) , \tag{13}$$

where $V(r)$ is a spherically symmetric interaction potential, and thus

$$\eta_l(\infty) = 0 . \tag{14}$$

Obviously, equation (13) is only valid if the integral on the right-hand side exists, which is not the case for potentials with a $1/r$ singularity or stronger. In this paper we shall extend this result to the case where the potential at the origin may be as singular as $1/r^{2-0}$ or less, including the obviously important case $1/r$. At infinity the potential is assumed to vanish faster than $1/r$. The result is

$$\eta_l(k) \xrightarrow[k\to\infty]{} k\int_0^\infty \mathrm{d}r \left[\sqrt{1 - \frac{2m}{k^2}V(r)} - 1\right] , \tag{15}$$

which still implies $\eta_l(\infty) = 0$ and which reduces to (13) for potentials less singular than $1/r$ at the origin. In the case of a Dirac particle the Schrödinger result $\eta_l(\infty) = 0$ does not hold in general. Instead it was shown by Parzen [12] that

$$\eta_{\epsilon\kappa}(k) \xrightarrow[k\to\infty]{} -\frac{\epsilon}{k}\int_0^\infty \mathrm{d}r\, V(r) = -\frac{\epsilon}{|\epsilon|}\int_0^\infty \mathrm{d}r\, V(r) , \tag{16}$$

where $\epsilon = \pm\sqrt{k^2 + m^2}$. In general, the right-hand side of (16) is a constant which yields $\eta_{\pm\infty\kappa}(\infty) = 0$ only for a special type of potential. As was the case with (13) the result (16) only holds if the integral on the right-hand side exists. This is not the case for $V(r) \sim 1/r$ at the origin. In this paper we shall derive (16) more rigorously than was done in [12], and we shall generalize the result to the case of a potential behaving like $1/r$ at the origin. Unlike the Schrödinger case there is no reason to treat more singular potentials since the scattering wave functions do not behave well in this case. The result we shall prove is

$$\eta_{\epsilon\kappa}(k) \xrightarrow[k\to\infty]{} k\int_0^\infty \mathrm{d}r \left[\sqrt{1-\frac{2\epsilon}{k^2}V(r)}-1\right], \tag{17}$$

which reduces to (16) if V is less singular than $1/r$ at the origin.

As an application of the above results we shall investigate the following set of equations

$$\begin{aligned} u'_{1\epsilon\kappa} + \frac{\kappa}{r}u_{1\epsilon\kappa} - (m_0+\epsilon+\varphi)\,u_{2\epsilon\kappa} &= 0 \\ u'_{2\epsilon\kappa} - \frac{\kappa}{r}u_{2\epsilon\kappa} - (m_0-\epsilon-\varphi)\,u_{1\epsilon\kappa} &= 0, \end{aligned} \tag{18}$$

$$\varphi'' + \frac{2}{r}\varphi' = \frac{e_0^2}{4\pi}\frac{1}{r^2}\sum_{\kappa=1}^{\infty}\kappa\left(\varrho_\kappa+\varrho_{-\kappa}\right), \tag{19}$$

$$\begin{aligned} \delta(r-r')\,\delta_{ij} = \sum_{0\le\epsilon_\kappa\le m_0} u_{i\epsilon_\kappa\kappa}(r)\,u_{j\epsilon_\kappa\kappa}(r') + \sum_{0<\epsilon_\kappa\le m_0} u_{i,-\epsilon_\kappa\kappa}(r)\;u_{j,-\epsilon_\kappa\kappa}(r') \\ + \int_{0+}^{\infty}\frac{dk}{2\pi}\left[u_{i\varepsilon\kappa}(r)\,u_{jE\kappa}(r') + u_{i,-\varepsilon\kappa}(r)\,u_{j,-\varepsilon\kappa}(r')\right], \end{aligned} \tag{20}$$

where $i = 1,2$, $j = 1,2$, $\kappa = \pm1, \pm2, \ldots$, $u_{i,\pm\epsilon_\kappa\kappa}$ are bound state and $u_{i,\pm\varepsilon\kappa}$ are scattering state solutions of (18), $\epsilon = \pm\epsilon_\kappa$, $0 \le \epsilon_\kappa \le m_0$, are bound state and $\epsilon = \pm\varepsilon$, $\varepsilon \equiv \sqrt{m_0^2+k^2}$, are scattering state energies and

$$\begin{aligned} \varrho_\kappa = \sum_{0\le\epsilon_\kappa\le m_0}\left(u_{1\epsilon_\kappa\kappa}^2 + u_{2\epsilon_\kappa\kappa}^2\right) - \sum_{0<\epsilon_\kappa\le m_0}\left(u_{1,-\epsilon_\kappa\kappa}^2 + u_{2,-\epsilon_\kappa\kappa}^2\right) \\ + \int_{0+}^{\infty}\frac{\mathrm{d}k}{2\pi}\left(u_{1\varepsilon\kappa}^2 + u_{2\varepsilon\kappa}^2 - u_{1,-\varepsilon\kappa}^2 - u_{2,-\varepsilon\kappa}^2\right). \end{aligned} \tag{21}$$

For the sake of simplicity we assume that there are no threshold resonances and hence in (20) and (21) the region of integration excludes $k = 0$. These equations are subject to certain boundary conditions which are explained in the text. Equation (18) is the radial Dirac equation, (19) is one of the Maxwell equations (Poisson equation) and (20) is the completeness relation for radial Dirac wave functions. Equations (18)-(20) arise as a spherically symmetric special case of more general equations in a recently proposed generalized interaction picture of quantum electrodynamics (QED). The derivation of these equations from QED goes beyond the framework of the present paper and we refer the reader to the forthcoming paper [13]. In the present paper, using the above results, we shall prove that for any solution of (18)-(20), which has a finite number of bound states, the total charge vanishes:

$$Q_0 = 0\,, \tag{22}$$

where the charge density is defined by the right-hand side of (19) (in units of $-e_0^2$). Furthermore, the coupling constant $e_0^2/4\pi$ is not a free parameter but rather must have a numerical value for which

$$\int_0^\infty \mathrm{d}r\, \varphi(r) = 0\,. \tag{23}$$

2. NORMALIZATION OF SCATTERING STATES

2.1 SCHRÖDINGER CASE

Consider the radial Schrödinger equation

$$u_{kl}'' - \left[\frac{l\,(l+1)}{r^2} + 2mV - k^2\right] u_{kl} = 0\,, \tag{24}$$

for a scattering state characterized by the reduced radial wave function $u_{kl}(r)$ subject to the boundary conditions

$$u_{kl}(0) = 0\,, \quad u_{kl}(r) \xrightarrow[r\to\infty]{} 2\sin\left(kr - \frac{\pi l}{2} + \eta_l(k)\right)\,, \tag{25}$$

where $\eta_l(k)$ is the phase shift. Here we assume that the potential $V(r)$ is less singular at the origin than $1/r^2$ and that it vanishes at infinity faster than $1/r$. The boundary conditions (25) determine the normalization of the wave functions:

$$\begin{aligned} \int_0^\infty \mathrm{d}r\, u_{kl}(r)\, u_{k'l}(r) &= 2\pi\delta(k-k') + \Delta(k,k') \\ &\quad - (-1)^l \left\{2\pi\delta(k+k')\cos\left[\eta_l(k) + \eta_l(k')\right] + \Delta(k,-k')\right\}\,, \end{aligned} \tag{26}$$

where

$$\Delta(k,k') = \begin{cases} 2\eta_l'(k)\,, & k = k' \\ 0\,, & k \neq k' \end{cases} \tag{27}$$

and $\eta_l'(k) = \partial_k \eta_l(k)$. Notice that in the physical region where both k and k' are positive the last two terms in (26) vanish identically. Moreover, when integrated over positive values of k or k', only the first delta-function contributes. Thus in most cases one could drop all terms except the first. Then, however, one has lost the valuable information about the phase shifts η_l contained in the $\Delta(k,k')$ term. Therefore it is especially desirable to look into situations where only the diagonal terms in (26) are essential and the delta-functions do not contribute. For instance, subtracting from (26) its noninteracting counterpart the delta-functions cancel and we obtain

$$\int_0^\infty \mathrm{d}r \left[u_{kl}^2(r) - v_{kl}^2(r)\right] = 2\eta_l'(k) + (-1)^l 2\pi\delta(k)\sin^2\eta_l(k), \qquad v_{kl}(r) = 2krj_l(kr), \tag{28}$$

where $j_l(kr)$ are the spherical Bessel functions. This equation turns out to be quite useful, as will be shown below. Also notice that the extra terms on the right-hand side of (26) cannot be cancelled by changing the normalization in (25).

To derive equation (26) we multiply (24) by $u_{k'l}$ and the corresponding equation for $u_{k'l}$ by u_{kl}. Subtracting the resulting equations from one another and integrating using $u_{kl}(0) = u_{k'l}(0) = 0$, we obtain

$$\int_0^R \mathrm{d}r\, u_{kl}(r)\, u_{k'l}(r) = \frac{u_{kl}(R)\, u_{k'l}'(R) - u_{kl}'(R)\, u_{k'l}(R)}{k^2 - k'^2}, \tag{29}$$

where $u_{kl}'(R) = \partial_R u_{kl}(R)$. For large enough R one can evaluate the right-hand side of (29) using the asymptotic expression (25) and obtain

$$\begin{aligned}\frac{1}{2}\int_0^R \mathrm{d}r\, u_{kl}(r)\, u_{k'l}(r) = {}& \frac{\sin[(k-k')R]}{k-k'}\cos[\eta_l(k) - \eta_l(k')] + \frac{\sin[\eta_l(k) - \eta_l(k')]}{k-k'}\cos[(k-k')R] \\ & - (-1)^l\left\{\frac{\sin[(k+k')R]}{k+k'}\cos[\eta_l(k) + \eta_l(k')] + \frac{\sin[\eta_l(k) + \eta_l(k')]}{k+k'}\cos[(k+k')R]\right\}.\end{aligned} \tag{30}$$

Using $\eta_l(-k) = -\eta_l(k)$ (see ref. [14] for a proof), equation (26) follows as $R \to \infty$.

It is instructive to consider a somewhat different derivation. Taking the derivative of (24) with respect to k and multiplying the result by u_{kl}, then multiplying (24) by $\partial_k u_{kl}$, subtracting the resulting two equations from one another and integrating, we obtain

$$\int_0^R \mathrm{d}r\, u_{kl}^2(r) = \frac{1}{2k}\left[u_{kl}'(R)\,\partial_k u_{kl}(R) - u_{kl}(R)\,\partial_k u_{kl}'(R)\right]. \tag{31}$$

For a large enough R we can use the asymptotics (25) to evaluate the right-hand side of (31). The result

$$\int_0^R \mathrm{d}r\, u_{kl}^2(r) = 2R + 2\eta_l'(k) - (-1)^l \frac{1}{k}\sin[2kR + 2\eta_l(k)] \tag{32}$$

was first obtained by Lüders [15]. Equation (32) is exact if the potential $V(r)$ vanishes for $r > R$ and is valid asymptotically otherwise. From (32) one easily recovers the diagonal terms of (26).

2.2 DIRAC CASE

Consider now the reduced radial Dirac equations

$$\begin{aligned} u'_{1\epsilon\kappa} + \frac{\kappa}{r} u_{1\epsilon\kappa} - (\epsilon + m - V)\, u_{2\epsilon\kappa} &= 0 \\ u'_{2\epsilon\kappa} - \frac{\kappa}{r} u_{2\epsilon\kappa} + (\epsilon - m - V)\, u_{1\epsilon\kappa} &= 0\,, \end{aligned} \tag{33}$$

where ϵ is the energy, $V(r)$ is the time component of a vector potential and $\kappa = \pm 1, \pm 2, \ldots$. The quantum number κ is the standard parametrization of the total angular momentum $j = |\kappa| - 1/2$ and of the relative orientation between the spin and the orbital angular momentum. The appropriate boundary conditions are

$$u_{1\epsilon\kappa}(0) = 0\,, \quad u_{1\epsilon\kappa}(r) \xrightarrow[r\to\infty]{} \sqrt{\frac{\epsilon + m}{2\epsilon}}\, 2\sin\left(kr - \frac{\pi l}{2} + \eta_{\epsilon\kappa}(k)\right), \tag{34}$$

$$u_{2\epsilon\kappa}(0) = 0\,, \quad u_{2\epsilon\kappa}(r) \xrightarrow[r\to\infty]{} \sqrt{\frac{\epsilon + m}{2\epsilon}}\, \frac{\kappa_0 k}{\epsilon + m}\, 2\sin\left(kr - \frac{\pi \bar{l}}{2} + \eta_{\epsilon\kappa}(k)\right), \tag{35}$$

where $k = \pm\sqrt{\epsilon^2 - m^2}$, $\kappa_0 = \kappa/|\kappa|$, $l = |\kappa| - (1 - \kappa_0)/2$, $\bar{l} = l - \kappa_0$, and $\eta_{\epsilon\kappa}(k)$ is the phase shift. To ensure the consistency of (34) and (35) with (33) we assume that $V(r)$ behaves like or less singularly than $1/r$ at the origin and that it vanishes at infinity faster than $1/r$. Thus the Yukawa potential $e^{-\mu_0 r}/r$ is allowed but the Coulomb potential is excluded. The normalization of the wave functions resulting from the boundary conditions (34) and (35) is

$$\int_0^\infty \mathrm{d}r\, \left[u_{1\epsilon\kappa}(r)\, u_{1\epsilon'\kappa}(r) + u_{2\epsilon\kappa}(r)\, u_{2\epsilon'\kappa}(r)\right] = \begin{cases} 2\pi\delta(k - k') + \Delta(k, k') \\ \quad - (-1)^l \left\{2\pi\delta(k + k') \cos\left[\eta_{\epsilon\kappa}(k) + \eta_{\epsilon\kappa}(k')\right] \right. \\ \qquad \left. + \Delta(k, -k')\right\}, \quad \epsilon = \epsilon' \\ 0\,, \quad \epsilon \neq \epsilon' \end{cases} \tag{36}$$

where $\Delta(k, k')$ is the same function as in (27), except that the phase shift η_l is replaced by $\eta_{\epsilon\kappa}$. Notice the similarity of (36) to the corresponding Schrödinger case (26). As in that case we can extract the information on the phase shifts $\eta_{\epsilon\kappa}$ by subtracting from (36) the corresponding equation for the noninteracting case, and we obtain

$$\int_0^\infty \mathrm{d}r\, \left[u^2_{1\epsilon\kappa}(r) + u^2_{2\epsilon\kappa}(r) - v^2_{1\epsilon\kappa}(r) - v^2_{2\epsilon\kappa}(r)\right] = 2\eta'_{\epsilon\kappa}(k) + (-1)^l\, 2\pi\delta(k) \sin^2\eta_{\epsilon\kappa}(k)\,, \tag{37}$$

where

$$v_{1\epsilon\kappa}(r) = \sqrt{\frac{\epsilon+m}{2\epsilon}}\, 2kr\, j_l(kr)\,, \quad v_{2\epsilon\kappa}(r) = \sqrt{\frac{\epsilon+m}{2\epsilon}}\, \frac{\kappa_0 k}{\epsilon+m}\, 2kr\, j_{\bar{l}}(kr) \tag{38}$$

is the regular free-particle solution of the Dirac equation (33), which obeys (34), (35) and (36) with $\eta_{\epsilon\kappa}(k)=0$. Contrary to the case of the Schrödinger equation the energy can now be either positive or negative and we can use $u_{i,-\epsilon\kappa}$ instead of $v_{i\epsilon\kappa}$ to extract the diagonal terms in (36). The result is

$$\begin{aligned}
&\int_0^\infty \mathrm{d}r\, \left[u_{1\epsilon\kappa}^2(r) + u_{2\epsilon\kappa}^2(r) - u_{1,-\epsilon\kappa}^2(r) - u_{2,-\epsilon\kappa}^2(r)\right] \\
&\quad = 2\left[\eta'_{\epsilon\kappa}(k) - \eta'_{-\epsilon\kappa}(k)\right] + (-1)^l\, 2\pi\delta(k) \sin\left[\eta_{\epsilon\kappa}(k) + \eta_{-\epsilon\kappa}(k)\right] \sin\left[\eta_{\epsilon\kappa}(k) - \eta_{-\epsilon\kappa}(k)\right] .
\end{aligned} \tag{39}$$

To derive (36) we multiply the Dirac equation (33) by $(-u_{2\epsilon'\kappa}, u_{1\epsilon'\kappa})$ and the Dirac equation for ϵ' by $(-u_{2\epsilon\kappa}, u_{1\epsilon\kappa})$ and subtract the results. Upon integration we obtain

$$\int_0^R \mathrm{d}r\, \left[u_{1\epsilon\kappa}(r)\, u_{1\epsilon'\kappa}(r) + u_{2\epsilon\kappa}(r)\, u_{2\epsilon'\kappa}(r)\right] = \frac{u_{1\epsilon\kappa}(R)\, u_{2\epsilon'\kappa}(R) - u_{1\epsilon'\kappa}(R)\, u_{2\epsilon\kappa}(R)}{\epsilon-\epsilon'} . \tag{40}$$

For a large enough R the right-hand side of (40) can be evaluated using the asymptotic wave functions (34) and (35). The result is

$$\begin{aligned}
&\int_0^R \mathrm{d}r\, \left[u_{1\epsilon\kappa}(r)\, u_{1\epsilon'\kappa}(r) + u_{2\epsilon\kappa}(r)\, u_{2\epsilon'\kappa}(r)\right] \\
&= A\left\{\frac{\sin\left[(k-k')\,R\right]}{k-k'} \cos\left[\eta_{\epsilon\kappa}(k) - \eta_{\epsilon'\kappa}(k')\right] + \frac{\sin\left[\eta_{\epsilon\kappa}(k) - \eta_{\epsilon'\kappa}(k')\right]}{k-k'} \cos\left[(k-k')\,R\right]\right\} \\
&- (-1)^l\, B\left\{\frac{\sin\left[(k+k')\,R\right]}{k+k'} \cos\left[\eta_{\epsilon\kappa}(k) + \eta_{\epsilon'\kappa}(k')\right] + \frac{\sin\left[\eta_{\epsilon\kappa}(k) + \eta_{\epsilon'\kappa}(k')\right]}{k+k'} \cos\left[(k+k')\,R\right]\right\} .
\end{aligned} \tag{41}$$

where

$$\begin{aligned}
A &= \left(\frac{\epsilon}{|\epsilon|} k\sqrt{\frac{\epsilon'+m}{\epsilon\epsilon'(\epsilon+m)}} + \frac{\epsilon'}{|\epsilon'|} k'\sqrt{\frac{\epsilon+m}{\epsilon\epsilon'(\epsilon'+m)}}\right) \frac{\epsilon+\epsilon'}{k+k'}\,, \\
B &= \left(\frac{\epsilon}{|\epsilon|} k\sqrt{\frac{\epsilon'+m}{\epsilon\epsilon'(\epsilon+m)}} - \frac{\epsilon'}{|\epsilon'|} k'\sqrt{\frac{\epsilon+m}{\epsilon\epsilon'(\epsilon'+m)}}\right) \frac{\epsilon+\epsilon'}{k-k'} .
\end{aligned} \tag{42}$$

Equation (36) is now easily recovered as $R \to \infty$.

As in the Schrödinger case the diagonal terms of (36) can be obtained somewhat differently. We derive the Dirac equation (33) with respect to ϵ, multiply the resulting equation by $(-u_{2\epsilon\kappa}, u_{1\epsilon\kappa})$ and subtract from the result the Dirac equation multiplied by $(-\partial_\epsilon u_{2\epsilon\kappa}, \partial_\epsilon u_{1\epsilon\kappa})$. Upon integration we obtain

$$\int_0^R \mathrm{d}r\, \left[u_{1\epsilon\kappa}^2(r) + u_{2\epsilon\kappa}^2(r)\right] = u_{2\epsilon\kappa}(R)\, \partial_\epsilon u_{1\epsilon\kappa}(R) - u_{1\epsilon\kappa}(R)\, \partial_\epsilon u_{2\epsilon\kappa}(R) . \tag{43}$$

Taking R large and inserting the asymptotic wave functions (34) and (35) on the right-hand side, we obtain

$$\int_0^R \mathrm{d}r\,\left[u_{1\epsilon\kappa}^2(r)+u_{2\epsilon\kappa}^2(r)\right]=2R+2\eta'_{\epsilon\kappa}(k)-(-1)^l\,\frac{m}{\epsilon k}\sin\left[2kR+2\eta_{\epsilon\kappa}(k)\right] \tag{44}$$

From (44) one easily recovers the diagonal terms of (36). Notice the close similarity of (44) to the corresponding result for the Schrödinger case (32). In particular for small energies ($m/\epsilon\to 1$) both results coincide.

3. HIGH ENERGY LIMIT

3.1 SCHRÖDINGER CASE

It is a well known result (see ref. [11] p. 352) that

$$\eta_l(k)\xrightarrow[k\to\infty]{}-\frac{m}{k}\int_0^\infty \mathrm{d}r\,V(r) \tag{45}$$

and thus

$$\eta_l(\infty)=0\,. \tag{46}$$

Obviously, equation (45) is only valid if the integral on the right-hand side exists, which is not the case for potentials with a $1/r$ singularity or stronger. In this section we want to extend this result to the case where the potential at the origin may be as singular as $1/r^{2-0}$ or less, including the obviously important case $1/r$. At infinity the potential is assumed to vanish faster than $1/r$. The result we shall now prove is

$$\eta_l(k)\xrightarrow[k\to\infty]{}k\int_0^\infty \mathrm{d}r\,\left[\sqrt{1-\frac{2m}{k^2}V(r)}-1\right], \tag{47}$$

which still implies (46) and which reduces to (45) for potentials less singular than $1/r$ at the origin.

We introduce a new variable $\bar r$ and a new wave function $\chi_{kl}(\bar r)$

$$u_{kl}(r)=\frac{\chi_{kl}(\bar r)}{\sqrt{F}},\qquad \bar r=\int_0^r \mathrm{d}r'\,F(r')\,,\qquad F(r)=\sqrt{1-\frac{2m}{k^2}V(r)}\,. \tag{48}$$

Putting this into the Schrödinger equation (24) we get

$$\ddot\chi_{kl}-\left[\frac{l(l+1)}{\bar r^2}\left(1+\frac{1}{k}A\right)-\frac{m}{2k^2}B-\frac{3m}{4k^4}C-k^2\right]\chi_{kl}=0\,, \tag{49}$$

where

$$A=\frac{k\frac{\bar{r}^2-r^2}{r^2}+\frac{2m}{k}V}{1-\frac{2m}{k^2}V}\,,\quad B=\frac{\ddot{V}}{1-\frac{2m}{k^2}V}\,,\quad C=\left(\frac{\dot{V}}{1-\frac{2m}{k^2}V}\right)^2 \tag{50}$$

and where the dots mean the derivatives with respect to the new variable $\bar{r}$. Consider now a sphere of radius $\bar{r}=\sqrt{m/k}$ around the origin, k being large, and assume the case of the strongest allowed singularity $V\sim 1/r^{2-0}$. Then everywhere outside of the sphere the terms proportional to A, B and C in (49) are bounded by certain positive powers of m/k. Hence as $k\to\infty$, we obtain

$$\ddot{\chi}_{kl}-\left[\frac{l\,(l+1)}{\bar{r}^2}-k^2\right]\chi_{kl}=0\,, \tag{51}$$

of which the physical solution is $\chi_{kl}(\bar{r})=2k\bar{r}j_l(k\bar{r})$. Therefore as $k\to\infty$, from (48) we have

$$u_{kl}(r)\xrightarrow[r\to\infty]{}2\sin\left(kr-\frac{\pi l}{2}+k\int_0^\infty \mathrm{d}r\left[\sqrt{1-\frac{2m}{k^2}V(r)}-1\right]\right) \tag{52}$$

and hence (47).

3.2 DIRAC CASE

In the case of a Dirac particle the Schrödinger result (46) in general does not hold. Instead it was shown by Parzen [12] that

$$\eta_{\epsilon\kappa}(k)\xrightarrow[k\to\infty]{}-\frac{\epsilon}{k}\int_0^\infty \mathrm{d}r\;V(r)=-\frac{\epsilon}{|\epsilon|}\int_0^\infty \mathrm{d}r\;V(r)\,, \tag{53}$$

where $\epsilon=\pm\sqrt{k^2+m^2}$. In general, the right-hand side of (53) is a constant which yields $\eta_{\pm\infty\kappa}(\infty)=0$ only for a special type of potential. As was the case with (45), the result (53) only holds if the integral on the right-hand side exists. This is not the case for $V(r)\sim 1/r$ at the origin. In this section we want to rederive (53) in a more rigorous way than was done in [12] and to extend the result to the case of a potential behaving like $1/r$ at the origin. Unlike the Schrödinger case there is no reason to treat more singular potentials since the scattering wave functions do not behave well in this case. The result we shall prove is

$$\eta_{\epsilon\kappa}(k)\xrightarrow[k\to\infty]{}k\int_0^\infty \mathrm{d}r\left[\sqrt{1-\frac{2\epsilon}{k^2}V(r)}-1\right]\,, \tag{54}$$

which reduces to (53) if V is less singular than $1/r$ at the origin.

Eliminating $u_{2\epsilon\kappa}$ from (33), we obtain

$$u_{1\epsilon\kappa}''-\left[\frac{\kappa(\kappa+1)}{r^2}-\frac{\kappa}{r}\frac{V'}{\epsilon+m-V}-V^2+2\epsilon V-k^2\right]u_{1\epsilon\kappa}+\frac{V'}{\epsilon+m-V}u_{1\epsilon\kappa}'=0\,. \tag{55}$$

Eliminating $u_{1\epsilon\kappa}$ from (33) leads to

$$u''_{2\epsilon\kappa} - \left[\frac{\kappa(\kappa-1)}{r^2} + \frac{\kappa}{r}\frac{V'}{\epsilon-m-V} - V^2 + 2\epsilon V - k^2\right] u_{2\epsilon\kappa} + \frac{V'}{\epsilon-m-V} u'_{2\epsilon\kappa} = 0\,. \tag{56}$$

Equations (55) and (56) are equivalent to the Dirac equation (33) provided the boundary conditions (34) and (35) are imposed. Actually it is not necessary to solve (55) and (56) simultaneously. For instance, if (55) is solved for $u_{1\epsilon\kappa}$ one gets $u_{2\epsilon\kappa}$ through the first of equations (33). In order to get rid of the last term in (55) and (56) we introduce the new wave functions $(w_{1\epsilon\kappa}, w_{2\epsilon\kappa})$ defined through

$$u_{1\epsilon\kappa}(r) = \sqrt{\frac{\epsilon+m-V(r)}{2\epsilon}}\, w_{1\epsilon\kappa}(r)\,, \quad u_{2\epsilon\kappa}(r) = \frac{\epsilon k \kappa}{|\epsilon||k||\kappa|}\sqrt{\frac{\epsilon-m-V(r)}{2\epsilon}}\, w_{2\epsilon\kappa}(r)\,. \tag{57}$$

Putting these in (55) and (56), we obtain

$$w''_{1\epsilon\kappa} - \left[\frac{l(l+1)}{r^2} - \frac{\kappa}{r}\frac{V'}{\epsilon+m-V} + \frac{1}{2}\frac{V''}{\epsilon+m-V} + \frac{3}{4}\left(\frac{V'}{\epsilon+m-V}\right)^2 - V^2 + 2\epsilon V - k^2\right] w_{1\epsilon\kappa} = 0\,, \tag{58}$$

$$w''_{2\epsilon\kappa} - \left[\frac{\bar{l}(\bar{l}+1)}{r^2} + \frac{\kappa}{r}\frac{V'}{\epsilon-m-V} + \frac{1}{2}\frac{V''}{\epsilon-m-V} + \frac{3}{4}\left(\frac{V'}{\epsilon-m-V}\right)^2 - V^2 + 2\epsilon V - k^2\right] w_{2\epsilon\kappa} = 0\,, \tag{59}$$

where we used $\kappa(\kappa+1) = l(l+1)$ and $\kappa(\kappa-1) = \bar{l}(\bar{l}+1)$ which are readily obtained from $l = |\kappa| - (1-\kappa_0)/2$ and $\bar{l} = l - \kappa_0$, $\kappa_0 = \kappa/|\kappa|$. Equations (58) and (59) are of the Schrödinger-type except that the potential depends on the energy. Solving (58) and (59) is equivalent to solving the original Dirac equation (33) provided the boundary conditions

$$w_{1\epsilon\kappa}(0) = 0\,, \quad w_{1\epsilon\kappa}(r) \xrightarrow[r\to\infty]{} 2\sin\left(kr - \frac{\pi l}{2} + \eta_{\epsilon\kappa}(k)\right)\,, \tag{60}$$

$$w_{2\epsilon\kappa}(0) = 0\,, \quad w_{2\epsilon\kappa}(r) \xrightarrow[r\to\infty]{} 2\sin\left(kr - \frac{\pi\bar{l}}{2} + \eta_{\epsilon\kappa}(k)\right) \tag{61}$$

are met. We now turn to the limit $k \to \infty$. To perform this limit we can use either (58) or (59), the result will be the same. As in the Schrödinger case, considering a small sphere of radius $(m/k)^{1/4}$, we observe that everywhere outside of the sphere the second, third and fourth terms in the parentheses of (58) and (59) are bounded by positive powers of m/k as $k \to \infty$ and hence can be neglected. The term V^2 behaves as $1/r^2$ at the origin and vanishes faster than $1/r^2$ at infinity. Hence it does alter the form of the wave function at the origin, but at large distances it contributes only to the phase of the wave function, which remains a Bessel function. However, V^2 is of order zero in k so that, according to the preceding section, it does not contribute to the asymptotic limit $\eta_{\epsilon\kappa}(\infty)$ and, in particular, cannot compete with the term $2\epsilon V$ which is of order one in k. Hence as $k \to \infty$ we neglect it and obtain from (58)

$$w''_{1\epsilon\kappa} - \left[\frac{l\,(l+1)}{r^2} + 2\epsilon V - k^2\right] w_{1\epsilon\kappa} = 0\,, \tag{62}$$

which is subject to the boundary condition (60). Thus the high energy limit of the Dirac equation is dominated by the Schrödinger equation (24) in which the mass m is replaced by the energy $\epsilon = \pm\sqrt{k^2+m^2}$. It is easy to check that, despite this alteration of the Schrödinger equation, the arguments of the preceding section are still valid and we can apply (47) replacing m by ϵ. The result is given in (54).

4. ZERO ENERGY LIMIT: LEVINSON'S THEOREM

4.1 SCHRÖDINGER CASE

The set of all physical solutions of the Schrödinger equation (24) constitutes a complete set in the sense that for each $l = 0, 1, \ldots$

$$\sum_{\epsilon_l<0} u_{\epsilon_l l}\,(r)\, u_{\epsilon_l l}\,(r') + \int_0^\infty \frac{\mathrm{d}k}{2\pi}\, u_{kl}\,(r)\, u_{kl}\,(r') = \delta\,(r-r')\,, \tag{63}$$

where $u_{\epsilon_l l}$ are bound state solutions of (24) normalized according to

$$\int_0^\infty \mathrm{d}r\; u^2_{\epsilon_l l}\,(r) = 1 \tag{64}$$

and u_{kl} are scattering state solutions (25). With respect to the completeness relation we have to distinguish two cases. In the first case, if there exists a zero-energy solution of the Schrödinger equation (24), which vanishes at the origin and is finite at large distances (we will call it finite), it is not normalizable in the sense of (64). Such a solution, clearly, is not a bound state (it is called a half-bound state [11] or a zero-energy resonance [16] since it becomes a bound state after an arbitrarily small increase in the strength of the potential). It is part of the continuum and is responsible for the delta-function in (28). Hence the sum over bound states on the left-hand side of (63) does not include the zero-energy solution and the integral over k is understood as including the value $k = 0$. This is the meaning of the completeness relation (63). In the second case, if a finite, zero-energy, solution exists, it is normalizable. Such a solution is a bound state and must be included in the sum over bound states on the left-hand side of (63) and, consequently, the integral over k is understood as excluding the value $k = 0$. The completeness relation for this case is

$$\sum_{\epsilon_l\le 0} u_{\epsilon_l l}\,(r)\, u_{\epsilon_l l}\,(r') + \int_{0+}^\infty \frac{\mathrm{d}k}{2\pi}\, u_{kl}\,(r)\, u_{kl}\,(r') = \delta\,(r-r')\,. \tag{65}$$

Notice that, if no finite zero-energy solution exists, then one can use either one of the completeness relations. In case a finite zero-energy solution exists, it is necessarily a zero-energy resonance if $l = 0$, and a bound state if $l \geq 1$. This is easily seen by examining the Schrödinger equation (24) at large distances for potentials which vanish faster than $1/r^2$, and noticing that a finite zero-energy solution behaves as $1/r^l$. If the potential does not vanish faster than $1/r^2$ at infinity, then finite, zero-energy, solutions do not exist.

Obviously the completeness relation also holds for a free particle, except that in this case there are no bound states and hence (63) and (65) are identical. We now proceed with the second case above using (65). Subtracting from (65) the corresponding equation for the noninteracting case the delta-functions cancel and we obtain

$$\sum_{\epsilon_l \leq 0} u_{\epsilon_l l}(r)\, u_{\epsilon_l l}(r') + \int_{0+}^{\infty} \frac{\mathrm{d}k}{2\pi} \left[u_{kl}(r)\, u_{kl}(r') - v_{kl}(r)\, v_{kl}(r')\right] = 0\,, \tag{66}$$

where v_{kl} are the free particle solutions. Thus the diagonal part of (66) reads

$$\sum_{\epsilon_l \leq 0} u^2_{\epsilon_l l}(r) + \int_{0+}^{\infty} \frac{\mathrm{d}k}{2\pi} \left[u^2_{kl}(r) - v^2_{kl}(r)\right] = 0\,. \tag{67}$$

Integrating over r and substituting (28), we obtain

$$\eta_l(0) = \eta_l(\infty) + n_l \pi \tag{68}$$

where n_l is the number of bound states having angular momentum l (not counting the $2l+1$ degeneracy). Finally substituting (46), we get

$$\eta_l(0) = n_l \pi\,. \tag{69}$$

Equation (69) is known as Levinson's theorem [1]. It is valid whenever there is no zero-energy resonance and this, as explained above, is the case for all $l \geq 1$. This is, of course, a well known result.

We now return to the first case where a finite zero-energy solution, if it exists, is not normalizable and where we have to use (63) instead of (65). Since a zero-energy resonance can occur only for $l = 0$ we do not need to consider higher angular momentum states. Because the region of integration in (63) contains the value $k = 0$, the steps preceding (69) remain the same except that now the delta-function on the right-hand side of (28) contributes, and we obtain

$$\eta_0(0) = \eta_0(\infty) + n_0 \pi + \frac{\pi}{2} \sin^2 \eta_0(0)\,. \tag{70}$$

Substituting (46), we get

$$\eta_0(0) = n_0 \pi + \frac{\pi}{2} \sin^2 \eta_0(0)\,. \tag{71}$$

This version of Levinson's theorem was first derived by Ni [9]. Equation (71) can be solved for $\eta_0(0)$ and there are only three solutions:

$$\eta_0(0) = \begin{cases} n_0 \pi \\ \left(n_0 + \frac{1}{4}\right)\pi \\ \left(n_0 + \frac{1}{2}\right)\pi . \end{cases} \tag{72}$$

The second and third solutions correspond to the case with a zero-energy resonance, whereas the first solution corresponds to the case with no such state. The third solution is a result obtained by Newton [7]. Equation (72) is the most general statement of Levinson's theorem possible. The only input in our derivation is the completeness relation (63) and the boundary conditions (25). Although we do not have an example for the second solution in (72) there is little doubt that it can be realized.

Levinson's theorem (69) can be proved in a number of different ways (see ref. [17] and [18], for instance). The present proof has the advantage of being very general and extremely simple and also allows us some additional insights.

4.2 DIRAC CASE

A further advantage of the above proof is that it can be taken over to the case of the Dirac equation almost without change. In this section we will first rederive the result of Ma and Ni [10], which is the original correct statement of Levinson's theorem for Dirac particles, and which is valid for the sum of positive and negative energy phase shifts. Then we will prove a stronger statement of Levinson's theorem, valid for positive and negative energies separately.

The zero-energy resonance of the preceding chapter is now called threshold resonance (its meaning is still the same: $k=0$). As in the Schrödinger case we distinguish two cases: with and without threshold resonance. However, there is now a slight complication - the threshold resonance can have either a positive or negative energy, or there could exist two resonances simultaneously, one with positive and the other with negative energy. For the sake of simplicity we will consider only two cases; the gap will be filled at the end of this section where we consider the positive and negative energies separately. In the first case any finite threshold solution (which does not necessarily exist) of the Dirac equation (33) is a resonance and not a bound state. The completeness relation in this case reads

$$\begin{aligned} \delta(r-r')\,\delta_{ij} = \sum_{-m<\epsilon_\kappa<m} & u_{i\epsilon_\kappa\kappa}(r)\, u_{j\epsilon_\kappa\kappa}(r') \\ & + \int_0^\infty \frac{\mathrm{d}k}{2\pi} \left[u_{i\epsilon\kappa}(r)\, u_{j\epsilon\kappa}(r') + u_{i,-\epsilon\kappa}(r)\, u_{j,-\epsilon\kappa}(r')\right] , \end{aligned} \tag{73}$$

where $i = 1,2$, $j = 1,2$, $u_{i\epsilon_\kappa\kappa}$ are bound state solutions of (33), $\epsilon = \sqrt{k^2+m^2}$ and where the region of integration includes $k=0$, so that a term with a delta-function $\delta(k)$ would contribute. The bound states are normalized according to

$$\int_0^\infty \mathrm{d}r \left[u^2_{1\epsilon_\kappa\kappa}(r) + u^2_{2\epsilon_\kappa\kappa}(r)\right] = 1\,. \tag{74}$$

In the second case any finite threshold solution (which does not necessarily exist) is a bound state. The corresponding completeness relation is

$$\begin{aligned}\delta(r-r')\,\delta_{ij} = &\sum_{-m\le\epsilon_\kappa\le m} u_{i\epsilon_\kappa\kappa}(r)\,u_{j\epsilon_\kappa\kappa}(r') \\ &+ \int_{0+}^\infty \frac{\mathrm{d}k}{2\pi}\left[u_{i\epsilon\kappa}(r)\,u_{j\epsilon\kappa}(r') + u_{i,-\epsilon\kappa}(r)\,u_{j,-\epsilon\kappa}(r')\right]\,,\end{aligned} \tag{75}$$

where the region of integration does not include $k=0$, so that a term with a delta-function $\delta(k)$ would not contribute. The rest of the derivation is identical to the Schrödinger case, except that equation (37) has to be used instead of (28). The result following from (75) is

$$\eta_{m\kappa}(0) + \eta_{-m,\kappa}(0) = \left(N^+_\kappa + N^-_\kappa\right)\pi\,, \tag{76}$$

whereas the one following from (73) is

$$\eta_{m\kappa}(0) + \eta_{-m,\kappa}(0) = \left(N^+_\kappa + N^-_\kappa\right)\pi + (-1)^l\,\frac{\pi}{2}\left[\sin^2\eta_{m\kappa}(0) + \sin^2\eta_{-m,\kappa}(0)\right]\,, \tag{77}$$

where $l=|\kappa|-1$ for $\kappa=-1,-2,\ldots$ and $l=\kappa$ for $\kappa=1,2,\ldots$ is the orbital angular momentum, N^+_κ is the number of positive and N^-_κ is the number of negative energy bound states of (33). In deriving (77) we used $\eta_{\infty\kappa}(\infty) = -\eta_{-\infty,\kappa}(\infty)$ which follows from (54). Equation (77) is Levinson's theorem for Dirac particles first obtained by Ma and Ni [10]. Above we derived equations (55) and (56) which, if subjected to the boundary conditions (34) and (35), are equivalent to the Dirac equation (33). An inspection of these equations at threshold ($k=0$) and for large r, shows that a threshold resonance can occur only if $\kappa=\pm1$. Therefore (76) is valid for all $\kappa=\pm2,\pm3,\ldots$ and for $\kappa=\pm1$ if there is no threshold resonance, whereas (77) is valid for $\kappa=-1$ ($l=0$, $\bar{l}=1$) and $\kappa=1$ ($l=1$, $\bar{l}=0$).

One may ask oneself whether (76) and (77) are perhaps valid for positive and negative energies separately. In fact, in some of the initial work (see refs. [19] and [9]) this was claimed to be true but later was found incorrect [10]. Yet, intuitively, by a number of reasons we expect that an extension of (76) and (77), for positive and negative energies separately, should be possible. We now show that this is indeed the case. The basic observation which we need is the fact that the set of Schrödinger-like equations (58) and (59) subject to the boundary conditions (60) and (61) is fully equivalent to the original Dirac equation (33) subject to the boundary conditions (34) and (35). Equations (58) and (59) are useful because they are not coupled and hence the phase shift $\eta_{\epsilon\kappa}(k)$ can be computed using any one of them, without reference to the other and for each of the positive and negative energies ϵ separately. Certainly we cannot apply Levinson's theorem to (58) or (59) directly since the potential in these equations depends on the energy and hence the completeness relation does not have the form (63). However, consider the following equations

$$w_{kl}^{+\prime\prime} - \left[\frac{l\,(l+1)}{r^2} - \frac{\kappa}{r}\frac{V'}{2m-V} + \frac{1}{2}\frac{V''}{2m-V} + \frac{3}{4}\left(\frac{V'}{2m-V}\right)^2 - V^2 + 2mV - k^2\right] w_{kl}^{+} = 0\,, \tag{78}$$

$$w_{k\bar{l}}^{-\prime\prime} - \left[\frac{\bar{l}\,(\bar{l}+1)}{r^2} - \frac{\kappa}{r}\frac{V'}{2m+V} - \frac{1}{2}\frac{V''}{2m+V} + \frac{3}{4}\left(\frac{V'}{2m+V}\right)^2 - V^2 - 2mV - k^2\right] w_{k\bar{l}}^{-} = 0\,, \tag{79}$$

which are subject to the boundary conditions

$$w_{kl}^{+}(0) = 0\,, \quad w_{kl}^{+}(r) \xrightarrow[r\to\infty]{} 2\sin\left(kr - \frac{\pi l}{2} + \eta_l^{+}(k)\right)\,, \tag{80}$$

$$w_{k\bar{l}}^{-}(0) = 0\,, \quad w_{k\bar{l}}^{-}(r) \xrightarrow[r\to\infty]{} 2\sin\left(kr - \frac{\pi \bar{l}}{2} + \eta_{\bar{l}}^{-}(k)\right)\,. \tag{81}$$

At threshold ($k=0$) (78) and (80) coincide with (58) and (60) for $\epsilon = m$, and similarly (79) and (81) coincide with (59) and (61) for $\epsilon = -m$. Moreover, both sets of equations and boundary conditions are analytical near the threshold. Therefore

$$\eta_l^{+}(0) = \eta_{m\kappa}(0)\,, \quad \eta_{\bar{l}}^{-}(0) = \eta_{-m,\kappa}(0)\,. \tag{82}$$

Actually one would expect an ambiguity in both equations (82), each in terms of an additive integer multiple of 2π. However, it is easy to see that both integers (say n_1 and n_2) must be zero. This follows from the fact that the simultaneous change of m to $-m$ and κ to $-\kappa$ is a symmetry operation, which implies $n_1 = n_2$. Equation (76) (or (77)), on the other hand, implies $n_1 = -n_2$, and hence both integers are zero. Equations (78) and (79) are just usual Schrödinger equations, so that we can apply Levinson's theorem (69) and (72) and obtain

$$\eta_{m\kappa}(0) = \begin{cases} n_l^{+}\pi & l = 0, 1, \ldots \\ \left(n_0^{+} + \frac{1}{4}\right)\pi & l = 0 \\ \left(n_0^{+} + \frac{1}{2}\right)\pi & l = 0\,, \end{cases} \tag{83}$$

$$\eta_{-m,\kappa}(0) = \begin{cases} n_{\bar{l}}^{-}\pi & \bar{l} = 0, 1, \ldots \\ \left(n_0^{-} + \frac{1}{4}\right)\pi & \bar{l} = 0 \\ \left(n_0^{-} + \frac{1}{2}\right)\pi & \bar{l} = 0\,, \end{cases} \tag{84}$$

where n_l^+ is the number of bound state solutions ($k^2 < 0$) of (78) and $n_{\bar{l}}^-$ is the number of bound state solutions of (79). In (83) and (84) the first case refers to a situation without a threshold resonance and the other two cases to a situation with a threshold resonance. Equations (83) and (84) constitute Levinson's theorem for Dirac particles. As a consequence of (76) and (83), (84) we have

$$N_\kappa^+ + N_\kappa^- = n_l^+ + n_{\bar{l}}^- \,, \tag{85}$$

whereas in general $N_\kappa^+ \neq n_l^+$ and $N_\kappa^- \neq n_{\bar{l}}^-$. It is an interesting fact to notice that (78) and (79) do not correspond to the usual expansion based on the Foldy-Wouthuysen scheme (see [20]). The above trick of "freezing" the energy of the second order Dirac equation was used for a different purpose in ref. [21].

5. APPLICATION TO A NONPERTURBATIVE QED

Consider the following set of equations

$$\begin{aligned} u'_{1\epsilon\kappa} + \frac{\kappa}{r} u_{1\epsilon\kappa} - (m_0 + \epsilon + \varphi)\, u_{2\epsilon\kappa} = 0 \\ u'_{2\epsilon\kappa} - \frac{\kappa}{r} u_{2\epsilon\kappa} - (m_0 - \epsilon - \varphi)\, u_{1\epsilon\kappa} = 0 \,, \end{aligned} \tag{86}$$

$$\varphi'' + \frac{2}{r}\varphi' = \frac{e_0^2}{4\pi} \frac{1}{r^2} \sum_{\kappa=1}^{\infty} \kappa \left(\varrho_\kappa + \varrho_{-\kappa}\right) \,, \tag{87}$$

$$\begin{aligned} \delta(r - r')\, \delta_{ij} = \sum_{0 \le \epsilon_\kappa \le m_0} u_{i\epsilon_\kappa\kappa}(r)\, u_{j\epsilon_\kappa\kappa}(r') + \sum_{0 < \epsilon_\kappa \le m_0} u_{i,-\epsilon_\kappa\kappa}(r)\, u_{j,-\epsilon_\kappa\kappa}(r') \\ + \int_{0+}^{\infty} \frac{\mathrm{d}k}{2\pi} \left[u_{i\epsilon\kappa}(r)\, u_{jE\kappa}(r') + u_{i,-\epsilon\kappa}(r)\, u_{j,-\epsilon\kappa}(r')\right] \,, \end{aligned} \tag{88}$$

where $i = 1,2$, $j = 1,2$, $\kappa = \pm 1, \pm 2, \ldots$, $u_{i,\pm\epsilon_\kappa\kappa}$ are bound state and $u_{i,\pm\epsilon\kappa}$ are scattering state solutions of (86), $\epsilon = \pm\epsilon_\kappa$, $0 \le \epsilon_\kappa \le m_0$, are bound state and $\epsilon = \pm\varepsilon$, $\varepsilon \equiv \sqrt{m_0^2 + k^2}$, are scattering state energies and

$$\begin{aligned} \varrho_\kappa = \sum_{0 \le \epsilon_\kappa \le m_0} \left(u_{1\epsilon_\kappa\kappa}^2 + u_{2\epsilon_\kappa\kappa}^2\right) - \sum_{0 < \epsilon_\kappa \le m_0} \left(u_{1,-\epsilon_\kappa\kappa}^2 + u_{2,-\epsilon_\kappa\kappa}^2\right) \\ + \int_{0+}^{\infty} \frac{\mathrm{d}k}{2\pi} \left(u_{1\epsilon\kappa}^2 + u_{2\epsilon\kappa}^2 - u_{1,-\epsilon\kappa}^2 - u_{2,-\epsilon\kappa}^2\right) . \end{aligned} \tag{89}$$

For the sake of simplicity we assume that there are no threshold resonances and hence in (88) and (89) the region of integration excludes $k = 0$. The boundary conditions are

$$|\varphi(0)| < \infty \,, \qquad \varphi(\infty) = 0 \tag{90}$$

for the field φ, and the usual boundary conditions

$$u_{i,\pm\epsilon_\kappa\kappa}(0)=0\,,\qquad u_{i,\pm\epsilon_\kappa\kappa}(\infty)\xrightarrow[r\to\infty]{} c_{i,\pm\epsilon_\kappa\kappa}\,\mathrm{e}^{-\gamma_\kappa r}\,, \tag{91}$$

hold for the bound states, where $c_{i,\pm\epsilon_\kappa\kappa}$ are real constants and $\gamma_\kappa=\sqrt{m_0^2-\epsilon_\kappa^2}\geq 0$, and

$$u_{1\epsilon\kappa}(0)=0\,,\quad u_{1\epsilon\kappa}(r)\xrightarrow[r\to\infty]{}\sqrt{\frac{\epsilon+m_0}{2\epsilon}}\,2\sin\left(kr-\frac{\pi l}{2}+\eta_{\epsilon\kappa}(k)\right) \tag{92}$$

$$u_{2\epsilon\kappa}(0)=0\,,\quad u_{2\epsilon\kappa}(r)\xrightarrow[r\to\infty]{}\sqrt{\frac{\epsilon+m_0}{2\epsilon}}\,\frac{\kappa_0 k}{\epsilon+m_0}\,2\sin\left(kr-\frac{\pi\bar{l}}{2}+\eta_{\epsilon\kappa}(k)\right) \tag{93}$$

for the scattering states, where $l=|\kappa|-(1-\kappa_0)/2$, $\bar{l}=l-\kappa_0$ and $\kappa_0=\kappa/|\kappa|$. The bound states are normalized according to

$$\int_0^\infty \mathrm{d}r\left[u^2_{1,\pm\epsilon_\kappa\kappa}(r)+u^2_{2,\pm\epsilon_\kappa\kappa}(r)\right]=1\,. \tag{94}$$

Notice that (86)-(88) is a closed system of equations. Also notice that any solution of this system constitutes a complete orthonormal set of functions and, therefore, Pauli's exclusion principle is built in. Equations (86)-(88) arise as a spherically symmetric special case of more general equations in a recently proposed generalized interaction picture of quantum electrodynamics (QED). This generalized interaction picture is useful, since it allows for a new nonperturbative approach to QED. The derivation of these equations from QED and more details on their properties will be given in a forthcoming paper [13]. Here we want to apply the results of the preceding sections to the investigation of self-consistency of equations (86)-(88). We shall prove in this section that for any solution of (86)-(88) with a finite number of bound states the total charge vanishes: $Q_0=0$, where the charge density is defined by the right-hand side of (87) (in units of $-e_0^2$). Furthermore, the coupling constant $e_0^2/4\pi$ is not a free parameter but rather must have a numerical value for which $\int_0^\infty \mathrm{d}r\,\varphi(r)=0$.

Firstly we notice that there exists at least one solution. In fact, if we assume that there are no bound states then

$$u_{1\epsilon\kappa}=v_{1\epsilon\kappa}\,,\qquad u_{2\epsilon\kappa}=v_{2\epsilon\kappa} \tag{95}$$

is a solution of (86)-(88), where

$$v_{1\epsilon\kappa}(r)=\sqrt{\frac{\epsilon+m}{2\epsilon}}\,2kr\,j_l(kr)\,,\quad v_{2\epsilon\kappa}(r)=\sqrt{\frac{\epsilon+m}{2\epsilon}}\,\frac{\kappa_0 k}{\epsilon+m}\,2kr\,j_{\bar{l}}(kr) \tag{96}$$

and $j_l(kr)$, $j_{\bar{l}}(kr)$ are the spherical Bessel functions. In general, however, a solution of (86)-(88) will contain a number of positive and a number of negative bound states. While the possibility of an infinite number of bound states cannot be ruled out on simple grounds, we want to examine the consistency conditions for a finite number of bound states.

If we multiply (87) by r^2 and integrate the resulting equation we obtain

$$\varphi'(r) = -\frac{e_0^2}{4\pi}\frac{Q_0}{r^2} - \frac{e_0^2}{4\pi}\frac{1}{r^2}\sum_{\kappa=1}^{\infty}\kappa\int_r^{\infty}\mathrm{d}r'\left[\varrho_\kappa(r') + \varrho_{-\kappa}(r')\right], \tag{97}$$

where

$$Q_0 = -\sum_{\kappa=1}^{\infty}\kappa\int_0^{\infty}\mathrm{d}r'\left[\varrho_\kappa(r') + \varrho_{-\kappa}(r')\right]. \tag{98}$$

At large r we have

$$\begin{aligned}\varrho_\kappa(r) \xrightarrow[r\to\infty]{} & \sum_{0\le\epsilon_\kappa\le m_0}\left(c^2_{1\epsilon_\kappa\kappa} + c^2_{2\epsilon_\kappa\kappa}\right)\mathrm{e}^{-\gamma_\kappa r} - \sum_{0<\epsilon_\kappa\le m_0}\left(c^2_{1,-\epsilon_\kappa\kappa} + c^2_{2,-\epsilon_\kappa\kappa}\right)\mathrm{e}^{-\gamma_\kappa r} \\ & - (-1)^l 4m\int_{0+}^{\infty}\frac{\mathrm{d}k}{2\pi}\frac{1}{\varepsilon}\cos\left[\eta_{\epsilon\kappa}(k) - \eta_{-\epsilon\kappa}(k)\right]\cos\left[2kr + \eta_{\epsilon\kappa}(k) + \eta_{-\epsilon\kappa}(k)\right]\end{aligned} \tag{99}$$

and hence

$$\begin{aligned}\int_r^{\infty}\mathrm{d}r'\varrho_\kappa(r') \xrightarrow[r\to\infty]{} & \sum_{0\le\epsilon_\kappa\le m_0}\frac{c^2_{1\epsilon_\kappa\kappa} + c^2_{2\epsilon_\kappa\kappa}}{\gamma_\kappa}\mathrm{e}^{-\gamma_\kappa r} - \sum_{0<\epsilon_\kappa\le m_0}\frac{c^2_{1,-\epsilon_\kappa\kappa} + c^2_{2,-\epsilon_\kappa\kappa}}{\gamma_\kappa}\mathrm{e}^{-\gamma_\kappa r} \\ & + (-1)^l 2m\int_{0+}^{\infty}\frac{\mathrm{d}k}{2\pi}\frac{1}{\varepsilon k}\cos\left[\eta_{\epsilon\kappa}(k) - \eta_{-\epsilon\kappa}(k)\right]\sin\left[2kr + \eta_{\epsilon\kappa}(k) + \eta_{-\epsilon\kappa}(k)\right].\end{aligned} \tag{100}$$

It now follows from (97) and (100) that

$$\varphi(r) \xrightarrow[r\to\infty]{} -\frac{e_0^2}{4\pi}\frac{Q_0}{r} + O\left(\mathrm{e}^{-ar}\right), \quad a > 0. \tag{101}$$

Now, if $Q_0 > 0$ then φ acts as an attractive potential for the positive energy states and as a repulsive potential for the negative energy states. Similarly, if $Q_0 < 0$ then φ acts as an attractive potential for the negative energy states and as a repulsive potential for the positive energy states. Consequently, in both cases φ supports an infinite number of bound states, like any attractive potential, which vanishes at infinity not faster than $1/r^2$. Thus $Q_0 > 0$ and $Q_0 < 0$ are inconsistent with a finite number of bound states. On the other hand, if $Q_0 = 0$ then there will be at most a finite number of bound states, since φ acts as a short range potential with nonvanishing repulsive and attractive parts. The repulsive part is due to the electrostatic self-interaction of bound states, whilst the attractive part is provided by the scattering states, which fully compensate the repulsive part. Thus the consistency condition for the existence of a finite number of bound states is

$$Q_0 = 0\,. \tag{102}$$

This consistency condition implies a restriction on φ. Combining (98) and (89), we obtain

$$Q_0 = -\sum_{\kappa=-\infty}^{\infty} |\kappa| \left\{ N_\kappa^+ - N_\kappa^- + \int_{0+}^{\infty} \frac{\mathrm{d}k}{2\pi} \int_0^{\infty} \mathrm{d}r \left[u_{1\epsilon\kappa}^2(r) + u_{2\epsilon\kappa}^2(r) - u_{1,-\epsilon\kappa}^2(r) - u_{2,-\epsilon\kappa}^2(r) \right] \right\}\,. \tag{103}$$

where N_κ^+ and N_κ^- are the number of positive and negative energy bound states of (86) respectively. Substituting (39), we get

$$Q_0 = -\sum_{\kappa=-\infty}^{\infty} |\kappa| \left\{ N_\kappa^+ - N_\kappa^- - \left[\eta_{m\kappa}(0) - \eta_{-m\kappa}(0)\right] \frac{1}{\pi} + \left[\eta_{\infty\kappa}(\infty) - \eta_{-\infty\kappa}(\infty)\right] \frac{1}{\pi} \right\}\,. \tag{104}$$

Since the boundary conditions for φ prohibit a singularity at the origin, we can use (53) for $\eta_{\pm\infty}(\infty)$ and obtain

$$Q_0 = -\sum_{\kappa=-\infty}^{\infty} |\kappa| \left\{ N_\kappa^+ - N_\kappa^- - n_l^+ + n_l^- + \frac{2}{\pi} \int_0^{\infty} \mathrm{d}r\, \varphi(r) \right\}, \tag{105}$$

where we used Levinson's theorem (84), and where n_l^+ and n_l^- are the number of bound state solutions of (78) and (79) with $V = -\varphi$ and $m = m_0$ respectively. Since the last term in (105) is independent of κ it must vanish, otherwise Q_0 would become infinite. Hence we conclude that

$$\int_0^{\infty} \mathrm{d}r\, \varphi(r) = 0 \tag{106}$$

must hold for any solution of (86)-(88) having a finite number of bound states. Notice that if all of the bound states have either positive or negative energies, then (106) implies (102), which follows from (85). Also notice that $\int_0^\infty \mathrm{d}r\, \varphi(r)$ is a dimensionless quantity and therefore does not depend on the bare mass parameter m_0 and is a function of the coupling constant $e_0^2/4\pi$ only. Hence, due to (106), the coupling constant $e_0^2/4\pi$ becomes an eigenvalue of (86)-(88), i.e. we expect that (106) holds only if $e_0^2/4\pi$ acquires one or more specific numerical values. To illuminate this point we consider the following iteration procedure. As the initial step we make a reasonable guess of φ, which satisfies (106) and which we denote by φ_0. Then we solve the Dirac equation (86) with $\varphi = \varphi_0$ and obtain a complete set of bound and scattering states. At this stage $e_0^2/4\pi$ is a free parameter. Now we fix it by requiring that with this complete set the solution of (87), which we denote by φ_1, satisfies (106). If there is no value of $e_0^2/4\pi$ for which (106) is satisfied, then we start again trying to make a better choice of φ_0. If, however, there is such a value of $e_0^2/4\pi$, then we have completed the first iteration and can start the second one, now with φ_1 instead of φ_0. Assume that this iteration procedure is convergent, then it is clear that, as a result of (106), the coupling constant will emerge, fixed at one or several numerical values.

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