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Transition from Discrete to Continuous Spectra*

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The stationary states of a system bound in a spherical box and additionally subjected to a perturbation of finite range are studied in the limit as the box radius becomes infinite. The transition from formal discrete-spectrum theory to formal scattering theory is carried out explicitly by two different methods. It is shown quite generally (i.e., even when the total Hamiltonian is not separable) that the level shift produced by the perturbation is proportional to the corresponding scattering phase shift.

I. INTRODUCTION

An attempt has recently been made by Reifman and Newton, in collaboration with the author,[1] to justify a procedure of Brueckner[2] which attempts to deal with nuclear many-body bound-state problems in the language of scattering theory, by imagining that the nuclear radius is sufficiently large so that the stationary two-body states are quasi-continuous. In particular, the attempt was made to justify Brueckner's use of the principal-value Green's function and the tangent of the phase shift in his self-consistent calculation of nuclear binding energies.

Two facts affecting this work have subsequently become apparent. First, it is unlikely that the nuclear problem can actually be attacked strictly from a scattering-theoretical point of view. The reason for this, which was not fully appreciated at the beginning, is as follows[3]: Owing to the Fermi statistics and the degenerate nature of the nuclear system, intermediate-state summations occurring in calculations of the level-shift contributions from individual two-body encounters must be extended only over regions well removed from the energy shell. This has the result that although the two-body level-shift operator for the nuclear system is then identical with a certain two-body "reactance" operator, as Brueckner and Levinson have shown,[4] the latter operator has nothing in common with the reactance operator for free scattering. Only for systems of low density or at temperatures sufficiently high so that particle statistics may be ignored can the scattering-theoretical viewpoint be profitably retained.

Secondly, the formal arguments of reference 1, which are now seen to be of interest only in the low-density case, are actually in error, as has been pointed out by Fukuda and Newton.[5] These authors show in special cases that the level shift produced on a quasi-continuous state by a perturbation of finite range becomes, in the limit as boundary walls recede to infinity, proportional simply to the corresponding phase shift, *not* to its tangent.

It is curious that this result, which seems to have been known more or less privately for some time by various individuals, has not previously achieved the dignity of a special statement in the literature.† In the case of a spherically symmetric potential it can be very readily inferred simply by using a spherical boundary of radius R and then examining the asymptotic behavior as $R\rightarrow\infty$ of stationary state wave functions of given angular momentum which vanish on the boundary. It is the purpose of the present paper to provide a correct formal proof in the general case.

II. SUMMARY OF SCATTERING THEORY

The S matrix has the well-known form[6]

$$\begin{aligned} S_{ba}&=(\varphi_b,S\varphi_a)\\ &=\delta_{ba}-2\pi i\delta(E_b-E_a)R_{ba}(E_a+i0), \end{aligned}\tag{1}$$

where the φ_a are orthonormalized eigenvectors of the unperturbed Hamiltonian H_0 (with spectrum E_a) and the operator $R(E)$ is given by

$$R(E)=H_1[1+G_0(E)R(E)]=H_1[1-G_0(E)H_1]^{-1},\tag{2}$$

$$G_0(E)=(E-H_0)^{-1},\tag{3}$$

H_1 being the perturbation which produces the scattering. The operator $G_0(E)$ is variously known as the unperturbed "resolvent" or Green's function. The resolvent $G(E)$ of the total Hamiltonian

$$H=H_0+H_1\tag{4}$$

may be expressed in the forms

$$G(E)=(E-H)^{-1}=G_0(E)+G_0(E)R(E)G_0(E)\tag{5a}$$

$$=G_0(E)[1+H_1G(E)].\tag{5b}$$

With use of the formal identity

$$G_0(E\pm i0)=\mathcal{P}(E-H_0)^{-1}\mp\pi i\delta(E-H_0),\quad E\text{ real},\tag{6}$$

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[1] Reifman, DeWitt, Newton, Phys. Rev. **101**, 877 (1956).
[2] K. A. Brueckner, Phys. Rev. **97**, 1353 (1955); see also references cited in this work.
[3] K. A. Brueckner (private communication).
[4] K. A. Brueckner and C. A. Levinson, Phys. Rev. **97**, 1344 (1955); Appendix B.
[5] N. Fukuda and R. G. Newton, Phys. Rev. **103**, 1558 (1956), preceding paper. Although Brueckner was therefore wrong in using the tangent of the phase shift, this, because of the now recognized inapplicability of the scattering picture in his problem, does not mean that his calculations can be corrected simply by replacing the tangents by the phase shifts themselves.

† See however reference 7.
[6] See, for example, B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950).

where the symbol $\mathcal{P}$ denotes the "principal value" when appearing in a summation (integration), Eq. (2) may be split up in the form

$$[1-H_1\mathcal{P}(E-H_0)^{-1}]R(E+i0) = H_1[1-\pi i\delta(E-H_0)R(E+i0)]. \quad (7)$$

Removal of the factor on the left and multiplication by a delta function in energy gives the Heitler integral equation

$$2\pi\delta(E_b-E_a)R_{ba}(E_a+i0) = K_{ba}-\pi i\sum_c K_{bc}\delta(E_c-E_a)R_{ca}(E_a+i0), \quad (8)$$

where

$$K_{ba}=2\pi\delta(E_b-E_a) \times(\varphi_b,\, H_1[1-\mathcal{P}(E_a-H_0)^{-1}H_1]^{-1}\varphi_a). \quad (9)$$

K is the reactance operator. Its relation to the scattering operator S follows from Eqs. (1) and (8):

$$S=\frac{1-\frac{1}{2}iK}{1+\frac{1}{2}iK}=e^{2i\delta}, \quad (10)$$

$$K=-2\tan\delta, \quad (11)$$

where δ is the "phase shift" operator. The unitarity of S follows from the obvious Hermitian character of K.

A unitary matrix can (in principle) be diagonalized by a unitary transformation. The S matrix is already diagonal in energy. Therefore it will be convenient to make the transformation of basis

$$\varphi_a\rightarrow\varphi_{E'\lambda'}, \quad H_0\varphi_{E'\lambda'}=E'\varphi_{E'\lambda'}, \quad (12)$$

where λ' denotes the remaining labels necessary to complete the diagonalization process

$$(\varphi_{E''\lambda''},S\varphi_{E'\lambda'})=\exp[2i\delta_{\lambda'}(E')]\delta_{E''E'}\delta_{\lambda''\lambda'}. \quad (13)$$

Attention should be called to the fact that the normalization condition,

$$(\varphi_{E''\lambda''},\varphi_{E'\lambda'})=\delta_{E''E'}\delta_{\lambda''\lambda'}, \quad (14)$$

on the eigenvectors of H_0 actually requires us to place the system in a box which is finite, however large. This means we are already, in effect, working with a quasi-continuous spectrum. In the case of spherical symmetry, in which λ' represents the ordinary angular momentum quantum numbers l, m, the appropriate box shape is obviously spherical. It is almost as obvious (see Appendix) that this is also the appropriate shape in the general case (e.g., tensor forces or nonspherical potentials), at least when the box is sufficiently large and the perturbation H_1 has finite range. If we denote the radius of the box by R then the level separation in the quasi-continuous spectrum near E' is given by

$$dE'=\pi\hbar v'/R, \quad (15)$$

where v' is the scattering velocity corresponding to energy E'.

Use of the normalization condition (14) implies that matrix elements like $(\varphi_{E''\lambda''},H_1\varphi_{E'\lambda'})$ are of order $(dE''dE')^{\frac{1}{2}}$. Intermediate-state summations in perturbation formulas therefore have the general form $\sum_{E'}f(E')dE'$ and become ordinary integrations in the limit $R\rightarrow\infty$, $dE'\rightarrow 0$. When dealing with discrete summations involving the delta function, one may employ the formal identity

$$\delta(E''-E')dE'=\delta_{E''E'}. \quad (16)$$

III. THE SEPARABLE CASE AND THE FREDHOLM DETERMINANT[7]

In the most familiar cases (e.g., spherical symmetry), the perturbation H_1 is itself diagonal in the labels λ'. The total Hamiltonian is then said to be separable, for it can be written in the form

$$H=\sum_{\lambda'}(H_{0\lambda'}+H_{1\lambda'}), \quad (17)$$

where

$$H_{0\lambda'}=\sum_{E'}\ \varphi_{E'\lambda'}\rangle E'\langle\varphi_{E'\lambda'}, \quad (18)$$

$$H_{1\lambda'}=\sum_{E''E'}\ \varphi_{E''\lambda'}\rangle(\varphi_{E''\lambda'},H_1\varphi_{E'\lambda'})\langle\varphi_{E'\lambda'}, \quad (19)$$

and all work can be carried out within a single subspace corresponding to a fixed value of λ'. We shall drop the prime on the λ to indicate that the equations to follow are independent of the choice of subspace. The notation will otherwise be obvious.

We introduce the Fredholm determinant

$$D_\lambda(E)=\det{}_\lambda[1-G_{0\lambda}(E)H_{1\lambda}] =\det{}_\lambda[1-H_{1\lambda}G_{0\lambda}(E)]. \quad (20)$$

The question of how to define such a determinant in the presence of a continuous spectrum is usually answered by generalizing from the case of finite matrices via the identity $|A|=\exp(\mathrm{tr}\log A)$, and expanding the logarithm, thereby reducing the problem to one of evaluating traces and checking certain convergence conditions on the operator $G_{0\lambda}(E)H_{1\lambda}$. However, since we are here working with a quasi-continuous spectrum, we may (ignoring convergence questions) write formally

$$D_\lambda(E)=\det{}_\lambda[(E-H_{0\lambda})^{-1}(E-H_\lambda)] =\prod_{E'}(E-E')^{-1}(E-E'-\Delta E'_\lambda), \quad (21)$$

where $\Delta E'_\lambda$ is the shift in the unperturbed level E' due to the perturbation $H_{1\lambda}$.

Two facts about the level shifts will be important for future reference. First, $\Delta E'_\lambda\rightarrow 0$ as $dE'\rightarrow 0$, except in the case of the *true* bound states, which are in effect peeled off the bottom of the set of (quasi) continuum states and whose level shifts remain finite in the limit. Secondly, the unperturbed level separation dE', when sufficiently small, is also effectively the level separation

[7] The method of this section is based on material contained in a paper by J. Schwinger [Phys. Rev. **94**, 1362 (1954)] which treats the special case of a Dirac electron in an impressed time-independent electromagnetic field. The line of reasoning, however, has been somewhat altered so as to avoid explicit use of the coordinate representation.

in the *perturbed* spectrum (the true bound levels again excluded). Thus, if the zero point of energy be taken (as usual) at the bottom of the quasi-continuum, the spectral distribution along any small portion of the positive real axis in the complex E plane has an invariant form similar to that pictured in Fig. 1. The circles in the figure indicate the unperturbed spectrum and the crosses the perturbed spectrum. The pictured level shift $\Delta E'_\lambda$ corresponds to a situation in which the perturbed level in each case has shifted down past three unperturbed levels.

The level shifts may be related to the phase shifts by means of the identity

$$D_\lambda(E+i0)^*/D_\lambda(E+i0)=\exp[2i\delta_\lambda(E)], \quad E \text{ real}, \tag{22}$$

the proof of which is fairly straightforward. One writes

$$\begin{aligned} D_\lambda(E+i0)^*/D_\lambda(E+i0) &= \det{}_\lambda\{[1-G_{0\lambda}(E-i0)H_{1\lambda}][1-G_{0\lambda}(E+i0)H_{1\lambda}]^{-1}\} \\ &= \det{}_\lambda\{1+[G_{0\lambda}(E+i0)-G_{0\lambda}(E-i0)] \\ &\qquad \times H_{1\lambda}[1-G_{0\lambda}(E+i0)H_{1\lambda}]^{-1}\} \\ &= |\delta_{E''E'}-2\pi i\delta(E-E'')R_{\lambda E''E'}(E+i0)|, \end{aligned} \tag{23}$$

where use has been made of (2) and (6). The final determinant has nonvanishing elements only along the principal diagonal and along the row $E''=E$. Comparison of Eqs. (1), (13) and (23) therefore leads immediately to (22), with $\delta_\lambda(E)=n\pi$ for $E<0$.[8]

From Eq. (22) it follows that

$$\operatorname{Im}\log D_\lambda(E+i0)=-\delta_\lambda(E), \quad E \text{ real}. \tag{24}$$

Next observe from Eq. (21) that

$$\lim_{E\to-\infty} D_\lambda(E)=\lim_{H_1\to 0} D_\lambda(E)=1, \tag{25}$$

and hence

$$\lim_{E\to-\infty} \delta_\lambda(E)=\lim_{H_1\to 0} \delta_\lambda(E)=0. \tag{26}$$

Now if we let E increase from $-\infty$ along the negative real axis, the phase shift $\delta_\lambda(E)$ remains zero until we reach the first true bound level (if any), which is a zero of $D_\lambda(E)$. At this point, the instruction "$E+i0$" tells us that we must pass around the zero in the clockwise sense in the upper half-plane thereby adding $-\pi$ to the phase of $D_\lambda(E)$, or π to $\delta_\lambda(E)$. Continuing in this manner we add π to $\delta_\lambda(E)$ each time we pass a bound level until we reach the origin, where we have[9]

$$\delta_\lambda(0)=N_\lambda\pi, \tag{27}$$

N_λ being the number of true bound states with quantum numbers λ.

As we pass onto the positive real axis, the situation changes completely. At first sight one might be led to think that the phase shift undergoes rapid oscillations, increasing by π each time we pass one of the zeros $E'+\Delta E'_\lambda$, and decreasing by π each time we pass a pole E'. However, we must remember that the instruction "$E+i0$" is to be taken in the sense "$\lim_{\epsilon\to 0}(E+i\epsilon)$" where ϵ is a small positive quantity. In order that the use of ϵ give the correct causal description of the scattering process (i.e., be able to make the distinction between retarded and advanced waves), the limit $\epsilon\to 0$ must be accompanied by (or preceded by) a swelling of the spherical box of such a nature that

$$dE'/\epsilon\to 0, \tag{28}$$

so that summations over intermediate states [e.g., in the expansion of $R_\lambda(E)$] become, in the limit of infinite box, integrations over contours which pass definitely to one side or the other of poles introduced by the Green's function $G_{0\lambda}(E)$. Correspondingly, in the determination of $\delta_\lambda(E)$ the function $D_\lambda(E)$ must be viewed from a point far enough above the real axis so that the rapid oscillations in phase will be smoothed out to some average value.

It is shown in the Appendix that the smoothed-out value is just equal to the average value along the real axis. Suppose $\Delta E'_\lambda=-(n+x)dE'$, where n is an integer and $0\leqq x<1$. Then referring to Fig. 1, one sees that $\operatorname{Im}\log D_\lambda(E)$ is equal to $-n\pi$ between points 1 and 2 and to $-(n+1)\pi$ between points 2 and 3. The average value is evidently

$$\begin{aligned} \langle \operatorname{Im}\log D_\lambda(E')\rangle_{\text{Av}} &= -(1-x)n\pi-x(n+1)\pi \\ &= \pi(\Delta E'_\lambda/dE'), \end{aligned} \tag{29}$$

and hence

$$\Delta E'_\lambda=-\frac{1}{\pi}\delta_\lambda(E')dE'. \tag{30}$$

This, for the separable case, is the result announced in the introduction. It is worth pointing out that its derivation depends only on the assumption, pictured

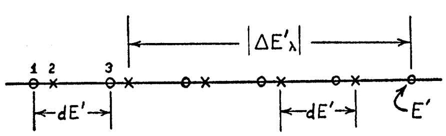

FIG. 1. Spectral distribution along a small portion of the positive real axis. Circles indicate the unperturbed spectrum and crosses the perturbed spectrum.

[8] Equation (22) is originally due to R. Jost and A. Pais, Phys. Rev. 82, 840 (1951). [See especially Eqs. (32) and (43) of their paper.] In drawing inferences from this formula, however, one should be cautioned that Jost and Pais work in the complex k-plane, k being the wave number and related quadratically to E, whereas Eq. (22) here has meaning only for real E. It is especially important to remember this when E is negative.

[9] Strictly speaking we should write $\delta_\lambda(-0)=N_\lambda\pi$ to distinguish this value from the limit $\delta_\lambda(+0)$ as E approaches the origin along the positive real axis. $\delta_\lambda(E)$ will be continuous at the origin only if $\lim_{E'\to+0}R_{\lambda E'E'}(E'+i0)=0$, and the latter condition can be verified only by a quite separate investigation. This condition is known to be valid in the three-dimensional spherical case [except when the lower-most continuum state is "just barely" bound, in which case $\delta_\lambda(+0)=(N_\lambda+\frac{1}{2})\pi$ [see R. Jost, Helv. Phys. Acta 20, 256 (1947)], although it does not generally hold in two- or one-dimensional problems.

in Fig. 1, of fine-grained spectral invariance. Conversely, one may argue from the known smooth behavior of phase shifts to the validity of the spectral invariance assumption.

IV. THE GENERAL CASE

For the general case we shall use an alternative method of procedure based directly on ordinary discrete-spectrum perturbation theory We introduce the projection operators

$$P_{E'}=\sum_{\lambda'}\varphi_{E'\lambda'}\rangle\langle\varphi_{E'\lambda'}. \quad (31)$$

Then, making use of Eq. (5b), we write

$$\begin{aligned}P_{E''}G(E)P_{E'}&=(E-E'')^{-1}[P_{E'}\delta_{E''E'}+P_{E''}H_1P_{E'}G(E)P_{E'}\\&\qquad+P_{E''}H_1(1-P_{E'})G(E)P_{E'}]\\&=(E-E'')^{-1}[P_{E'}\delta_{E''E'}+P_{E''}\Sigma(E)P_{E'}G(E)P_{E'}], \quad (32)\end{aligned}$$

where

$$\begin{aligned}P_{E''}\Sigma(E)P_{E'}&=P_{E''}H_1P_{E'}+P_{E''}H_1(1-P_{E'})G_0(E)\Sigma(E)P_{E'} \quad (33a)\\&=P_{E''}H_1[1-(1-P_{E'})G_0(E)H_1]^{-1}P_{E'}. \quad (33b)\end{aligned}$$

Setting $E''=E'$ in Eq. (32), we get

$$P_{E'}G(E)P_{E'}=\frac{P_{E'}}{E-E'-P_{E'}\Sigma(E)P_{E'}}, \quad (34)$$

which will lead us to a familiar expression for the level shifts.

First, however, one must observe that Eqs. (1) and (13) imply

$$\lim_{E\to E'+i0}(\varphi_{E'\lambda''},R(E)\varphi_{E'\lambda'})=0 \quad \text{for} \quad \lambda''\neq\lambda', \quad (35)$$

and hence [see Eq. (5a)]

$$\lim_{E\to E'+i0}(\varphi_{E'\lambda''},G(E)\varphi_{E'\lambda'})=0 \quad \text{for} \quad \lambda''\neq\lambda'. \quad (36)$$

In virtue of the essential continuity of orthogonality properties when the spherical box is sufficiently large, Eq. (36) may equally well be written in the form

$$\lim_{E\to E'+\Delta E'_{\lambda'}}(\varphi_{E'\lambda''},G(E)\varphi_{E'\lambda'})=0 \quad \text{for} \quad \lambda''\neq\lambda', \quad (37)$$

valid for dE' finite though small. This, combined with Eq. (34) and the observation that the perturbed spectrum is given by the poles of $G(E)$, then yields

$$(\varphi_{E'\lambda''},\Sigma(E'+\Delta E'_{\lambda'})\varphi_{E'\lambda'})=\Delta E'_{\lambda'}\delta_{\lambda''\lambda'}, \quad (38)$$

which is the basic formula of discrete spectrum theory.

In order to connect this formula with scattering theory it is necessary to determine what form the operator $(1-P_{E'})G_0(E'+\Delta E'_{\lambda'})$ takes in the limit $dE'\to 0$. Now this operator leads to intermediate-state summations of the form

$$\sum_{\substack{E''\lambda''\\E''\neq E'}}\frac{f(E'',\lambda'')dE''}{E'+\Delta E'_{\lambda'}-E''}=\sum_{E''\lambda''}\frac{f(E'',\lambda'')dE''}{E'+\Delta E'_{\lambda'}-E''}-\frac{dE'}{\Delta E'_{\lambda'}}\sum_{\lambda''}f(E',\lambda''). \quad (39)$$

If dE' (and hence also the $\Delta E'_{\lambda'}$) is sufficiently small, an $\epsilon\gg dE'$, $\Delta E'_{\lambda'}$ may be found such that $f(E'',\lambda'')$ and dE'' are essentially constant in the range $E'-\epsilon<E''<E'+\epsilon$. The first sum on the right of Eq. (39) is then conveniently separated into two parts, one including only those terms for which $|E''-E'|<\epsilon$, and the other the remaining terms. (Here we again envisage an eventual limiting procedure $\epsilon\to 0$, $dE'\to 0$ such that $dE'/\epsilon\to 0$.) The latter part contributes an amount which is essentially the same as that given by a principal value integration, namely

$$\sum_{\lambda''}\mathcal{P}\int\frac{f(E'',\lambda'')dE''}{E'-E''}; \quad (40)$$

while the former part contributes an amount which reflects the asymmetry of position of the level $E'+\Delta E'_{\lambda'}$ with respect to the unperturbed levels, and which may be computed with the help of the appendix, Eq. (A.7), namely

$$\sum_{\lambda''}f(E',\lambda'')\sum_{n=-\infty}^{\infty}\frac{dE'}{\Delta E'_{\lambda'}-ndE'}=\frac{\pi}{\tan(\pi\Delta E'_{\lambda'}/dE')}\sum_{\lambda''}f(E',\lambda''). \quad (41)$$

One may therefore infer

$$(1-P_{E'})G_0(E'+\Delta E'_{\lambda'})\to\mathcal{P}\frac{1}{E'-H_0}+\left[\frac{\pi}{\tan(\pi\Delta E'_{\lambda'}/dE')}-\frac{dE'}{\Delta E'_{\lambda'}}\right]\delta(E'-H_0). \quad (42)$$

Brueckner's assumption[2,4] that $(1-P_{E'})G_0(E'+\Delta E'_{\lambda'})\to\mathcal{P}(E'-H_0)^{-1}$ is therefore seen to be incorrect for low-density problems in which the scattering picture is valid.

Using Eqs. (33a) and (42), we may write

$$\left(1-H_1\mathcal{P}\frac{1}{E'-H_0}\right)\Sigma(E'+\Delta E'_{\lambda'})P_{E'}=H_1\left\{1+\left[\frac{\pi}{\tan(\pi\Delta E'_{\lambda'}/dE')}-\frac{dE'}{\Delta E'_{\lambda'}}\right]\times\delta(E'-H_0)\Sigma(E'+\Delta E'_{\lambda'})\right\}P_{E'}, \quad (43)$$

where

$$2\pi\delta(E''-E')(\varphi_{E''\lambda''},\Sigma(E'+\Delta E'_{\lambda'})\varphi_{E'\lambda'})$$
$$=(\varphi_{E''\lambda''},K\varphi_{E'\lambda'})+\left[\frac{\pi}{\tan(\pi\Delta E'_{\lambda'}/dE')}-\frac{dE'}{\Delta E'_{\lambda'}}\right]$$
$$\times\sum_{E'''\lambda'''}(\varphi_{E''\lambda''},K\varphi_{E'''\lambda'''})\delta(E'''-E')$$
$$\times(\varphi_{E'''\lambda'''},\Sigma(E'+\Delta E'_{\lambda'})\varphi_{E'\lambda'}). \quad (44)$$

Taking the diagonal element of this equation, and using Eqs. (11), (16), and (38), we get

$$2\pi\frac{\Delta E'_{\lambda'}}{dE'}=-2\tan\delta_{\lambda'}(E')$$
$$\times\left\{1+\left[\frac{\pi}{\tan(\pi\Delta E'_{\lambda'}/dE')}-\frac{dE'}{\Delta E'_{\lambda'}}\right]\frac{\Delta E'_{\lambda'}}{dE'}\right\}$$
$$=-2\pi\frac{\Delta E'_{\lambda'}}{dE'}\frac{\tan\delta_{\lambda'}(E')}{\tan(\pi\Delta E'_{\lambda'}/dE')}, \quad (45)$$

which leads immediately to the completely general result

$$\Delta E'_{\lambda'}=-\frac{1}{\pi}\delta_{\lambda'}(E')dE'. \quad (46)$$

Appeal may also be made in the general case to the Fredholm determinant. Here, since the Hamiltonian is not necessarily separable, we must work with the total determinant[10]

$$D(E)=\det[1-G_0(E)H_1]$$
$$=\prod_{E'\lambda'}(E-E')^{-1}(E-E'-\Delta E'_{\lambda'}). \quad (47)$$

In actuality the total determinant is divergent (except in one-dimensional problems). We may, however, work with it purely formally.[11] Proceeding as in Eq. (23), one obtains

$$D(E+i0)^*/D(E+i0)$$
$$=|\delta_{E''E'}\delta_{\lambda''\lambda'}-2\pi i\delta(E-E'')R_{E''\lambda''E'\lambda'}(E+i0)|. \quad (48)$$

Here the determinant is conveniently arranged in blocks according to the labels λ'. The diagonal blocks have exactly the same form as the determinant of Eq. (23); i.e., they have nonvanishing elements along the principal diagonal and along the rows $E''=E$. The off-diagonal blocks, however, have nonvanishing elements only along the rows $E''=E$ *except*, owing to Eq. (35), that these rows have zeros in the columns $E'=E$. The off-diagonal blocks therefore contribute nothing to the determinant, and we have

$$\frac{D(E+i0)^*}{D(E+i0)}=\exp[2i\sum_{\lambda'}\delta_{\lambda'}(E)]. \quad (49)$$

which leads, with Eq. (47), to[12]

$$\sum_{\lambda'}\Delta E'_{\lambda'}=-\frac{1}{\pi}\sum_{\lambda'}\delta_{\lambda'}(E')dE'. \quad (50)$$

V. THE PERTURBED STATE VECTORS

For the sake of completeness and of further demonstrating the internal consistency of the arguments presented here, we include a final section on the construction of the stationary perturbed-state vectors.

In discrete-spectrum theory, the perturbed state vectors may be defined by[13]

$$Z_{E'\lambda'}^{\frac{1}{2}}\psi_{E'\lambda'}=\lim_{E\to E'+\Delta E'_{\lambda'}}(E-E'-\Delta E'_{\lambda'})G(E)\varphi_{E'\lambda'}. \quad (51)$$

Here one simply observes that the operator acting on $\varphi_{E'\lambda'}$ on the right is a projection operator on the eigenstate of H corresponding to the eigenvalue $E'+\Delta E'_{\lambda'}$.[14] $Z_{E'\lambda'}$ is a normalization factor representing the probability of finding $\varphi_{E'\lambda'}$ in $\psi_{E'\lambda'}$. From Eq. (37), one infers that

$$(\varphi_{E'\lambda''},\psi_{E'\lambda'})=Z_{E'\lambda'}^{\frac{1}{2}}\delta_{\lambda''\lambda'}. \quad (52)$$

Using Eq. (32), one may rewrite (51) in the forms

$$Z_{E'\lambda'}^{\frac{1}{2}}\psi_{E'\lambda'}=\lim_{E\to E'+\Delta E'_{\lambda'}}(E-E'-\Delta E'_{\lambda'})G_0(E)$$
$$\times[1+\Sigma(E)P_{E'}G(E)]\varphi_{E'\lambda'}$$
$$=Z_{E'\lambda'}G_0(E'+\Delta E'_{\lambda'})$$
$$\times\Sigma(E'+\Delta E'_{\lambda'})\varphi_{E'\lambda'}. \quad (53)$$

In passing to the second form, one observes that the limiting procedure in the first form picks out only the pole of $G(E)$ corresponding to $\psi_{E'\lambda'}$ and that the residue at this pole is $Z_{E'\lambda'}$. One finally uses Eqs. (33b) and

[10] Since the labels λ' are determined in the general case solely by asymptotic requirements, they are not well defined for the true bound states unless appeal is made to an adiabatic switching procedure. The diagonalizing vectors $\varphi_{E'\lambda'}$ will vary continuously as the perturbation is switched off. Thus the labels λ' will have a physical significance which is a continuously varying function (constant in the separable case) of both energy and perturbation strength, and each true bound state may be assigned a unique set of labels λ' at the moment it passes over into the continuum. Such an assignment is implied in Eq. (47).

[11] One may instead work with the function $D'(E)=D(E)\times\exp[\mathrm{tr}G_0(E)H_1]$ from which the divergent asymptotic high-energy contributions to $D(E)$ are removed. $D'(E)$ is convergent in most cases of interest.

[12] Eqs. (47) and (50) together yield a canonical form for the Fredholm determinant:

$$D(E)=\prod_{E_B}\left(1-\frac{E_B}{E}\right)\exp\frac{1}{\pi}\sum_{\lambda'}\int\frac{\delta_{\lambda'}(E')}{E-E'}dE'$$

where the E_B are the levels of the true bound states.

[13] B. S. DeWitt, Phys. Rev. **100**, 905 (1955).

[14] The notation is slightly confusing. $\psi_{E'\lambda'}$ corresponds to the eigenvalue $E'+\Delta E'_{\lambda'}$, *not* E'.

(38) to write

$$\psi_{E'\lambda'} = Z_{E'\lambda'}{}^{\frac{1}{2}}[1+(1-P_{E'})G_0(E'+\Delta E'_{\lambda'})\Sigma(E'+\Delta E'_{\lambda'})]\varphi_{E'\lambda'}$$
$$= Z_{E'\lambda'}{}^{\frac{1}{2}}[1-(1-P_{E'})G_0(E'+\Delta E'_{\lambda'})H_1]^{-1}\varphi_{E'\lambda'}. \quad (54)$$

In continuum theory, on the other hand, the perturbed state vectors are defined by

$$\psi_{E'\lambda'}{}^{\pm} = \lim_{E\to E'\pm i0} (E-E')G(E)\varphi_{E'\lambda'} \quad (55a)$$
$$= [1+G_0(E'\pm i0)R(E'\pm i0)]\varphi_{E'\lambda'} \quad (55b)$$
$$= [1-G_0(E'\pm i0)H_1]^{-1}\varphi_{E'\lambda'}. \quad (55c)$$

When the perturbation H_1 has finite range, this definition can be shown[13] to lead to normalized vectors $\psi_{E'\lambda'}{}^{\pm}$. The difference between Eqs. (51) and (55a) is significant. In Eq. (51) the variable E is allowed to approach the pole of $G(E)$ while dE' is still finite, whereas in Eq. (55a), owing to the requirement $dE'/\epsilon\to 0$, the spectrum is first allowed to become continuous so that the approach is no longer to a pole but to a branch line along the positive real axis, from above or below. In the limit $dE'\to 0$, however, $\psi_{E'\lambda'}$ and $\psi_{E'\lambda'}{}^{\pm}$ must differ only by phase factors. We now confirm this.

First rewrite Eq. (42) in the form

$$(1-P_{E'})G_0(E'+\Delta E'_{\lambda'}) \to G_0(E'\pm i0) - \pi\left[\frac{1}{\tan\delta_{\lambda'}(E')} - \frac{1}{\delta_{\lambda'}(E')} \mp i\right]\delta(E'-H_0), \quad (56)$$

and then combine Eqs. (54) and (55c) to get

$$\psi_{E'\lambda'}{}^{\pm} = Z_{E'\lambda'}{}^{-\frac{1}{2}}[1-G_0(E'\pm i0)H_1]^{-1} \times[1-(1-P_{E'})G_0(E'+\Delta E'_{\lambda'})H_1]\psi_{E'\lambda'}$$
$$= Z_{E'\lambda'}{}^{-\frac{1}{2}}\left\{\psi_{E'\lambda'} + \pi\left[\frac{1}{\tan\delta_{\lambda'}(E')} - \frac{1}{\delta_{\lambda'}(E')} \mp i\right] \times \sum_{E''\lambda''}\psi_{E''\lambda''}{}^{\pm}\,\delta(E'-E'')(\varphi_{E''\lambda''}, H_1\psi_{E'\lambda'})\right\}$$
$$= Z_{E'\lambda'}{}^{-\frac{1}{2}}\psi_{E'\lambda'} - \delta_{\lambda'}(E')\left[\frac{1}{\tan\delta_{\lambda'}(E')} - \frac{1}{\delta_{\lambda'}(E')} \mp i\right]\psi_{E'\lambda'}{}^{\pm}, \quad (57)$$

in which use has been made of the relation

$$\delta(E'-E'')(\varphi_{E''\lambda''}, H_1\psi_{E'\lambda'}) = Z_{E'\lambda'}{}^{\frac{1}{2}}\delta(E''-E')(\varphi_{E''\lambda''}, \Sigma(E'+\Delta E'_{\lambda'})\varphi_{E'\lambda'})$$
$$= Z_{E'\lambda'}{}^{\frac{1}{2}}(\Delta E'_{\lambda'}/dE')\delta_{E''E'}\delta_{\lambda''\lambda'}$$
$$= -Z_{E'\lambda'}{}^{\frac{1}{2}}\pi^{-1}\delta_{\lambda'}(E')\delta_{E''E'}\delta_{\lambda''\lambda'}. \quad (58)$$

Equation (57) is readily solved, giving

$$\psi_{E'\lambda'}{}^{\pm} = \exp[\pm i\delta_{\lambda'}(E')]\psi_{E'\lambda'}, \quad (59)$$

with

$$Z_{E'\lambda'}{}^{\frac{1}{2}} = \sin\delta_{\lambda'}(E')/\delta_{\lambda'}(E') \leqq 1. \quad (60)$$

The result expressed by Eq. (59) is quite consistent with the definition of the S matrix,

$$(\varphi_{E''\lambda''}, S\varphi_{E'\lambda'}) = (\psi_{E''\lambda''}{}^{-}, \psi_{E'\lambda'}{}^{+}). \quad (61)$$

In conclusion, the author is happy to acknowledge a stimulating correspondence with Professor R. G. Newton and Professor K. A. Brueckner.

APPENDIX

Comments On the Use of Box Shapes Other than Spherical

It is helpful to realize that the physical process which a bound system undergoes is one of *multiple* scattering. The discrete stationary states of the system are those in which the waves produced by repeated scatterings reinforce one another.

The author's attention has been called[15] to the fact that the level shift operator $\Sigma(E)$ for plane waves is not identical with that for spherical waves, as may be easily shown by expanding one type of wave in terms of the other. This confusing point has its explanation in the fact that the appropriate boundary for a plane-wave eigenbasis is a rectangular box, and the bound state problem then corresponds to the problem of scattering by an infinite lattice formed by endless reflections of this box.

In order to describe *single* scattering only, within the rectangular framework, the scattering process must be allowed to last no longer than L/v, where L is the length of the box and v is the scattering velocity. This means that the energy shell within which one works has a thickness of order $\hbar v/L$. But the individual level shifts in the plane-wave case are of order $1/L^3$, and therefore the energy shell for single scattering is not sufficiently refined to sort out the various degeneracy-removals and permit a diagonalization of the S matrix for the whole lattice.

Only the spherical box (with spherical waves) is suitable for establishing a connection between single scattering processes and discrete-spectrum theory, for only then are the individual level shifts of the same order as the energy shell thickness. This is because multiple scattering inside a sphere is redundant. Spherical waves yield essentially complete scattering information after their first transit from the spherical boundary to the scattering region and back again, and repeated reflections contribute nothing new. The spherical waves which diagonalize the S matrix can be determined from the results of the first "bounce."

The Smoothed-Out Value for $\delta_\lambda(E')$

If $\Delta E'_\lambda = -(n+x)dE'$, where n is an integer and $0\leqq x<1$, then, for arbitrary ζ,

$$\delta_\lambda(E') = \lim_{dE'/\epsilon\to 0}\{n\pi + \sum_{m=-\infty}^{\infty}[\cot^{-1}(m-\zeta)dE'/\epsilon - \cot^{-1}(m+x-\zeta)dE'/\epsilon]\}, \quad (A.1)$$

the limit being actually independent of ζ and hence smooth. To evaluate the limit, make use of the identity

$$\cot^{-1}x - \cot^{-1}y = \tan^{-1}[(y-x)/(1+xy)], \quad (A.2)$$

and write

$$\delta_\lambda(E') = \lim_{dE'/\epsilon\to 0}(n\pi + \sum_{m=-\infty}^{\infty}\tan^{-1} \times\{(xdE'/\epsilon)/[1+(m-\zeta)(m+x-\zeta)(dE'/\epsilon)^2]\})$$
$$= n\pi + x\int_{\infty}^{\infty}(1+y^2)^{-1}dy = (n+x)\pi$$
$$= -\pi(\Delta E'_\lambda/dE'). \quad (A.3)$$

[15] K. A. Brueckner (private communication).

Evaluation of an Infinite Series

Let

$$f(x)=\pi e^{iax}/\sin\pi a, \tag{A.4}$$

and note that

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}e^{-inx}f(x)dx=\frac{(-1)^n}{a-n}. \tag{A.5}$$

This means that

$$f(x)=\sum_{n=-\infty}^{\infty}\frac{(-1)^n}{a-n}e^{inx}\quad\text{for}\quad -\pi<x<\pi, \tag{A.6}$$

and also

$$\sum_{n=-\infty}^{\infty}\frac{1}{a-n}=\tfrac{1}{2}[f(\pi)+f(-\pi)]=\frac{\pi}{\tan(\pi a)}. \tag{A.7}$$

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Nonlinear Spinor Field*

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A classical spinor field is defined by a variational principle on a Lagrangian with quadratic Dirac and quartic Fermi terms. Localized (particle-like) solutions are found within a class of comparison functions which make the angular momentum stationary for a given charge. It is found that the existence of eigensolutions depends in a radical way on the parameters of the Lagrangian, but that the observable properties of those solutions which do exist depend little on these parameters.

INTRODUCTION

New knowledge of the elementary particles is currently recorded by simply adding new terms to the Lagrangian of the total field. Although there is no doubt that this procedure is only provisional, attempts to make inferences about the intrinsic structure of the total field have, except for some efforts to guess new symmetries,[1] been unrelated to experiment. Nevertheless these theories[2] have attracted wide interest, and in any case the problem remains. By considering a very simple model, we shall attempt to present some results on one of the well-known questions which these theories raise, namely: can all the elementary particles be represented as eigenstates of a single underlying field?

The different fundamental theories appearing in the literature have in common the feature (a) that the equations of motion are *nonlinear* partial differential equations. They may be classified by (b) the group of the theory, e.g., the Lorentz group, or some wider group, like that of general relativity, or the generalized theory of gravitation.[2] They may be further classified by (c) their relation to quantum theory: most are quantized in the conventional Hamiltonian way. On the other hand, as is well known, Einstein expected that it would not be necessary to supplement the complete classical field equations with quantum postulates. The recent literature contains several papers in which similar and other unconventional views of the quantum theory are discussed.[3–7] The model to be discussed here will be characterized by (a) nonlinear equations of motion and (b) Lorentz rather than general covariance. We do not discuss point (c); however, the following analysis will be entirely classical.

Dirac has rather recently proposed a new classical theory of the electron.[8] Schrödinger has shown how this theory may be described as a Klein-Gordon-Schrödinger field coupled to a Maxwell field in the usual way, although with a particular choice of gauge.[9] It had been pointed out earlier that there is a class of classical field theories which may be arrived at in this same way—by coupling different representations of the Lorentz group through Lorentz-invariant interactions—i.e., simply by interpreting as classical and unitary precisely the total fields ordinarily considered only in terms of quantum field theory.[10] As a consequence of Schrödinger's remark, Dirac's new field may be related to this class.

Another example belonging to this same class may be arrived at by coupling the Maxwell field to the spinor field; this procedure leads to the differential equations of quantum electrodynamics, except that now the amplitudes are regarded as unquantized. Then, by eliminating the photon field, one obtains[10–12]

$$\gamma_\mu\partial_\mu\psi+\kappa\psi+e^2\int d^4x'[\bar{\psi}(x')\gamma_\mu\psi(x')]\times D_F(x'-x)\gamma_\mu\psi(x)=0,$$

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