Application of the Variation Method to Field Quantization*

L. I. SCHIFF
Department of Physics, Institute of Theoretical Physics, Stanford University, Stanford, California
(Received 29 November 1962)

The object of this paper is the application of the variation method to a simple field theory. A representation is found in which the state functions are emphasized. Variational trial forms are chosen for these, and optimized by making the expectation value of the field Hamiltonian stationary. Only the simplest case of a neutral, spin-zero, boson field with a fourth-power self-coupling term is considered here, but it is hoped that with further elaboration this may in the future lead to a description of the multipion resonances. The variation method has the advantage of avoiding any limitation on the strength of the self-coupling. Explicit results are obtained for the vacuum, single-particle, and two-particle (scattering and bound) states, and comparison is made with the determinantal method. Finally, a criterion for the variational stability of the vacuum state is obtained.

I. INTRODUCTION

THE existence of well-defined resonances, or quasi-bound states, of the two-pion and three-pion systems has now been established by experimental observation.[1] Several theoretical attempts have been directed toward relating these resonances with each other[2]; none of these has provided an exact solution within the framework of any definite model, nor are the limitations of the approximations completely understood. The simplest field-theoretical model is that in which only pions (no nucleons) are present, and the interaction between pions is represented by a nonbilinear self-coupling term in the field Lagrangian. Such a term appears after renormalization of the pion-nucleon coupling,[3] and the classical theory of this model was discussed many years ago in an attempt to account for the saturation of nuclear forces.[4] Quantization was carried through in a lattice space, with the field-gradient (kinetic energy) term being treated as a perturbation[5]; the object of this approach was to take strong self-couplings into account without approximation. Lattice quantization led to physically plausible lowest (vacuum) and first excited (single-particle) states. More complicated self-couplings have also been introduced in attempts to account for other properties of elementary particles.[6-8] The particular case of the fourth-power self-coupling has been treated most fully by means of the determinantal method[9]; this work provides an important standard with which new theoretical approaches, such as that developed below, can be compared.

The present paper starts with a representation in which the state functions are emphasized.[10] The variation method then provides a technique for improving these functions, and a criterion for gauging the degree of improvement that is attained. It also avoids any limitation on the strength of the self-coupling. Only the simplest case of a neutral, spin-zero, boson field with a fourth-power term in the Lagrangian is considered here, although the same methods can be applied to the self-coupled pion (unit isospin) field.[11] The work reported here is also limited to separable, or nearly separable, variational trial functions. While the results obtained evidently cannot be compared with experiment, they are promising enough to warrant extension to more elaborate trial functions.

II. GENERAL FORMALISM

We start with the Lagrangian density (in units such that $\hbar=c=1$)

$$\tfrac{1}{2}\dot{\phi}^2-\tfrac{1}{2}(\nabla\phi)^2-\tfrac{1}{2}\mu_0^2\phi^2-\tfrac{1}{4}\lambda_0\phi^4,$$

which is Lorentz invariant if the field amplitude ϕ is a scalar or pseudoscalar function of the coordinates and time. The canonical quantization procedure[12] then leads to the Hamiltonian

$$H=\int[\tfrac{1}{2}\pi^2+\tfrac{1}{2}(\nabla\phi)^2+\tfrac{1}{2}\mu_0^2\phi^2+\tfrac{1}{4}\lambda_0\phi^4]d^3r, \quad (1)$$

the commutation relations

$$[\phi(\mathbf{r},t),\pi(\mathbf{r}',t)]=i\delta(\mathbf{r}-\mathbf{r}'), \quad (2)$$

and the total momentum operator

$$\mathbf{G}=-\frac{1}{2}\int[\pi(\nabla\phi)+(\nabla\phi)\pi]d^3r. \quad (3)$$

It is easily seen that $\mathbf{G}$ commutes with H, so that the

* Supported in part by the U. S. Air Force through the Air Force Office of Scientific Research.

[1] For a summary of the experimental results, see the report by G. Puppi presented in the *Proceedings of the International Conference on High-Energy Physics at CERN, 1962* (CERN, Geneva, 1962), p. 713.

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[12] See, for example, G. Wentzel, *Quantum Theory of Fields* (Interscience Publishers, Inc., New York, 1949), Sec. 6.

states of the system may be classified according to values of the total energy and total momentum. Since Eqs. (1) and (2) are also invariant with respect to the substitution $\phi \rightarrow -\phi$, $\pi \rightarrow -\pi$, we expect the states to possess a multiplicative quantum number (equal to ± 1) that we shall call the amplitude parity.[13]

The integration volume in (1) and (3) is chosen at first to be a rectangular box of volume Ω with periodic boundary conditions at the edges; Ω is later allowed to become arbitrarily large. It is then convenient to expand the field amplitudes in terms of the normal modes of the box,

$$\phi=\Omega^{-1/2}\sum q_k \exp(i\mathbf{k}\cdot\mathbf{r}), \quad \pi=\Omega^{-1/2}\sum p_k \exp(-i\mathbf{k}\cdot\mathbf{r}).$$

The $\mathbf{k}$'s are three vectors whose rectangular components are integer multiplies of 2π divided by the corresponding length of the box; for notational simplicity, their vectorial character will not be indicated in the subscripts. The commutation relations (2) become $[q_k,p_{k'}]=i\delta_{k,k'}$ with other pairs commuting. Further, since we are dealing with a neutral field, the unquantized ϕ is real; then the quantized ϕ and π are Hermitian, so that

$$q_k^*=q_{-k}, \quad p_k^*=p_{-k}. \tag{4}$$

In the usual quantization procedure,[12] the q's and p's are expressed in terms of non-Hermitian creation and destruction operators. Since we wish to emphasize the state functions rather than the operators, we express the q's and p's in terms of Hermitian operators in the following way:

$$q_k\equiv 2^{-1/2}(x_k+iy_k), \quad p_k\equiv 2^{-1/2}(X_k-iY_k).$$

The new commutation relations, $[x_k,X_{k'}]=[y_k,Y_{k'}]=i\delta_{k,k'}$ with other pairs commuting, make it possible to adopt the representation

$$X_k=-i\partial/\partial x_k, \quad Y_k=-i\partial/\partial y_k.$$

Thus, H can be expressed in terms of the x's, y's, and their derivatives. However, it is slightly more convenient to define "cylindrical" coordinates

$$x_k\equiv z_k\cos\theta_k, \quad y_k\equiv z_k\sin\theta_k,$$

and express H and $\mathbf{G}$ in terms of the z's, θ's, and their derivatives:

$$H=\sum H_k^0+(\lambda_0/\Omega^2)\int[\sum z_k\cos(\mathbf{k}\cdot\mathbf{r}+\theta_k)]^4 d^3r, \tag{5}$$

$$H_k^0=-\tfrac{1}{2}\left[\frac{1}{z_k}\frac{\partial}{\partial z_k}\left(z_k\frac{\partial}{\partial z_k}\right)+\frac{1}{z_k^2}\frac{\partial^2}{\partial\theta_k^2}\right]+\tfrac{1}{2}\omega_k^2 z_k^2, \tag{6}$$

$$\mathbf{G}=\sum i\mathbf{k}\frac{\partial}{\partial\theta_k}. \tag{7}$$

Here, $\omega_k^2\equiv\mathbf{k}^2+\mu_0^2$.

Since Eqs. (4) are satisfied if $x_k=x_{-k}$ and $y_k=-y_{-k}$, or if $z_k=z_{-k}$ and $\theta_k=-\theta_{-k}$, it is only necessary to sum over half the $\mathbf{k}$ space. The summations in Eqs. (5) and (7), and all subsequent summations over $\mathbf{k}$, are written with coefficients so chosen that they do, in fact, extend over half the $\mathbf{k}$ space. This has the advantage that the field variables are not duplicated within a summation. While it is desirable to exploit the discreteness of the $\mathbf{k}$ space throughout most of the calculation, final results are only of interest for arbitrarily large Ω. A summation can then be replaced by an integration, which for convenience will be taken over the entire $\mathbf{k}$ space; we, thus, have the correspondence

$$\sum[\ ]\rightarrow\frac{\Omega}{16\pi^3}\int[\ ]d^3k. \tag{8}$$

III. SEPARABLE TRIAL FUNCTIONS

An exact solution of the equation $H\psi=E\psi$, where ψ is a function of the z's and θ's, would give the energy levels E of the quantized field. We shall apply the variation principle to the approximate determination of ψ, by choosing a trial function with some flexibility, and regarding the optimal form as that which makes the expectation value of H stationary. We first choose, for simplicity, a separable trial function that is written as a product of arbitrary functions of the normal mode variables:

$$\psi=\prod f_k(z_k,\theta_k). \tag{9}$$

The product in (9), like the sums in (5) and (7), extends over half the $\mathbf{k}$ space. The f's are assumed to be normalized:

$$\int|f_k|^2 d\tau_k\equiv\int_0^\infty z_k dz_k\int_0^{2\pi}\frac{d\theta_k}{2\pi}|f_k|^2=1.$$

The invariance of H with respect to change in sign of the field amplitude implies that it is invariant with respect to replacement of each θ_k by $\theta_k+\pi$. Thus, we expect each f_k to have definite amplitude parity, and each $|f_k|^2$ to remain unchanged under this substitution. This means that when the expectation value of H is computed with ψ, the only terms in the expansion of the fourth power of the summation in (5) that contribute are

$$\sum z_k^4\cos^4(\mathbf{k}\cdot\mathbf{r}+\theta_k)+3\sum\sum{}' z_k^2 z_l^2\cos^2(\mathbf{k}\cdot\mathbf{r}+\theta_k)\times\cos^2(\mathbf{l}\cdot\mathbf{r}+\theta_l). \tag{10}$$

The prime on the last summation indicates that $\mathbf{l}\neq\mathbf{k}$. Furthermore, after the $\mathbf{r}$ integration is performed, the θ dependence of (10) disappears. We, thus, obtain

$$\langle H\rangle\equiv(\psi H\psi)=\sum(f_k H_k^0 f_k)+(3\lambda_0/8\Omega)\sum(f_k z_k^4 f_k)+(3\lambda_0/4\Omega)\sum\sum{}'(f_k z_k^2 f_k)(f_l z_l^2 f_l), \tag{11}$$

where we have used the notation

$$(f_k H_k^0 f_k)\equiv\int\bar{f}_k H_k^0 f_k d\tau_k.$$

[13] This quantum number, introduced in reference 10, has been discussed further by G. Barton (to be published).

The condition that (11) be stationary for an arbitrary variation of the complex functions f_k, subject to the condition that they be normalized, is

$$\frac{\delta\langle H\rangle}{\delta f_k}=H_k{}^0 f_k+\left(\frac{3\lambda_0}{8\Omega}\right)z_k{}^4 f_k + \left(\frac{3\lambda_0}{2\Omega}\right)[\sum{}'(f_l z_l{}^2 f_l)]z_k{}^2 f_k=E_k f_k, \quad (12)$$

where E_k is a Lagrange multiplier. Comparison between the variational equation with respect to f_k and the complex conjugate of (12) shows that E_k is real.

The group of equations (12) for all $\mathbf{k}$ constitutes a particularly simple set of coupled nonlinear equations. We write them in the form

$$[H_k{}^0+(3\lambda_0 A/2\Omega)z_k{}^2]f_k + (3\lambda_0/8\Omega)[z_k{}^4-4(f_k z_k{}^2 f_k)z_k{}^2]f_k=E_k f_k, \quad (13)$$

where $A\equiv\sum(f_k z_k{}^2 f_k)$. Since it follows from (8) that each summation is proportional to Ω, it is apparent that the second bracket term in (13) is of order $1/\Omega$ compared to the first bracket term. Thus, a zero-order solution may be obtained with A as a parameter. The correction to this, which has the relative order of magnitude of the arbitrarily small quantity $1/\Omega$, can then be found by perturbation theory when the unperturbed f_k is inserted in the second bracket term of (13).

The variational energy $\langle H\rangle$ can be expressed in terms of the E's by multiplying (12) through by $\hat{f}_k$, integrating over z_k and θ_k, and summing over $\mathbf{k}$. Equation (11) may then be written as

$$\langle H\rangle=\sum E_k-(3\lambda_0 A^2/4\Omega)+(3\lambda_0/4\Omega)\sum(f_k z_k{}^2 f_k)^2. \quad (14)$$

We are interested in the value of $\langle H\rangle$ when Ω is arbitrarily large. Owing to the summation in the first term of (14), E_k must be known to relative order $1/\Omega$ if the Ω-independent part of $\langle H\rangle$ is to be obtained correctly. In similar fashion, the f_k must be known to relative order $1/\Omega$ if A is to be found with sufficient accuracy to give the Ω-independent part of the second term of (14) correctly. On the other hand, the unperturbed f's can be used to calculate the last term of (14).

It can be shown that the corrections of relative order $1/\Omega$ are zero for all the cases considered in this paper. While a simple proof of this result would be desirable, it has not been found, and the required calculations are sufficiently lengthy and uninteresting that they have been omitted. The subsequent work, therefore, ignores the $1/\Omega$ corrections.

Lowest State—Physical Vacuum

The leading terms of Eq. (13), together with the form of $H_k{}^0$ given in (6), shows that the unperturbed f's are two-dimensional harmonic oscillator functions. Then the unperturbed $E_k=(n_k+1)\epsilon_k$, where n_k is zero or a positive integer and

$$\epsilon_k{}^2=\omega_k{}^2+(3\lambda_0 A/\Omega), \quad A=\sum[(n_k+1)/\epsilon_k]. \quad (15)$$

Suppose now that we start with some set of n_k, and imagine that changes to $n_k+\delta n_k$ are made. Then if the corresponding fractional change in A is small, which implies that only a finite number of the n's are changed, the change in ϵ_k is given approximately by $\delta\epsilon_k=(3\lambda_0\delta A/2\Omega\epsilon_k)$. The variational energy

$$\langle H\rangle=\sum(n_k+1)\epsilon_k-(3\lambda_0 A^2/4\Omega),$$

given by the leading terms of (14), then changes by the amount

$$\delta\langle H\rangle=\sum\epsilon_k\delta n_k. \quad (16)$$

Thus, a moderate increase in the n's increase $\langle H\rangle$. It is reasonable, then, to expect the smallest value of $\langle H\rangle$ to be attained when each n_k is zero. This lowest state corresponds to the physical vacuum. The corresponding normalized unperturbed eigenfunctions of Eq. (13) are

$$f_k(z_k,\theta_k)=(2\epsilon_k)^{1/2}\exp(-\tfrac{1}{2}\epsilon_k z_k{}^2). \quad (17)$$

The vacuum state is defined by Eqs. (9) and (17); it has zero total momentum and even amplitude parity (equal to $+1$).

If we regard A as an undetermined parameter in the first of Eqs. (15), the second equation shows that A is quadratically divergent in the following sense: For a finite $\mathbf{k}$ space with dimensions of order Λ, A is of order $\Omega\Lambda^2$. This suggests that mass renormalization be introduced by replacing the square of the unrenormalized rest mass, $\mu_0{}^2$, by $\mu^2-\delta\mu^2$ in the original Lagrangian density; here, $\delta\mu^2\equiv 3\lambda_0 A/\Omega\propto\lambda_0\Lambda^2$ is the mass counter term. The first of Eqs. (15) then becomes

$$\epsilon_k{}^2=\mathbf{k}^2+\mu^2, \quad (18)$$

and we shall see that μ is to be interpreted as the physical particle rest mass.

First Excited States—Single Particles

The first excited states of the field are evidently obtained when each of the n's is zero except for one of them which is equal to unity. The state function is given by (9), where each of the f's has the form (17) except for one, which is a first excited oscillator state:

$$f_k(z_k,\theta_k)=2^{1/2}\epsilon_k z_k\exp(\pm i\theta_k-\tfrac{1}{2}\epsilon_k z_k{}^2). \quad (19)$$

It follows from (7) that this state is an eigenfunction of the total momentum operator $\mathbf{G}$ with eigenvalue $\mp\mathbf{k}$; it also has odd amplitude parity (equal to -1). Equation (16) shows that the energy of this state exceeds that of the vacuum by ϵ_k. Thus, if we regard the vacuum energy as being unobservable, Eq. (18) shows that the first excited states correspond to single relativistic particles of rest mass μ. It should be noted that even though $\mathbf{k}$ is restricted to half of the space, the twofold degeneracy of (19), indicated by the $\pm$ sign, yields particles of all momenta.

We have shown in this section that the state functions defined by Eqs. (9), (17), and (19) are optimal from the point of view of the variation principle provided only that the trial function is of separable form. The same final result for the particle energy and momentum can be obtained by applying the Bogoliubov transformation to the non-Hermitian creation and destruction operators usually defined in terms of the q's and p's.[11] However, this procedure *assumes* that the transformed operators correspond to oscillator states, and it is much more difficult in the Bogoliubov formalism to show that oscillator states are actually optimal.

IV. SECOND EXCITED STATES

The second excited states of the field may be described by separable trial functions of the form (9) in which either (a) each of the n's is zero except for two of them which are equal to unity, or (b) each of the n's is zero except for one of them which is equal to two. In case (a), the θ dependence is of the form $\exp(\pm i\theta_k \pm i\theta_l)$, which corresponds to total momentum $\mp\mathbf{k}\mp\mathbf{l}$. Since we must have $\mathbf{k}\neq\mathbf{l}$, the total momentum cannot be zero; we can nevertheless arrive at a c.m. (center-of-mass) coordinate system by a limiting process. It is somewhat simpler to make use of case (b), in which case there are three second excited states, which may be chosen to be proportional to $\exp(\pm 2i\theta_k)$, or independent of θ_k. The first two of these have total momentum $\mp 2\mathbf{k}$ and even amplitude parity, and describe two particles each with momentum $\mp\mathbf{k}$. The third state has zero total momentum and even amplitude parity, and describes a pair of particles with equal and opposite momenta ($\mathbf{k}$ and $-\mathbf{k}$). This representation of the c.m. system is used in the following; however, the same results can be obtained from case (a) by means of the limiting process mentioned above.

Wave Packet Trial Function

The second excited state just described [case (b)] is degenerate in a way in which the first excited state of Sec. III is not. First excited states for all vectors $\mathbf{k}$ of the same magnitude have the same energy and amplitude parity; but since they have different momenta and $\mathbf{G}$ commutes with H, matrix elements of H between different states are all zero. On the other hand, second excited states for all vectors $\mathbf{k}$ of the same magnitude have the same energy, amplitude parity, and momentum; hence they may, and in fact do, have nonvanishing matrix elements of H between them. It is necessary, therefore, to work with a wave packet: a sum of separable products of the form (9).

We, thus, choose our trial function in the form

$$\psi_2=\sum a_k g_k(z_k,\theta_k)\prod{}' f_l(z_l,\theta_l), \tag{20}$$

where the f's and g's are normalized and have even amplitude parity, and f_k and g_k are orthogonal to each other; again, the prime indicates that $l\neq k$. Normalization of ψ_2 requires that $\sum|a_k|^2=1$. It then follows from (8) that unless a limited set of the a's is involved in (20), which turns out not to be the case, each a_k is of order $\Omega^{-1/2}$. We do *not* assume at this point that the f's and g's are oscillator functions. Our object is to determine the optimal function of the form (20) that has the quantum numbers of the vacuum (zero total momentum and even amplitude parity), and is orthogonal to the vacuum trial function. Since it turns out that the f's and g's in (20) are, in fact, oscillator functions of the kind considered in Sec. III, the orthogonality requirement is automatically fulfilled. For the present, however, we do not make this assumption.

The argument leading to Eq. (10) is still valid, and we find that the expectation value of H is

$$\begin{aligned}\langle H\rangle_2=&\sum(f_kH_k^0f_k)+(3\lambda_0A^2/4\Omega)\\&+\sum|a_k|^2\{(g_k[H_k^0+(3\lambda_0A/2\Omega)z_k^2]g_k)-(f_k[H_k^0+(3\lambda_0A/2\Omega)z_k^2]f_k)\}\\&+(3\lambda_0/2\Omega)|\sum a_k(f_kz_k^2g_k)|^2+(3\lambda_0/8\Omega)\sum[(f_kz_k^4f_k)-2(f_kz_k^2f_k)^2]\\&+(3\lambda_0/8\Omega)\sum|a_k|^2[(g_kz_k^4g_k)-(f_kz_k^4f_k)+4(f_kz_k^2f_k)^2-4|(f_kz_k^2g_k)|^2\\&\qquad-4(g_kz_k^2g_k)(f_kz_k^2f_k)].\end{aligned} \tag{21}$$

The terms in Eq. (21) have been grouped so that those in the first line are of order Ω, those in the next two lines are independent of Ω, and those in the last two lines are of order $1/\Omega$; A is again defined as $\sum(f_kz_k^2f_k)$. In analogy with Eq. (12), the variational equations associated with (21) may be written as

$$\begin{aligned}&\delta\langle H\rangle_2/\delta\bar{f}_k=E_kf_k+\xi_kg_k,\\&\delta\langle H\rangle_2/\delta\bar{g}_k=E_k'g_k+\zeta_kf_k,\\&\delta\langle H\rangle_2/\delta\bar{a}_k=\alpha a_k.\end{aligned} \tag{22}$$

The Lagrange multipliers E_k, E_k', and α are associated with the normalization of f_k, g_k, and ψ_2, respectively; ξ_k and ζ_k are associated with the orthogonality of f_k and g_k. From a comparison between the variational equations with respect to f_k, g_k, a_k, and the complex conjugates of Eqs. (22), it is readily seen that E_k, E_k', and α are real, and that $\xi_k=\bar{\zeta}_k$.

We ignore the last two lines of (21) in what follows. Then the first of Eqs. (22) consists of two parts, one of which is of order Ω compared to the other; the leading (unperturbed) part is just the oscillator equation [first part of (13)]. The second of Eqs. (22) is all of the same order, and is an inhomogeneous equation that relates g_k to the unperturbed f's. It may be solved by expanding g_k in oscillator functions; it then follows that only one of

the even excited states appears, and we take this to be the second. The third of Eqs. (22) is

$$\{(g_k[H_k^0+(3\lambda_0 A/2\Omega)z_k^2]g_k) - (f_k[H_k^0+(3\lambda_0 A/2\Omega)z_k^2]f_k)\}a_k + (3\lambda_0/2\Omega)(g_k z_k^2 g_k)\sum(f_l z_l^2 f_l)a_l=\alpha a_k. \quad (23)$$

If we multiply this through by $\bar{a}_k$ and sum over k, the right side is equal to α. The left side can be shown to be equal to $\langle H\rangle_2$ minus the vacuum energy found in Sec. III, if only terms that fail to vanish as Ω becomes arbitrarily large are retained. Thus, if we again regard the vacuum energy as being unobservable, α is the energy of the second excited state.

Equation (23) determines α and the a's. It is sufficient now to use the unperturbed f's, in which case (23) becomes

$$2\epsilon_k a_k+(3\lambda_0/2\Omega\epsilon_k)[\sum(a_l/\epsilon_l)]=\alpha a_k. \quad (24)$$

The physical meaning of Eq. (24) may be inferred in the following way: If λ_0 were zero, then a_k could be different from zero only if $\alpha=2\epsilon_k$. Thus, for arbitrarily large but finite Ω, there would be a discrete set of energy levels that correspond to noninteracting pairs of particles with equal and opposite momenta; for given magnitude of the momenta, each level would be degenerate with respect to direction. Since λ_0 is not equal to zero, the spectrum of α does not have this simple form, but is still discrete. The a's are mixed together, and the displaced α's correspond to wave packets that describe two-particle scattering. The displacement of α can be related to the scattering phase shift in a well-known way.[14–16]

Two-Particle Scattering

We define $B\equiv\sum(a_l/\epsilon_l)$, and rewrite Eq. (24) as

$$(\alpha-2\epsilon_k)a_k=3\lambda_0 B/2\Omega\epsilon_k. \quad (25)$$

There are two kinds of nontrivial solutions of (25): Either a_k is spherically symmetric with respect to the direction of the vector $\mathbf{k}$ and $B\neq 0$, or else $B=0$ and $\alpha=2\epsilon_k$. The first case describes S-wave scattering, and the second describes higher partial waves in the c.m. system for which there is no energy displacement and hence no scattering. We are interested only in S-wave scattering, in which case the equation for α is easily seen to be

$$\sum\frac{1}{\epsilon_k^2(\alpha-2\epsilon_k)}=\frac{2\Omega}{3\lambda_0}. \quad (26)$$

The summation in (26) is over the vectors $\mathbf{k}$, and may be written as a summation over the magnitudes and directions of these vectors. Because of the spherical symmetry of the summand, we may write this

$$\sum_k\sum_{\theta,\phi}=\sum_k C(k), \quad (27)$$

where $\mathbf{k}\equiv(k,\theta,\phi)$. It is convenient then to imagine that the volume Ω is of spherical shape with radius R, so that $\Omega=4\pi R^3/3$. Then we may use spherical waves instead of the plane waves of Sec. II; for any partial wave, the summation over k can be replaced in the limit of arbitrarily large Ω or R by R/π times an integration over k. The function $C(k)$ can be determined by writing the limit of the complete summation in (27) either as $(R/\pi)\int C(k)dk$, or from Eq. (8) as $(\Omega/16\pi^3)\int 4\pi k^2 dk$. It follows that

$$C(k)=k^2R^2/3. \quad (28)$$

Except in the immediate neighborhood of the value of k for which the denominator of the summand vanishes, the left side of (26) may be replaced by the principal value of the integral over k. From (27) and (28), this is

$$P\int\frac{(k^2R^2/3)(R/\pi)dk}{\epsilon_k^2(\alpha-2\epsilon_k)}. \quad (29)$$

The discreteness of the summation must of course be taken into account when ϵ_k is close to $\frac{1}{2}\alpha$. Let ϵ_K be the value of ϵ_k that is closest to $\frac{1}{2}\alpha$, and K be the corresponding value of k. Then the denominator of the summand of (26) can be written to sufficient approximation

$$-2\epsilon_K^2[(\epsilon_K-\tfrac{1}{2}\alpha)+(K/\epsilon_K)(n\pi/R)],$$

where n ranges from $-\infty$ to $+\infty$ in integer steps. This substitution, together with (27) and (28), then gives for this part of the left side of (26):

$$-\frac{KR^3}{6\epsilon_K}\cot\frac{(\epsilon_K-\frac{1}{2}\alpha)\epsilon_K R}{K}. \quad (30)$$

In the argument of the cotangent, $\epsilon_K-\frac{1}{2}\alpha$ is the negative of the displacement of the energy of a particle caused by the interaction, and $(K/\epsilon_K)(\pi/R)$ is the separation of adjacent unperturbed particle energies; thus, this argument is just the scattering phase shift δ.[14–16]

Combining Eqs. (26), (29), and (30), we obtain

$$\frac{\pi K}{\epsilon_K}\cot\delta=-\frac{16\pi^2}{3\lambda_0}-P\int\frac{k^2dk}{\epsilon_k^2(\epsilon_k-\epsilon_K)}, \quad (31)$$

where we have replaced $\frac{1}{2}\alpha$ by ϵ_K in the integral. This integral is logarithmically divergent, which means that δ is infinitesimally close to zero or an integer multiple of π if λ_0 is finite. We may, however, assume that λ_0 is infinitesimally negative in such a way that the first term on the right side of (31) cancels the divergent part of the integral, leaving a finite remainder that determines δ. One way of accomplishing such a coupling constant renormalization is to add and subtract $\int(k^2/\epsilon_k^3)dk$ on the right side of (31), and define the renormalized coupling constant λ by the relation

$$\frac{16\pi^2}{3\lambda}=\frac{16\pi^2}{3\lambda_0}+\int\frac{k^2}{\epsilon_k^3}dk. \quad (32)$$

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Equation (31) then becomes, after a change in variable of integration from k to ϵ_k:

$$\frac{\pi K}{\epsilon_K}\cot\delta=-\frac{16\pi^2}{3\lambda}-\epsilon_K\cdot P\int_\mu^\infty\frac{kd\epsilon_k}{\epsilon_k^2(\epsilon_k-\epsilon_K)}. \tag{33}$$

The last term in (33), ϵ_K times the principal value of the integral, may be evaluated in an elementary way and is equal to

$$1+\frac{\pi}{2w}-\frac{(w^2-1)^{1/2}}{w}\ln[w+(w^2-1)^{1/2}],\quad w\equiv\frac{\epsilon_K}{\mu}>1.$$

We, thus, have a closed expression for the differential scattering cross section in the c.m. system, $(1/K^2)\sin^2\delta$; it decreases monotonically with increasing particle energy.

Two-Particle Bound State

Equation (26) may also have a solution for which $\alpha<2\mu$, which corresponds to a bound state of the two-particle system. In this case, the summation on the left side is equal to the integral (29), of course without taking the principal value. We use the same renormalization as for the scattering problem, replace α by $2\epsilon_0$, and find that (33) is replaced by

$$-\frac{16\pi^2}{3\lambda}=\epsilon_0\int_\mu^\infty\frac{kd\epsilon_k}{\epsilon_k^2(\epsilon_k-\epsilon_0)}=1+\frac{\pi}{2v}-\frac{(1-v^2)^{1/2}}{v}(\tfrac{1}{2}\pi+\sin^{-1}v),$$

where $v\equiv\epsilon_0/\mu<1$ is the ratio of the total energy of the system to the rest mass of two free particles, and the value of the arcsine lies between 0 and $\frac{1}{2}\pi$. There is no bound state unless λ is negative and $16\pi^2/3|\lambda|<1+\frac{1}{2}\pi$; as $|\lambda|$ increases from this minimum value to infinity, ϵ_0 decreases monotonically from μ to zero.

Connection with the Determinantal Method

A formalism such as that developed in this paper must conserve probability, since it is set up in terms of normalized state functions. It is expected, then, that the S matrix will be unitary, and this is demonstrated in the case of two-particle scattering by the existence of the real phase shift given in (33). It is also of some interest to rewrite (33) in a form that brings it into correspondence with the determinantal method,[9,16] which also leads to an S matrix that is automatically unitary. The result is

$$\begin{gathered}\frac{1}{\pi}-e^{i\delta}\sin\delta=\frac{r(K)}{D(K)},\quad r(K)=-\frac{3\lambda K}{16\pi^2\epsilon_K},\\ D(K)=1-\epsilon_K\int_\mu^\infty\frac{r(k)d\epsilon_k}{\epsilon_k(\epsilon_k-\epsilon_K-i\eta)},\end{gathered} \tag{34}$$

where η is a positive infinitesimal.

Equation (34) is very similar to the first-order result obtained by Baker and Zachariasen,[9] which differs from (34) mainly through the appearance of the squared energy rather than the energy in the integrand of D. This is a characteristic difference between covariant and noncovariant dispersion relations; indeed, Auvil[11] has shown that (34) can be obtained from a summation of graphs in which the propagation is entirely forward in time, not forward and backward as with Feynman graphs. However, it has not proved possible to derive the covariant version of (34) from a variation principle by the methods developed in this paper, so it is not clear that the first-order Baker-Zachariasen expression for δ is superior to (33) or (43).

V. STABILITY OF THE VACUUM STATE

The variation principle has been used in this paper in the sense that the expectation value of the field Hamiltonian for a given class of trial functions is to be made stationary. The stationary point should in addition be a minimum, and we investigate this now to see whether or not the vacuum state found in Sec. III is stable with respect to small variations in the f's. Our procedure consists in calculating $\langle H\rangle$, given by (11), when f_k of (17) is replaced by

$$F_k\equiv(f_k+g_k)\Big[1+\int|g|^2d\tau_k\Big]^{-1/2};$$

here g_k is orthogonal to f_k, so that F_k is normalized. The smallness of the variation implies that $\int|g_k|^2d\tau_k\ll1$, and we shall keep only quantities of second order in the g's.

Retaining only the leading terms, of order Ω, we find after some calculation that $\langle H\rangle$ is replaced by $\langle H\rangle+\delta\langle H\rangle$, where

$$\begin{aligned}\delta\langle H\rangle=&\sum(g_k[H_k^0+(3\lambda_0A/2\Omega)z_k^2-\epsilon_k]g_k)\\&+(3\lambda_0/4\Omega)\{\sum[(g_kz_k^2f_k)+(f_kz_k^2g_k)]\}^2.\end{aligned} \tag{35}$$

Since ϵ_k is the smallest eigenvalue of the operator $H_k^0+(3\lambda_0A/2\Omega)$, and the square bracket in the second term is real, it is evident that $\delta\langle H\rangle$ is positive so long as λ_0 is positive and g_k is nonzero. Thus, the vacuum state is stable if $\lambda_0>0$. However, the discussion following Eq. (31) shows that there is no two-particle interaction in this case. We should, therefore, investigate stability when λ_0 is negative.

This is most readily accomplished by expanding g_k in higher oscillator states f_{kn}, which are assumed to be normalized:

$$g_k=\sum_{n=1}^\infty b_{kn}f_{kn},\quad[H_k^0+(3\lambda_0A/2\Omega)]f_{kn}=(n+1)\epsilon_kf_{kn}.$$

In this notation, f_{k0} is given by (17) and f_{k1} by (19). Only f_{k2} contributes to the second term of (35), and it is

easily seen that

$$(f_{k2}z_k^2 f_k)=\beta_k/\epsilon_k, \quad |\beta_k|\leqq 1;$$

the value of β_k depends on the particular linear combination of the three degenerate second excited oscillator states that is chosen for f_{k2}. Substitution into (35) then gives

$$\delta\langle H\rangle=\sum \epsilon_k(|b_{k1}|^2+2|b_{k2}|^2+3|b_{k3}|^2+\cdots) + (3\lambda_0/4\Omega)[\sum(b_{k2}\beta_k+\bar{b}_{k2}\bar{\beta}_k)/\epsilon_k]^2. \quad (36)$$

For negative λ_0, $\delta\langle H\rangle$ is algebraically smallest when all of the b's are zero except for b_{k2}. Further, if only a finite set of the b_{k2} differ from zero, the first term of (36) is of order unity and the second term is of order $1/\Omega$, so that $\delta\langle H\rangle$ is positive. Thus, we obtain the severest test of stability if we assume that b_{k2} is real and β_k is equal to unity, and then take the limit of arbitrarily large Ω so that b_{k2} can be replaced by a continuous function $b(k)$. Equation (36) then becomes

$$\delta\langle H\rangle=\frac{\Omega}{2\pi^2}\int \epsilon_k b^2(k)k^2dk-\frac{3|\lambda_0|\Omega}{16\pi^4}\left[\int \frac{b(k)}{\epsilon_k}k^2dk\right]^2, \quad (37)$$

where we have explicitly recognized that λ_0 is negative.

We must now choose $b(k)$ so as to maximize the ratio

$$\left[\int \frac{b(k)}{\epsilon_k}k^2dk\right]^2 \Big/ \int \epsilon_k b^2(k)k^2dk. \quad (38)$$

Variation of (38) with respect to the form of $b(k)$ shows that it is stationary when $b(k)=\text{constant}/\epsilon_k^2$; further analysis shows that this stationary point is a maximum. It then follows from (37) that $\delta\langle H\rangle$ is positive with this form for $b(k)$ if

$$|\lambda_0|<\frac{8\pi^2}{3}\left(\int \frac{k^2}{\epsilon_k^3}dk\right)^{-1}. \quad (39)$$

The inequality (39) is the stability criterion for the vacuum state when it has the separable form (9) and it is assumed that λ_0 is negative. The integral in (39) is logarithmically divergent; if the **k** space is spherical and has radius Λ, then (39) becomes approximately

$$|\lambda_0|<\frac{8\pi^2}{3\ln(2\Lambda/\mu)}, \quad \Lambda\gg\mu. \quad (40)$$

It is interesting to see what conclusions can be drawn concerning the renormalized coupling constant λ from (32) and (39).

We see that

$$\frac{16\pi^2}{3\lambda}=-\frac{16\pi^2}{3|\lambda_0|}+\int \frac{k^2}{\epsilon_k^3}dk<-\frac{8\pi^2}{3|\lambda_0|},$$

from which it follows that λ is negative for stability, and also that $|\lambda|<2|\lambda_0|$. Together with (40), this leads to the stability criterion

$$|\lambda|<\frac{16\pi^2}{3\ln(2\Lambda/\mu)}, \quad (41)$$

which for large Λ means that the renormalized two-particle interaction is very weak.[17] As an example, there is no bound state of the two-particle system if $\Lambda>6.6\mu$.

VI. CONCLUDING REMARKS

We have shown how the system described by Eqs. (1) and (2) can be formulated in terms of state functions that can be approximated by means of the variation principle. This method does not impose any limitation on the magnitude of λ_0. Optimal trial functions of separable form have been found that correspond to the vacuum and to single-particle states, and which require the introduction of mass renormalization. Optimal wave packets that describe two-particle scattering and binding have been constructed, and these lead naturally to coupling constant renormalization. The variational stability of the vacuum state has been examined, and yields the rather unsatisfactory criterion (41). This suggests that attention should be focused on more elaborate trial functions, particularly for the vacuum state, rather than on the introduction of isotopic spin or the solution of the three-particle problem.[11]

Although it is not shown in this paper, we have also found that a sum of separable products of the form (9), in each of which a finite number of the f's are permitted to differ from the lowest oscillator function (17), does not change the leading term in the vacuum energy, which is of order Ω. It seems likely that improvement can be achieved only by abandoning the separable form (9), perhaps by expressing ψ as a function of collective variables that involve all of the z's and θ's. The variation formalism is well adapted to attempts of this kind, and these are now under way.

ACKNOWLEDGMENTS

The writer takes pleasure in thanking P. R. Auvil, Jr., and M. Baker for stimulating conversations on matters connected with this paper.

[17] Owing to an error of a factor 2 in the earlier derivation of the stability criterion, this result was incorrectly stated in reference 10.