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Renormalization of trial wave functionals using the effective potential

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We introduce a procedure for renormalizing trial variational wave functionals in Fermi and Bose field theories in terms of zero-momentum n-point functions. The method relies on a variational calculation of the effective potential. Two model field theories, $\lambda\phi^4$ and $g\bar{\psi}\psi\phi$, are treated explicitly with simple trial wave functionals for the Fermi and Bose vacuums.

I. INTRODUCTION

The idea of treating the search for solutions of quantum field theories as a variational problem is not a new one. In the 1960's papers by Schiff[1] and Rosen,[2] in particular, attempted to find approximate solutions to several model theories variationally, though with mixed success. The procedure followed in all of these papers, which we shall adopt here, is to write the (functional) Schrödinger equation which an energy eigenstate of the field theory must satisfy. An ansatz for the vacuum state is written which has a number of free parameters, and these are determined by minimization of the expectation value of the Hamiltonian. Once the vacuum state is obtained, it is straightforward to search for the excited states variationally. All this is completely analogous to the variational approach, familiar to us from simple quantum-mechanical problems.

All of these papers had two essential weaknesses which contributed to the decline of interest in variational calculations in the late 1960's. The first was the lack of a functional description for fermions, which precluded any treatment of a field theory involving fermions.[3] Clearly, any calculational scheme which cannot be used for fermions is of very limited applicability. Fortunately, physicists have recently discovered how to use Grassmann variables, and the required description of Fermi state vectors as Grassmann functionals has been developed.[4,5] The remaining weakness of the earlier variational calculations was the problem of renormalization. In a typical variational calculation one encounters divergent integrals which somehow must be absorbed in bare parameters in the Lagrangian, so that physically measurable quantities become their finite observed values. Quite simply, it was not clear just what a reasonable definition of the physical coupling constant or even the mass was, given some variational ansatz for the vacuum. The schemes for absorbing divergences which were employed suffered from this uncertainty in physical interpretation, and thus tended to be rather arbitrary. This is in contrast with the situation in perturbation theory, in which one could construct given n-point functions perturbatively and relate simple properties of these functions to quantities such as physical masses and coupling constants, which allowed renormalization to proceed unambiguously. As with the first weakness of variational calculations, this problem may now be avoided by making use of a new technique in field theory, based on the effective potential.[6,7]

Starting from the effective potential one may easily construct n-point functions which may be used in renormalization, as is conventionally done in perturbation theory. The relevant observation here is that the variational calculation of the effective potential is a straightforward exercise and uses an ansatz of which the vacuum trial ansatz is a special case. This allows the development of a renormalization scheme which employs the same approximation in treating the n-point functions as in finding the vacuum state, and in which the physical interpretation of the renormalized quantities is clear and unambiguous. The application of this renormalization scheme to variational calculations of the state vectors of Bose and Fermi-Bose interacting theories is the principal new contribution of this paper.

The text of the paper is organized in the following way. First, we show how the effective potential may be obtained and used in a simple quantum-mechanical problem in one dimension. Rather than discuss the effective-potential formalism in detail in this paper, we instead refer the interested reader to a concise review of its properties,[7] which we shall use without explicit justification. Next, we consider the familiar problem of a scalar field with quartic self-coupling, and find the vacuum, one-particle, and two-particle states in a simple vacuum ansatz. The effective-potential-based renormalization is carried out for this model, which leads to an interpretation of the variational ansatz for the n-point functions derived from the effective potential as sums of all Feynman diagrams of a certain type. Finally, we treat a model Fermi-Bose interacting theory variationally and discuss the applicability of our approach to physically interesting theories such as quantum electrodynamics (QED) and quantum chromodynamics (QCD).

II. QUANTUM MECHANICS

In this section we illustrate our approach to variational problems by considering a simple model which avoids the complexity of the infinite number of degrees of freedom in field theory. The model we choose is a one-dimensional simple harmonic oscillator with a quartic term in the potential energy. The Schrödinger equation, which energy eigenstates of this theory must satisfy, is

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+\frac{\mu^2}{2}x^2+\lambda_0 x^4\right)|\psi(x)\rangle = E\,|\psi(x)\rangle\,. \tag{2.1}$$

With no perturbation, $\lambda_0=0$, the ground state of this theory is simply a Gaussian,

$$|\psi_0(x)\rangle = \left(\frac{\mu}{\pi}\right)^{1/4} e^{-\mu x^2/2}\,, \tag{2.2}$$

$$E_0=\tfrac{1}{2}\mu\,. \tag{2.3}$$

For $\lambda_0>0$, a simple trial vacuum wave function one might choose is

$$|\psi(x)\rangle = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}\,. \tag{2.4}$$

The expectation value of the energy of this trial function is

$$E(\alpha)=\frac{1}{4}\left(\alpha+\frac{\mu^2}{\alpha}\right)+\frac{3\lambda_0}{4\alpha^2}\,. \tag{2.5}$$

The value of α which minimizes $E(\alpha)$ is the solution of

$$\alpha=+\left(\mu^2+\frac{6\lambda_0}{\alpha}\right)^{1/2}\,, \tag{2.6}$$

which approaches $+\mu$ as $\lambda_0\to 0$.

Now we consider the effective potential for this problem. Here we define the effective potential $V(x_0)$ as the minimum value of the energy in the set of all normalized state vectors in which x has the expectation value x_0:

$$V(x_0)=\min\{\langle x_0|H|x_0\rangle\}\,, \tag{2.7}$$

with

$$\langle x_0|x|x_0\rangle = x_0\,, \tag{2.8}$$

$$\langle x_0|x_0\rangle = 1\,. \tag{2.9}$$

To calculate $V(x_0)$ variationally, we need only consider a set of states $\{|x_0\rangle\}$ with some parametrization, and we minimize $\langle x_0|H|x_0\rangle$ with respect to these parameters. A set which has (2.4) as a special case is

$$|\alpha,x_0\rangle = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha(x-x_0)^2/2}\,. \tag{2.10}$$

Clearly, the requirements (2.8) and (2.9) are satisfied. To find $V(x_0)$ we simply minimize $\langle H\rangle$ with respect to α, with H given by (2.1). $\langle H\rangle$ is explicitly

$$\begin{aligned}\langle\alpha,x_0|H|\alpha,x_0\rangle &\equiv V(\alpha,x_0)\\ &=\frac{1}{4}\left(\alpha+\frac{\mu^2}{\alpha}\right)+\frac{3\lambda_0}{4\alpha^2}+\frac{1}{2}\mu^2x_0^2\\ &\quad+\lambda_0x_0^4+\frac{3\lambda_0}{\alpha}x_0^2\,.\end{aligned} \tag{2.11}$$

So the value of α which minimizes $V(\alpha,x_0)$ is

$$\alpha(x_0)=+\left[\mu^2+\frac{6\lambda_0}{\alpha(x_0)}+12\lambda_0x_0^2\right]^{1/2}\,. \tag{2.12}$$

We obtain the effective potential $V(x_0)$, which results from the Gaussian ansatz (2.10), by solving the implicit Eq. (2.12) and substituting $\alpha(x_0)$ for α in (2.11). The value of this is that we may now obtain the renormalized mass m and coupling λ from the effective potential,

$$m^2=\left.\frac{d^2V}{dx_0^2}\right|_{\min}\,, \tag{2.13}$$

$$\lambda=\frac{1}{4!}\left.\frac{d^4V}{dx_0^4}\right|_{\min}\,. \tag{2.14}$$

The derivatives are evaluated at the value of x_0 given by $dV/dx_0=0$, $d^2V/dx_0^2>0$, which is the value of x_0 in the vacuum state. From (2.12) it is clear that $\alpha(x_0)$ is even, and the solution of $dV/dx_0=0$ we require is $x_0=0$. At this point we may evaluate derivatives of $V(x_0)$ to obtain

$$\left.\frac{d^2V}{dx_0^2}\right|_{x_0=0}=\mu^2+\frac{6\lambda_0}{\alpha}=m^2\,, \tag{2.15}$$

$$\frac{1}{4!}\left.\frac{d^4V}{dx_0^4}\right|_{x_0=0}=\lambda_0\frac{1-6\lambda_0/m^3}{1+3\lambda_0/m^3}=\lambda\,. \tag{2.16}$$

The meaning of (2.15) is clear. If we define m, the renormalized mass, by $E_1-E_0\equiv m$, it is easy to prove that $m=\alpha$. This shows that the mass obtained from the effective potential (2.15) agrees with the mass obtained variationally in (2.6). The variational first excited state used to obtain this result is

$$|\,\alpha, 1\rangle = \frac{\sqrt{2}\alpha^{3/4}}{\pi^{1/4}} x e^{-\alpha x^2/2}\,. \tag{2.17}$$

We construct this state by acting on the vacuum with the adjoint of the vacuum annihilation operator,

$$A^\dagger(\alpha) = \frac{1}{\sqrt{2\alpha}}\left(\alpha x - \frac{d}{dx}\right). \tag{2.18}$$

The energy of an n-particle state constructed in this fashion is

$$E_n = (n + \tfrac{1}{2})\alpha + [2n(n-1) - 1]\frac{3\lambda_0}{4\alpha^2}, \tag{2.19}$$

from which $E_1 - E_0 \equiv m = \alpha$.

Renormalization consists of the elimination of unmeasurable parameters in the theory (here μ, λ_0) in favor of physically measurable ones, such as m and λ. We have not given an interpretation to the renormalized coupling constant λ [(2.16)], but it may presumably be related to the quantum-mechanical analogs of n-point functions in field theory. For example, we might relate it to the amplitude to go from the asymptotic state $|1\rangle$ to $|3\rangle$ under the interaction λx^4. Assuming that such an interpretation may be found, the renormalized version of the Hamiltonian in (2.1) is

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}m^2\left(1 - \frac{1}{2}\left\{1 - \frac{3\lambda}{m^3} - \left[\left(1 - \frac{3\lambda}{m^3}\right)^2 - 24\frac{\lambda}{m^3}\right]^{1/2}\right\}\right)x^2 + \frac{m^3}{12}\left\{1 - \frac{3\lambda}{m^3} - \left[\left(1 - \frac{3\lambda}{m^3}\right)^2 - 24\frac{\lambda}{m^3}\right]^{1/2}\right\}x^4\,, \tag{2.20}$$

and the n-particle energy is

$$E_n = \left(n + \frac{1}{2} + \frac{[2n(n-1) - 1]}{16}\left\{1 - \frac{3\lambda}{m^3} - \left[\left(1 - \frac{3\lambda}{m^3}\right)^2 - 24\frac{\lambda}{m^3}\right]^{1/2}\right\}\right)m\,. \tag{2.21}$$

Although this corresponds to the conventional renormalization scheme in terms of coupling constants and one-particle masses, the fact that we know the higher excited-state energies lets us renormalize in terms of these masses only. For example, in terms of $m \equiv E_1 - E_0$ and $m_2 \equiv E_2 - E_0$ we find

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}[m^2 - 2m(m_2 - 2m)]x^2 + \frac{m^2}{3}(m_2 - 2m)x^4\,, \tag{2.22}$$

$$m_n \equiv E_n - E_0 = m\left[n + \left(\frac{m_2}{2m} - 1\right)n(n-1)\right]. \tag{2.23}$$

In terms of simplicity, the second choice of physical renormalized parameters is obviously preferable.

We have now completed the desired objective of calculating the particle spectrum in terms of renormalized quantities variationally, using the effective potential. Naturally, one could further improve the variational ansatz [(2.4), (2.10)] by introducing more parameters, and thereby obtain better approximate wave functions and energies, but we would encounter no new conceptual difficulties. Hence, we shall proceed directly to the scalar-field-theory problem.

III. A SCALAR QUANTUM FIELD THEORY

Now we treat the problem of the variational determination and renormalization of energy eigenstates of a nontrivial model field theory described by the Lagrangian

$$\mathcal{L} = \tfrac{1}{2}(\partial_\mu\phi)^2 - \tfrac{1}{2}\mu^2\phi^2 - \lambda_0\phi^4\,. \tag{3.1}$$

The state vectors may be written as wave functions $\Omega[\phi]$, which give the amplitude for the field ϕ to be found at a point $\phi(\vec{x})$ in function space.[1,2] The Schrödinger equation satisfied by $\Omega[\phi]$ is in this case[2]

$$\int d\vec{x}\left[-\frac{1}{2}\frac{\delta^2}{\delta\phi(\vec{x})^2} + \frac{1}{2}|\vec{\nabla}\phi|^2 + \frac{1}{2}\mu^2\phi^2 + \lambda_0\phi^4\right]\Omega[\phi] = E\,\Omega[\phi]\,. \tag{3.2}$$

It is this functional Schrödinger equation which we shall treat variationally.

First, it helps to know the solutions of the free theory with $\lambda_0 = 0$ in (3.2). One may easily check that the vacuum state is the Gaussian functional

$$|\,\Omega_0[\phi]\rangle = \eta\exp\left[-\frac{1}{2}\int d\vec{x}\,\phi(\vec{x})(\mu^2 - \nabla^2)^{1/2}\phi(\vec{x})\right] \tag{3.3}$$

with the usual zero-point energy [defining $\omega_{\vec{k}} \equiv (\mu^2 + \vec{k}^2)^{1/2}$]

$$E_0=\int\frac{d\vec{k}}{(2\pi)^3}\tfrac{1}{2}\,\omega_{\vec{k}}=\sum_{\vec{k}}\tfrac{1}{2}\,\omega_{\vec{k}}\,. \tag{3.4}$$

(We suppress the trivial time dependence e^{-iE_0t} in Ω.) Excited states may be constructed from this vacuum wave functional by repeated application of the creation operator $A^\dagger(\vec{p})$:

$$A^\dagger(\vec{p})=\frac{1}{[(2\pi)^3 2\omega_{\vec{p}}]^{1/2}}\int d\vec{x}\,e^{-i\vec{p}\cdot\vec{x}}\left((\mu^2-\nabla^2)^{1/2}\phi(\vec{x})-\frac{\delta}{\delta\phi(\vec{x})}\right). \tag{3.5}$$

If we write an n-particle state functional $|\Omega(\vec{p}_1,\ldots,\vec{p}_n)\rangle$ in terms of the Fourier components $a(\vec{k})$ of $\phi(\vec{x})$, we obtain a more familiar looking result, which is a Hermite polynomial in $a(\vec{p})$ times a Gaussian in $\sum_{\vec{k}}|a(\vec{k})|^2$. As the free scalar theory is a collection of uncoupled harmonic oscillators, one for each $\vec{p}$, this result is exactly what we expect for the excited states.

To approximate the ground state of (3.1) variationally, we need an ansatz for the vacuum functional $\Omega[\phi]$. By analogy with the choice (2.4) as a generalization of (2.2), we choose here to generalize the functional matrix $(\mu^2-\nabla^2)^{1/2}$ which appears in the free-theory ground state (3.3). Our trial vacuum is

$$|\Omega_f[\phi]\rangle\equiv|0_f\rangle=\eta_f\exp\left[-\frac{1}{2}\iint d\vec{x}\,d\vec{y}\;\phi(\vec{x})f(\vec{x}-\vec{y})\phi(\vec{y})\right]. \tag{3.6}$$

Translational invariance of the vacuum requires that f be a function of $\vec{x}-\vec{y}$. We could write f as a differential operator, but the kernel form we give here is both easier to manipulate and completely equivalent to an operator f. The normalization constant is understood to normalize Ω_f to unity,

$$\eta_f^{\,2}\int D\phi\,\exp\left[-\iint d\vec{x}\,d\vec{y}\;\phi(\vec{x})\,f(\vec{x}-\vec{y})\phi(\vec{y})\right]=1\,, \tag{3.7}$$

and the functional integral $\int D\phi$ is over all functions $\phi(\vec{x})$ at some fixed time t.

Having found a suitable normalized ansatz for the vacuum, we proceed to find the expectation value of the Hamiltonian $E[f]$ as a functional of $f(\vec{x}-\vec{y})$. The necessary matrix elements are easily derived by considering a vacuum with a source term added,

$$|0_f\rangle_J=\eta_f\exp\left[-\frac{1}{2}\iint d\vec{x}\,d\vec{y}\;\phi(\vec{x})f(\vec{x}-\vec{y})\phi(\vec{y})+\int\phi(\vec{x})J(\vec{x})d\vec{x}\right]. \tag{3.8}$$

The scalar product of this state and the regular trial vacuum is

$$\langle 0_f|0_f\rangle_J=\eta_f^{\,2}\int d\phi\;e^{-\phi f\phi+J\phi}\,. \tag{3.9}$$

Here we have suppressed an understood summation over the indices $\vec{x}$, $\vec{y}$. Completing the square in (3.9) gives the result

$$\begin{aligned}\langle 0_f|0_f\rangle_J&=\exp\left[\tfrac{1}{4}\iint d\vec{x}\,d\vec{y}\,J(\vec{x})g(\vec{x}-\vec{y})J(\vec{y})\right]\\&=e^{JgJ/4}\,,\end{aligned} \tag{3.10}$$

where g is the functional matrix inverse of f,

$$gf=\int d\vec{z}\,g(\vec{x}-\vec{z})f(\vec{z}-\vec{y})\equiv\delta(\vec{x}-\vec{y})\,. \tag{3.11}$$

Taking functional derivatives of (3.9) with respect to J and using (3.10), we may easily derive useful matrix elements of ϕ between trial vacuum states. For example,

$$\begin{aligned}\langle 0_f|\phi(\vec{x})\phi(\vec{y})|0_f\rangle&=\left(\frac{\delta^2}{\delta J(\vec{x})\delta J(\vec{y})}\langle 0_f|0_f\rangle_J\right)\bigg|_{J=0}\\&=\left(\frac{\delta^2}{\delta J(\vec{x})\delta J(\vec{y})}e^{JgJ/4}\right)\bigg|_{J=0}\\&=\tfrac{1}{2}g(\vec{x}-\vec{y})\,.\end{aligned} \tag{3.12}$$

Proceeding similarly, we may find the matrix element $\langle 0_f|H|0_f\rangle=E[f]$. This we choose to express in terms of the Fourier component $f(\vec{p})$ of f, defined as follows:

$$f(\vec{x}-\vec{y})=f_{\mathrm{op}}(\vec{\nabla}_x)\delta(\vec{x}-\vec{y})\,, \tag{3.13}$$

$$f(\vec{p})\equiv f_{\mathrm{op}}(\vec{\nabla}_x)e^{-i\vec{p}\cdot\vec{x}}\big|_{x=0}\,. \tag{3.14}$$

For example, if $f_{\mathrm{op}}=(\mu^2-\nabla^2)^{1/2}$, then $f(\vec{p})=(\mu^2+\vec{p}^{\,2})^{1/2}=\omega_{\vec{p}}$. This has the advantage that the Fourier component of the functional matrix $g(\vec{x}-\vec{y})$ is simply $g(\vec{p})=1/f(\vec{p})$. In terms of $f(\vec{p})$, the energy is

$$E[f]=\langle 0_f|H|0_f\rangle=\left[\tfrac{1}{4}\int d\vec{p}\,f(\vec{p})\left(1+\frac{\omega_{\vec{p}}^{\,2}}{f(\vec{p})^2}\right)+\frac{3\lambda_0}{4(2\pi)^3}\left(\int\frac{d\vec{p}}{f(\vec{p})}\right)^2\right]\delta_p(\vec{0})\,. \tag{3.15}$$

The $\delta_p(\vec{0})=V/(2\pi)^3$ is simply a divergent constant proportional to the volume of space, as expected in the zero-point energy. We now vary E with respect to f to find the best trial vacuum:

$$\frac{\delta E[f]}{\delta f(\vec{q})}=\frac{1}{4}\left(1-\frac{\omega_{\vec{q}}^{\,2}}{f(\vec{q})^2}\right)-\frac{3\lambda_0}{2(2\pi)^3}\frac{1}{f(\vec{q})^2}\int\frac{d\vec{p}}{f(\vec{p})}=0\,, \tag{3.16}$$

$$f(\vec{q})^2=\omega_{\vec{q}}^{\,2}+\frac{6\lambda_0}{(2\pi)^3}\int\frac{d\vec{p}}{f(\vec{p})}\,. \tag{3.17}$$

First we naturally check the case $\lambda_0=0$ to see that we recover the free vacuum (3.3). In this case we have

$$f(\vec{q})^2=\omega_{\vec{q}}^{\,2}=\mu^2+\vec{q}^{\,2}, \tag{3.18}$$

$$f_{op}(\vec{\nabla}_x)=(\mu^2-\nabla_x^{\,2})^{1/2}, \tag{3.19}$$

$$f(\vec{x}-\vec{y})=(\mu^2-\nabla_x^{\,2})^{1/2}\delta(\vec{x}-\vec{y}). \tag{3.20}$$

Inserting this in the ansatz (3.6), we see that we do indeed recover the free vacuum wave functional.

If $\lambda_0\neq 0$, the result we find for f is surprisingly similar to the free case. The integral on the RHS of (3.17) is clearly just a constant depending on μ and λ_0, so we may write $f(\vec{q})$ as

$$f(\vec{q})^2=\vec{q}^{\,2}+\mu^2+\frac{6\lambda_0}{(2\pi)^3}\kappa(\lambda_0,\mu). \tag{3.21}$$

The two constant terms may be identified with a new mass m:

$$m^2=\mu^2+\frac{6\lambda_0}{(2\pi)^3}\int\frac{d\vec{p}}{(m^2+\vec{p}^{\,2})^{1/2}}. \tag{3.22}$$

The form of $f(\vec{q})$ tells us that the best trial vacuum solution of (3.2) of the general form (3.6) is simply the vacuum of a free theory with a new mass m, given by (3.22).

At this point, two questions occur to us regarding the results (3.21) and (3.22). First, we might ask whether or not the new mass parameter m which appears in the best trial vacuum wave functional is equal to the energy of a rest particle minus the vacuum energy. As m is merely a parameter in the vacuum state, this is not obviously the case. Second, we might wonder whether the mass renormalization (3.22) can be related to some approximation to the ϕ propagator in terms of keeping a certain class of Feynman diagrams. The answer to both these questions, as we shall show explicitly, is in the affirmative.

Taking the second question first, we ask what approximation to the propagator results from (3.22). An obvious step is to rewrite the momentum integral in four dimensions:

$$m^2=\mu^2+\frac{12i\lambda_0}{(2\pi)^4}\int\frac{d^4p}{p^2-m^2}. \tag{3.23}$$

One may show that this approximates the propagator as a free mass μ line corrected by bubbles of mass m attached sequentially along the μ line, or equivalently, as all possible growths of nonoverlapping bubbles of mass μ (Fig. 1). Thus, the Gaussian approximation to $\lambda_0\phi^4$ sums all diagrams without overlapping divergences in the propagator.

Now we treat the question of the physical particle mass. As in the quantum-mechanical problem, we find the one-particle state by acting on the vacuum with the adjoint of the vacuum annihilation operator

$$A_f^\dagger(\vec{p})=\frac{1}{[(2\pi)^3 2f(\vec{p})]^{1/2}}\times\int d\vec{x}\,e^{-i\vec{p}\cdot\vec{x}}\left(\int d\vec{y}\,f(\vec{x}-\vec{y})\phi(\vec{y})-\frac{\delta}{\delta\phi(\vec{x})}\right). \tag{3.24}$$

For the free theory one may show that this becomes the correct creation operator for a particle of mass μ, momentum $\vec{p}$. The normalization is chosen so that

$$[A_f(\vec{p}),A_f^\dagger(\vec{p}\,')]=\delta(\vec{p}-\vec{p}\,'). \tag{3.25}$$

The expectation value of H between two such one-particle states is easily shown to be

$$\begin{aligned}\frac{\langle\vec{p}_f^{\,\prime}|H|\vec{p}_f\rangle}{\langle\vec{p}_f^{\,\prime}|\vec{p}_f\rangle}&=\langle 0_f|A_f(\vec{p}\,')HA_f^\dagger(\vec{p})|0_f\rangle/\delta(\vec{p}-\vec{p}\,')\\&=\left\{\left[\tfrac{1}{4}\int d\vec{q}\,f(\vec{q})\left(1+\frac{\omega_{\vec{q}}^{\,2}}{f(\vec{q})^2}\right)+\frac{3\lambda_0}{4(2\pi)^3}\left(\int\frac{dq}{f(\vec{q})}\right)^2\right]\delta_p(\vec{0})+\left[\tfrac{1}{2}f(\vec{p})\left(1+\frac{\omega_{\vec{p}}^{\,2}}{f(\vec{p})^2}\right)+\frac{3\lambda_0}{(2\pi)^3 f(\vec{p})}\int\frac{d\vec{q}}{f(\vec{q})}\right]\right\}\frac{\delta(\vec{p}-\vec{p}\,')}{\delta(\vec{p}-\vec{p}\,')}.\end{aligned} \tag{3.26}$$

There are two contributions to the energy. The first is exactly the divergent vacuum energy we found previously, and the second is an additional contribution to the one-particle-state energy. Minimizing this expression gives the same function $f(\vec{p})$ we found in treating the vacuum problem (3.21) and (3.22). If we subtract off the vacuum energy and set $\vec{p}=\vec{p}\,'=\vec{0}$, the one-particle energy we find using the f of (3.21) is

$$\begin{aligned}E_1-E_0&=\tfrac{1}{2}m\left(1+\frac{\mu^2}{m^2}\right)+\frac{3\lambda_0}{(2\pi)^3 m}\int\frac{d\vec{q}}{(m^2+\vec{q}^{\,2})^{1/2}}\\&=\tfrac{1}{2}m\left(1+\frac{\mu^2}{m^2}\right)+\frac{m^2-\mu^2}{2m}=m.\end{aligned} \tag{3.27}$$

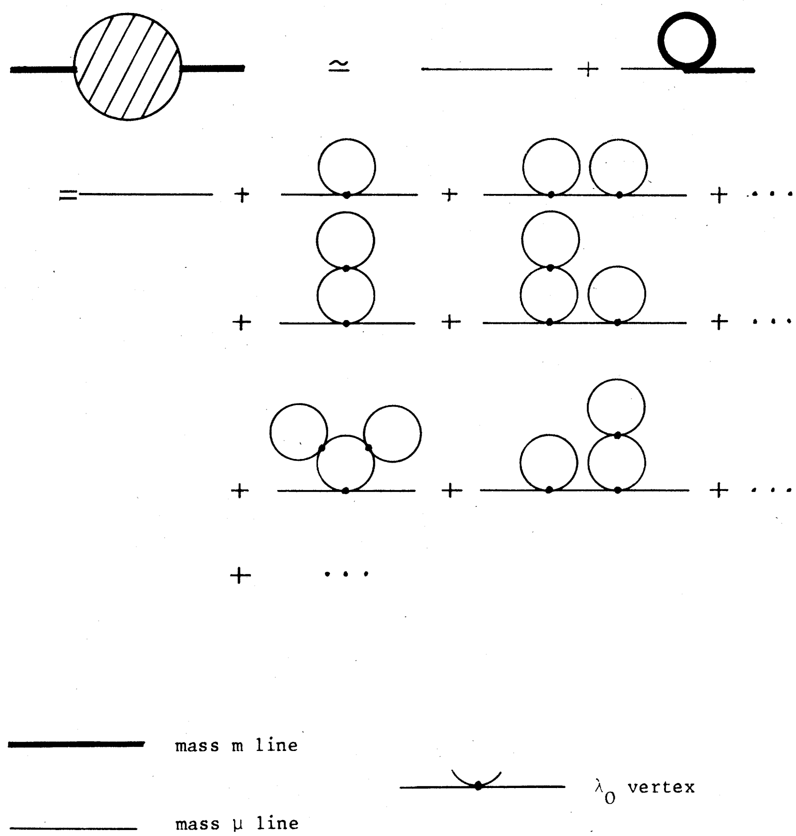

FIG. 1. Gaussian approximation to the two-point function in $\lambda_0\phi^4$ theory.

This shows that the variational one-particle mass is indeed the parameter m in the vacuum state. Note that a cancellation must occur between the contribution of the H_0 and $\lambda_0\phi^4$ terms in the Hamiltonian to bring this about. For a boosted state, we may also show that

$$E_1(\vec{p}) - E_0 = (m^2 + \vec{p}^{\,2})^{1/2}, \tag{3.28}$$

exactly as it should be.

Having constructed the variational vacuum and one-particle states, we naturally turn to the bound-state problem. First we look for a positroniumlike state of two quanta of the renormalized mass m,

$$|2\rangle = \int d\vec{p}\,\Sigma(\vec{p})\,|\vec{p}, -\vec{p}\rangle_m, \tag{3.29}$$

where $\Sigma(\vec{p})$ is the Fourier transform of the relative wave function of the two mass-m quanta. In terms of mass-μ quanta, this is no more a two-particle state that is the vacuum $|0\rangle_m$ a pure vacuum state. It is instead a superposition of 0, 2, 4, ... of the mass-μ quanta, chosen variationally to have the lowest energy. The energy of the trial state (3.29) is

$$\begin{aligned} E_2 &= \frac{\langle 2|H|2\rangle}{\langle 2|2\rangle} \\ &= E_0 + \frac{\int d\vec{p}\,2E_{\vec{p}}\Sigma(\vec{p})^2 + [3\lambda_0/(2\pi)^3][\int d\vec{p}\,\Sigma(\vec{p})/E_{\vec{p}}]^2}{\int d\vec{p}\,\Sigma(\vec{p})^2}\,. \end{aligned} \tag{3.30}$$

Here $E_{\vec{p}} \equiv (m^2 + \vec{p}^{\,2})^{1/2}$. We find the wave function $\Sigma(\vec{p})$ by varying the energy again, this time with respect to $\Sigma(\vec{p})$. We find an integral equation for $\Sigma(\vec{p})$

$$(E_{\vec{p}} - \tfrac{1}{2}m_2)\Sigma(\vec{p}) + \frac{3\lambda_0}{(2\pi)^3 2E_{\vec{p}}}\int \frac{d\vec{\kappa}\,\Sigma(\vec{\kappa})}{E_{\vec{\kappa}}} = 0\,. \tag{3.31}$$

The Lagrange multiplier m_2 is just the energy of the bound state above the vacuum $|0\rangle_m$. As this is an integral equation with a separable kernel, the solution is trivial:

$$\Sigma(\vec{p}) = \frac{c}{E_{\vec{p}}(E_{\vec{p}} - \frac{1}{2}m_2)}\,. \tag{3.32}$$

Resubstituting this result into (3.31) gives a relation between the bare coupling λ_0 and the energy of the bound state m_2. The integral in (3.31) diverges, so we introduce a cutoff $|\vec{\kappa}| = \Lambda$ in the momentum integral. The coupling λ_0 which allows a bound state of energy $m_2 = 2m\eta$ ($\eta < 1$) is

$$\lambda_0 = \frac{-8\pi^2/3}{\ln(\Lambda^2/m^2) + 2\ln 2 + (\pi/\eta)[1-(1-\eta^2)^{1/2}] - 2(1-\eta^2)^{1/2}\sin^{-1}(\eta)/\eta + O((\Lambda/m)^{-1})}\,. \tag{3.33}$$

This constraint on λ_0 has two objectionable features. Obviously λ_0 is negative, which leads us to suspect that there is no ground state at all for this value of λ_0. Another problem is that λ_0 goes to zero as the cutoff is removed in a fashion which is independent of the bound-state energy to the leading order in $\ln(\Lambda^2/m^2)$. This unusual constraint on λ_0, if we are to obtain a bound state, may be found in the literature; in particular, both the bound-state wave function (3.32) and the asymptotic part of the behavior of λ_0 were previously found in a similar fashion by Schiff.[1] One possible way out of the problems of λ_0 is to note that the bare coupling has no direct physical significance and could be anything; we only care about the renormalized, physically measurable λ. This is the point at which Schiff's early work becomes *ad hoc*, as his renormalization scheme is an arbitrary subtraction of the logarithmic divergence of λ_0^{-1}. Here we instead construct the effective potential for this model variationally, as we did for the quantum-mechanical problem in Sec. II. This allows us to derive the renormalized mass m and coupling constant λ in a unified fashion.

The effective potential $V(\phi_0)$ is the expectation value of the Hamiltonian in a normalized state $|\phi_0\rangle$ which has a constant expectation value of the field ϕ, $\langle\phi\rangle = \phi_0$, and for which $V(\phi_0)$ is a minimum:

$$V(\phi_0) = \min(\langle\phi_0|H|\phi_0\rangle)\,, \tag{3.34}$$

with

$$\langle\phi_0|\phi(\vec{x})|\phi_0\rangle = \phi_0\,, \tag{3.35}$$

$$\langle\phi_0|\phi_0\rangle = 1\,. \tag{3.36}$$

The value of this object is that it is the generating function of connected Green's functions with no external legs and zero external momenta, so that we can obtain two- and four-point functions directly from $V(\phi_0)$. As in the quantum-mechanical problem, we choose an ansatz for a set of states $\{|\boldsymbol{\phi_0}\rangle\}$ of which the previous vacuum ansatz (3.6) is a special case. Here we choose

$$|\phi_0\rangle_f = \eta_f \exp\left\{-\tfrac{1}{2}\iint d\vec{x}\,d\vec{y}[\phi(\vec{x})-\phi_0] \times f(\vec{x}-\vec{y};\phi_0)[\phi(\vec{y})-\phi_0]\right\}. \tag{3.37}$$

Once again, we calculate the expectation value of H for such a state and minimize $E[f,\phi_0]$ with respect to f, this time with ϕ_0 a nonzero constant. Again, we find that the optimal $f(\vec{x}-\vec{y};\phi_0)$ is the vacuum f [(3.20)] with a new mass, but this time the mass depends on the shift ϕ_0. Explicitly, we find

$$m^2(\phi_0) = \mu^2 + 12\lambda_0\phi_0^2 + 6\lambda_0 G(\phi_0)\,, \tag{3.38}$$

where the divergent constant $G(\phi_0)$ is defined by

$$G(\phi_0) \equiv \frac{1}{(2\pi)^3}\int \frac{d\vec{\kappa}}{[\vec{\kappa}^2 + \mu^2 + 12\lambda_0\phi_0^2 + 6\lambda_0 G(\phi_0)]^{1/2}} \tag{3.39}$$

$$= \frac{1}{(2\pi)^3}\int \frac{d\vec{\kappa}}{[\vec{\kappa}^2 + m(\phi_0)^2]^{1/2}}\,. \tag{3.40}$$

The results (3.38) may be understood as the same sum of diagrams we found previously for $m^2(\phi_0 = 0)$ with the additional complication that the bare mass is shifted from μ^2 to $\mu^2 + 12\lambda_0\phi_0^2$ by the vacuum expectation value of ϕ^2 in the interaction term $\lambda_0\phi^4$.

Having found the function $f(\vec{x}-\vec{y};\phi_0)$, we may resubstitute it in (3.34) to obtain $V(\phi_0)$. The result is

$$V(\phi_0) = \tfrac{1}{2}\mu^2\phi_0^2 + \lambda_0\phi_0^4 + \tfrac{1}{2}F(\phi_0) - \frac{3\lambda_0}{4}G(\phi_0)^2 \tag{3.41}$$

and the new function $F(\phi_0)$ we have introduced is defined by

$$F(\phi_0) \equiv \frac{1}{(2\pi)^3}\int d\vec{\kappa}[\vec{\kappa}^2 + m(\phi_0)^2]^{1/2}\,. \tag{3.42}$$

To get as far as the four-point function, we need here the expansion of $V(\phi_0)$ only to ϕ_0^4. This is easily carried out, and the mass and coupling constant we find are

$$m^2 = \frac{d^2V}{d\phi_0^2}\bigg|_{\min} = \frac{d^2V}{d\phi_0^2}\bigg|_{\phi_0=0} = \mu^2 + 6\lambda_0 G(\phi_0 = 0)\,, \tag{3.43}$$

$$\lambda = \frac{1}{4!}\frac{d^4V}{d\phi_0^4}\bigg|_{\min} = \frac{1}{4!}\frac{d^4V}{d\phi_0^4}\bigg|_{\phi_0=0} = \lambda_0\frac{1-6\lambda_0 I(m)}{1+3\lambda_0 I(m)}\,, \tag{3.44}$$

where

$$I(m) = \frac{1}{(2\pi)^3}\int \frac{d\vec{\kappa}}{[\vec{\kappa}^2 + m^2]^{3/2}}\,. \tag{3.45}$$

The derivatives are evaluated at the value ϕ_0 takes on in the physical vacuum state, determined by

$$\frac{dV}{d\phi_0}\bigg|_{\text{vac}} = 0\,. \tag{3.46}$$

This is easily seen to be $\phi_0 = 0$. The mass we obtain from this effective potential (3.43) is identical to the mass we found previously in minimizing the energy of the unshifted vacuum (3.22). The renormalized coupling λ is new and may be compared with the expression which we obtained in treating the $\lambda_0 x^4$ problem (2.16). It should not come as a surprise that this value of λ is obtained by approximating the four-point function with zero external momenta by the set of graphs in Fig. 2. We have no explanation as to why this particular set of diagrams should be summed by the Gaussian ansatz, although one interesting observation is that these are the same sets of diagrams one sums to leading order in the $1/N$ expansion[8] in models with N internal degrees of freedom for the scalar field.[9,10] Some of the results familiar from the study of these models, such as the existence of a bound state for negative λ_0 and the cutoff behavior $\lambda_0 \sim C \ln(\Lambda^2/m^2)^{-1}$ (Ref. 9), are clearly due to the close relation of the two approximations. We suspect that one learns more about why the $1/N$ expansion is summable to leading order (it leads to a trivial Gaussian vacuum wave functional) from this correspondence than one learns about why this set of diagrams arises from the Gaussian wave functional.

Returning to the renormalization of the coupling constant λ_0, we note that the restriction to zero external momenta in the four-point function is not a problem in the massive ϕ theory, and the renormalization group can be used to determine values of λ at other values of these momenta. Had we been treating a massless ϕ theory we would have a problem here, as the $p_i = 0$ point is a stable fixed point for this theory and the renormalized coupling λ is zero there. For the massive case we expect this λ to be a nonzero constant.[11]

The relation between λ and λ_0 found from the effective potential (3.44) allows us to determine the renormalized λ which produces the bound state (3.32) of energy $m_2 = 2m\eta$. Inserting the expression (3.33) in (3.44) and defining $I(m)$ with the same ultraviolet cutoff $\vec{k}^2 = \Lambda^2$ used for λ_0, we find

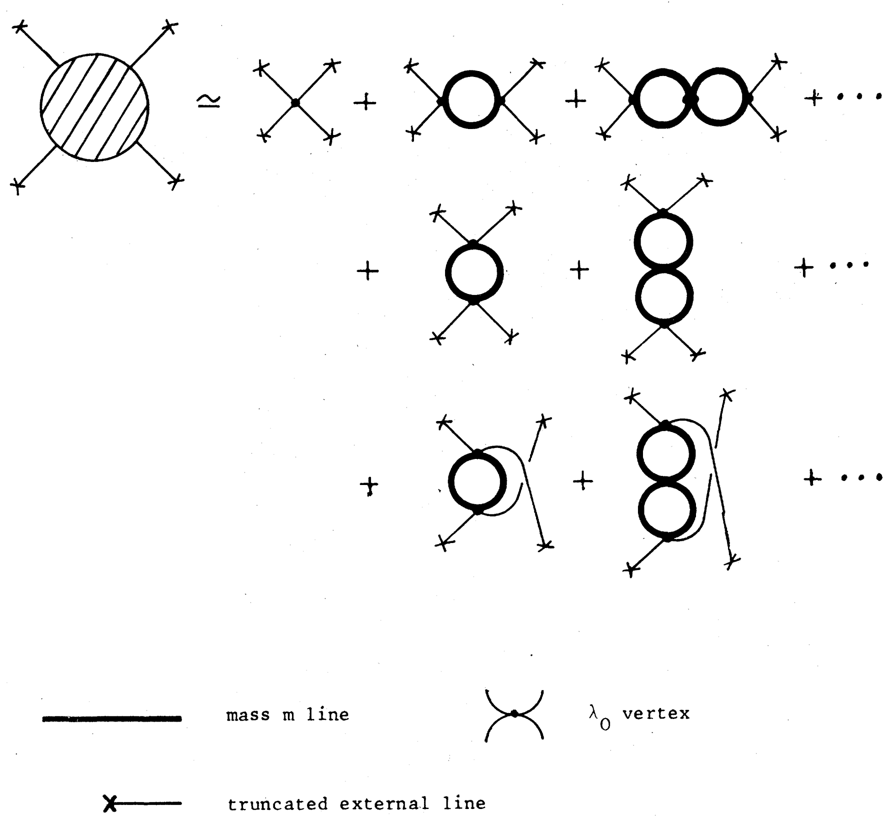

FIG. 2. Gaussian approximation to the four-point function in $\lambda_0\phi^4$ theory. (All mass-m lines have the expansion of Fig. 1 in terms of the bare mass μ.)

$$\lambda = \frac{40\pi^2}{3\ln(\Lambda^2/m^2)} + O(\ln(\Lambda^2/m^2)^{-2})\,. \qquad (3.47)$$

This λ is positive, unlike λ_0, which avoids the problem of the existence of the vacuum alluded to earlier. However, as the cutoff Λ goes to infinity, the renormalized λ goes to zero, which is contrary to our expectations. Although we have no explanation for this result, we note that it depends critically on the bound-state wave function (3.32). For example, if this were changed so that λ_0 behaved as

$$\lambda_0 = \frac{-4\pi^2/3}{\ln(\Lambda^2/m^2) + f(\eta)}\,, \qquad (3.48)$$

we would have a cancellation of the logarithms when we calculated λ, leaving λ a finite function of the bound-state energy $m_2 = 2m\eta$. Consequently, we suggest that the surprising and unphysical result (3.47) is an artifact of the overly simplified ansatz (3.6) we originally chose for the vacuum. It would be instructive to improve this vacuum ansatz by the inclusion of more functional parameters and to observe the effect on the bound-state spectrum and the renormalized coupling constant λ. Owing to the mathematical complexity of the task, we do not consider it at this time.

An interesting point is that the behavior of the renormalized coupling λ bears some resemblance to the behavior of the one-loop renormalization-group-improved four-point function in massless $\lambda_0\phi^4$ theory. Starting from the Callan-Symanzik equation

$$\left[\mu\frac{\partial}{\partial\mu} + \beta(\lambda)\frac{\partial}{\partial\lambda} + n\gamma(\lambda)\right]\Gamma^{(n)} = 0\,, \qquad (3.49)$$

and approximating the two- and four-point proper vertex functions by the one-loop results (Fig. 3),

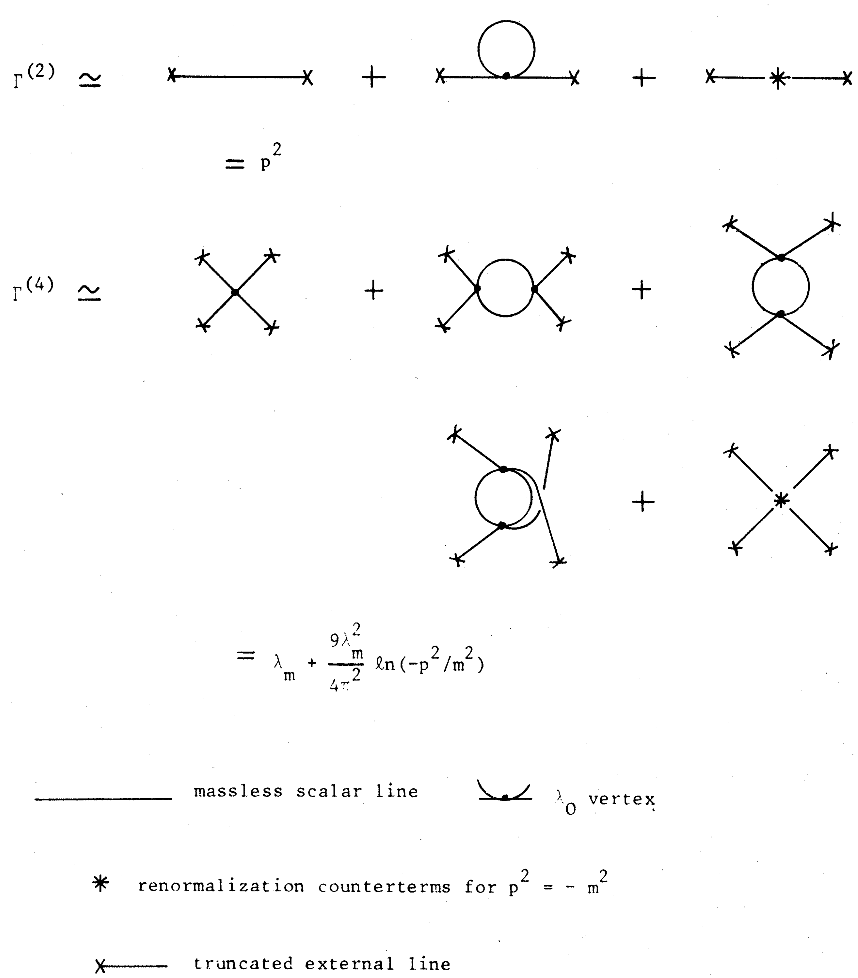

FIG. 3. One-loop approximation to $\lambda_0\phi^4$ vertex functions.

we may derive the β and γ functions to this order as

$$\beta(\lambda)=\frac{9}{2\pi^2}\lambda^2\,,\quad \gamma(\lambda)=0\,. \tag{3.50}$$

If the four-point vertex function has been renormalized to $\lambda(\mu_0)$ at some Euclidean momenta $p^2=-\mu_0^2$, $p_i\cdot p_j=-\frac{1}{3}\mu_0^2$, $i\neq j$, the renormalization-group-improved four-point vertex at a different p^2 is given by

$$\Gamma^{(4)}(p^2)=\frac{\lambda(\mu_0)}{1-[9\lambda(\mu_0)/4\pi^2]\ln(-p^2/\mu_0^2)}\,. \tag{3.51}$$

As this theory is asymptotically free in the infrared, we may smoothly take the limit $-p^2\to 0_+$, starting from some small but finite $\lambda(\mu_0)$ at $-p^2=\mu_0^2$. For $|-p^2|\ll\mu_0^2$, we find

$$\Gamma^{(4)}(|-p^2|\ll\mu_0^2)=-\frac{4\pi^2}{9\ln(-p^2/\mu_0^2)}-\frac{16\pi^4}{81\lambda(\mu_0)\ln^2(-p^2/\mu_0^2)}+\cdots\,. \tag{3.52}$$

The leading asymptotic approach to the infrared point with $\Gamma^{(4)}=0$ is independent of the value of $\lambda(\mu_0)$ at the renormalization point; to see the initial value of $\lambda(\mu_0)$, we have to go to next order in the asymptotic form. The similarity of (3.47) and (3.52) is suggestive, but not particularly useful, as we are comparing two different functions [cutoff and renormalized $\Gamma^{(4)}$] for two different theories (massless and massive $\lambda\phi^4$). Ideally, we should like to variationally calculate $\Gamma^{(4)}(p^2)$ [(3.51)]. This exercise obviously requires a variational treatment of the effective action, which we shall consider in an upcoming paper.

IV. A FERMI-BOSE COUPLED FIELD THEORY

The really interesting problems in nature involve field theories with Fermi and Bose fields interacting. To treat the solutions of such theories variationally, we must introduce wave functionals of classical Fermi fields,[4] just as we have used wave functionals of a classical Bose field to treat a scalar field theory. These classical anticommuting Fermi fields, otherwise known as Grassmann fields, have a number of important mathematical properties which may be unfamiliar to many physicists. Consequently, we have given some of their more important properties, together with properties of the wave functionals of the free Dirac theory, in the Appendix. Other useful properties of these objects may be found in the literature.[12]

The particular model we shall treat is a scalar interacting with a Dirac spinor through a Yukawa coupling:

$$\mathcal{L}=\bar{\psi}(i\not{\partial}-m_0)\psi+\tfrac{1}{2}[(\partial_\mu\phi)^2-\mu_0^2\phi^2]-g_0\bar{\psi}\psi\phi\,. \tag{4.1}$$

The functional Hamiltonian for this model is easily obtained using results derived elsewhere[4]:

$$H=\int d\vec{x}\left(-\frac{1}{2}\frac{\delta^2}{\delta\phi(\vec{x})^2}+\tfrac{1}{2}|\vec{\nabla}\phi(\vec{x})|^2+\tfrac{1}{2}\mu_0^2\phi(\vec{x})^2 - [-i\vec{\alpha}\cdot\vec{\nabla}+\beta m_0+\beta g_0(\phi(\vec{x}))]_{ab}\psi_b(\vec{x})\frac{\delta}{\delta\psi_a(\vec{x})}\right). \tag{4.2}$$

Next, we need an ansatz for the vacuum state. We choose a wave functional in which the Fermi and Bose variables are separated as a simple first-trial vacuum and we use the familiar Gaussian (3.6) for the Bose part:

$$|0\rangle=\eta_f\exp\left[-\tfrac{1}{2}\iint d\vec{x}\,d\vec{y}\,\phi(\vec{x})\times f(\vec{x}-\vec{y})\phi(\vec{y})\right]\Omega_0[\psi]\,. \tag{4.3}$$

The Fermi wave functional is not so easy to generalize, as the free Fermi vacuum is a δ functional rather than a Gaussian.[4] However, we shall proceed by taking a cue from the result found throughout the last section, and assume that the Fermi vacuum is a true vacuum with the mass m left as a free parameter:

$$\Omega_0[\psi]=\delta[\psi_+]_m\,. \tag{4.4}$$

Calculating $f(\vec{x}-\vec{y})$ variationally as previously, we find

$$f(\vec{x}-\vec{y})=(\mu_0^2-\nabla_x^2)^{1/2}\delta(\vec{x}-\vec{y})\,, \tag{4.5}$$

which seems to indicate that there is no mass renormalization of the ϕ quanta, an obviously invalid result. When we consider the effective potential, however, we shall see that reading the ϕ mass naively from (4.5) is wrong. This is the first place we have required the effective potential to obtain the mass renormalization; in all previous cases it could be read directly from the analog of (4.5). Shifting the scalar field in (4.3) by a constant ϕ_0, and minimizing the energy $E[f,\phi_0]$, we again obtain (4.5) and the effective potential becomes

$$V(\phi_0)=\tfrac{1}{2}\int\frac{d\vec{k}}{(2\pi)^3}(\vec{k}^2+\mu_0^2)^{1/2}+\tfrac{1}{2}\mu_0\phi_0^2 - 2\int\frac{d\vec{k}}{(2\pi)^3}\left((\vec{k}^2+m^2)^{1/2}+\frac{(m_0+g_0\phi_0-m)m}{(\vec{k}^2+m^2)^{1/2}}\right). \tag{4.6}$$

The unfamiliar second integral is the expectation value of the Fermi and interaction parts of the energy in the Fermi vacuum state with an undetermined mass m. Minimizing with respect to the parameter m gives

$$\frac{\partial V(\phi_0)}{\partial m} = -2\int \frac{d\vec{\kappa}}{(2\pi)^3}\,\frac{\vec{\kappa}^2}{(\vec{\kappa}^2+m^2)^{3/2}}\,(m_0+g_0\phi_0-m) = 0\,, \tag{4.7}$$

so the renormalized mass $m(\phi_0)$ is

$$m(\phi_0) = m_0 + g_0\phi_0\,. \tag{4.8}$$

With this optimum mass, the effective potential becomes

$$V(\phi_0) = \int \frac{d\vec{\kappa}}{(2\pi)^3}\Big\{\tfrac{1}{2}(\vec{\kappa}^2+\mu_0^2)^{1/2} - 2[\vec{\kappa}^2+(m_0+g_0\phi_0)^2]^{1/2}\Big\} + \tfrac{1}{2}\mu_0^2\phi_0^2\,. \tag{4.9}$$

The new feature here is that ϕ has a nonzero vacuum expectation value in the physical vacuum. This expectation value we find as usual by imposing the condition

$$\frac{dV(\phi_0)}{d\phi_0}\bigg|_{\text{physical vacuum}} = 0\,, \tag{4.10}$$

which leads to a value of ϕ_0 given by

$$\phi_0 = \frac{2g_0}{\mu_0^2}(m_0+g_0\phi_0)\int \frac{d\vec{\kappa}}{(2\pi)^3[\vec{\kappa}^2+(m_0+g_0\phi_0)^2]^{1/2}} = \phi_{\text{vac}}\,. \tag{4.11}$$

Since ϕ_0 has a vacuum expectation value, there is a fermion mass renormalization, given by (4.8). Explicitly,

$$m = m_0 - \frac{4ig_0^2 m}{\mu_0^2}\int \frac{d^4\kappa}{(2\pi)^4(\kappa^2-m^2)}\,. \tag{4.12}$$

Diagrammatically, this corresponds to approximating the fermion propagator as the sum of all tadpole attachments with no overlapping divergences (Fig. 4).

The ϕ two-point function we find as usual from the effective potential,

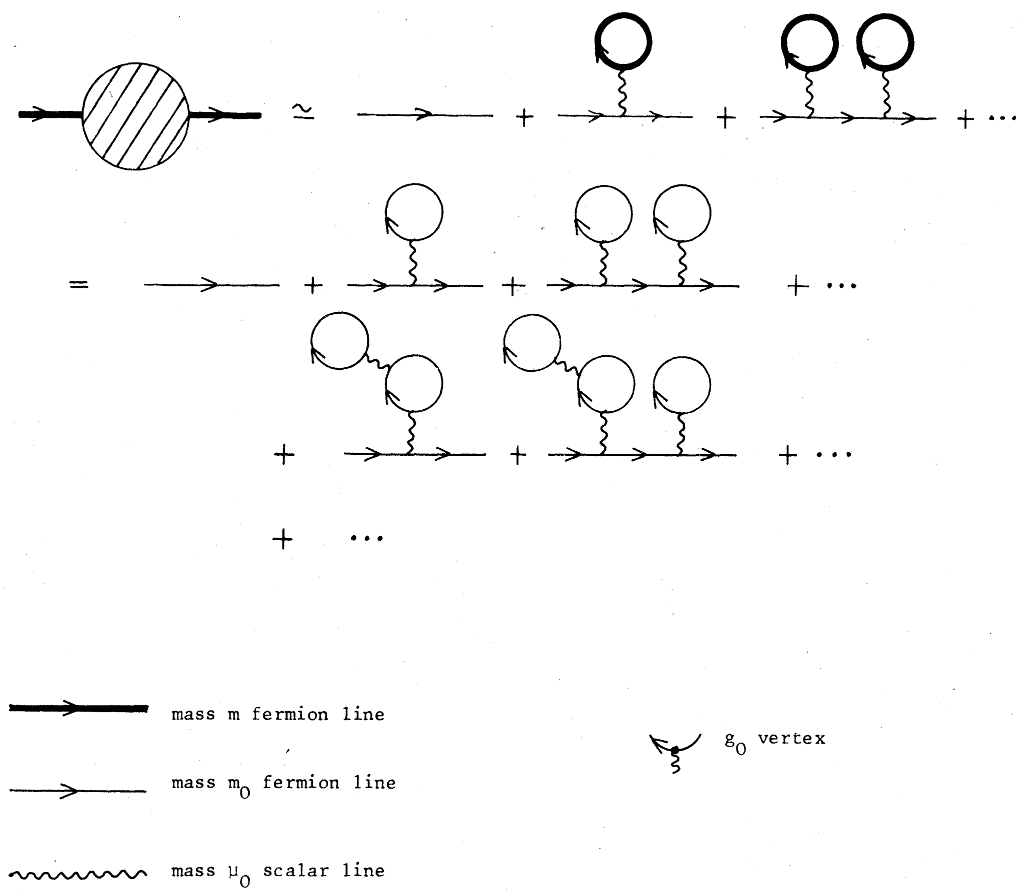

FIG. 4. Variational approximation to the fermion propagator in the Yukawa model $g_0\bar{\psi}\psi\,\phi$.

$$-\Delta_\phi(0)^{-1} = \left.\frac{d^2V}{d\phi_0{}^2}\right|_{\phi_0=\phi_{\text{vac}}}$$
$$= \mu_0{}^2 - 2g_0{}^2 \int \frac{d\vec{\kappa}}{(2\pi)^3} \frac{\vec{\kappa}^2}{(\vec{\kappa}^2 + m^2)^{3/2}}, \qquad (4.13)$$

which is an approximation to the propagator resulting from the insertion of all nonoverlapping bubbles in the ϕ propagator (Fig. 5). This is not, however, the mass of the ϕ quanta with respect to the vacuum, as there is a wave-function renormalization in the ϕ propagator which we have not disentangled from the mass renormalization. (See the comments in this regard in Sec. V.) The actual ϕ mass may be obtained either by a variational calculation of the one-particle state, or through the use of the effective action, as we shall discuss later.

As a final comment on these mass shifts, we note that the fermion mass may be derived from a generalized effective potential $V(\phi_0, \psi_0)$, in which the spinor field ψ is given a constant spinor expectation value ψ_0. This $V(\phi_0, \psi_0)$ is derived using shifted Fermi vacuum states in the trial wave functional of the form

$$\Omega[\psi] = \delta[(\psi - \psi_0)_+]_m, \qquad (4.14)$$

and for this model turns out to be

$$V(\phi_0, \psi_0) = V(\phi_0) + (m_0 + g_0\phi_0)\bar{\psi}_0\psi_0. \qquad (4.15)$$

Clearly, the fermion mass matrix is

$$m^{ab} = \left.\frac{d^2V(\phi_0, \psi_0)}{d\psi_0^b d\bar{\psi}_0^a}\right|_{\psi_0=\bar{\psi}_0=0}$$
$$= (m_0 + g_0\phi_0)\delta^{ab} = m\delta^{ab}. \qquad (4.16)$$

Higher pure Fermi n-point functions with zero external momenta vanish in this approximation.

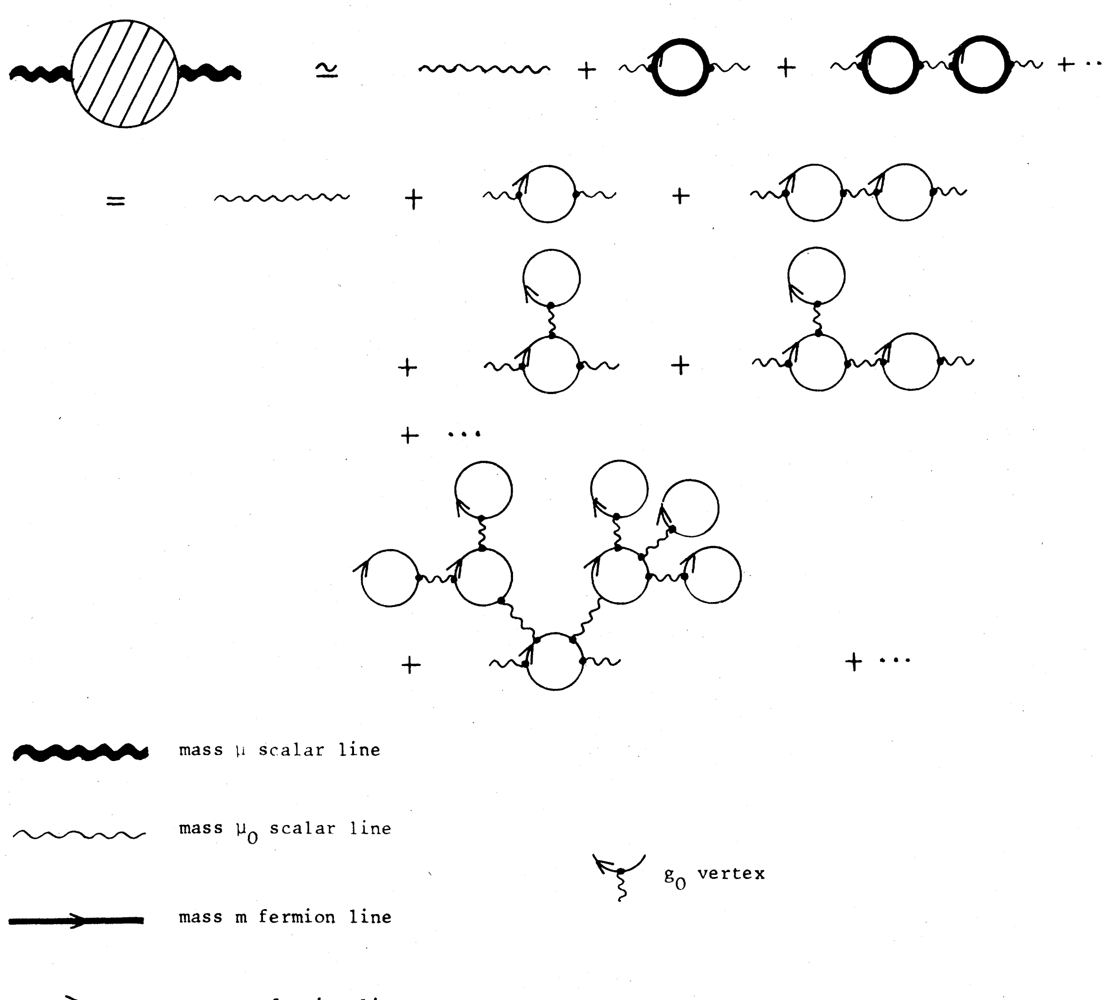

FIG. 5. Variational approximation to the boson propagator in $g_0\bar{\psi}\psi\phi$.

We may also see from $V(\phi_0, \psi_0)$ that the Yukawa coupling constant g_0 is not renormalized here.

At this point we could proceed to search for bound states of various types ($|\phi\phi\rangle$, $|\psi\bar{\psi}\rangle$, $|\psi\psi\rangle$, ...) in the model, and perhaps compare them with results obtained from potential problems describing the exchange of relevant quanta. We might also learn something about the strange behavior of λ in the $\lambda\phi^4$ problem by finding the constraints imposed on the coupling constant g_0 by the bound states. These are very interesting problems which undoubtedly deserve further attention. However, the much more relevant exercise of a variational calculation of the vacuum and bound-state wave functionals of a Fermi-Bose gauge theory is also possible using this formalism, and it is this topic which we shall introduce in the next section.

V. QED, QCD, THE EFFECTIVE ACTION, AND MORE THEORY

There is no obvious reason why the methods used here to approximate the vacuum and bound-state spectrum cannot be applied to QED. The real problem is that the trial wave functionals used in the Yukawa model are found to be a bad approximation for QED. For example, consider the diagrams we sum to give the fermion propagator (Fig. 4). In QED all the corrections are identically zero. The same is true in QCD. The photon propagator does slightly better, being the sum of all in-line chains of e^+e^- loops, but there is simply no mass renormalization in either case. What is needed for QED is an ansatz for the vacuum functional which sums relevant diagrams, i.e., mixed Fermi-Bose and overlapping divergences. The search for such an ansatz is currently underway.

To treat QCD, we are faced with the problem of infrared divergences in boson n-point functions which make the effective potential an awkward object to use in renormalization. We can get around this problem by developing a variational treatment of the effective action, i.e., the generating functional of connected n-point functions with arbitrary external momenta. This necessary formal development is also currently under consideration.

Finally, we note that the effective action is actually necessary to do the renormalization calculations presented in the text of the paper, and we have only been able to use the effective potential through a fortunate coincidence. In general, we expect a renormalized propagator (for example) to have the form

$$\Delta(p^2) = \frac{Z(p^2)}{p^2 - m^2},$$

where $Z(p^2)$ is the wave-function renormalization. At zero external momenta, this is

$$\Delta(0) = -Z(0)/m^2 .$$

The quantity we calculate from the effective potential is[7]

$$\left.\frac{d^2V(\phi_0)}{d\phi_0^{\,2}}\right|_{\phi_0=\phi_{\text{vac}}} = -\Delta(0)^{-1} = \frac{m^2}{Z(0)}.$$

So the mass and wave function renormalizations are inextricably mixed in the effective potential. Fortunately, the wave-function renormalization constant $Z(p^2)$ due to tadpole attachments, such as we have often encountered, is unity; we do indeed recover the renormalized mass in this special case. To separate out the $Z(p^2)$ part of the propagator generally, we require the effective action.

One development of the understanding of the variational approach which would be very valuable is to establish the connection between the wave-functional ansatz and the Feynman diagrams summed in renormalization. Although we have shown the connection for the special cases considered, we have no such general understanding. This kind of insight clearly would be an important guide in the selection of a trial wave functional for a given theory.

ACKNOWLEDGMENTS

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APPENDIX

In this appendix we briefly review some of the properties of Grassmann functions and functionals which are employed in the text. Grassmann functions are anticommuting c numbers whose properties under integration and differentiation are summarized by

$$\{\psi^a(\vec{x}), \psi^b(\vec{y})\} = 0 , \tag{A1}$$

$$\left\{\frac{\delta}{\delta\psi^a(\vec{x})}, \psi^b(\vec{y})\right\} = \delta^{ab}\delta(\vec{x}-\vec{y}) , \tag{A2}$$

$$\int d\psi^a(\vec{x}) = 0\,, \tag{A3}$$

$$\int \psi^a(\vec{x})d\psi^b(\vec{y}) = \delta^{ab}\delta(\vec{x}-\vec{y})\,. \tag{A4}$$

The Grassmann δ functional is a frequently encountered object

$$\delta[\psi] = \prod_a \prod_x \psi^a(\vec{x}) \tag{A5}$$

which satisfies the definition

$$\int f(\psi^a(\vec{x}))\delta[\psi-\chi]D\vec{\psi} \equiv f(\chi^a(\vec{x}))\,. \tag{A6}$$

The measure $D\psi$ is

$$D\psi = \prod_b \prod_y d\psi^b(\vec{y})\,. \tag{A7}$$

Notice that one must use care in defining the ordering of factors in the measure and in the δ functional; once a convention is chosen it must be adhered to rigorously.

A useful integral representation of the δ functional is

$$\delta[\psi] = \int \exp\left[\sum_a \int d\vec{x}\,\eta^a(\vec{x})\psi^a(\vec{x})\right]D\eta\,, \tag{A8}$$

where η is also a Grassmann variable.

Fermi state vectors may be easily represented as functionals of Grassmann variables. First, the functional Hamiltonian is obtained from the classical field theory Hamiltonian by the substitution $\pi_\psi \to i\delta/\delta\psi$ (Ref. 4);

$$H = \int d\vec{x}[-i\pi_a(\vec{x})(-i\vec{\alpha}\cdot\vec{\nabla}+\beta m)_{ab}\psi_b(\vec{x})]$$

$$= -\int d\vec{x}(-i\vec{\alpha}\cdot\vec{\nabla}+\beta m)_{ab}\psi_b(\vec{x})\frac{\delta}{\delta\psi_a(\vec{x})}\,. \tag{A9}$$

This operator becomes more transparent when exhibited in momentum space, with Grassmann momentum-space components $a_{\vec{\kappa}\lambda}$ defined by

$$\psi^a(\vec{x}) = \sum_{\lambda=1}^{4} \int d\vec{\kappa}\left[\frac{m}{(2\pi)^3\omega_{\vec{\kappa}}}\right]^{1/2} a_{\vec{\kappa}\lambda} w^a_{\vec{\kappa}\lambda} e^{i\vec{\kappa}\cdot\vec{x}}\,. \tag{A10}$$

The spinor $w_{\vec{\kappa}\lambda}$ is related to the Bjorken and Drell spinors $w^{\rm BJD}_{\vec{\kappa},\lambda}$ (Ref. 13) by $w_{\vec{\kappa},\lambda} = w^{\rm BJD}_{\epsilon_\lambda\vec{\kappa},\lambda}$. In terms of the $\{a_{\vec{\kappa}\lambda}\}$ the Hamiltonian is

$$H = \sum_{\lambda=1}^{4} \int d\vec{\kappa}\left(-\epsilon_\lambda \omega_{\vec{\kappa}} a_{\vec{\kappa}\lambda}\frac{\delta}{\delta a_{\vec{\kappa}\lambda}}\right). \tag{A11}$$

By inspection, the lowest energy eigenstate of (A11) is

$$\Omega_0[\psi] = \prod_{\lambda=1}^{2}\prod_{\vec{\kappa}} a_{\vec{\kappa}\lambda} = \prod_{\lambda=1}^{2}\delta[a_\lambda] \equiv \delta[\psi_+]\,, \tag{A12}$$

where the ψ_+ refers to the positive-energy $(\lambda = 1, 2)$ part of ψ. In going from the infinite product to the δ functional we have used the Grassmann identity (A5).

The adjoint vacuum functional is easily seen to be

$$\Omega_0^\dagger[\psi] = \prod_{\lambda=3}^{4}\prod_{\vec{\kappa}} a_{\vec{\kappa}\lambda} \equiv \delta[\psi_-]\,, \tag{A13}$$

so that we satisfy

$$\int \Omega_0^\dagger[\psi]\Omega_0[\psi]D\psi = 1\,. \tag{A14}$$

The correct fermion zero-point energy arises from the action of H on $\Omega_0[\psi]$.

To construct excited states of the free theory, one may use the functional analogs of the electron (b) and positron (d) creation and annihilation operators (the d operators given in Ref. 4 are incorrect);

$$b^\dagger_{\vec{\kappa},\uparrow} = \frac{\delta}{\delta a_{\vec{\kappa},1}}\,,\quad b_{\vec{\kappa},\uparrow} = a_{\vec{\kappa},1}\,,$$

$$b^\dagger_{\vec{\kappa},\downarrow} = \frac{\delta}{\delta a_{\vec{\kappa},2}}\,,\quad b_{\vec{\kappa},\downarrow} = a_{\vec{\kappa},2}\,, \tag{A15}$$

$$d^\dagger_{\vec{\kappa},\uparrow} = a_{-\vec{\kappa},4}\,,\quad d_{\vec{\kappa},\uparrow} = \frac{\delta}{\delta a_{-\vec{\kappa},4}}\,,$$

$$d^\dagger_{\vec{\kappa},\downarrow} = -a_{-\vec{\kappa},3}\,,\quad d_{\vec{\kappa},\downarrow} = \frac{-\delta}{\delta a_{-\vec{\kappa},3}}\,. \tag{A16}$$

It is straightforward to show that the matrix elements obtained from this functional description are identical to the matrix elements obtained using the more familiar second-quantized field and state-vector description of fermions. Thus, the two descriptions are completely equivalent.

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