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Numerical Methods in Calculating Boson and Fermion Loop Corrections

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We present accurate numerical methods for calculating the one boson and the one fermion loop energy in a static, spherically symmetric background field for a simple theory of fermions interacting with bosons through Yukawa coupling. Various FORTRAN codes have been developed and tested for the calculations. The methods presented here should be useful in general problems involving one loop quantum corrections, and in other problems where one needs to calculate the Green's function for a particle moving in a background field.

I. INTRODUCTION

The calculation of loop corrections in strong-coupling Fermi–Bose field theories requires extreme accuracy. We have developed precision methods for such purposes and have applied them, as a special case, to the Friedberg–Lee nontopological soliton model [1].

One-loop corrections to the energy require summing the negative energy states of the (deformed) Dirac sea and the normal mode energies of the Bose field. The energies for the non-interacting field must be subtracted, and further subtractions which yield renormalization of the coupling constants are required to obtain physical results. These subtractions of large quantities to obtain small remainders require extreme precision; subtraction of analytic from numerical quantities should be avoided. Subtraction of numerical from numerical quantities are best done for quantities calculated with the same algorithm.

The methods presented here involve the construction of Fermi and Bose Green's functions for imaginary energy. Energy sums are executed by a contour integration

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along the imaginary axis. Other properties of the system can be evaluated from appropriate integrations of the Green's functions thus obtained.

The general methods for calculating loop corrections using Green's functions evaluated along the imaginary energy axis are well known [2, 8]. The present work contains novel methods which, the authors believe, yield high accuracy and efficiency and therefore may be of considerable value to practitioners in the field.

In the following, we divide our discussions into four sections. In Section II, we use the Friedberg–Lee soliton model as an example to introduce the general formalism. In Section III, we discuss how to calculate the full boson and fermion Green's functions. In Section IV, we discuss how to evaluate the boson and fermion renormalization subtractions. Finally in Section V, we present some sample results.

II. The Friedberg–Lee Model as an Example

The Friedberg–Lee non-topological soliton model is an example of a system of (strongly) interacting massless Fermi and non-linear Bose fields. For the present paper, we ignore the gluon field (which is actually at the crux of color confinement). The Lagrangian is given by

$$\mathscr{L} = \tfrac{1}{2}(\partial_\mu \phi)^2 - U(\phi) + \bar{\psi}(i\partial\!\!\!/ - g\phi)\psi + \text{counterterms}, \tag{2.1}$$

where

$$U(\phi) = \frac{a}{2!}\phi^2 + \frac{b}{3!}\phi^3 + \frac{c}{4!}\phi^4 + B. \tag{2.2}$$

The self-energy term $U(\phi)$ is chosen to terminate in fourth order for renormalizability, even though the ϕ-field is to be regarded as an effective one, and loop corrections may not be appropriate. Here we utilize quantum corrections in this model as a test of the methods.

The one-loop correction to the energy is given by

$$E = \sum_i (n_i \varepsilon_i - n_{0i}\varepsilon_{0i}) + \tfrac{1}{2}\sum_j (h_j - h_{0j}), \tag{2.3}$$

where ε_{0i}, ε_i, h_{0j}, and h_j are defined below. The first sum is the fermion energy. The occupation number n_i is taken to be 0 or 1, to allow for the presence of valence quarks; for the vacuum, $n_{0i} = 1$ if $\varepsilon_{0i} < 0$ and $n_{0i} = 0$ if $\varepsilon_{0i} > 0$. The second sum is the zero-point energy of the Bose field. Written in this form the energy still contains infinities which, however, depend on ϕ, in the same form as the original Lagrangian and are canceled by the counterterms.

Let $\phi_c = \langle \phi \rangle$, which is assumed to be time-independent and spherically

symmetric throughout this paper. The fermion energies, ε_i, are determined by the Dirac equation

$$(-i\alpha\cdot\nabla+\beta g\phi_c)\,\psi_i=\varepsilon_i\psi_i, \tag{2.4}$$

and the Bose eigenvalues satisfy

$$(-\nabla^2+W(\phi_c))\,\phi_j=h_j^2\phi_j, \tag{2.5}$$

where $W(\phi_c)=d^2U/d\phi_c^2$. The corresponding Green's functions satisfy

$$(\nabla^2+\omega^2-W(\phi_c))\,D(\omega,\mathbf{r},\mathbf{r}')=\delta^3(\mathbf{r}-\mathbf{r}'), \tag{2.6}$$

$$(i\alpha\cdot\nabla+\omega-\beta g\phi_c(r))\,\gamma_0 S(\omega,\mathbf{r},\mathbf{r}')=\delta^3(\mathbf{r}-\mathbf{r}'). \tag{2.7}$$

The corresponding free Green's functions satisfy the same equations with the replacement of W and ϕ_c by W_0 and ϕ_0, where ϕ_0 is the minimum of $U(\phi)$ and $W_0=W(\phi_0)$. The fermion energy can also be expressed as

$$\frac{1}{2\pi i}\int_C \omega\,d\omega\,\mathrm{Tr}\,\gamma^0 S(\omega,\mathbf{r},\mathbf{r}) \tag{2.8}$$

and the boson energy as

$$-\frac{1}{2\pi i}\int_C \omega^2\,d\omega\,\mathrm{Tr}\,D(\omega,\mathbf{r},\mathbf{r}), \tag{2.9}$$

where the trace "Tr" is taken on spatial variables (i.e., spatial integration) and Dirac indices for the fermion case. In the fermion case, the contour encloses the poles of the occupied sea plus valence states and runs from $-\infty$ to $+\infty$ along the real ω-axis. It is convenient to separate out the valence states explicitly and deform the contour to the imaginary axis, so that $\omega=iy$ and $-\infty<y<+\infty$. In the Bose case, the contour is the same as in the fermion case, without enclosing any valence states and is again deformed to the imaginary axis.

Infinities are removed in the usual way by expanding S and D and identifying the divergences with the negative of counter terms in the standard way. We then obtain a finite expression for the energy [3, 4],

$$\begin{aligned}E=&\sum_{\text{(valence)}}\varepsilon_i+\int_{-\infty}^{+\infty}y^2\frac{dy}{2\pi}\,\mathrm{Tr}\{D(iy)-D_0(iy)-D_0^2(iy)\,\tilde{W}-D_0^3(iy)\,\tilde{W}^2\}\\&+i\int_{-\infty}^{+\infty}y\frac{dy}{2\pi}\,\mathrm{Tr}\,\gamma^0\{S(iy)-S_0(iy)-S_0^2(iy)(g\tilde{\phi}_c)-S_0^3(iy)(g\tilde{\phi}_c)^2\\&-S_0^4(iy)(g\tilde{\phi}_c)^3-S_0^5(iy)((g\tilde{\phi}_c)^4-(g\nabla\tilde{\phi}_c)^2)\},\end{aligned} \tag{2.10}$$

where $\tilde{\phi}_c=\phi_c-\phi_0$, $\tilde{W}=W-W_0$.

We use the fact that ϕ_c is spherically symmetric, $\phi_c(\mathbf{r}) = \phi_c(r)$, and make a partial wave decomposition of the Green's functions. With the definition

$$D(iy, \mathbf{r}, \mathbf{r}') \equiv \frac{1}{rr'} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} D_l(y, r, r')\, Y_{lm}(\theta, \phi)\, Y^*_{lm}(\theta', \phi'), \tag{2.11}$$

we have

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - y^2 - W\right) D_l(y, r, r') = \delta(r - r'). \tag{2.12}$$

One can expand D_0 in the same fashion as D is expanded. In this case, D_l is replaced by D_{0l} which satisfies Eq. (2.12) with W replaced by W_0. Similarly, we can make a partial wave decomposition of the fermion Green's functions. Defining

$$G(y, \mathbf{r}, \mathbf{r}') \equiv -\gamma_0 S(iy, \mathbf{r}, \mathbf{r}') \tag{2.13}$$

and expanding

$$G(y, \mathbf{r}, \mathbf{r}') = \frac{1}{rr'} \sum_{\kappa, m} G_\kappa(y, r, r') \otimes \mathcal{Y}_{\kappa m}(\theta, \phi)\, \mathcal{Y}^\dagger_{\kappa m}(\theta', \phi'), \tag{2.14}$$

we have

$$\begin{pmatrix} g\phi_c(r) - iy & -d/dr - \kappa/r \\ d/dr - \kappa/r & -g\phi_c(r) - iy \end{pmatrix} G_\kappa(y, r, r') = \delta(r - r'), \tag{2.15}$$

where the spinor harmonics are

$$\mathcal{Y}_{\kappa m}(\theta, \phi) \equiv \mathcal{Y}^l_{jm}(\theta, \phi) = \sum_{m_l m_s} \langle l m_l \tfrac{1}{2} m_s | jm \rangle\, Y_{lm_l}(\theta, \phi)\, \chi_{m_s}. \tag{2.16}$$

The $\langle l m_l \frac{1}{2} m_s | jm \rangle$ are Clebsch–Gordon coefficients,

$$\chi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \chi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{2.17}$$

are the 2-components Pauli spinors, and j is the total angular momentum. κ is the Dirac quantum number, $\kappa = (-1)^{j-l+1/2}(j + \frac{1}{2})$. For the free Green's function, we define

$$G_0(y, \mathbf{r}, \mathbf{r}') \equiv -\gamma_0 S_0(iy, \mathbf{r}, \mathbf{r}'). \tag{2.18}$$

One can make a partial wave expansion for G_0 that is identical to Eq. (2.14) with G_κ being replaced by $G_{0\kappa}$, which satisfy Eq. (2.15) with ϕ_c replaced by ϕ_0.

We use the property

$$G_{-\kappa}(y, r, r') = -\sigma_1 G_\kappa(-y, r, r')\, \sigma_1, \tag{2.19}$$

to see that

$$trG_{-\kappa}(y, r, r') = -trG_{\kappa}(-y, r, r'), \tag{2.20}$$

where σ_1 is the first Pauli matrix. Then we obtain from Eq. (2.10) [3, 4],

$$E = \sum_{\text{(valence)}} \varepsilon_i + \sum_{l=0}^{\infty} (2l+1)\, E_{Bl} + 4 \sum_{\kappa=1}^{\infty} \kappa E_{F\kappa}, \tag{2.21}$$

where

$$E_{Bl} = \int_{-\infty}^{+\infty} y^2 \frac{dy}{2\pi} \int_0^{\infty} dr \{ D_l(y, r, r) - D_{0l}(y, r, r) - D_{0l}^2(y, r, r)\, \tilde{W} - D_{0l}^3(y, r, r)\, \tilde{W}^2 \}, \tag{2.22}$$

with $D_{0l}^n(y, r, r) \equiv \langle r |\, D_{0l}^n(y)\, | r \rangle$,

$$E_{F\kappa} = \int_{\infty}^{+\infty} y^2 \frac{dy}{2\pi} \int_0^{\infty} dr\, ir \left\{ \frac{1}{y} \operatorname{Im} G_{\kappa}(y, r, r) + \tilde{G}_{0\kappa} + \tilde{G}_{0\kappa}^2 \times \{ (g\phi_c)^2 - (g\phi_0)^2 \} + \tilde{G}_{0\kappa}^3 \{ [(g\phi_c)^2 - (g\phi_0)^2]^2 + [g\phi_c'(r)]^2 \} \right\}. \tag{2.23}$$

Here we have

$$\tilde{G}_{0\kappa} = \begin{pmatrix} D_{0|\kappa-1|}(y, r, r) & 0 \\ 0 & D_{0|\kappa|}(y, r, r) \end{pmatrix}, \tag{2.24}$$

where

$$D_{0\kappa}^{-1} = \frac{d^2}{dr^2} - \frac{\kappa(\kappa+1)}{r^2} - (g\phi_0)^2 - y^2. \tag{2.25}$$

From the above equations, we see that the fermion renormalization subtractions for a κ partial wave component can be constructed exactly as the boson renormalization subtractions, except that they are actually equivalent to the sum of the subtractions for a 2-component boson. This observation simplifies our later numerical calculations.

The numerical evaluation of E in Eq. (2.21) involves three steps. First, one needs to calculate the Fermi valence eigenvalues, ε_i. There exist standard methods for this purpose [3, 5]. Second, one needs to calculate the boson loop energy. Finally, one needs to calculate the fermion loop energy. The essential steps in calculating boson and fermion loop energies include constructing the full Green's functions and calculating the various renormalization counterterms. These basic steps are by no means limited to the calculation of the one loop energy. In fact, all the one-body properties at the one loop level can be calculated similarly, and higher order loop

calculations require the initial calculation of the same Green's functions used here. For example, the one loop contribution to the soliton (hadron) static observables, such as the magnetic moment, charge density and charge radius, etc., can in general be reduced to evaluating the expression,

$$\sum_{\kappa} \kappa \int F(y) \frac{dy}{2\pi} \mathrm{Tr}(MG_{\kappa}), \tag{2.26}$$

where $F(y)$ is a polynomial in y and M is a matrix acting on internal variables. In the above, renormalization counterterms must be subtracted. The number of subtractions needed to render each observable finite varies, but never exceeds the number required for the one loop energy. Also, G_{κ} can be generalized to include a vector potential that is static and spherically symmetric [8]. Thus, it should be emphasized that the techniques and methods described in this paper have much wider applications than just calculating the one loop energy.

III. Constructing the Full Green's Functions

1. *The Full Boson Green's Function*

Denote by $u_l(y, r)$ and $v_l(y, r)$ the solutions of the equation

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - W(r) - y^2\right)\phi = 0 \tag{3.1}$$

which are regular at $r=0$ and at $r=\infty$, respectively. D_l then can be constructed from these two solutions [6],

$$D_l(y, r, r') = \frac{1}{w_l(y)} [u_l(y, r)\, v_l(y, r')\theta(r'-r) + v_l(y, r) u_l(y, r')\theta(r-r')], \tag{3.2}$$

where $\theta(r)$ is the step function with $\theta(0) = \frac{1}{2}$ and

$$w_l(y) = u_l(y, r)\frac{d}{dr} v_l(y, r) - v_l(y, r)\frac{d}{dr} u_l(y, r) \tag{3.3}$$

is the Wronskian. Because of the various renormalization subtractions, we need to construct $D_l(y, r, r')$ numerically with very high accuracy. We use the following scheme. Let $u_{l0}(y, r)$ and $v_{l0}(y, r)$ be the two independent solutions that satisfy Eq. (3.1) with $W(r)$ replaced by W_0, that are regular at $r=0$ and $r=\infty$, respectively. They are known analytically and are related to modified spherical Bessel functions of the first and second kind, i_l and k_l,

$$u_{l0}(y, r) = r i_l(a_y r), \qquad v_{l0}(y, r) = r k_l(a_y r), \tag{3.4}$$

where $a_y = (y^2 + W_0)^{1/2}$. D_{0l} is given by (3.2) with u_{l0} and v_{l0} replacing u_l and v_l. Define

$$u_l(y, r) \equiv u_{l0}(y, r) f_l(y, r), \qquad v_l(y, r) \equiv v_{l0}(y, r)\, g_l(y, r). \tag{3.5}$$

Then from Eq. (3.1) we find that $f_l(y, r)$ and $g_l(y, r)$ satisfy the equations,

$$\left[\frac{d^2}{dr^2} + 2\frac{u'_{l0}(y, r)}{u_{l0}(y, r)}\frac{d}{dr} - \tilde{W}(r)\right] f_l(y, r) = 0, \tag{3.6a}$$

$$\left[\frac{d^2}{dr^2} + 2\frac{v'_{l0}(y, r)}{v_{l0}(y, r)}\frac{d}{dr} - \tilde{W}(r)\right] g_l(y, r) = 0. \tag{3.6b}$$

The boundary conditions for f_l and g_l are chosen so that both are very smooth functions of r, since the singular behavior of u_l and v_l at $r = 0$ and $r = \infty$ has been filtered out through the transformation (3.5).

Since (3.6a) and (3.6b) are linear second-order differential equations, each has two linearly independent solutions. Of these two independent solutions, one may be chosen to be well behaved and, in practice, is very smooth. The other is rapidly varying and singular at either $r = 0$ or $r = \infty$.

In order to generate the desired solutions it is necessary to integrate (3.6a) for f_l from 0 to ∞ [10]. The inside boundary condition is chosen to be

$$f_l(0) = 1, \qquad f'_l(0) = 0. \tag{3.7}$$

As $r \to \infty$, f_l approaches a constant, C_l.

It is necessary to integrate (3.6b) for g_l from ∞ to 0. The outside boundary condition is similarly chosen to be

$$g_l(r) = 1, \qquad g'_l(r) = 0, \qquad r \to \infty. \tag{3.8}$$

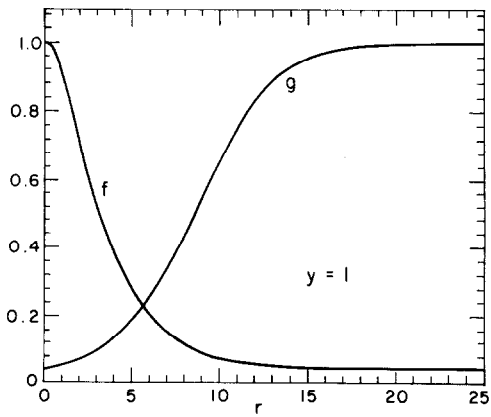

FIG. 1. The solutions f_l and g_l for the boson full Green's function. The plot is for the same case as in Table I ($l = 1$, $R = 10$, $T = 2$, $\phi_0 = 1$, and $\phi_b = 0.2$) for $y = 1$. For ease of presentation, we have multiplied f_l by a scale factor that can always be absorbed into the Wronskian. Both f_l and g_l are monatonic in r. As y gets larger, f_l and g_l approach unity (see Figs. 2 and 3).

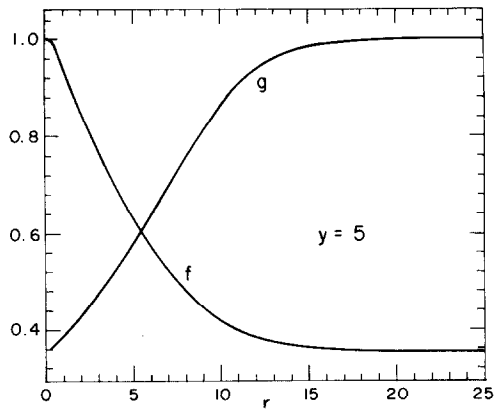

FIG. 2. Same as Fig. 1 with $y = 5$.

Then g_l goes to a constant as $r \to 0$. Note that f_l and g_l both approach unity as either $y \to \infty$ or $l \to \infty$. The leading order term for E_{Bl} is

$$\int y^2 \frac{dy}{2\pi} \int_0^\infty dr\, u_{l0} v_{l0} [f_l g_l - 1]. \tag{3.9}$$

Thus we see that the accuracy is governed by the accuracy of f_l and g_l with respect to unity. Some examples of solutions f_l and g_l are plotted in Figs. 1–3.

2. THE FULL FERMION GREEN'S FUNCTION

With minor added complications, the fermion Green's function, $G_\kappa(y, r, r')$, can be constructed similarly with high accuracy. In order to construct the fermion

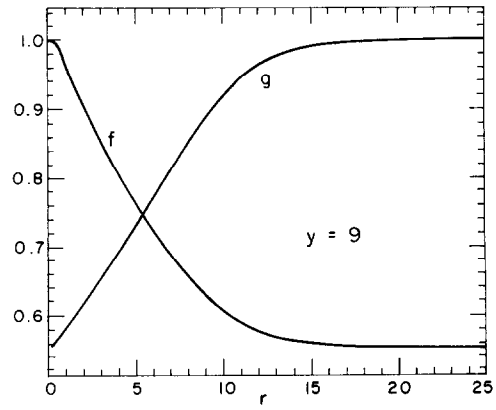

FIG. 3. Same as Fig. 1 with $y = 9$.

Green's function, let $U_\kappa(y, r)$ and $V_\kappa(y, r)$, which are regular at $r=0$ and at $r=\infty$, respectively, be two independent solutions of the equation

$$\begin{pmatrix} g\phi_c(r)-iy & -d/dr-\kappa/r \\ d/dr-\kappa/r & -g\phi_c(r)-iy \end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}=0, \tag{3.10}$$

with

$$U_\kappa=\begin{pmatrix}U_\kappa^1\\ U_\kappa^2\end{pmatrix}, \qquad V_\kappa=\begin{pmatrix}V_\kappa^1\\ V_\kappa^2\end{pmatrix}. \tag{3.11}$$

G_κ can be constructed from the two solutions as follows [6, 8],

$$G_\kappa(y, r, r')=\frac{1}{j_\kappa(y)}\{U_\kappa(y, r)\, V_\kappa^{\mathrm{T}}(y, r')\theta(r'-r)+V_\kappa(y, r)\, U_\kappa^{\mathrm{T}}(y, r')\theta(r-r')\}, \tag{3.12}$$

where

$$j_\kappa(y)=U_\kappa^1(y, r)\, V_\kappa^2(y, r)-U_\kappa^2(y, r)\, V_\kappa^1(y, r) \tag{3.13}$$

is the Wronskian.

Define

$$U_\kappa^1=U_{0\kappa}^1\,\tilde{U}_\kappa^1, \qquad U_\kappa^2=U_{0\kappa}^2\,\tilde{U}_\kappa^2, \tag{3.14}$$

where $(U_{0\kappa}^1, U_{0\kappa}^2)$ satisfy Eq. (3.10) with $\phi_c(r)$ replaced by ϕ_0. Then we have

$$\begin{pmatrix} (g\phi_c(r)-iy)\, U_{0\kappa}^1/U_{0\kappa}^2 & -d/dr-(g\phi_0-iy)\, U_{0\kappa}^1/U_{0\kappa}^2 \\ d/dr+(g\phi_0+iy)\, U_{0\kappa}^2/U_{0\kappa}^1 & -(g\phi_c(r)+iy)\, U_{0\kappa}^2/U_{0\kappa}^1 \end{pmatrix}\begin{pmatrix}\tilde{U}_\kappa^1\\ \tilde{U}_\kappa^2\end{pmatrix}=0. \tag{3.15}$$

The boundary conditions are chosen so that $\tilde{U}_\kappa^1$ and $\tilde{U}_\kappa^2$ are very smooth functions of r. $U_{0\kappa}^1$ and $U_{0\kappa}^2$ are known exactly and can be expressed in terms of the modified spherical Bessel functions,

$$U_{0\kappa}^1=r i_{\kappa-1}(c_y r), \tag{3.16a}$$

$$U_{0\kappa}^2=\frac{r c_y i_\kappa(c_y r)}{g\phi_0+iy}, \tag{3.16b}$$

where $c_y=[y^2+(g\phi_0)^2]^{1/2}$. The solutions for $(\tilde{U}_\kappa^1, \tilde{U}_\kappa^2)$ are complex. Similarly, we can define

$$V_\kappa^1=V_{0\kappa}^1\,\tilde{V}_\kappa^1, \qquad V_\kappa^2=V_{0\kappa}^2\,\tilde{V}_\kappa^2, \tag{3.17}$$

where $(\tilde{V}_\kappa^1, \tilde{V}_\kappa^2)$ satisfy a similar equation as $(\tilde{U}_\kappa^1, \tilde{U}_\kappa^2)$, and

$$V_{0\kappa}^1=r k_{\kappa-1}(c_y r), \tag{3.18a}$$

$$V_{0\kappa}^2=-\frac{r c_y k_\kappa(c_y r)}{g\phi_0+iy}. \tag{3.18b}$$

$\tilde{V}_\kappa^1$ and $\tilde{V}_\kappa^2$ are also complex.

In analogy with the boson case discussed in the previous section, in order to obtain the desired solutions for $\tilde{U}^1_\kappa$ and $\tilde{U}^2_\kappa$, one needs to start from $r=0$ and solve the coupled differential equation (3.15) from *inside out*. The boundary conditions can be easily determined using (3.15) and by setting $\phi_c = \phi_c(0)$. These are given by

$$\tilde{U}^1_\kappa(0) = 1, \tag{3.19a}$$

$$\tilde{U}^2_\kappa(0) = \frac{g^2\phi_c(0)\,\phi_0 + y^2 + iy[g\phi_c(0) - g\phi_0]}{c_y^2}. \tag{3.19b}$$

Similarly, in order to obtain the desired solutions for $\tilde{V}^1_\kappa$ and $\tilde{V}^2_\kappa$, one needs to specify the boundary conditions for $\tilde{V}^1_\kappa$ and $\tilde{V}^2_\kappa$ at $r \to \infty$ and solve the coupled differential equations obeyed by $\tilde{V}^1_\kappa$ and $\tilde{V}^2_\kappa$ from *outside in*. The boundary conditions in this case are simply

$$\tilde{V}^1_\kappa(r \to \infty) = 1, \qquad \tilde{V}^2_\kappa(r \to \infty) = 1. \tag{3.20}$$

The resulting solutions to the coupled differential equations for $(\tilde{U}^1_\kappa, \tilde{U}^2_\kappa)$ and $(\tilde{V}^1_\kappa, \tilde{V}^2_\kappa)$ are rather smooth everywhere, and solutions with high accuracy can be obtained with the aid of a good library [7] subroutine.

IV. Calculating the Subtraction Terms

In order to calculate the renormalization subtraction terms for both the boson loop and the fermion loop, we need to calculate the matrix elements

$$\langle r|\, D^n_{0l}\, |r\rangle, \tag{4.1}$$

with $n = 1$, 2, and 3. This can be done most easily by noting that the formal solution of the equation defining D_{0l} can be written

$$D_{0l}(y, r, r') = -\sum_i \frac{\phi_{0i}(r)\,\phi^\dagger_{0i}(r')}{y^2 + h^2_{0i}}, \tag{4.2}$$

where ϕ_{0i} is a complete set of eigenfunctions for the equation

$$\left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + W_0\right)\phi_{0i} = h^2_{0i}\phi_{0i}, \tag{4.3}$$

which are normalized to

$$\int_0^\infty dr\, \phi^\dagger_{0i}(r)\,\phi_{0j}(r) = \delta_{ij}, \tag{4.4a}$$

and satisfy the completeness relation

$$\sum_i \phi_{0i}(r)\,\phi^\dagger_{0i}(r') = \delta(r - r'). \tag{4.4b}$$

From Eqs. (4.2), (4.4a), and (4.4b), it is easy to derive [3]

$$D^n_{0l}(y, r, r') \equiv \langle r| D^n_{0l} |r'\rangle = (-1)^n \sum_i \frac{\phi_{0i}(r)\, \phi^\dagger_{0i}(r')}{(y^2 + h^2_{0i})^n}$$

$$= \frac{1}{(n-1)!} \left(\frac{d}{dy^2}\right)^{n-1} D_{0l}(y, r, r'). \tag{4.5}$$

Using the solution of D_{0l} in terms of the modified Bessel functions, we finally arrive at

$$D^n_{0l}(y, r, r) = \frac{1}{(n-1)!} \left(\frac{1}{2a_y} \frac{d}{da_y}\right)^{n-1} \{-a_y r^2 i_l(a_y r)\, k_l(a_y r)\}. \tag{4.6}$$

The Appendix gives the detailed forms of the various matrix elements in terms of the modified spherical Bessel functions and their derivatives.

V. Some Illustrative Results

Combining all the above ideas, we have developed and tested relevant FORTRAN codes to calculate the energy E. Our codes mainly consist of four subroutines, BESSEL, BOSON, FERMION, and COUNTER. BESSEL is a subroutine that calculates the modified spherical Bessel functions with high accuracy using standard procedures. BOSON and FERMION are subroutines that calculate the full boson and fermion Green's functions. COUNTER is a subroutine that calculates the various renormalization subtraction terms for both the boson and fermion loop.

The numerical work involved in the calculations is extensive; associated with any extensive numerical project is the question of how trustworthy the results are, since it is easy to make a programming mistake.

The subroutine BESSEL can be checked by comparison of its results with accurate tables of Bessel functions. There are several ways to check BOSON, FERMION, and COUNTER. First, in numerical studies of physical systems, we always put the systems inside a large but finite space volume and then use finite grids to discretize the volume. It is, therefore, necessary to make sure that numerical results are stable against changes of the size of the volume and the number of grid points. The artifacts introduced by the effects of finite volume and grids should be negligible for physical results. We used several different sizes of the volume and numbers of grid points so that our final results for the numerically constructed Green's functions are stable against changes of both. We also checked to make sure that the Wronskians are constant for fixed y. Second, the y-integration should converge after renormalization subtractions. This requires precise cancellations for each of the subtractions. More importantly, our results have been checked by two other means, which makes us confident that they are correct. First of all, for smooth

solitons, where the derivative expansion [3, 4, 11] works, we demonstrated that the expansions clearly converge to the numerically calculated full one-loop energies, thus indicating that our numerical results are correct. Second, the fermion loop energy, which is more difficult to calculate than the boson loop energy and has similar subtraction terms as the boson loop energy, can be calculated differently. Instead of using the Green's function method, one can simply calculate the fermion negative energy eigenvalues [9]. One can then use the same subtraction scheme as in the Green's function method to renormalize the theory. For soliton configurations that have been studied using both methods, the results always agree up to several digits; and in particular, all results presented below agree to all but the last digit shown.

For the purpose of illustration, we present some sample results in Tables I–III. For definiteness, we take a Wood–Saxon form for ϕ_c,

$$\phi_c = \phi_0 - \frac{\phi_b}{1+\exp((r-R)/T)}, \tag{5.1}$$

$$W = 3\phi_c^2 - \phi_0^2. \tag{5.2}$$

R controls the radius of ϕ_c, T its surface thickness, and ϕ_b the depth of ϕ_c at the origin. In Table I, we present the results for the $l=1$ component of the boson loop with $\phi_0=1$, $\phi_b=0.2$, $R=10$, and $T=2$. The first entry gives the value of $\int y^2\,dy/2\pi \int_0^\infty dr\, D_l(y, r, r)$. Although this quantity should be infinite, we truncate the y-integration and insist that after subtracting the counter terms the results are insensitive to the cutoff. The cutoff we used for the y-integration that produced the data of Tables I and II is $y=40$. The second entry gives the corresponding value after the first renormalization subtraction, that is, $\int y^2\,dy/2\pi \int_0^\infty dr$ $\{D_l(y, r, r) - D_{0l}(y, r, r)\}$. The third entry gives the value after the second subtraction, $\int y^2\,dy/2\pi \int_0^\infty dr\{D_l(y, r, r) - D_{0l}(y, r, r) - D_{0l}^2(y, r, r)\,\tilde{W}\}$. Finally, the last entry gives the value of the renormalized energy, Eq. (2.22). In Table II, we present the results for the $\kappa=2$ component of the fermion loop. Here we take $R=10$, $T=2$, $\phi_0=1$, $\phi_b=1$, and $g=1$. Similar to the boson case, the first entry gives the value $-4\int y\,dy/2\pi \int_0^\infty dr\, tr\ \mathrm{Im}\, G_\kappa(y, r, r)$. The second entry gives the value after the first subtraction, $-4\int (y^2\,dy/2\pi) \int_0^\infty dr\, tr\{(1/y)\ \mathrm{Im}\, G_\kappa(y, r, r) + \tilde{G}_{0\kappa}(y, r, r)\}$, and so on. The final entry gives the value of the renormalized energy, Eq. (2.23). We have varied the box size in which the system is contained from $L=15$ (L is the radius

TABLE I

The Values of the $l=1$ Component for the Boson Loop Energy after Various Renormalization Subtractions with $R=10$, $T=2$, $\phi_0=1$, and $\phi_b=0.2$

Unrenormalized	1st subtraction	2nd subtraction	3rd subtraction
−7910.56021	−3.15144	−0.09206	−0.01387

TABLE II

The Values of the $\kappa = 2$ Component for the Fermion Loop Energy after Various Renormalization Subtractions with $R = 10$, $T = 2$, $\phi_0 = 1$, and $\phi_b = 1$

Unrenormalized	1st subtraction	2nd subtraction	3rd subtraction
15826.41549	7.58564	0.45408	0.14875

of the box size) to $L = 25$. The first four digits of our final results for the energy of each partial wave after renormalization subtractions are insensitive to the variation. From the results, we see clearly that we need high accuracy in the calculations. After various renormalization subtractions, the significant digits of the starting values are reduced from 9 to 4 for the boson loop and from 10 to 5 for the fermion loop. Table III presents the energies of different partial waves for the fermion loop in one soliton configuration and their corresponding values of leading order in the derivative expansion [4]. For $\kappa = 2$, the value of $E_\kappa = 0.14875$ is to be compared with the value obtained through the eigenvalue method [9], 0.14876. Also it takes approximately 13 h of CPU time on a VAX 11/780 to obtain the results of E_κ, $\kappa = 1, 2, ..., 12$ in Talbe III. The $\kappa = 1$ takes 25 min CPU time, $\kappa = 2$ takes 30 min, and $\kappa = 13$ takes about 2 h. In the last column of Table III, we give the CPU times in seconds that are required for calculating the energy of each partial wave on a CRAY X-MP48 machine.

Finally, we discuss summing the various partial waves to obtain the total loop energies. Since it is impossible to calculate all partial waves, we have to use

TABLE III

The Fermion Loop Energy and the Two Leading Terms in Its Derivative Expansion for Various Partial-Waves with $R = 10$, $T = 2$, $\phi_0 = 1$, and $\phi_b = 1$

κ	$E_{F\kappa}$	$\int d^3r\, V_F$	$\int d^3r(V_F + \frac{1}{2}Z_F(\nabla\phi_c)^2)$	CPU Time (s)
1	0.221800	0.216104	0.224060	24.0
2	0.148746	0.144800	0.149616	27.9
3	0.102324	0.099552	0.102758	28.9
4	0.071774	0.069802	0.072022	29.8
5	0.051212	0.049790	0.051364	30.7
6	0.037118	0.036082	0.037218	31.7
7	0.027304	0.026540	0.027372	32.6
8	0.020370	0.019800	0.020418	33.8
9	0.015400	0.014972	0.015438	34.9
10	0.011792	0.011464	0.011818	36.1
11	0.009138	0.008886	0.009159	36.9
12	0.007160	0.006961	0.007173	37.8

Note. The last column gives CPU times used in calculating E_κ for each partial wave using a CRAY X-MP machine. The data are obtained by using grids of $N_r = 500$ along the spatial r-direction, and $N_y = 64$ along the y-direction.

extrapolation [10] to obtain the total sum over all the partial waves. Assuming for large l, $E_{Bl}=\sum_{i=0}^{m}\alpha_i/l^{i+n}$, one can determine n using the known results at l and $l+1$ so that $l^n E_{Bl}\simeq(l+1)^n E_{Bl+1}$, then one can determine α_i by using the known results of $l, ..., l+m$ and solving a set of coupled linear algebraic equations. One can improve the extrapolation by using several known consecutive E_{Bl}'s to calculate the total sum, and then perform repeated extrapolation [10] using these sums. Similar methods apply to the fermion energy as well. This extrapolation, however, can only be applied to cases in which the energies of the last several partial waves are in the asymptotic region to a good extent. That is, the first few coefficients in the expansion series of E_{Bl} (or $E_{F\kappa}$) in terms of the inverse powers of l (or κ) should approximately have the same values for the last several partial waves.

If for a soliton configuration the convergence of the partial wave sum is not fast, such as the case of Table III, results from the extrapolation would not be very accurate. For such cases, we will use the following method to obtain the energy. Even when the derivative expansion [4] does not work well for the total energy, it becomes accurate for higher partial waves, much as the Born approximation improves as energy is increased. Since the major contributions to the total sum of the energy come from the lower partial waves, we can get a good estimate of the total energy by using the first few terms in the derivative expansion to approximate the energies of higher partial waves. The total sum of all the partial waves for the leading terms of the derivative expansion can be easily calculated. They are given by the spatial integrations of the analytically known expressions (such as for $V_F(\phi_c)$ and $Z_F(\phi_c)$). For example, for the one fermion loop we have

$$E_F=4\sum_{\kappa=1}^{\infty}\kappa E_{F\kappa}=\int d^3r\left(V_F(\phi_c)+\frac{1}{2}Z_F(\phi_c)(\nabla\phi_c)^2\right), \tag{5.3}$$

where $E_{F\kappa}$ is given by Eq. (2.23), and

$$V_F=-\frac{1}{16\pi^2}\left\{(g\phi_c)^4\ln\frac{\phi_c^2}{\phi_0^2}-\frac{1}{2}((g\phi_c)^2-(g\phi_0)^2)(3(g\phi_c)^2-(g\phi_0)^2)\right\}, \tag{5.4}$$

$$Z_F(\phi_c)=-\frac{g^2}{8\pi^2}\ln\frac{\phi_c^2}{\phi_0^2}-\frac{g^2}{12\pi^2}. \tag{5.5}$$

Under this approximation, the sum of all the partial waves with l (or κ) greater than a certain integer n will be the total sum minus the sum of the partial waves up to n. The leading terms of the derivative expansion for each partial wave can be calculated with high accuracy [4].

We apply the method to the case presented in Table III. From Table III, we know empirically that for each partial wave, the energy is always greater than the effective potential alone and less than the sum of the effective potential with the second derivative contributions. By using the higher partial waves V_F to approximate the energy, we will get a lower bound for the total energy. Similarly, by using the higher partial waves of $V_F+\frac{1}{2}Z_F(\nabla\phi_c)^2$ we will obtain an upper bound

for the total energy. From the analytical forms of $V_F(\phi_c)$ and $Z_F(\phi_c)$ given by Eqs. (5.4) and (5.5), we obtain $\int d^3r\, V_F = 12.018$, and $\int d^3r\, \frac{1}{2} Z_F(\nabla\phi_c)^2 = 0.377$. The sum of lower partial waves for both can be obtained using the data given in Table III. Similarly, the sum of lower partial waves of $E_{F\kappa}$, κ from 1 to 12, can be done ($4\sum_{\kappa=1}^{\kappa=12} E_{F\kappa}$). From these, we get $12.279 < E_F < 12.356$. Notice that the error for E_F estimated from the bounds is less than 1%. It would also be possible to maintain a running extrapolation, and then empirically extrapolate this derivative expansion improved running sum. In all cases one requires stability as the crucial test of when an extrapolation has stabilized.

Besides extrapolations based on the empirically determined dependence of the energy on κ (or l) and the derivative expansion, at this moment we have no other means to estimate the energy contribution from higher partial waves. The former extrapolation only starts to work when the dependence of higher partial waves on l (or κ) enters the asymptotic region, while the latter is best suited for smooth soliton configurations where the derivative expansion is valid. In fact, this latter method cannot be applied to solitons for which the effective potential becomes imaginary and higher order terms blow up. This happens for all topological solitons in $1+1$ dimensions, as an important example [12]. Better ways to estimate the remainders need to be further investigated.

Appendix

From Section IV, we can express the matrix elements, $\langle x|\, D_{0l}^n(y)\, |x\rangle$, in terms of the modified spherical Bessel functions and their derivatives through the formula

$$\begin{aligned}\langle x|\, D_{0l}^n(y)\, |x\rangle &= \frac{1}{(n-1)!}\left(\frac{1}{2a_y}\frac{d}{da_y}\right)^{n-1} D_{0l}(y, x, x) \\ &= \frac{1}{(n-1)!}\left(\frac{1}{2a_y}\frac{d}{da_y}\right)^{n-1} \{-a_y i_l(a_y x)\, k_l(a_y x)\}. \end{aligned} \tag{1}$$

Defining $\zeta = a_y x$,

$$(i_l(\zeta)\, k_l(\zeta))' = \frac{d}{d\zeta}(i_l(\zeta)\, k_l(\zeta)), \qquad (i_l(\zeta)\, k_l(\zeta))'' = \frac{d^2}{d\zeta^2}(i_l(\zeta)\, k_l(\zeta)), \tag{2}$$

and

$$(i_l(\zeta)\, k_l(\zeta))^{(n)} = \frac{d^n}{d\zeta^n}(i_l(\zeta)\, k_l(\zeta)), \qquad n \geqslant 3, \tag{3}$$

we obtain

$$\begin{aligned}&\langle x|\, D_{0l}^2(y)\, |x\rangle \\ &\quad = -\frac{1}{2a_y}\{i_l(\zeta)\, k_l(\zeta) + \zeta(i_l(\zeta)\, k_l(\zeta))'\}, \end{aligned} \tag{4}$$

$$\langle x|\, D_{0l}^{3}(y)\,|x\rangle$$

$$= -\frac{1}{(2a_y)^3}\{-i_l(\zeta)\,k_l(\zeta)+\zeta(i_l(\zeta)\,k_l(\zeta))'+\zeta^2(i_l(\zeta)\,k_l(\zeta))''\}, \tag{5}$$

$$\langle x|\, D_{0l}^{4}(y)\,|x\rangle$$

$$= -\frac{1}{48a_y^5}\{3i_l(\zeta)\,k_l(\zeta)-3\zeta(i_l(\zeta)\,k_l(\zeta))'+\zeta^3(i_l(\zeta)\,k_l(\zeta))^{(3)}\}, \tag{6}$$

$$\langle x|\, D_{0l}^{5}(y)\,|x\rangle$$

$$= -\frac{1}{384a_y^7}\{-15i_l(\zeta)\,k_l(\zeta)+15\zeta(i_l(\zeta)\,k_l(\zeta))'-3\zeta^2(i_l(\zeta)\,k_l(\zeta))''$$

$$-2\zeta^3(i_l(\zeta)\,k_l(\zeta))^{(3)}+\zeta^4(i_l(\zeta)\,k_l(\zeta))^{(4)}\}. \tag{7}$$

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REFERENCES

1. R. FRIEDBERG AND T. D. LEE, *Phys. Rev. D* **15**, 1694 (1977); **16**, 1096 (1977); R. GOLDFLAM AND L. WILETS, *Phys. Rev. D* **25**, 1951 (1982); L. WILETS, *Nontopological Solitons* (World Scientific, Singapore, 1989). The one loop energy has also been studied for chiral solitons. See, for example, S. KAHANA AND G. RIPKA, *Phys. Lett. B* **155**, 327 (1985); V. SONI, *Phys. Lett. B* **183**, 91 (1987).
2. A. L. FETTER AND J. D. WALECKA, *Quantum Theory of Many Particle Systems*, (McGraw-Hill, New York, 1971); L. P. KADANOFF AND G. BAYM, *Quantum Statistical Mechanics* (Benjamin, New York, 1962).
3. M. LI, Ph.D. thesis, University of Washington, 1987 (unpublished).
4. M. LI AND R. PERRY, *Phys. Rev. D* **37**, 1670 (1988).
5. R. HORN, R. GOLDFLAM, AND L. WILETS, *Comput. Phys. Commun.* **42**, 105 (1986).
6. R. COURANT AND D. HILBERT, *Methods of Mathematical Physics* (Interscience, New York, 1962).
7. International Mathematical and Statistical Libraries, Inc., Houston, Texas.
8. E. H. WICHMANN AND N. M. KROLL, *Phys. Rev.* **101**, 843 (1956); M. GYULASSY, *Nucl. Phys. A* **244**, 497 (1975).
9. R. PERRY, *Nucl. Phys. A* **467**, (1987).
10. G. DAHLQUIST AND A. BJÖRCK, *Numerical Methods* (Prentice-Hall, Englewood Cliffs, NJ 1974).
11. L. H. CHAN, *Phys. Rev. Lett.* **54**, 1222 (1985); **56**, 404 (1986); C. M. FRASER, *Z. Phys. C* **28**, 101 (1985); O. CHEYETTE, *Phys. Rev. Lett.* **55**, 2394 (1985).
12. R. J. PERRY AND M. LI, *Mod. Phys. Lett. A* **2**, 353 1987; M. LI, R. J. PERRY, AND L. WILETS, *Phys. Rev. D* **36**, 596 (1987).