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MONTE CARLO APPROACHES TO EFFECTIVE FIELD THEORIES

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INTRODUCTION

In this paper, we explore the application of continuum Monte Carlo methods to effective field theory models. Effective field theories, in this context, are those in which a Fock space decomposition of the states is useful. These problems arise both in nuclear and condensed matter physics. In nuclear physics, much work has been done on effective field theories of mesons and baryons. While the theories are not fundamental, they should be able to describe nuclear properties at low energy and momentum scales. After describing the methods, we solve two simple scalar field theory problems; the polaron and two nucleons interacting through scalar meson exchange.

The methods presented here are rather straightforward extensions of methods used to solve quantum mechanics problems. Monte Carlo methods are used to avoid the truncation inherent in a Tamm-Dancoff approach and its associated difficulties (such as cluster separability). Nevertheless, the methods will be most valuable when the Fock space decomposition of the states is useful. Hence, while they are not intended for *ab initio* studies of QCD, they may prove valuable in studies of light nuclei, or for systems of interacting electrons and phonons. In these problems a Fock space decomposition can be used to reduce the number of degrees of freedom and to retain the rotational symmetries exactly. These symmetries can be recovered in a lattice approach, but only at the cost of a very large number of degrees of freedom, most of which may be physically irrelevant.

The problems we address here are comparatively simple, but offer useful initial tests of the method. We present results for the polaron¹ (a slow electron in a polar crystal) and two non-relativistic nucleons interacting through scalar meson exchange. In each case, it is possible to integrate out the boson degrees of freedom exactly, and obtain a retarded form of the action that depends only upon the fermion paths. Here we keep the explicit bosons, though, since (1) we would like to retain information about the boson components of the states and (2) it will be necessary to keep these components in order to treat non-scalar or interacting bosonic fields. We conclude with a few remarks on future applications of the method.

HAMILTONIAN AND METHODS

We consider a simple Hamiltonian consisting of free-particle energies for mesons and baryons plus a simple interaction term:

$$H = \int d\mathbf{k} \, \omega_f(k) \, a^\dagger(\mathbf{k})a(\mathbf{k}) + \int d\mathbf{k} \, \omega_b(k) \, b^\dagger(\mathbf{k})b(\mathbf{k}) + \left[\int d\mathbf{k}d\mathbf{q} \, \beta(\mathbf{q}) \, a^\dagger(\mathbf{k}-\mathbf{q})a(\mathbf{k})b^\dagger(\mathbf{q}) + h.c. \right], \quad (1)$$

where the $a(\mathbf{k})$ ($b(\mathbf{k})$) are the fermion (boson) destruction operators, and $a^\dagger(\mathbf{k})$ ($b^\dagger(\mathbf{k})$) the creation operators. The function $\omega_f(k)$ describes the free fermion propagator, and $\omega_b(k)$ the boson propagator. The coupling term involving $\beta(k)$ is linear here, creating or destroying one boson at a time. While this feature may not be essential, it is necessary that the theory not include fermion loops. Relativistic extensions incorporating only Z-graphs do seem feasible, however. These 'quenched' theories are used to describe the polaron, and may be useful for hadronic effective field theories due to the composite nature of the nucleons.

The problems discussed in this paper involve only scalar bosons and one or two fermions, hence the sign problem does not arise. Of course, it will appear for systems with more fermions, in which case transient estimation or fixed node methods can be employed. It is also possible that the methods proposed elsewhere in this volume by Kalos for handling the fermion sign problem for few-body systems will prove useful here.

We employ a momentum space description here, although conversion to coordinate space is straightforward. The expressions in momentum space are highly non-local, but in coordinate space the non-locality is governed by the form factors at the vertices. Each representation has advantages and disadvantages. For example, momentum space is useful in determining the self-energy and effective mass of one fermion, while coordinate space may prove more useful in studying few-fermion systems. This would be particularly true if, for example, a contact nucleon-nucleon term was added to the Hamiltonian to represent part of the repulsive core.

A simple variational (trial) wave function for one fermion and many bosons is:

$$\Psi_t = P(\mathbf{K}) \int d\mathbf{k}_f g(\mathbf{k}_f, \mathbf{K}) a^\dagger(\mathbf{k}_f) \exp\left[\int d\mathbf{k} f(k) b^\dagger(\mathbf{k})\right] |0\rangle. \quad (2)$$

The operator $P(\mathbf{K})$ is a projection on total momentum $\mathbf{K}$, $g(\mathbf{k}_f, \mathbf{K})$ describes the fermion wave function, and $f(k)$ describes the bosons. This wave function describes independent mesons multiplied by a fermion wave function, which is appropriate to the problems studied here.

Variational Monte Carlo can be performed as a random walk in both coordinate and Fock space, using the Metropolis method² to obtain points distributed with a density distribution proportional to the square of a trial wave function. Three types of moves are employed in the algorithm; creation, destruction, and diagonal moves. The diagonal moves are those that do not create or destroy mesons; they can be treated in the standard fashion. The creation and destruction moves must be constructed to satisfy detailed balance. The condition may be written generically as:

$$|\Psi(\mathbf{K}_{n+1})|^2 T(\mathbf{K}_{n+1} \rightarrow \mathbf{K}_n) A(\mathbf{K}_{n+1} \rightarrow \mathbf{K}_n) = |\Psi(\mathbf{K}_n)|^2 T(\mathbf{K}_n \rightarrow \mathbf{K}_{n+1}) A(\mathbf{K}_n \rightarrow \mathbf{K}_{n+1}), \quad (3)$$

where $T(a \rightarrow b)$ represents the probability of proposing a move from configuration a to configuration b , and A represents the acceptance probability for that move. The arguments $\mathbf{K}_n$ indicate the momenta of each of the particles, n of which are bosons. For a wave function of the form of Eq. 2,

$$|\Psi(\mathbf{K}_n)|^2 = g^2(\mathbf{k}_f) \prod_{i=1}^n f^2(k_i) / n!. \quad (4)$$

Many valid choices of the transition and acceptance probabilities exist. For simple wave functions, it is possible to obtain very efficient Metropolis algorithms. Of course, the wave function must be symmetric under the exchange of any two boson momenta. Also, some care must be undertaken when constructing the detailed balance condition, since in going from the $n+1$ to the n boson state there are $n+1$ possible choices of the meson to destroy. For other than 1-body problems, there is also the choice of which fermion absorbs the destroyed meson's momentum. Given this algorithm, variational methods can be applied to determine approximate ground state properties.

The Green's function Monte Carlo method^{3,4} projects out the true ground state by applying $\exp(-H\tau)$ to the trial wave function. This method can be thought of as corresponding to time-ordered perturbation theory, where the 'time' variable is a euclidean time. For Hamiltonians of the form of equation 1, no time-step error need be associated with the calculation.

The method is most easily described algorithmically. We assume some familiarity with standard Green's function or Diffusion Monte Carlo methods.^{3,4} The variational Monte Carlo algorithm can be used to generate a set of configurations drawn with probability proportional to the square of the trial wave function. Each configuration consists of the coordinates of the fermions plus a set of coordinates for the bosons. In order to propagate the configurations in imaginary time, we first calculate the following quantities for each configuration:

$$E_{diag} = \omega_f(k_f) + \sum_i \omega_b(k_i), \quad (5)$$

$$E_{cre} = \frac{\int d\mathbf{q} \langle \Psi_t(\mathbf{K}_{n+1}) | \beta(q) b^\dagger(\mathbf{q}) a^\dagger(k-q) a(k) | \Psi_t(\mathbf{K}_n) \rangle}{\langle \Psi_t(\mathbf{K}_n) | \Psi_t(\mathbf{K}_n) \rangle}, \quad (6)$$

$$E_{des} = \frac{\sum_i \langle \Psi_t(\mathbf{K}_{n-1}) | \beta(q) b(\mathbf{q}) a^\dagger(k+q) k | \Psi_t(\mathbf{K}_n) \rangle}{\langle \Psi_t(\mathbf{K}_n) | \Psi_t(\mathbf{K}_n) \rangle}. \quad (7)$$

$$(8)$$

The first quantity E_{diag} is just the sum of boson and meson energies. The 'creation energy' E_{cre} involves an integral over all momenta for a created meson. The vector $\Psi_t(\mathbf{K}_{n+1})$ indicates a state with n boson momenta equal to the original configuration, and one additional boson of momentum q . The fermion must lose the created boson's momentum. For the simple wave functions used here, this integral can be performed analytically. The 'destruction energy' E_{des} sums over all possible destroyed mesons. Generalizations of these expressions to systems with more than one fermion are straightforward, and involve sums over the fermions that absorb or destroy mesons. We assume everywhere that the occupation probability for bosons of any specific momentum q goes as the inverse of the volume.

Once we have calculated these quantities, a configuration can be propagated without any time step error. The probability per unit time of creating or destroying a meson is given by $|E_{cre}| + |E_{des}|$. The time until the next creation or destruction can then be sampled from an exponential distribution

$$\delta\tau = \frac{-1}{|E_{cre}| + |E_{des}|} \log(\zeta), \quad (9)$$

where ζ is a random number distributed uniformly between 0 and 1. The growth per unit time of the population is

$$R = |E_{cre}| + |E_{des}| - E_{diag} - E_t, \quad (10)$$

where E_t is an arbitrary constant added to the Hamiltonian to keep the size of the population stable. After choosing $\delta\tau$, the weight of the configuration is multiplied by $R\delta\tau$.

At this point either a creation or destruction move must be made, with probabilities:

$$P_{cre} = |E_{cre}| / [|E_{cre}| + |E_{des}|] \quad (11)$$

$$P_{des} = |E_{des}| / [|E_{cre}| + |E_{des}|]. \quad (12)$$

If a creation move is chosen, the weight is multiplied by the sign of $-E_{cre}$ and a momentum for the new boson is picked with relative probability proportional to the creation energy for a boson of momentum q . If a destruction move is chosen, one of the bosons is destroyed with a relative probability governed by the destruction energy for that boson. In this case the weight of the configuration is multiplied by the sign of $-E_{des}$. In the problems discussed here, these signs are always positive. Each configuration can be propagated until it has reached a specified imaginary time. Note that different numbers of steps will be required for each configuration. At this point, the branching technique is used to retain equal weights for all the configurations.

Alternative formulations of the Green's function method are possible. The method outlined above requires that the creation energy E_{cre} be evaluated exactly for each configuration in order to eliminate time step errors. If this is not feasible, one can employ iteration schemes where the interaction term of the Hamiltonian enters linearly, allowing one to sample them directly. Such a method would be essentially a Monte Carlo implementation of Rayleigh-Schroedinger perturbation theory.

THE POLARON

In this section we briefly review the polaron,¹ and discuss some of the results we have obtained. The polaron has been studied extensively; a review is given in reference 5. For this reason, it offers a valuable testing ground for our method. The Hamiltonian is of the form of equation 1 for a slow electron interacting with a field of phonons. The free-particle energies and coupling are:

$$\omega_f(k) = k^2/2 \quad \omega_b(k) = 1 \quad \beta(k) \propto \sqrt{\alpha}/k. \quad (13)$$

The electron mass and phonon energy have been absorbed into the coupling constant. Note that the phonon energy is independent of momentum in this Hamiltonian.

A variety of variational schemes have been employed to study this problem.⁵ While I cannot list them all, I will try to illustrate the most important features. The variational wave functions presented here are very simple, but they serve to illustrate the two limits.

At weak coupling (small α), the ground state wave function can be written in the form of equation 2, with

$$g(\mathbf{k}) = 1 \quad f(\mathbf{k}) \propto \frac{\sqrt{\alpha}}{k} \left(\frac{1}{2 + k^2} \right) \quad (14)$$

A wave function of this form gives an $E(\alpha) = -\alpha$, and an expectation value of $\alpha/2$ for the number of bosons. Better wave functions give corrections of order α^2 .

At strong coupling this wave function is inadequate because the large number of uncorrelated phonons in the trial wave function leads to large fermion kinetic energies. The simplest, but by no means most accurate, strong coupling wave function assumes that g and f are both gaussians. Neglecting momentum conservation, the parameters of the gaussians can be optimized to yield an energy of $E = -\alpha^2/(3\pi)$ and an average value of $2\alpha^2/(3\pi)$ bosons. The variational method described above can be used to project out a state of zero total momentum, which lowers the energy. Note that before the projection on zero momentum this wave function confines the electron. Once the projection is introduced, though, the electron is not confined since the no-phonon component of the state is a delta function in momentum space.

As mentioned previously, the phonons can be integrated out exactly. The result, due to Feynman,⁶ is an effective action for the electron which contains a retarded interaction:

$$S_{eff} = \int_0^\beta dt \frac{\dot{\mathbf{x}}^2}{2} + \frac{\alpha}{2} \int_0^\beta dt \int_0^t d\tau \frac{\exp(-[t - \tau])}{|\mathbf{x}(t) - \mathbf{x}(\tau)|} \quad (15)$$

From the action, the ground state energy can be obtained through the path integral:

$$Z(\beta) \equiv \int d\mathbf{x}_0 \int_0^{\mathbf{x}(\beta)=\mathbf{x}_0} \mathcal{D}[\mathbf{x}] \exp(-S[\mathbf{x}]) \xrightarrow{\beta \rightarrow \infty} \exp[-\beta E_0] \quad (16)$$

The integral over the end-point $\mathbf{x}_0$ is a projection onto the zero-momentum state. Of course, in principle this is not necessary in the infinite β limit, but it greatly improves the convergence in numerical calculations.

This retarded interaction cannot be treated analytically, so various approximations and numerical methods have been employed. Feynman constructed a gaussian trial action which can be explicitly evaluated to determine an upper bound to the ground state energy:

$$S_T = \int_0^\beta dt \frac{\dot{\mathbf{x}}^2}{2} + C \int_0^\beta dt \int_0^t d\tau \exp(-w[t - \tau]) [\mathbf{x}(t) - \mathbf{x}(\tau)]^2 \quad (17)$$

This form contains two variational parameters, w and C . These can be optimized numerically for any value of the coupling constant; the results are given in table 1.

The second-order corrections to this trial action have also been evaluated,⁷ essentially through calculating moments of the path integral. The results of this calculation are also given in the table. Note that these corrections do not necessarily preserve the upper bound property for the estimated ground state energy.

Finally, the effective action can be evaluated numerically to achieve an 'exact' result. Alexandrou, Fleischer, and Rosenfelder⁸ have recently done this by breaking the path integral into fourier components. The lowest M components (with M as large as 19) are treated by Monte Carlo integration, while Feynman's trial action is used for the higher components. This approach requires one to extrapolate to the $\beta \rightarrow \infty, M \rightarrow \infty$ limit, while keeping $M \gg \beta$.

In order to compare the methods, we have computed the ground state energy at the same coupling constants as Alexandrou, et al.⁸ Note that the Feynman trial action (column 1) gives a result correct to within a few per cent for all values of the coupling constant. The next column adds the second order corrections to Feynman's trial action. The third and fourth columns indicate the results of the Fourier decomposition and our GFMC results, respectively. The sum of statistical and systematic errors are indicated in brackets. At small coupling constants these two numerical methods give results identical within their statistical errors. As the coupling constant increases, though, the results begin to disagree.

Table 1: Polaron Ground-State Energy

α	S_T	+pert	Fourier	GFMC
1.0	-1.013	-1.0135	-1.0166[20]	-1.0167[2]
3.0	-3.133	-3.161	-3.153[9]	-3.168[2]
5.0	-5.440	-5.523	-5.484[24]	-5.555[15]

The two methods have somewhat different weaknesses. The effective action technique has the equivalent of a finite time-step error, and requires an extrapolation to infinite β limit. The extrapolations become more difficult as the coupling constant increases; these extrapolations are described in their paper.

Any errors in the GFMC results are likely due to the bias caused by fluctuating populations. This bias increases with coupling constant due to the fairly primitive trial wave functions used here. We have checked our results by varying the population size and by using different trial functions which are linear superpositions of the weak and strong coupling wave functions. In the future, we will use more accurate trial wave functions, which will reduce both the bias and the statistical error of the results.

We now examine some properties of the phonons, as that was one of the reasons for keeping these variables explicitly in the first place. Figure 1 shows the probability of different numbers of bosons for the case $\alpha = 3$. The solid line is the result of calculations with the weak coupling wave function, and the circles are mixed estimates obtained in the GFMC calculations, using the weak coupling wave function as the importance function. Mixed estimates are defined as $\langle O \rangle_M = \langle \Psi_T | O | \Psi_0 \rangle$. Linear extrapolation can be used to approximate the true ground state expectation value. I have not done that in this case since the differences in probabilities can be quite large when the number of phonons is large, and the extrapolation procedure is likely to be inadequate. Undoubtedly this could be cured with more accurate trial wave functions.

Figure 1) Probability for different numbers of phonons

In the second figure, we plot the expectation value of the square of the momentum vs. the number of phonons, again for $\alpha = 3$. For the bosons, the sum of the squares of the individual momenta are plotted. The weak coupling results are a straight line since the phonons are uncorrelated in this approximation. In our GFMC results (again mixed estimates are plotted), the fermion has on average a smaller momenta than the weak coupling limit, while the bosons momenta are larger. These results are due to correlations induced between the phonons by the fermion kinetic energy; the system prefers phonons with anti-correlated momenta.

Figure 2) Expectation value of P^2 vs. the number of phonons

In the near future, these calculations will be extended to larger coupling constants and to finite momentum. To improve the accuracy of the calculations, the trial wave functions should be improved, but the methods are basically unchanged. A variety of polaron problems have been studied in the literature (for example, polarons bound in a well); exact GFMC calculations are also feasible for these problems.

NUCLEONS AND SCALAR MESONS

In this section, we look at solutions for one and two nucleons interacting through scalar meson exchange. This problem is similar to that studied initially by Serot, Koonin, and Negele.⁹ They treated a one-dimensional system of nucleons interacting with scalar and vector meson fields using a lattice approach. Eventually one would like to include interacting scalar, vector, and pion fields (and perhaps a contact interaction) in three dimensions. The hope is that eventually one will be able to treat effects such as exchange currents, three-body forces, meson-nucleon scattering and meson production in a more consistent manner.

Although we are still a long way from that goal, perhaps we can gain some insight in even these very simple models. Here we treat a Hamiltonian in the form of Equation 1, with:

$$\omega_f(k) = k^2/(2M) \quad \omega_b(k) = \sqrt{m^2 + k^2} \quad \beta(k) = \alpha N(\alpha) \frac{\exp(-k^2/k_0^2)}{\sqrt{\omega_b(k)}}, \quad (18)$$

where we take a ‘nucleon’ mass of 1 GeV, a scalar mass of 0.1 GeV, and two different sets of values for the coupling:

$$\text{set}[A] \quad g = 0.04 \quad k_0 = 1.0 fm^{-1} \quad (19)$$

$$\text{set}[B] \quad g = 0.35 \quad k_0 = 4.0 fm^{-1}. \quad (20)$$

$$(21)$$

In each case, the factor N is a normalization factor: $N = [1/(k_0\sqrt{\pi})]^{3/2}$. Parameter set A corresponds to a weak-coupling situation and gives total energies at a nuclear physics scale (tens of MeV). Set B is an intermediate coupling, but due to the lack of short range repulsion in this model, gives very large total energies (hundreds of MeV).

We compare the nucleon self-energies in the static approximation to the GFMC results in table 2. In the static approximation, one solves for the state in the $M \rightarrow \infty$ limit, and adds the kinetic energy of the fermion as a perturbation. As one can see from the table, the static approximation is very accurate at weak coupling but somewhat less accurate at intermediate coupling.

Table 2: Nucleon Self-Energy

Weak Coupling			
Self Energy (GeV)		$\langle b^\dagger b \rangle$	
Static	GFMC	Static	GFMC
-0.018807	-0.018865[3]	0.1297	0.1247[3]
Intermediate Coupling			
Self Energy (GeV)		$\langle b^\dagger b \rangle$	
Static	GFMC	Static	GFMC
-0.1672	-0.1751[6]	0.681	0.599[1]

In the static approximation, one can also construct a potential from the relation:

$$V_{NN}(\text{static}) = - \int dk \quad \frac{|\beta(k)\rho(k)|^2}{\omega_b(k)} + \Delta E_{\text{recoil}} - 2\Delta E_1. \quad (22)$$

The nucleon density is indicated by ρ , and the last two terms are the recoil kinetic energy in the two-body system and twice the recoil energy of an isolated nucleon, respectively. The resulting potential and recoil correction are shown for the weak-coupling case in figure 3.

Figure 3) Nucleon-Nucleon potential in the static approximation.

We can compute the solution of the Schroedinger equation with this static potential and compare to the solution of the full two-nucleon problem. For weak coupling (case A), the Schroedinger equation gives an energy of -12.3 MeV, with a contribution of approximately +0.8 MeV from the recoil terms. We have used a somewhat simplified variational form for the two-nucleon state in the full calculation; it has the solution of the Schroedinger equation built into the fermion sector but the bosonic wave function is simplified. Treating the full static approximation to the wave function is computationally expensive in momentum space. Nevertheless, the Variational Monte Carlo result for the simplified wave function is -9.6 MeV. The Green's function Monte Carlo method gives a slightly lower energy of -13 ± 0.1 MeV.

For the intermediate coupling problem, the variational result for the difference between two interacting nucleons and two isolated nucleons is 145 MeV, while the GFMC result is 150 ± 2 MeV. Thus the variational result is surprisingly close to the correct answer. Of course the difference is larger (approximately 20 MeV) in terms of absolute energies, but it appears that the error is largely in the one-body self-energy.

The errors made in the static approximation here are 5 to 10 %, similar to those found in reference 9. When making detailed comparisons of particular expectation values the error may be larger, however. Of course, this picture is much too simplified for even primitive comparisons with nuclear physics. At a minimum, a repulsive core must be added, either through a vector meson exchange or a contact interaction. In addition, the full field theory should be compared with a potential model that gives the same two-nucleon phase shifts, not simply with the static approximation, since conventional NN interactions are obtained through fits to experimental data.

CONCLUSION

We have introduced Monte Carlo methods applicable to effective field theories and used them to study the polaron and nucleon plus scalar meson problems. The GFMC method gives the exact ground state energy for these field theories, and also the self-energy as a function of the momentum. There are several interesting yet straightforward applications of the method that remain to be carried out. These include further studies of polaron problems (higher coupling, bound polarons, ...) and nuclear systems with repulsive cores.

More interesting, though, are solutions of effective field theories with pion degrees of freedom. These are more complicated due to the nature of the pi-nucleon coupling. It is not yet clear if these approaches will be successful in dealing with this problem.

If a method can be developed, though, a great deal of interesting physics could be studied in this context. The pion provides a very large fraction of the interaction in potential models and is essential for a realistic description of light nuclei. Calculations of π -N scattering are the first natural candidates for this approach, and also comparisons of deuteron form factors in the field theory picture compared to the traditional potential plus exchange current model. Of course, one would hope eventually to be able to tie together much of medium-energy physics in this way, including general models of exchange currents, and three nucleon interactions that arise in potential models due to the resonance structure of the nucleon. We are currently pursuing work along these lines.

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