Feynman-Goldstone diagrams in a time-dependent basis

Michel Baranger and Ismail Zahed
Center for Theoretical Physics, Laboratory for Nuclear Science and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
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A generalization of many-fermion Feynman-Goldstone diagrams is derived based on a time-dependent unperturbed Hamiltonian along with a time-dependent reference state. In lowest order, the time-dependent Hartree-Fock equations follow immediately from the same arguments which lead to static Hartree-Fock when the basis is time independent. Systematic corrections to the time-dependent Hartree-Fock mean-field approximation are obtained through higher order diagrams.

[NUCLEAR STRUCTURE Generalization of Feynman-Goldstone diagrams to a time-dependent reference state. Diagrammatic derivation of the time-dependent Hartree-Fock equations and their systematic corrections.]

I. INTRODUCTION

It will be shown in this paper that the usual perturbation expansion for a many-fermion system in terms of Feynman-Goldstone diagrams can be extended to the case where the unperturbed single-particle Hamiltonian is time dependent. The lines of the diagrams, then, cannot be single-particle stationary states; instead, they represent arbitrary solutions of the unperturbed single-particle Schrödinger equation.

Some obvious applications suggest themselves. For instance, the time-dependent Hartree-Fock (TDHF) equation has long been used to approximate collective motion; with the present method, TDHF appears as the zeroth order in an explicit perturbation expansion which is, in principle, exact. Applications to heavy ion scattering are also natural.

This formalism can be very useful for a *time-independent* total Hamiltonian H, which one breaks up into two *time-dependent* parts, $H=H_0(t)+H_1(t)$, where $H_0(t)$ is the unperturbed Hamiltonian and $H_1(t)$ the perturbation. As is often the case with other broken symmetries, this breaking of the time-translation symmetry can lead to new insights and shortcuts.

II. A TIME-DEPENDENT UNPERTURBED HAMILTONIAN

Consider one of the standard derivations of time-dependent perturbation theory and Feynman diagrams, for instance that of Ref. 1. The usual custom is to write $H=H_0+H_1$, where H_0 is time independent and H_1 possibly time dependent. But actually the argument goes through just as well, with very little change, if H_0 is time dependent. We show this now.

The first step is to write the exact propagator $K(t,t')$ as a product of many propagators over infinitesimal time intervals:

$$K(t,t')=\lim_{\substack{\epsilon\to 0\\ N\to\infty\\ N\epsilon=t-t'}} K(t,t-\epsilon)K(t-\epsilon,t-2\epsilon)\cdots K(t'+\epsilon,t')\ ,\quad N \text{ factors}\ . \tag{1}$$

Then each propagator is expanded in powers of H_1. One possibility is

$$K(\tau+\epsilon,\tau)=1-i\epsilon H_0\left[\tau+\frac{\epsilon}{2}\right]-i\epsilon H_1\left[\tau+\frac{\epsilon}{2}\right], \tag{2}$$

which is correct for infinitesimal ϵ. It is better, however, to keep a unitary form for the zero-order part of (2), hence to write

$$K(\tau+\epsilon,\tau)=K_0(\tau+\epsilon,\tau)-i\epsilon H_1\left[\tau+\frac{\epsilon}{2}\right], \tag{3}$$

where K_0 is the unperturbed propagator. The next step is to carry expansion (3) into (1) and to collect terms according to their order in H_1. The products of unperturbed propagators are recombined into single propagators and one obtains the following perturbation expansion of $K(t,t')$, which is the usual one except for the fact that $K_0(\tau,\tau')$ is calculated with a time-dependent H_0:

$$K(t,t')=K_0(t,t')-i\int_{-\infty}^{+\infty}dt_1K_0(t,t_1)H_1(t_1)K_0(t_1,t') +(-i)^2\int_{-\infty}^{+\infty}dt_1\int_{-\infty}^{+\infty}dt_2K_0(t,t_1)H_1(t_1)K_0(t_1,t_2)H_1(t_2)K_0(t_2,t')+\cdots . \tag{4}$$

The integrals extend from $-\infty$ to $+\infty$ because we are using the usual definition

$$K_0(t,t') \text{ and } K(t,t')=0 \text{ when } t-t'<0 . \tag{5}$$

Now we denote each term in expansion (4) by an unlabeled Feynman diagram, as shown in Fig. 1: each line stands for a $K_0(\tau,\tau')$, each vertex for an $H_1(\tau)$, and all intermediate times are to be integrated upon, with a factor $-i$ for each.

The next problem is that of choosing a basis to label the states. This is where things start to differ from the case where H_0 does not depend on time. In the latter case, the eigenstates of H_0 form a natural choice. Here, with H_0 depending on time, two possibilities come to mind. One is to use a completely arbitrary, time-independent basis, $|\mu\rangle$, $|\nu\rangle$, $|\rho\rangle$,.... Then, for example, the first-order term in $\langle\mu|K(t,t')|\nu\rangle$ is written

$$-i\int_{-\infty}^{+\infty}dt_1\sum_{\rho\sigma}\langle\mu|K_0(t,t_1)|\rho\rangle\langle\rho|H_1(t_1)|\sigma\rangle\langle\sigma|K_0(t_1,t')|\nu\rangle . \tag{6}$$

The other possibility is to use as a basis a complete orthonormal set of solutions of the time-dependent Schrödinger equation for H_0,

$$i\frac{d}{dt}|\phi(t)\rangle=H_0(t)|\phi(t)\rangle . \tag{7}$$

Because of the Hermiticity of H_0, which we assume, a basis which has been chosen orthonormal at one particular time remains orthonormal for all times. Let $|\alpha(t)\rangle$, $|\beta(t)\rangle$, etc.,..., be such a basis. Let us calculate terms in the perturbation expansion of $\langle\alpha(t)|K(t,t')|\beta(t')\rangle$. We can use for $\tau>\tau'$

$$K_0(\tau,\tau')|\gamma(\tau')\rangle=|\gamma(\tau)\rangle , \tag{8}$$

which simplifies things greatly; no matrix elements of propagators appear in the expansion at all, as long as we keep the integration times within the proper intervals. The expansion is then

$$\langle\alpha(t)|K(t,t')|\beta(t')\rangle=\langle\alpha|\beta\rangle-i\int_{t'}^{t}dt_1\langle\alpha(t_1)|H_1(t_1)|\beta(t_1)\rangle +(-i)^2\int_{t'}^{t}dt_1\int_{t'}^{t_1}dt_2\sum_{\gamma}\langle\alpha(t_1)|H_1(t_1)|\gamma(t_1)\rangle\langle\gamma(t_2)|H_1(t_2)|\beta(t_2)\rangle+\cdots . \tag{9}$$

This is the type of basis that will be used in the remainder of this paper. Essentially, it is the interaction representation, but for a time-dependent unperturbed Hamiltonian. Figure 2 shows how each term of expansion (9) can be denoted by a Feynman diagram in which we have labeled the intermediate states and the intermediate times. Each vertex contributes a matrix element of $H_1(t)$ in the time-dependent basis, but lines do not contribute anything, except limits for the time integrations.

One final note, when both H_0 and H_1 are time independent, which is a frequent occurrence, it makes sense to Fourier transform the propagator to get an "energy propagator." In a Feynman diagram associated with an energy propagator, there is an unperturbed propagator associated with each line, and this is usually some sort of "energy denominator." Calculations done with these energy denominators are usually quicker and more efficient than the calculation of the time integrals occurring in the time propagator, but this is not so here. If $H_0(t)$ or $|\alpha(t)\rangle$ are complicated functions of time, there is no reason to expect that a Fourier transformation will bring any simplification. The natural thing to do, therefore, is the obvious "time calculation" as defined by the integrals of Eq. (9). In some later papers, however, we shall apply the present formalism to the case of a "quasiperiodic" basis, for which each state of the basis reproduces itself after one period, except for a phase factor. Then it will make sense again to Fourier transform, with a Fourier series rather than a Fourier integral, and again something similar to an energy denominator will appear.

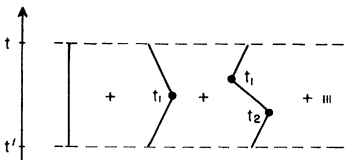

FIG. 1. Unlabeled Feynman diagrams occurring in the expansion of $K(t,t')$, Eq. (4).

III. MANY-BODY EXTENSION

Consider now a system composed of several particles, and suppose that the Hamiltonian H_0 is a sum of single-particle Hamiltonians, each of them time dependent, $h_{on}(t)$. We take a basis which is a product of single-

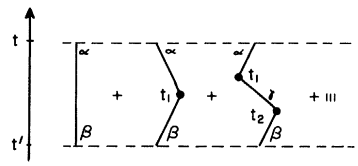

FIG. 2. Labeled Feynman diagrams contributing to $\langle\alpha(t)|K(t,t')|\beta(t')\rangle$, Eq. (9). The time-dependent unperturbed states $\alpha,\beta,\gamma,\ldots$, are solutions to the time-dependent Schrödinger equation (7).

particle bases, each of them time dependent in the appropriate Hamiltonian. We assume that H_1, which may also be time dependent, consists of few-body interactions: a one-body term, a two-body term, perhaps three- and four-body terms, but not much more. We are still calculating matrix elements of the exact propagator using expansion (9), but now $|\alpha\rangle$, $|\beta\rangle, \ldots,$ are many-body states.

Then it is obvious that each matrix element of H_1 in (9) involves only a few particles. This is reflected in the Feynman diagrams, provided that we draw a line for each particle, instead of a single line for the whole system. This is a good thing to do anyway, since it gives one a much more intuitive sense of the history of the system, which is what Feynman diagrams are for. Each one-body interaction in a Feynman diagram contributes a matrix element such as $\langle a(\tau)|H_1(\tau)|b(\tau)\rangle$; each two-body interaction contributes

$$\langle a(\tau)b(\tau)|H_1(\tau)|c(\tau)d(\tau)\rangle ,$$

etc.,. . . . As before, the lines of the diagram contribute nothing, except the ordering of the times at their extremities.

Examples of such diagrams are shown in Fig. 3. Two more things are obvious at this point. One is that a diagram may be the product of two independent contributions, each of which may be time integrated without reference to the other; this is true, for instance, of diagrams 3(a) and (c). The other is that a diagram does not always define a unique ordering of the intermediate times it contains. An example is diagram 3(d), in which the times t_3 and t_4 could be ordered either way. This means that this single diagram arises from two different terms in the fourth-order part of (9).

The conclusion is that many-body Feynman diagrams constitute a much more flexible and rich algebra than the "linear" algebra of equations like (9). From now on we shall use them in preference to the equations.

IV. FEYNMAN-GOLDSTONE DIAGRAMS

Suppose that the many-body system consists of N identical fermions. Then one can use Goldstone's idea,[2] saying that one picks a Fermi sea and one uses this Fermi sea as the "reference state." Then one draws diagrams showing only the difference between the actual state of the system and the reference state; these are the Feynman-Goldstone (FG) diagrams. A single particle which appears in the actual state, but not in the reference state, is represented by a "particle" line, with an arrow pointing up; a single particle appearing in the reference state, but not in the actual state, is represented by a "hole" line, with an arrow pointing down.

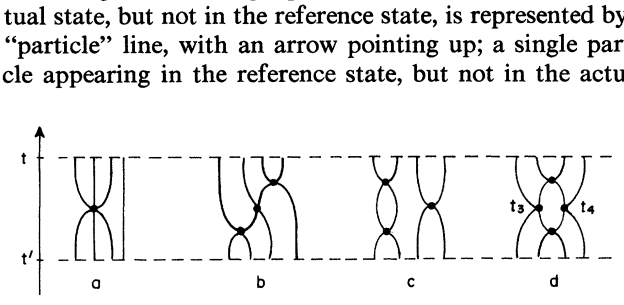

FIG. 3. Four Feynman diagrams occurring in the expansion of $K(t,t')$ for a four-particle system. Diagram (a) contains a three-body interaction; the others contain two-body interactions.

The big difference is that now the reference state, or the Fermi sea, is going to be time dependent. It will be made up of N orthonormal time-dependent single-particle orbitals, each of which is a solution of the time-dependent Schrödinger equation for the time-dependent single-particle Hamiltonian $h_0(t)$. Of course, it has no meaning now to pick the Fermi sea so as to fill the orbitals of lowest energy: the Fermi sea will be picked for convenience, depending on the problem. It may not be at all an approximation to the exact ground state of the system; it is just a convenient reference state.

The rules for calculating these diagrams are similar to the rules for FG diagrams in a time-independent basis, including the sign rule for hole lines and closed loops. There is one exception: The contribution of each line, particle or hole, is just unity; the entire time dependence is included in the matrix elements of the interaction. This has been shown in Sec. II, and the situation would be the same for the usual diagrams with a time-independent basis, if the basis was rendered time dependent by multiplying each eigenstate of H_0, $|\alpha\rangle$, by its harmonic time-dependence $e^{-iE_\alpha t}$. One does not usually do that; however, one includes $e^{-iE_\alpha t}$ with the propagator, and thus it contributes to a line.

Various arguments concerning the one-to-one correspondence between the original Feynman diagram and its FG equivalent, and concerning the Pauli principle, are the same in this case as they were for the time-independent basis.[1] In this latter case, it was also important to distinguish two ways of calculating diagrams: one with individual propagators (one propagator for each line), the other with global propagators (one propagator for each time interval of the whole system). Here this distinction disappears, since the lines do not contribute anything; all that remains is a question of limits of time integrations, and the number of diagrams to be dealt with is smaller if those limits are chosen as in the case of individual propagators, which is what was implied in the example of Fig. 3(d).

Some examples of FG diagrams in a time-dependent basis are shown in Fig. 4. The "vacuum-to-vacuum" diagrams 4(a) and (b) are contributions to the amplitude

$$\langle\phi_0(t)|K(t,t')|\phi_0(t')\rangle , \tag{10}$$

where $\phi_0(t)$ is the time-dependent reference state or Fermi sea, and $K(t,t')$ is the exact propagator. The "blank" diagram part of (10), i.e.,

$$\langle\phi_0(t)|K_0(t,t')|\phi_0(t')\rangle , \tag{11}$$

where $K_0(t,t')$ is the unperturbed propagator, is just equal to unity. The numerical value of diagram 4(a) is

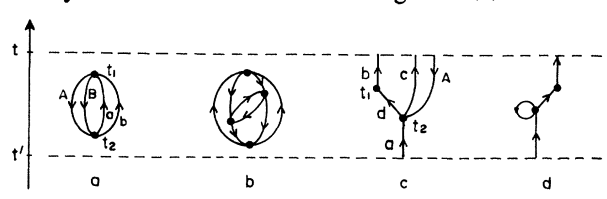

FIG. 4. Examples of unlabeled and labeled time-dependent based Feynman-Goldstone diagrams.

$$\frac{1}{4}\sum_{abAB}(-i)^2\int_{t'}^{t}dt_1\int_{t'}^{t_1}dt_2\langle A(t_1)B(t_1)\,|\,\tilde{V}\,|\,a(t_1)b(t_1)\rangle\langle a(t_2)b(t_2)\,|\,\tilde{V}\,|\,A(t_2)B(t_2)\rangle\ , \tag{12}$$

where $a,b,\ldots,$ are time-dependent unperturbed particle states, $A,B,\ldots,$ are hole states, and $\tilde{V}$ is an antisymmetrized two-body interaction, assumed time independent. Diagram 4(c) contributes to the amplitude

$$\langle b(t)c(t)A(t)\,|\,K(t,t')\,|\,a(t')\rangle\ . \tag{13}$$

Its numerical value is[3]

$$-\sum_{d}(-i)^2\int_{t'}^{t}dt_1\int_{t'}^{t_1}dt_2\langle b(t_1)\,|\,U(t_1)\,|\,d(t_1)\rangle\langle d(t_2)c(t_2)\,|\,\tilde{V}\,|\,a(t_2)A(t_2)\rangle\ , \tag{14}$$

where $U(t)$ is an assumed time-dependent one-body perturbation.

V. FIRST APPLICATION: THE TIME-DEPENDENT HARTREE-FOCK APPROXIMATION AND ITS CORRECTIONS

For this application, the total Hamiltonian is time independent and consists of a one-body kinetic energy K and a two-body interaction V,

$$H=K+V\ . \tag{15}$$

The idea is to have a *time-dependent one-body mean-field* $U(t)$ which one includes in the unperturbed Hamiltonian. Thus, one writes

$$H=H_0(t)+H_1(t)\ , \tag{16}$$

with

$$\begin{aligned}H_0(t)&=K+U(t)\ ,\\ H_1(t)&=V-U(t)\ .\end{aligned} \tag{17}$$

One determines $U(t)$ by demanding some convenient diagram cancellations. The simplest cancellation to ask for is that of Fig. 5 where the one-body vertex represents the $-U(t)$ part of $H_1(t)$. This means that all "Goldstone bubbles" and all $-U(t)$ vertices disappear from all FG diagrams, except for the two first order diagrams whose total cancellation is prevented by a factor $\frac{1}{2}$ in the "double bubble" (Fig. 6).

The algebraic expression of this cancellation is

$$\langle\beta(t)\,|\,U(t)\,|\,\alpha(t)\rangle=\sum_{A}\langle\beta(t)A(t)\,|\,\tilde{V}\,|\,\alpha(t)A(t)\rangle\ , \tag{18}$$

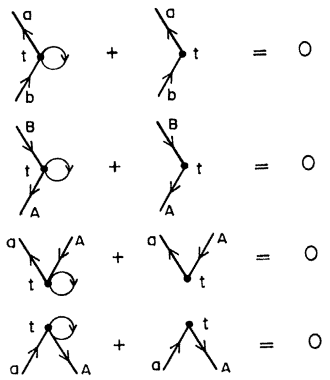

FIG. 5. Diagrammatic definition of the time-dependent Hartree-Fock one-body mean field.

where the sum extends over all hole states (all states of the Fermi sea) and α and β designate either particle or hole states. The single-particle basis is made up of solutions of the time-dependent Schrödinger equation for $H_0(t)$. In view of (18), this equation is

$$\begin{aligned}i\frac{d}{dt}\,|\,\alpha(t)\rangle&=K\,|\,\alpha(t)\rangle\\ &\quad+\sum_{\beta A}|\,\beta(t)\rangle\langle\beta(t)A(t)\,|\,\tilde{V}\,|\,\alpha(t)A(t)\rangle\ ,\end{aligned} \tag{19}$$

where the summation over β runs over the complete set, particles plus holes. This is just the time-dependent Hartree-Fock (TDHF) equation.

Thus, we have a perturbation formalism for which TDHF is the zeroth order. Corrections to TDHF can be obtained to any desired order by calculating the corresponding diagrams.

VI. FURTHER APPLICATIONS

The applications of this method are numerous and far ranging, extending much beyond the boundaries of nuclear physics. In the following paper, we begin to examine the use of periodic TDHF solutions to calculate energy levels associated with collective motion. Corrections to TDHF will be presented in later papers. Work has also been done on the description of highly collective scattering problems, such as collisions between heavy ions.

We shall not, at this point, try to make a definitive comparison with the method of functional integrals.[4] Let us just say that many things which have been derived by functional integrals can also be derived this way, and that the systematic calculation of corrections to a mean field approximation is often easier by the present method.

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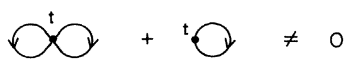

FIG. 6. The two noncanceling, first-order diagrams in the TDHF approximation. The first one involves a pair of equivalent hole lines, hence a $\frac{1}{2}$ symmetry factor.

[1]M. Baranger, in *Proceedings in the International School of Physics Enrico Fermi, Course 40, Varenna, 1967,* edited by M. Jean (Academic, New York, 1969).

[2]J. Goldstone, Proc. Phys. Soc. London, A 239, 267 (1957).

[3]M. B. Johnson and M. Baranger, Ann. Phys. (N.Y.) 62, 172 (1971).

[4]S. Levit, J. W. Negele, and Z. Paltiel, Phys. Rev. C 21, 1603 (1980); J. W. Negele, in *Proceedings in the International School of Physics Enrico Fermi, Course 77, Varenna, 1979,* edited by R. A. Broglia and R. A Ricci (North-Holland, Amsterdam, 1981); Rev. Mod. Phys. 54, 913 (1982).