Parquet notes

April 23, 2009

0.1 Formalism

0.1.1 vertex functions

These perturbative expansions attempt to describe all the scattering processes that take place in the system as one- or two-particle Feynman diagrams. In the one-particle formalism the self-energy describes the many-body processes that renormalize the motion of a particle in the interacting background of all the other particles. In the two particle context, with the aid of the parquet formalism, one is able to probe the interactions between particles in greater detail using the so-called vertex functions, which are matrices describing the two particle scattering processes. For example, the reducible two-particle vertex $F_h^{ph}(12;34)$ describes the amplitude of a particle-hole pair scattered from its initial state $|3,4>$ into the final state $|1,2>$. Here, $i = 1,2,3,4$ represents a set of indices which combines the momentum $\mathbf{k}_i$, the matsubara frequency $i\omega_{n_i}$ and, if needed, the spin σ_i and band index m_i.

In general, depending on how particles or holes are involved in the scattering processes, one can define three different two-particle scattering channels. These are the particle-hole (p-h) horizontal channel, the p-h vertical channel and the particle-particle (p-p) channel. For the Hubbard model, the spin degree of freedom further divides the particle-particle channel into triplet and singlet channels while the particle-hole is divided into density and magnetic channels.

One can further differentiate the vertices on the basis of their topology. Then one would end up with the reducible vertex noted F, the irreducible vertex Γ corresponding to a subclass of diagrams in F that can not be separated in two by breaking two horizontal Green's function lines, and the fully irreducible vertex which corresponds to the subclass of diagrams in Γ that can not be split in two parts by breaking two vertical Green's function lines. An illustration of these different types of vertices is provided in figure 1.

The Pauli exclusion principle produces the so-called crossing symmetries which in turn yields a relationship between these vertices in the different channels. This enables us to reduce the independent channels defined for the theory to the particle-particle and the particle-hole horizontal channel. The different classes of vertices are related by a set of equations which we will discuss next.

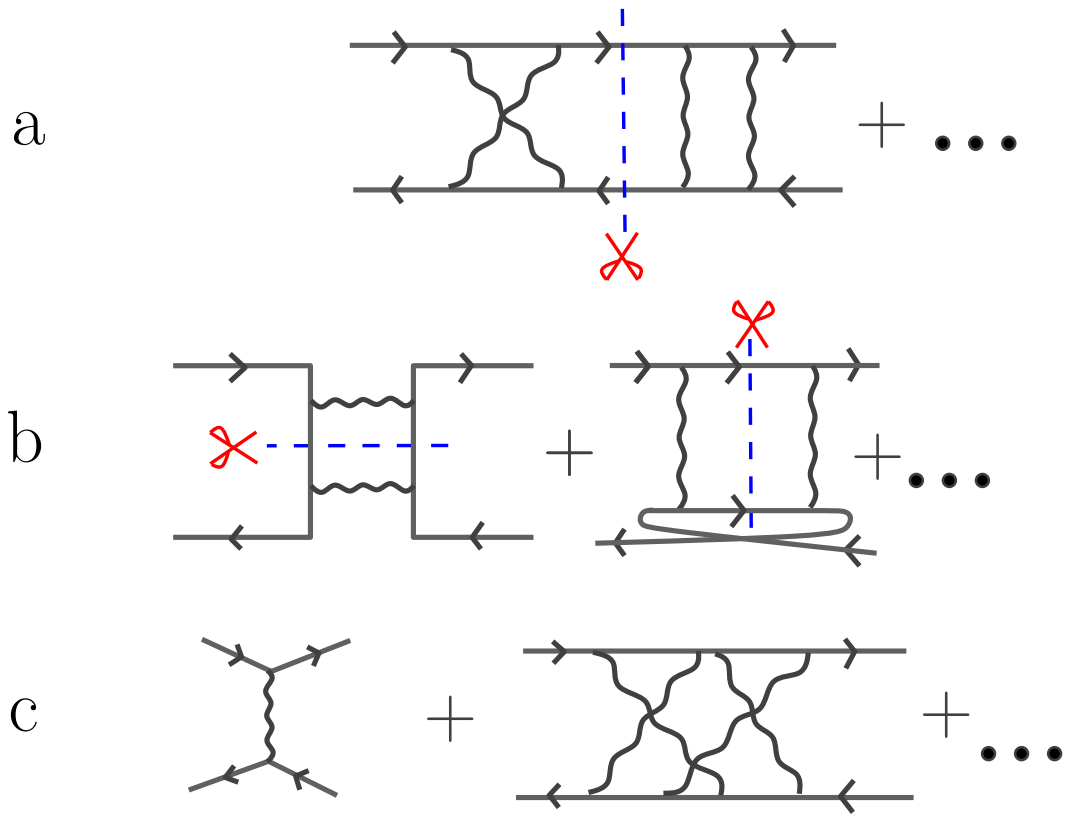

Figure 1: different classes of diagrams; the solid line represents the single particle Green's function and the wavy line represents the Coulomb interaction: here we use the p-h horizontal channel for illustration (a) reducible diagrams: can be separated into two parts by breaking two horizontal Green's function lines, (b) irreducible diagrams: can only be separated in two parts by breaking two Green's function lines in the other two channels, (c) fully irreducible diagrams : can not be split in two parts by breaking two Green's function lines in any channel

0.1.2 equations

The parquet formalism is self-consistent at both the one- and two-particle levels. The connection between the one- and two-particle quantities is through the Schwinger-Dyson equation which connects the reducible vertex F to the self-energy Σ. It is an exact equation derived

from the equation of motion and has the following form:

$$\begin{aligned}\Sigma(P) &= -\frac{UT^2}{4N}\sum_{P',Q}\{G(P')G(P'+Q)G(P-Q)(F_d(Q)_{P-Q,P'} - F_m(Q)_{P-Q,P'}) \\ &\quad +G(-P')G(P'+Q)G(-P+Q)(F_s(Q)_{P-Q,P'} + F_t(Q)_{P-Q,P'})\} \quad (1)\end{aligned}$$

where G is the single-particle Green's function, which itself can be calculated from the self-energy using the Dyson's equation:

$$G^{-1} = G_0^{-1} \; - \; \Sigma \quad (2)$$

The reducible and the irreducible vertices in a given channel are related by the Bethe-Salpeter equation. It has the following form:

$$F_{d/m}(Q)_{P,P'} = \Gamma_{d/m}(Q)_{P,P'} + \Phi_{d/m}(Q)_{P,P'} \quad (3)$$

$$F_{s/t}(Q)_{P,P'} = \Gamma_{s/t}(Q)_{P,P'} + \Psi_{s/t}(Q)_{P,P'} \quad (4)$$

where $r = d/m$ for the density and magnetic channels respectively and $r' = s/t$ for the singlet and triplet channels, and we are using the vertex ladders which are defined as:

$$\Phi_{d/m}(Q)_{P,P'} \equiv \sum_{P''} F_{d/m}(Q)_{P,P''}\chi_0^{ph}(Q)_{P''}\Gamma_{d/m}(Q)_{P'',P'} \quad (5)$$

$$\Psi_{s/t}(Q)_{P,P'} \equiv \sum_{P''} F_{s/t}(Q)_{P,P''}\chi_0^{pp}(Q)_{P''}\Gamma_{s/t}(Q)_{P'',P'} \quad (6)$$

χ_0 is the direct product of two single-particle Green's functions and is defined according to the particle-particle or the particle-hole channel.

In a similar manner, the irreducible vertex and the fully irreducible vertex are related by the parquet equation. This expresses the fact that the irreducible vertex in a given channel is still reducible in the other two channels. The parquet equation has the following form in the different channels:

$$\begin{aligned}\Gamma_d(Q)_{PP'} &= \Lambda_d(Q)_{PP'} - \frac{1}{2}\Phi_d(P'-P)_{P,P+Q} - \frac{3}{2}\Phi_m(P'-P)_{P,P+Q} \\ &\quad + \frac{1}{2}\Psi_s(P+P'+Q)_{-P-Q,-P} + \frac{3}{2}\Psi_t(P+P'+Q)_{-P-Q,-P} \quad (7)\\ \Gamma_m(Q)_{PP'} &= \Lambda_m(Q)_{PP'} - \frac{1}{2}\Phi_d(P'-P)_{P,P+Q} + \frac{1}{2}\Phi_m(P'-P)_{P,P+Q} \\ &\quad - \frac{1}{2}\Psi_s(P+P'+Q)_{-P-Q,-P} + \frac{1}{2}\Psi_t(P+P'+Q)_{-P-Q,-P} \quad (8)\end{aligned}$$

$$\Gamma_s(Q)_{PP'} = \Lambda_s(Q)_{PP'} + \frac{1}{2}\Phi_d(P'-P)_{-P',P+Q} - \frac{3}{2}\Phi_m(P'-P)_{-P',P+Q} + \frac{1}{2}\Phi_d(P+P'+Q)_{-P',-P} - \frac{3}{2}\Phi_m(P+P'+Q)_{-P',-P} \quad (9)$$

$$\Gamma_t(Q)_{PP'} = \Lambda_t(Q)_{PP'} + \frac{1}{2}\Phi_d(P'-P)_{-P',P+Q} + \frac{1}{2}\Phi_m(P'-P)_{-P',P+Q} - \frac{1}{2}\Phi_d(P+P'+Q)_{-P',-P} - \frac{1}{2}\Phi_m(P+P'+Q)_{-P',-P} \quad (10)$$

The Bethe-Salpeter equation and parquet equations are also exact and derived from the categorization of the Feynman diagrams.

The above description of the formalism is far from being exhaustive and is given for this paper to be reasonably self-contained. For a more detailed description of the parquet formalism, we refer the reader to Bickers et al [2][3]. Our goal is to solve these equations self-consistently for the Hubbard model on a two dimensional cluster. The algorithm for this solution is described in the next section.

0.2 Algorithm and computational challenge

The set of equations dicussed above are solved self-consistently as illustrated in the self-consistency loop in figure 2. One starts with a guess of the one-particle Green's function or self-energy. This can be taken from the second order approximation. The reducible and the irreducible vertices are also initialized with the bare interaction. The self-consistency loop can then be described as follows:
(i) first we calculte the bare susceptibility χ_0 which is just the product of two Green's functions
(ii) next this bare susceptibility is used to calculate F through the Bethe-Salpeter equation
(iii) we then proceed with solving the parquet equation which enables us to update the irreducible vertex Γ. This step requires the input of the fully irreducible vertex Λ which in the context of the parquet approximation is simply taken to be the bare interaction. It can also be derived from some more sophisticated methods.
(iv) it is followed by a calculation of the new F through the Bethe-Salpeter equation
(v) this value of F is then used to update the self-energy through the Schwinger Dyson equation
(vi) the Dyson's equation is then solved for the Green's function G.
This loop is repeated until convergence of the self-energy Σ is achieved within a reasonable criterion.

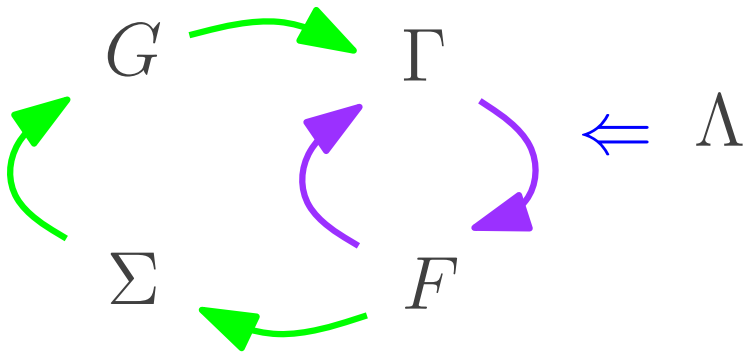

Figure 2: self-consistency loop

Unfortunately, this loop becomes unstable when the Coulomb interaction strength is increased or the temperature is lowered. This leads us to use some variations of the above scheme. One possibility is to start with an overestimated self-energy and to damp it along with the irreducible vertex between two iterations according to:

$$\Sigma = \alpha_1 \Sigma_{new} + (1 - \alpha_1)\Sigma_{old} \quad (11)$$

$$\Gamma = \alpha_2 \Gamma_{new} + (1 - \alpha_2)\Gamma_{old} \quad (12)$$

where α_1 and α_2 are some damping parameters.

The other possibility is to rewrite the coupled Bethe-Salpeter and parquet equations in the form of a Newton fixed-point problem. Then we can take advantage of the existing linear solvers such as BiCGS [7] or GMRES [6].

One major advantage that the parquet formalism has over Exact Diagonalization (ED) or Quantum Monte Carlo (QMC) is that it scales algebraically with the volume of the system in space-time as one can readily observe. The most time-consuming part of the formalism is the solution of the Bethe-Salpeter and the parquet equations, where the computational time scales as $O(nt^4)$ where $n_t = n_c \times n_f$, n_c being the number of sites on the cluster and n_f the number of Matsubara frequencies . Although the scaling is better than that of ED or QMC, one can see that when the system size grows, the problem quickly grows beyond the capacity of the usual desktops and becomes suitable for a distribution on a large number of processors on a supercomputer.

Our parallel scheme and our data distribution are based on the realization that the Bethe Salpeter equation is the most time-consuming part of our calculation. One can easily see that it decouples nicely with respect to the bosonic momentum-frequency index Q. This enables us to distribute the vertices across processors with respect to this third index and to solve the

Bethe-Salpeter equation with a local matrix inversion. However, this storage scheme puts a limit on the size of the problem that we can address. For a node with $2G$ of memory, the maximum value of n_t that we can use if our variables are complex double precision is about 2500. Unlike the Bethe-Salpeter equation, one can readily observe that the parquet equation doesn't decouple in terms of the third index. Solving this equation requires a rearrangement of the matrix elements across processors and this is the communication bottleneck in the algorithm. The rearrangement is necessary to obtain the form of the vertex ladder Φ or Ψ that is necessary in the parquet equation. For instance, in the d channel, we need $\Phi\left(P-P'\right)_{P,P+Q}$. This form of the vertex ladder is obtained in the three-step process described in equations 13, 14 and 15.

$$\Phi\left(Q\right)_{P,P'} \implies \Phi\left(Q\right)_{P,P-P'} \tag{13}$$
$$\Phi\left(Q\right)_{P,P-P'} \implies \Phi\left(P-P'\right)_{P,Q} \tag{14}$$
$$\Phi\left(P-P'\right)_{P,Q} \implies \Phi\left(P-P'\right)_{P,P+Q} \tag{15}$$

The first step in this transformation only moves data locally in memory. This doesn't require much time. The second step is actually just a 2D matrix transpose but with matrix elements spread on many nodes. This is where communication across nodes is required. It is achieved by using the standard MPI collective directives. The final step is also local and can equally be done very fast.

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