Hedin's equations and enumeration of Feynman diagrams

L. G. Molinari*

Dipartimento di Fisica dell'Università degli Studi di Milano and I.N.F.N. sezione di Milano, Via Celoria 16, I-20133 Milano, Italy (Received 17 September 2004; published 17 March 2005)

Hedin's equations are solved perturbatively in zero dimension to count Feynman graphs for self-energy, polarization, propagator, effective potential and vertex function in a many-body theory of fermions with two-body interaction. Counting numbers are also obtained in the *GW* approximation.

DOI: 10.1103/PhysRevB.71.113102

PACS number(s): 71.10.-w, 24.10.Cn, 11.10.Gh

I. INTRODUCTION

Consider a system of fermions described by the Hamiltonian $H = \sum_{i} h(i) + \sum_{i < i} v(i, j)$, where h is a single-particle operator and v is the two-particle interaction. In general, to obtain dressed correlators that describe quasiparticles and collective excitations, one must sum over classes of diagrams of all orders of perturbation theory in v. The random phase approximation for the effective potential or the ladder expansion for the vertex and the T matrix are two well known examples.¹ Iterative schemes are used in conserving approximations for the self-energy.^{2,3} The perturbative treatment of the electron gas requires a mixed approach, with partial resummations; a late step in the long history of the r_s expansion of correlation energy is the evaluation of third order diagrams.⁵ In these cases, it might be useful, or at least interesting, to know in advance how many diagrams are required at each order of the approximation, and how many are left out. The counting problem is much simpler than the original one, and is obtained by translating the recursive equations at hand to zero dimension. Properties other than loop content or perturbative numbers may also be evaluated: a notable example is diagram enumeration according to their topologies, that can be mapped to models of statistical mechanics on random lattices.4

In this report, I show how Feynman diagrams can be enumerated for the exact theory and its *GW* approximation. A useful starting point is the set of five Hedin's equations⁶ for the propagator G(1,2), the effective potential W(1,2), the proper self-energy $\Sigma(1,2)$, the polarization $\Pi(1,2)$, and the vertex $\Gamma(1;2,3)$

$$G(1,2) = g(1,2) + g(1,1')\Sigma(1',2')G(2',2),$$
(1)

$$W(1,2) = v(1,2) + v(1,1')\Pi(1',2')W(2',2), \qquad (2)$$

$$\Sigma(1,2) = i\Gamma(2';1,1')G(1',2)W(2',2), \tag{3}$$

$$\Pi(1,2) = -2i\Gamma(1;2',2'')G(2,2')G(2'',2), \qquad (4)$$

 $\Gamma(1;2,3) = \delta(1,2)\delta(1,3)$

+
$$\Gamma(1;2',3')G(2'',2')G(3',3'')\frac{\delta\Sigma(2,3)}{\delta G(2'',3'')}.$$
 (5)

Repeated primed space-time and internal variables are hereafter understood to be summed or integrated. g(1,2) is the Green function of the interacting system in the Hartree approximation, with exact particle density, so that Hartree-type insertion (tadpoles) is already accounted for. In the vertex equation, the Bethe–Salpeter kernel⁷ is specified as a functional derivative in the same quantities involved. Therefore, the five exact Hedin's equations are formally closed. A different functional closure of Schwinger–Dyson equations, leading to diagrammatic recursion schemes, was developed by Kleinert *et al.*^{8,9}

It is useful to restate Eq. (5) with the Hartree propagator g replacing the exact one, G

$$\Gamma(1;2,3) = \delta(1,2)\,\delta(1,3) + g(1',1)g(1,1'')\frac{\delta\Sigma(2,3)}{\delta g(1',1'')}.\tag{6}$$

It states that vertex diagrams are obtained from self-energy ones through the insertion of a bare vertex in a Hartree propagator line, in all possible ways. A derivation is given in the end. The formula can be advantageous when the selfenergy is approximated by some explicit expression of g and v, which are the free functional variables of the many-body problem.

To cope with the vertex equation is a formidable task.^{10,11} A strong nontrivial simplification is the *GW* approximation (*GWA*), where all corrections to the bare vertex $\Gamma^{(0)}(1;2,3) = \delta(1,2) \delta(1,3)$ are ignored. Eqs. (1)–(4), with Γ_0 replacing Γ , then become a closed set of integral equations.^{12,13}

The upmost difficulty of the problem of solving Hedin's or *GW* equations, vanishes in zero dimension of space-time, where the perturbative solution in the interaction v is a mean to count Feynman diagrams. The constraint of no Hartree-type insertions makes this approach much simpler than the usual one, based on the functional integral.^{14,15} Counting numbers are also evaluated in the *GWA*, and the omission of vertex corrections makes the number of diagrams grow with a power law, instead of factorially.

II. COUNTING FEYNMAN DIAGRAMS

In zero dimension of space-time, the four Hedin's Eqs. (1)–(4) become algebraic, with variables g and v, and the functional derivative in the vertex Eq. (6) is an ordinary one. After removing imaginary factors and replacing the factor (-2), due to the fermionic loop and spin summation, with a parameter ℓ that counts the same loops, Hedin's equations are

$$G = g + g\Sigma G, \quad W = v + v\Pi W, \tag{7}$$

$$\Sigma = GW\Gamma, \quad \Pi = \ell G^2 \Gamma, \quad \Gamma = 1 + g^2 \frac{\partial \Sigma}{\partial g}.$$
 (8)

By searching solutions as series expansions in the variables v and ℓ , one obtains coefficients that count all Feynman graphs, with weight one, that contribute to a perturbative order (specified by the power of v), with a given number of fermionic loops (the power of ℓ). I begin by solving for the self-energy. Elimination of G, W and Π gives

$$\Sigma (1 - g\Sigma)^2 = gv\Gamma[1 - (1 - \ell)g\Sigma].$$
(9)

It is useful to consider adimensional quantities, $\Sigma = gvs(x)$ and $x = g^2v$. After use of the equation for Γ one obtains a differential equation for s(x)

$$s(1-xs)^2 = \left(1+xs+2x^2\frac{\partial s}{\partial x}\right)\left[1-xs(1-\ell)\right].$$
 (10)

There is no standard solution of this (Abel) equation. The perturbative expansion is evaluated

$$\Sigma/vg = 1 + (2+\ell)x + (10+9\ell+\ell^2)x^2 + (74+91\ell+23\ell^2+\ell^3)x^3 + (706+1063\ell+416\ell^2+46\ell^3+\ell^4)x^4 + (8162+14193\ell+7344\ell^2+1350\ell^3+80\ell^4+\ell^5)x^5 + \dots$$
(11)

$$=1 + 3x + 20x^{2} + 189x^{3} + 2232x^{4} + 31130x^{5} + \dots$$
 (12)

The last line corresponds to $\ell = 1$. For example, in Eq. (12) we read that at order v^3 there are 20 self-energy diagrams; Eq. (11) gives the more detailed information that ten graphs come with no fermion loop, nine with a single loop and one with two loops. At each perturbative order there is a single diagram with the largest number of loops; the sum of such diagrams yields the ring approximation¹ $\Sigma_r = igW_r$, where the effective potential W_r is evaluated with ring insertions $\Pi_r = -2ig^2$.

The expansions for the vertex and the polarization are then obtained (I omit the propagator and the effective potential)

$$\Gamma = 1 + x + (6 + 3\ell)x^{2} + (50 + 45\ell + 5\ell^{2})x^{3}$$

+ (518 + 637\ell + 161\ell^{2} + 7\ell^{3})x^{4}
+ (6354 + 9567\ell + 3744\ell^{2} + 414\ell^{3} + 9\ell^{4})x^{5} + \dots(13)

$$=1 + x + 9x^{2} + 100x^{3} + 1323x^{4} + 20088x^{5}$$
(14)

$$\Pi/g^{2}\ell = 1 + 3x + (15 + 5\ell)x^{2} + (105 + 77\ell + 7\ell^{2})x^{3} + (945 + 1044\ell + 234\ell^{2} + 9\ell^{3})x^{4} + (10395 + 14784\ell + 5390\ell^{2} + 550\ell^{3} + 11\ell^{4})x^{5} + \dots$$
(15)

$$=1 + 3x + 20x^{2} + 189x^{3} + 2232x^{4} + 31130x^{5} + \dots$$
 (16)

Note that the counting numbers for the $\ell = 1$ expansions (12) and (16) of the self-energy and the polarization are the same. This occurs also in Q.E.D. though with smaller counting numbers, due to the cancellation of pairs of diagrams which differ by orientation of a fermionic loop with an odd number of propagators (Furry's theorem).¹⁶

I now evaluate the counting numbers in the *GWA*, which corresponds to $\Gamma = 1$ in Eq. (9). The equation for the self-energy becomes algebraic cubic, with solution

$$\Sigma_{GW}/vg = 1 + (1+\ell)x + (2+4\ell+\ell^2)x^2 + (5+15\ell+9\ell^2+\ell^3)x^3 + (14+56\ell+56\ell^2+16\ell^3+\ell^4)x^4 + (42+210\ell+300\ell^2+150\ell^3+25\ell^4+\ell^5)x^5 + \dots$$
(17)

$$=1 + 2x + 7x^{2} + 30x^{3} + 143x^{4} + 728x^{5} + \dots$$
 (18)

(20)

For $\ell = 1$, the cubic equation is $s(1-sx)^2 = 1$. By solving for the inverse function, $x(s) = s^{-1} - s^{-3/2}$, one locates a singular point for s'(x) in $x_c = 4/27$. The finite radius of convergence for the perturbative series (18) in *GWA* implies that the number of self-energy diagrams of order *n* grows with the power law $(27/4)^n$. In *GWA* the vertex function is trivial, and the polarization $\Pi_{GW} = -2iG_{GW}^2$ is the *GW*-dressed ring diagram

$$\Pi_{GW}/g^{2}\ell = 1 + 2x + (5 + 2\ell)x^{2} + (14 + 14\ell + 2\ell^{2})x^{3} + (42 + 72\ell + 27\ell^{2} + 2\ell^{3})x^{4} + (132 + 330\ell + 220\ell^{2} + 44\ell^{3} + 2\ell^{4})x^{5} + \dots$$
(19)

$$=1+2x+7x^2+30x^3+143x^4+728x^5+\ldots$$

The $\ell = 1$ expansions for the self-energy and the polarization are again the same, as one can show that Π/g^2 and *s* solve the same cubic equation.

By translating to zero dimension a closed system of equations for many-body correlators, one may enumerate the Feynman diagrams involved. I have shown this for the full theory of interacting fermions and the GW approximation, with the rule that a line is a Hartree propagator.

ACKNOWLEDGMENTS

This work was funded in part by the EU's 6th Framework Programme through the NANOQUANTA Network of Excellence (NMP4-CT-2004-500198)

APPENDIX A

I show that the vertex Eq. (5) can be written in the form (6); the simple proof is a modification of Hedin's construc-

tion, to which I refer. I recall the definition of the vertex function

$$\Gamma(1;2,3) = \delta(1,2)\,\delta(1,3) + \frac{\delta\Sigma(2,3)}{\delta V(1)}.$$
 (A1)

The potential *V* is the sum of an external potential (which is turned off at the end) and the Hartree potential $\int d2v(1,2)n(2)$, built with the exact particle density. Hedin's formula is obtained by writing the functional derivative in *V*, through the chain rule, as a derivative in the exact Green function *G*. It is admissible to do so in terms of *g*

$$\frac{\delta\Sigma(2,3)}{\delta V(1)} = \frac{\delta\Sigma(2,3)}{\delta g(1',1'')} \frac{\delta g(1',1'')}{\delta V(1)}$$

From the Hartree equation $(i\partial(t'_1) - h(1') - V(1'))g(1', 1'') = \delta(1', 1'')$, one evaluates the required functional derivative $\delta g(1', 1'') / \delta V(1) = g(1', 1)g(1, 1'')$. This ends the proof.

*Electronic address: luca.molinari@mi.infn.it

- ¹G. D. Mahan, *Many-Particle Physics*, 3rd ed. (Kluwer/Plenum, New York, 2000).
- ²Y. Takada, Phys. Rev. B **52**, 12 708 (1995).
- ³A. Schindlmayr, P. García-González, and R. W. Godby, Phys. Rev. B **64**, 235106 (2001).
- ⁴G. 'tHooft, Nucl. Phys. B **538**, 389 (1999).
- ⁵T. Endo, M. Horiuchi, Y. Takada, and H. Yasuhara, Phys. Rev. B **59**, 7367 (1999).
- ⁶L. Hedin, Phys. Rev. **139**, A796 (1965).
- ⁷J. D. Bjorken and S. D. Drell, *Relativistic Quantum Fields* (McGraw–Hill, New York, 1965), chap. 19.
- ⁸A. Pelster, H. Kleinert, and M. Bachmann, Ann. Phys. **297**, 363 (2002).
- ⁹A. Pelster and K. Glaum, Phys. Status Solidi B 237, 72 (2003).

- ¹⁰A. Schindlmayr and R. W. Godby, Phys. Rev. Lett. **80**, 1702 (1998).
- ¹¹G. Onida, L. Reining, and A. Rubio, Rev. Mod. Phys. **74**, 601 (2002).
- ¹²W. G. Aulbur, L. Jönsson, and J. W. Wilkins, *Solid State Physics*, edited by H. Ehrenreich and F. Spaepen (Academic, New York, 2000), Vol. 54.
- ¹³F. Aryasetiawan and O. Gunnarsson, Rep. Prog. Phys. **61**, 237 (1998).
- ¹⁴P. Cvitanovic, B. Lautrup, and R. B. Pearson, Phys. Rev. D 18, 1939 (1978).
- ¹⁵E. N. Argyres, A. F. W. van Hameren, R. H. P. Kleiss, and C. G. Papadopoulos, Eur. Phys. J. C **19**, 567 (2001).
- ¹⁶C. Itzykson and J. B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980), p. 466.