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A differential identity for Green functions

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Abstract

If P is a differential operator with constant coefficients, an identity is derived to calculate the action of e^P on the product of two functions. In many-body theory, P describes the interaction Hamiltonian and the identity yields a hierarchy of Green functions. The identity is first derived for scalar fields and the standard hierarchy is recovered. Then the case of fermions is considered and the identity is used to calculate the generating function for the Green functions of an electron system in a time-dependent external potential.

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1 Introduction

In spite of immense progress in the calculation of the properties of materials, some of them are still beyond our computational power. Systems containing both localized and delocalized electrons often belong to these hard problems. A particularly conspicuous example is the optical spectrum of molecules and solids containing transition metals. Brute force calculations involving a large number of configurations do not give satisfactory results for the colour of such familiar materials as blood [1] or grass [2]. In the solid state, non-perturbative Green function methods using the Bethe-Salpeter equation proved accurate for the colour of semiconductors [3, 4, 5] but not for transition metal compounds. On the other hand, the very simple ligand field formalism can be used to calculate the position of the spectral lines [6], but not their intensities. The success of non-perturbative Green function methods for semiconductors and of ligand field theory for the spectral line position makes it desirable to unify the Green function and the ligand field theories. The present paper describes a tool developed for this unification.

The main assumption of the Green function theory is that the eigenstate of the interacting system can be obtained as the adiabatic evolution of the ground state of the non-interacting system and that the latter can be written as a Slater determinant. A similar assumption is present in the Kohn-Sham approach to the density functional theory. On the contrary, the effectiveness of the ligand field approach comes from the fact that *several* initial states are taken into account. The ground state of the interacting system is then obtained by diagonalising an effective Hamiltonian representing the effect of the electron-electron interaction on these initial states [7]. The starting point of our unification is therefore to use non-perturbative Green function methods to set up an effective Hamiltonian for a small number of initial states. The standard Green function method is recovered when the number of initial states is one, the ligand field method is obtained as the first approximation of a hierarchy of equations for the Green functions [8].

To develop this theory, we used a mathematical tool initiated by Schwinger [9] and that was taken up by a few authors [10, 11, 12]. This approach is known as the theory of Green functions for open shells [13] and its development was rather slow because its combinatorial complexity is much larger than in the usual many-body theory. From a graphical point of view, the complexity comes from the fact that the Feynman diagrams must be drawn not only with the usual two-leg Feynman propagator but also with

$2k$-leg "propagators" where k goes from 1 to the number of initial states. These many-leg propagators describe the correlation between initial states. It turns out that quantum group methods are well suited to tame this complexity and help deriving an identity that yields a hierarchy of Green functions for open shells [14]. More precisely, if P is a differential operator with constant coefficients, the identity gives a closed formula for the action of e^P on the product of two functions fg.

For motivation, we show how this identity is used in many-body theory. The Green functions $G(x_1, \ldots, x_n)$ of an interacting system can be obtained from a generating function $Z(j)$ by functional derivatives with respect to the external source $j(x)$ ([15] p.212)

$$G(x_1, \ldots, x_n) \quad = \quad \frac{i^n}{Z} \frac{\delta^n Z}{\delta j(x_1) \ldots \delta j(x_n)}.$$

Therefore, in principle, $Z(j)$ provides a complete information on the system. The generating function $Z(j)$ is usually given by an equation of the type $Z(j) = \mathrm{e}^P \mathrm{e}^{W^0}$, where P is a polynomial in $\delta/\delta j(x)$ (the functional derivative with respect to the external source) and W^0 is a polynomial in j. In standard (i.e. closed shell) Green function theory, W^0 is bilinear in j:

$$W^0 \quad = \quad \frac{i}{2} \int \mathrm{d}x \mathrm{d}y j(x) G^0(x, y) j(y),$$

where $G^0(x, y)$ is the Green function of the non-interacting system. For the Green functions of open shells, the function $W^0(j)$ is a polynomial in j of degree larger than 2. This polynomial describes the initial state of the non-interacting system [16]. When we take the functional derivative of $Z(j)$ with respect to $j(x)$ and we denote $\delta Z(j)/\delta j(x)$ by $Z'(j)$, we find

$$Z'(j) \quad = \quad \frac{\delta}{\delta j(x)} \big(\mathrm{e}^P \mathrm{e}^{W^0}\big) = \mathrm{e}^P \Big(\frac{\delta \mathrm{e}^{W^0}}{\delta j(x)}\Big) = \mathrm{e}^P \big(W_0' \mathrm{e}^{W^0}\big),$$

where $W_0' = \delta W^0(j)/\delta j(x)$. The expression e^P is an infinite sum of differential operators $P^n/n!$ acting on the product $W_0' \mathrm{e}^{W^0}$. The role of the identity is to transform it into a *finite* sum of differential operators acting on $\mathrm{e}^P \mathrm{e}^{W^0} = Z(j)$. In other words, we obtain a non-trivial expression relating $Z'(j)$ to a differential operator D acting on $Z(j)$. This is indeed a hierarchy of Green functions, i.e. a relation between the one-point interacting Green function $Z'(j)$ and some n-point interacting Green functions generated by $DZ(j)$. Such a hierarchy is important because it provides non-perturbative equations that can be used to derive non-perturbative approximations [14]. In ref. [14], the identity was given without proof and no detail was given to explain how the hierarchy follows from the identity. The purpose of the present paper is to fill this gap by proving the main identity and by deriving in detail some of its applications.

The plan of the paper is as follows. After this introduction we show that the action of a differential operator P on a product of two functions fg can be described by a mathematical concept called a *coproduct*. Then we derive our main result which provides a way to calculate $\mathrm{e}^P(fg)$. As a simple application of the basic identity, we derive the hierarchy of Green functions for standard quantum field theory of the scalar field. We also describe the changes that are required when we consider fermions instead of bosons. As an application, we derive in detail the generating function Z in the presence of an external time-dependent potential. We conclude with some possible extensions of the basic identity to non-commutative algebras.

2 The coproduct of a differential operator

In this section we introduce the coproduct of a differential operator with constant coefficients. We start with the case of a one-dimensional problem and generalize it to the d-dimensional case. But first, we define the tensor product of functions and of differential operators, that will be crucial for the definition of the coproduct.

2.1 Tensor product

If f and g are functions of a variable x, the tensor product of f and g, denoted by $f \otimes g$, is a function of two variable defined by $(f \otimes g)(x, y) = f(x)g(y)$. From this definition, it follows that the tensor product

is linear: for any complex number λ and for any functions f, g and h we have $f\otimes(g+h)=f\otimes g+f\otimes h$, $(f+g)\otimes h=f\otimes h+g\otimes h$ and $\lambda(f\otimes g)=(\lambda f)\otimes g=f\otimes(\lambda g)$. Moreover, we can multiply the two tensor products $f\otimes g$ and $f'\otimes g'$ by the rule $(f\otimes g)(f'\otimes g')=(ff')\otimes(gg')$, where $(ff')(x)=f(x)f'(x)$ and $(gg')(y)=g(y)g'(y)$.

If the variable x runs over a d-dimensional space, we call differential operator a finite sum

$$P=\sum_{n_1,\ldots,n_d} a_{n_1\ldots n_d}\frac{\partial^{n_1}}{\partial x_1^{n_1}}\cdots\frac{\partial^{n_d}}{\partial x_d^{n_d}},$$

where $a_{n_1\ldots n_d}$ are complex numbers. If P and Q are differential operators acting on functions of x, the tensor product of P and Q, denoted by $P\otimes Q$ is the operator acting on the tensor product of two functions $f\otimes g$ by

$$(P\otimes Q)(f\otimes g)(x,y) \quad = \quad \big((Pf)\otimes(Qg)\big)(x,y)=(Pf)(x)(Qg)(y).$$

With this definition, it can be checked that the tensor product of differential operators is linear and that we can define the multiplication of tensor products of operators by $(P\otimes Q)(R\otimes S)=(PR)\otimes(QS)$. The tensor product is a familiar object in quantum physics to define an operator acting on a many-body state. For instance, if L is the angular momentum acting on a single particle, the angular momentum acting on two-particle wavefunctions is defined as $L\otimes 1+1\otimes L$.

2.2 The one-dimensional case

If $\partial=\mathrm{d}/\mathrm{d}x$, the action of ∂^n on the product of two functions of x is given by the Leibniz identity

$$\partial^n(fg) \quad = \quad \sum_{k=0}^{n}\binom{n}{k}(\partial^k f)(\partial^{n-k}g).$$

In this definition, the functions f and g are not really important and look more like dummy arguments. The coproduct is a way to calculate $\partial^n(fg)$ without mentioning f and g. The coproduct is denoted by Δ and defined by

$$\Delta\partial^n \quad = \quad \sum_{k=0}^{n}\binom{n}{k}\partial^k\otimes\partial^{n-k}.$$

For example

$$\begin{aligned}\Delta 1 &= 1\otimes 1,\\ \Delta\partial &= \partial\otimes 1+1\otimes\partial,\\ \Delta\partial^2 &= \partial^2\otimes 1+2\partial\otimes\partial+1\otimes\partial^2.\end{aligned}$$

More precisely, the relation between the coproduct and the derivative of fg is given by

$$\partial^n(fg)(x) \quad = \quad (\Delta\partial^n)(f\otimes g)(x,x).$$

At this stage, we need to define more accurately the algebraic structure we are using. Let $\mathcal{A}$ be the algebra of differential operators with constant coefficients (i.e. the algebra of polynomials in the variable ∂). Thus $P\in\mathcal{A}$ if and only if there is a finite number of complex numbers a_n such that $P=\sum_{n\geq 0}a_n\partial^n$. The product in $\mathcal{A}$ is the usual product of polynomials: if $P=\sum_{n\geq 0}a_n\partial^n$ and $Q=\sum_{m\geq 0}b_m\partial^m$ then $PQ=\sum_{n,m\geq 0}a_nb_m\partial^{n+m}$. Thus, $\mathcal{A}$ is a unitary commutative algebra. The coproduct appears when the differential operators act on a product of two functions. It is a linear map $\Delta:\mathcal{A}\to\mathcal{A}\otimes\mathcal{A}$ whose action on an element $P\in\mathcal{A}$ can be written $\Delta P=\sum_i R_i\otimes S_i$, so that $P(fg)=\sum_i(R_if)(S_ig)$. For example, for $P=\partial^2$ the coproduct is a sum of three terms described by $R_1=\partial^2$, $S_1=1$, $R_2=2\partial$, $S_2=\partial$ and $R_3=1$, $S_3=\partial^2$ (note that, by linearity of the tensor product, we can also choose $R_2=\partial$, $S_2=2\partial$). In general, we can use

$$P(fg) \quad = \quad \sum_{n\geq 0}a_n\sum_{k=0}^{n}\binom{n}{k}(\partial^k f)(\partial^{n-k}g),$$

to get

$$\Delta P = \sum_{n\geq 0} a_n \sum_{k=0}^{n} \binom{n}{k} \partial^k \otimes \partial^{n-k}. \tag{1}$$

In other words, the coproduct is just a way to denote which differential operators act on f and on g in $P(fg)$. The introduction of such a concept may look rather pedantic at this stage, but it will allow us to obtain very general results, valid for partial derivatives and even for functional derivatives. Note that the k-th derivative of ∂^n with respect to ∂ is $n!\partial^{n-k}/(n-k)!$ for $n \geq k$ and 0 for $n < k$, so that

$$\Delta P = \sum_{k\geq 0} \frac{\partial^k}{k!} \otimes P^{(k)}, \tag{2}$$

where $P^{(k)}$ is the k-th derivative of P with respect to ∂. The concept of a coproduct is unfamiliar, but it is very useful in quantum theory. For instance, it was needed to calculate matrix elements of many-body operators and density correlations [16]. In this paper we shall see that it is also quite useful to derive non-perturbative equations in Green function theory. We hope that the example of the coproduct of a differential operator makes this concept understandable. For convenience, we shall replace the notation $\Delta P = \sum_i R_i \otimes S_i$ by Sweedler's notation $\Delta P = \sum P_{(1)} \otimes P_{(2)}$, which is more common.

2.3 The d-dimensional case

In the d-dimensional case, we put $\partial_i = \partial/\partial x_i$ and we define the coproduct of $D = \prod_{i=1}^{d} \partial_i^{n_i}$ as

$$\Delta D = \sum_{k_1=0}^{n_1} \cdots \sum_{k_d=0}^{n_d} \binom{n_1}{k_1} \cdots \binom{n_d}{k_d} \partial_1^{k_1} \ldots \partial_d^{k_d} \otimes \partial_1^{n_1-k_1} \ldots \partial_d^{n_d-k_d}.$$

We can even define the coproduct of an infinite dimensional differential operator. If $\mathbf{r}_1, \ldots, \mathbf{r}_p$ are p points, the coproduct of the functional differential operator

$$D = \frac{\delta^{n_1+\cdots+n_p}}{\delta j(\mathbf{r}_1)^{n_1} \ldots \delta j(\mathbf{r}_p)^{n_p}} = \frac{\delta^{n_1}}{\delta j(\mathbf{r}_1)^{n_1}} \cdots \frac{\delta^{n_p}}{\delta j(\mathbf{r}_p)^{n_p}}$$

is defined by

$$\Delta D = \sum_{k_1=0}^{n_1} \cdots \sum_{k_p=0}^{n_p} \binom{n_1}{k_1} \cdots \binom{n_p}{k_p} \frac{\delta^{k_1+\cdots+k_p}}{\delta j(\mathbf{r}_1)^{k_1} \ldots \delta j(\mathbf{r}_p)^{k_p}} \otimes \frac{\delta^{n_1-k_1+\cdots+n_p-k_p}}{\delta j(\mathbf{r}_1)^{n_1-k_1} \ldots \delta j(\mathbf{r}_p)^{n_p-k_p}}.$$

2.4 Algebra morphism

Up to now, the coproduct is just a linear map from $\mathcal{A}$ to $\mathcal{A} \otimes \mathcal{A}$. The coproduct becomes a powerful tool if it has a property called *algebra morphism*. The coproduct is an algebra morphism if $\Delta 1 = 1 \otimes 1$ and, for any P and Q in $\mathcal{A}$, $\Delta(PQ) = (\Delta P)(\Delta Q)$ or, more explicitly

$$\begin{aligned} \Delta(PQ) &= \sum (PQ)_{(1)} \otimes (PQ)_{(2)} = \sum (P_{(1)} Q_{(1)}) \otimes (P_{(2)} Q_{(2)}) \\ &= \big(\sum P_{(1)} \otimes P_{(2)}\big)\big(\sum Q_{(1)} \otimes Q_{(2)}\big). \end{aligned}$$

To show that the coproduct of the algebra of differential operators is an algebra morphism, we consider for notational convenience the one-dimensional case. If we take $P = \partial^n$ and $Q = \partial^m$, then $PQ = \partial^{n+m}$ and

$$\begin{aligned} \Delta(PQ) &= \sum_{i=0}^{m+n} \binom{n+m}{i} \partial^i \otimes \partial^{n+m-i} = \sum_{k=0}^{n} \sum_{l=0}^{m} \binom{n}{k} \binom{m}{l} \partial^{k+l} \otimes \partial^{n+m-k-l} \\ &= \Big(\sum_{k=0}^{n} \binom{n}{k} \partial^k \otimes \partial^{n-k}\Big)\Big(\sum_{l=0}^{m} \binom{m}{l} \partial^l \otimes \partial^{m-l}\Big) = (\Delta P)(\Delta Q), \end{aligned}$$

where we used the Vandermonde convolution formula $\sum_{k+l=i} \binom{n}{k}\binom{m}{l} = \binom{n+m}{i}$. The d-dimensional case is proved similarly.

2.5 Reduced coproduct

For any element P of $\mathcal{A}$, the reduced coproduct of P is defined by

$$\underline{\Delta}P \quad = \quad \Delta P - P \otimes 1 - 1 \otimes P.$$

For example: $\underline{\Delta}\partial = 0$, $\underline{\Delta}\partial^2 = 2\partial \otimes \partial$,

$$\underline{\Delta}\partial^n \quad = \quad \sum_{k=1}^{n-1} \binom{n}{k} \partial^k \otimes \partial^{n-k},$$

for $n > 1$. We denote the reduced coproduct of P by $\underline{\Delta}P = \sum P_{(\underline{1})} \otimes P_{(\underline{2})}$. If the polynomial P is such that $P(0) = 0$, its coproduct ΔP contains the terms $P \otimes 1$ and $1 \otimes P$. The purpose of the reduced coproduct is to eliminate these terms. As a result of this operation, the degree of $P_{(\underline{1})}$ and $P_{(\underline{2})}$ is always greater than 0 and smaller than the degree of P.

3 The main identity

In this section, we prove the identity from which we can derive, among other things, the hierarchy of Green functions. Although this identity provides a powerful method to resum infinities of Feynman diagrams of the perturbation theory, its proof is very simple.

Proposition 3.1. *If $\mathcal{A}$ is a commutative algebra equipped with a coproduct Δ that is an algebra morphism and if $P \in \mathcal{A}$ then*

$$\Delta(\mathrm{e}^P) \quad = \quad \mathrm{e}^{\underline{\Delta}P}\big(\mathrm{e}^P \otimes \mathrm{e}^P\big), \tag{3}$$

where $\underline{\Delta}P = \Delta P - P \otimes 1 - 1 \otimes P$ and

$$\mathrm{e}^{\underline{\Delta}P} \quad = \quad 1 \otimes 1 + \sum_{n=1}^{\infty} \frac{1}{n!}(\underline{\Delta}P)^n = 1 \otimes 1 + \sum_{n=1}^{\infty} \frac{1}{n!}\Big(\sum P_{(\underline{1})} \otimes P_{(\underline{2})}\Big)^n$$

Proof. By linearity of the coproduct, we have

$$\Delta(\mathrm{e}^P) \quad = \quad \Delta(\sum_{n=0}^{\infty} \frac{1}{n!}P^n) = \sum_{n=0}^{\infty} \frac{1}{n!}\Delta(P^n) = \sum_{n=0}^{\infty} \frac{1}{n!}(\Delta P)^n = \mathrm{e}^{\Delta P},$$

where we used the fact that Δ is an algebra morphism to write $\Delta(P^n) = (\Delta P)^n$. In $\mathrm{e}^{\Delta P}$, the operator $M = \Delta P$ is considered as a linear operator from $\mathcal{A} \otimes \mathcal{A}$ to $\mathcal{A} \otimes \mathcal{A}$ defined by $M(Q \otimes R) = \sum (P_{(1)}Q) \otimes (P_{(2)}R)$. We decompose this operator M as $M = \underline{\Delta}P + P \otimes 1 + 1 \otimes P$ and we use the fact that the algebra $\mathcal{A}$ is commutative to write

$$\mathrm{e}^M \quad = \quad \mathrm{e}^{\underline{\Delta}P + P\otimes 1 + 1 \otimes P} = \mathrm{e}^{\underline{\Delta}P}\mathrm{e}^{P\otimes 1}\mathrm{e}^{1\otimes P}.$$

The proof is completed by noting that

$$\mathrm{e}^{P\otimes 1} \quad = \quad \sum_{n=0}^{\infty} \frac{1}{n!}(P \otimes 1)^n = \sum_{n=0}^{\infty} \frac{1}{n!}P^n \otimes 1 = \mathrm{e}^P \otimes 1.$$

Similarly, $\mathrm{e}^{1\otimes P} = 1 \otimes \mathrm{e}^P$, so that $\mathrm{e}^{P\otimes 1}\mathrm{e}^{1\otimes P} = (\mathrm{e}^P \otimes 1)(1 \otimes \mathrm{e}^P) = \mathrm{e}^P \otimes \mathrm{e}^P$. □

Note that $\underline{\Delta}$ is not an algebra morphism so that $(\underline{\Delta}P)^n \neq \underline{\Delta}(P^n)$. Thus, we will use a special notation to write the terms of $(\underline{\Delta}P)^n$. Namely,

$$(\underline{\Delta}P)^n \quad = \quad \sum P^n_{(1')} \otimes P^n_{(2')}.$$

With this notation, we can write the action of e^P on the product of two functions as

$$\mathrm{e}^P(fg) \quad = \quad (\mathrm{e}^P f)(\mathrm{e}^P g) + \sum_{n=1}^{\infty} \frac{1}{n!} \sum (P^n_{(1')}\mathrm{e}^P f)(P^n_{(2')}\mathrm{e}^P g). \tag{4}$$

4 Applications

We consider now some applications of the identity (4) of increasing complexity. The first application is a simple proof that $\mathrm{e}^{a\partial}f(x) = f(x+a)$, the second is a hierarchy of Green functions for closed shells.

4.1 The shift operator

For this very simple application, assume that you do not know Taylor's theorem and that you want to evaluate $\mathrm{e}^{a\partial}f(x)$ for an entire function f. To prove that $\mathrm{e}^{a\partial}f(x) = f(x+a)$ it is enough to show that $\mathrm{e}^{a\partial}x^n = (x+a)^n$. The proof will be recursive. For $n = 1$, $\partial^0 x = x$, $\partial^1 x = 1$ and $\partial^k x = 0$ for $k > 1$. Thus, $\mathrm{e}^{a\partial}x = (1 + a\partial)x = x + a$. Now take $n > 1$ and $P = a\partial$. We have $\Delta P = P \otimes 1 + 1 \otimes P$, so that $\underline{\Delta} P = 0$ and the identity (4) gives us $\mathrm{e}^P(fg) = (\mathrm{e}^P f)(\mathrm{e}^P g)$. Therefore, taking $f(x) = x^{n-1}$ and $g(x) = x$ we have $\mathrm{e}^P(x^n) = (\mathrm{e}^P x^{n-1})(\mathrm{e}^P x)$. The recursion hypothesis tells us that $\mathrm{e}^P x^k = (x+a)^k$ for all $k < n$, thus $\mathrm{e}^P(x^n) = (x+a)^{n-1}(x+a) = (x+a)^n$.

4.2 The standard hierarchy

In the quantum theory of the scalar field, the system is described by the action $A(\varphi) = A_0(\varphi) - V(\varphi)$, with

$$A_0(\varphi) \quad = \quad \frac{1}{2}\int \mathrm{d}x \partial_\mu \varphi(x)\partial^\mu \varphi(x) - m^2\varphi^2(x),$$

and $V(\varphi) = \int \mathrm{d}x F(\varphi(x))$, where $F(\varphi(x))$ is a polynomial such that $F(0) = F'(0) = 0$ (usually $\varphi^3(x)/3!$ or $\varphi^4(x)/4!$). The generating function of the Green functions of this theory can be obtained from the following formula (see [15] p. 445)

$$Z(j) \quad = \quad \mathrm{e}^{-iV(-i\delta_j)}\mathrm{e}^{\frac{i}{2}\int \mathrm{d}x\mathrm{d}y j(x)G^0(x,y)j(y)},$$

where δ_j is a short notation for the functional derivative $\delta/\delta j(x)$, and where $G^0(x,y)$ is the Green function of the free scalar field.

A hierarchy of Green functions is an exact relation between interacting Green functions. To obtain it, we first take the functional derivative of $Z(j)$ with respect to $j(x)$:

$$\begin{aligned}\frac{\delta Z(j)}{\delta j(x)} \quad &= \quad \mathrm{e}^{-iV(-i\delta_j)}\frac{\delta}{\delta j(x)}\mathrm{e}^{\frac{i}{2}\int \mathrm{d}z\mathrm{d}z' j(z)G^0(z,z')j(z')} \\ &= \quad i\mathrm{e}^{-iV(-i\delta_j)}\Big(\int \mathrm{d}y G^0(x,y)j(y)\mathrm{e}^{\frac{i}{2}\int \mathrm{d}z\mathrm{d}z' j(z)G^0(z,z')j(z')}\Big).\end{aligned}$$

Now we use equation (4) with $f = \int \mathrm{d}y G^0(x,y)j(y)$, $g = \mathrm{e}^{\frac{i}{2}\int \mathrm{d}z\mathrm{d}z' j(z)G^0(z,z')j(z')}$ and $P = -iV(-i\delta_j)$. We first calculate $(\mathrm{e}^P f) = \mathrm{e}^{-iV(-i\delta_j)}\int \mathrm{d}y G^0(x,y)j(y)$. From the fact that $F(0) = F'(0) = 0$, we see that no terms of F has a degree smaller than 2. Therefore, $V(-i\delta_j)\int \mathrm{d}y G^0(x,y)j(y) = 0$ because $\int \mathrm{d}y G^0(x,y)j(y)$ is of degree 1 in $j(x)$. This gives us

$$\mathrm{e}^{-iV(-i\delta_j)}\int \mathrm{d}y G^0(x,y)j(y) \quad = \quad \int \mathrm{d}y G^0(x,y)j(y).$$

Now we calculate the reduced coproduct $\underline{\Delta} V$. If $F(\varphi(x))$ is a polynomial in $\varphi(x)$, $F(-i\delta_j)$ is a polynomial in δ_j. Thus

$$\Delta V \quad = \quad \int \mathrm{d}y \sum_{k\geq 0}\frac{1}{k!}\delta^k_{j(y)} \otimes \frac{\partial^k F}{\partial \delta^k_{j(y)}} = \int \mathrm{d}y \sum_{k\geq 0}\frac{(-i)^k}{k!}\delta^k_{j(y)} \otimes F^{(k)}(-i\delta_{j(y)}).$$

Therefore,

$$\underline{\Delta} V \quad = \quad \int \mathrm{d}y \sum_{k\geq 1}\frac{(-i)^k}{k!}\delta^k_{j(y)} \otimes F^{(k)}(-i\delta_{j(y)}) - V \otimes 1.$$

The term $n = 1$ of the main identity (4) becomes

$$\int \mathrm{d}y \sum_{k\geq 1} \frac{(-i)^k}{k!} \big(\delta^k_{j(y)} f\big)\big(F^{(k)}(-i\delta_{j(y)})\mathrm{e}^P g\big) - (Vf)(\mathrm{e}^P g).$$

The fact that $f = \int \mathrm{d}y G^0(x,y)j(y)$ is of degree 1 in j implies that only the term $k = 1$ may give a non-zero contribution. Its value is

$$\int \mathrm{d}y(-i)\big(\delta_{j(y)} f\big)\big(F'(-i\delta_{j(y)})\mathrm{e}^P g\big) \quad = \quad -i\int \mathrm{d}y G^0(x,y)F'(-i\delta_{j(y)})Z(j).$$

Moreover, all terms coming from $(\underline{\Delta}V)^n$ with $n > 1$ in the main identity (4) give no contribution because they are of degree at least n in δ_j. This gives us the simple result

$$\frac{\delta Z(j)}{\delta j(x)} \quad = \quad i\int \mathrm{d}y G^0(x,y)j(y)Z(j) - i\int \mathrm{d}y G^0(x,y)F'(-i\delta_{j(y)})Z(j). \tag{5}$$

If we multiply this equation by $(\Box + m^2)$ we get the standard hierarchy (see [15] p. 447)

$$(\Box + m^2)\frac{\delta Z(j)}{\delta j(x)} \quad = \quad ij(x)Z(j) - iF'(-i\delta_{j(x)})Z(j), \tag{6}$$

which is usually obtained by path-integral methods. However, note that equation (6) does not imply equation (5) but

$$\frac{\delta Z(j)}{\delta j(x)} \quad = \quad i\int \mathrm{d}y G^0(x,y)j(y)Z(j) - i\int \mathrm{d}y G^0(x,y)F'(-i\delta_{j(y)})Z(j) + \phi(x),$$

where $\phi(x)$ is a solution of the scalar wave equation $(\Box + m^2)\phi(x) = 0$. Thus, equation (5) is a result stronger than (6).

5 The fermionic case

For applications to molecular or solid-state physics, we need to modify the equations to treat the case of fermions. The main difference with the previous case is in the definition of the tensor product.

5.1 Tensor product

The basic variables of the fermionic theories are the field operators $\psi(x)$ and $\psi^\dagger(x)$ and the fermionic sources $\eta(x)$ and $\bar{\eta}(x)$. These variables are assumed to anticommute: for example $\eta(x)\psi(y) = -\psi(y)\eta(x)$.

The functions f will be polynomials in these basic variables. If f is a monomial in the basic variables, we denote by $\deg(f)$ the degree of f. For example, if f is a basic variable, $\deg(f) = 1$. For $f = \psi^\dagger(\mathbf{r})\psi(\mathbf{r})$, $\deg(f) = 2$; for $f = \int \bar{\eta}(x)\psi(x)\mathrm{d}x$, $\deg(f) = 2$. The parity of a function f, denoted by $|f|$, is 0 if $\deg(f)$ is even and is 1 if $\deg(f)$ is odd. Moreover, a function f is said to be even if $|f| = 0$ and odd if $|f| = 1$. From the anticommutation of the basic variables, one can derive the following commutation relation of two functions f and g: $gf = (-1)^{|f||g|}fg$. Therefore, an even function commutes with all functions and two odd functions anticommute.

The differential operators are products of functional derivatives with respect to η or $\bar{\eta}$. The basic relations are

$$\begin{aligned}
\frac{\delta}{\delta\eta(x)}\eta(y) \quad &= \quad \delta(x-y), \quad \frac{\delta}{\delta\eta(x)}\bar{\eta}(y) = 0,\\
\frac{\delta}{\delta\bar{\eta}(x)}\bar{\eta}(y) \quad &= \quad \delta(x-y), \quad \frac{\delta}{\delta\bar{\eta}(x)}\eta(y) = 0.
\end{aligned}$$

If f and g are functions in the basic variable with a definite parity, then the functional derivative of the product fg is given by the modified Leibniz formula

$$\frac{\delta}{\delta\eta(x)}(fg) \quad = \quad \frac{\delta f}{\delta\eta(x)}g + (-1)^{|f|}f\frac{\delta g}{\delta\eta(x)}, \tag{7}$$

and the same equation for a functional derivative with respect to $\bar{\eta}(x)$. Equation (7) is known as Leibniz' rule.

The sources η and $\bar{\eta}$ anticommute, so the functional derivatives anticommute:

$$\frac{\delta^2}{\delta\eta(x)\delta\eta(y)} = -\frac{\delta^2}{\delta\eta(y)\delta\eta(x)}.$$

The degree of a monomial P in $\delta/\delta\eta(x)$ and $\delta/\delta\bar{\eta}(x)$ is denoted by $\deg(P)$ and the parity of P, denoted by $|P|$ is 0 if $\deg(P)$ is even and 1 if $\deg(P)$ is odd. The action of a differential operator on a product of two functions is given by

$$P(fg) = \sum(-1)^{|f||P_{(2)}|}(P_{(1)}f)(P_{(2)}g),$$

where the coproduct of terms of degree 1 is

$$\Delta\frac{\delta}{\delta\eta(x)} = \frac{\delta}{\delta\eta(x)}\otimes 1 + 1\otimes\frac{\delta}{\delta\eta(x)},$$
$$\Delta\frac{\delta}{\delta\bar{\eta}(x)} = \frac{\delta}{\delta\bar{\eta}(x)}\otimes 1 + 1\otimes\frac{\delta}{\delta\bar{\eta}(x)},$$

and the coproduct of a product of two monomials P and Q is calculated from the coproduct of P and Q by using the fact that the coproduct is an algebra morphism:

$$\Delta(PQ) = (\Delta P)(\Delta Q) = \sum(-1)^{|P_{(2)}||Q_{(1)}|}(P_{(1)}Q_{(1)})\otimes(P_{(2)}Q_{(2)}), \tag{8}$$

where we have used the fact that the multiplication of $P\otimes Q$ by $R\otimes S$ is $(-1)^{|Q||R|}(PR)\otimes(QS)$.

5.2 The main identity

With the conventions described in the last paragraph, the main identity (3) is valid without change for fermionic sources if P is even (i.e. if $|P| = 0$). The action on a product of two functions is now

$$\mathrm{e}^P(fg) = (\mathrm{e}^P f)(\mathrm{e}^P g) + \sum_{n=1}^{\infty}\frac{1}{n!}\sum(-1)^{|f||P^n_{(2')}|}\big(P^n_{(1')}(\mathrm{e}^P f)\big)\big(P^n_{(2')}(\mathrm{e}^P g)\big). \tag{9}$$

6 Application of the fermionic formula

The main application of the fermionic formula was the derivation of the hierarchy of Green functions for open shells [14]. It would be too long to give a detailed derivation of this hierarchy. So we consider the calculation of the generating function Z of the Green functions for a system in a time-dependent external potential. This generating function is useful in time-dependent density functional theory. We first describe some properties of fermionic sources, then we give the step by step derivation of the dependence of Z on η and $\bar{\eta}$, using the main identity. Finally, we use this identity again to obtain the exact expression of Z.

6.1 Fermion sources

The S-matrix of a fermionic system with external sources η and $\bar{\eta}$ and action $\mathcal{A}^{\mathrm{int}}$ is

$$S(\bar{\eta},\eta) = T\exp\big(-i\mathcal{A}^{\mathrm{int}} + i\int\bar{\eta}(x)\psi(x)\mathrm{d}x + i\int\psi^\dagger(x)\eta(x)\mathrm{d}x\big).$$

For a nonrelativistic fermion, $\psi(x)$ and $\psi^\dagger(x)$ have a spin index. Thus, the sources are also two-component vectors and

$$\bar{\eta}(x)\psi(x) = \sum_{s=1}^{2}\bar{\eta}_s(x)\psi_s(x), \qquad \psi^\dagger(x)\eta(x) = \sum_{s=1}^{2}\psi^\dagger_s(x)\eta_s(x).$$

To see how functional derivatives act with respect to the time-ordering operator, we first notice that the sources can be taken out of the time-ordering operator. For example, if $x^0 > y^0$

$$\begin{aligned} T(\bar{\eta}(x)\psi(x)\psi^\dagger(y)\eta(y)) &= \bar{\eta}(x)\psi(x)\psi^\dagger(y)\eta(y) = \bar{\eta}(x)\eta(y)\psi(x)\psi^\dagger(y) \\ &= \bar{\eta}(x)\eta(y)T(\psi(x)\psi^\dagger(y)), \end{aligned}$$

if $x^0 < y^0$

$$\begin{aligned} T(\bar{\eta}(x)\psi(x)\psi^\dagger(y)\eta(y)) &= \psi^\dagger(y)\eta(y)\bar{\eta}(x)\psi(x) = -\bar{\eta}(x)\eta(y)\psi^\dagger(y)\psi(x) \\ &= \bar{\eta}(x)\eta(y)T(\psi(x)\psi^\dagger(y)). \end{aligned}$$

Thus, the functional derivative with respect to $\eta(x)$ or $\bar{\eta}(x)$ commutes with the time-ordering operator. In particular [15]

$$\begin{aligned} \frac{\delta S(\bar{\eta},\eta)}{\delta\bar{\eta}(x)}|_{\bar{\eta}=\eta=0} &= iT\big(\psi(x)\mathrm{e}^{-i\mathcal{A}^{\mathrm{int}}}\big), \\ \frac{\delta S(\bar{\eta},\eta)}{\delta\eta(x)}|_{\bar{\eta}=\eta=0} &= -iT\big(\psi^\dagger(x)\mathrm{e}^{-i\mathcal{A}^{\mathrm{int}}}\big), \end{aligned}$$

where the minus sign in the last equation comes from the fact that the functional derivative must jump over $\psi^\dagger(x)$ to reach $\eta(x)$ in the definition of $S(\bar{\eta},\eta)$.

A standard result of the functional derivative approach [15, 17] is that the interacting S-matrix $S(\bar{\eta},\eta)$ can be obtained from the non-interacting S-matrix

$$S^0(\bar{\eta},\eta) = T\exp\big(i\int \bar{\eta}(x)\psi(x) + \psi^\dagger(x)\eta(x)\mathrm{d}x\big)$$

by the equation

$$S(\bar{\eta},\eta) = \exp\big(-i\int_{-\infty}^{\infty} H^{\mathrm{int}}(\frac{-i\delta}{\delta\bar{\eta}(x)},\frac{i\delta}{\delta\eta(x)})\mathrm{d}t\big)S^0(\bar{\eta},\eta),$$

where $H^{\mathrm{int}}(\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r},t))$ is the interaction Hamiltonian.

If $|\Phi_0\rangle$ is a non-degenerate eigenstate of H_0, the Green functions of the interacting system can be obtained from the generating function

$$Z(\bar{\eta},\eta) = \langle\Phi_0|S(\bar{\eta},\eta)|\Phi_0\rangle = \exp\big(-i\int_{-\infty}^{\infty} H^{\mathrm{int}}(\frac{-i\delta}{\delta\bar{\eta}(x)},\frac{i\delta}{\delta\eta(x)})\mathrm{d}t\big)Z^0(\bar{\eta},\eta),$$

where $Z^0 = \langle\Phi_0|S^0|\Phi_0\rangle$. If $|\Phi_0\rangle$ can be written as a Slater determinant, $|\Phi_0\rangle = b^\dagger_{i_N}\dots b^\dagger_{i_1}|0\rangle$, where $b^\dagger_n$ is the creation operator of the one-electron state $u_n(x)$ of the free Hamiltonian, we have [16]

$$Z^0(\bar{\eta},\eta) = \langle\Phi_0|T\exp\big(i\int \bar{\eta}(x)\psi(x) + \psi^\dagger(x)\eta(x)\mathrm{d}x\big)|\Phi_0\rangle = \mathrm{e}^{-i\int\bar{\eta}(x)G^0(x,y)\eta(y)\mathrm{d}x\mathrm{d}y},$$

where

$$G^0(x,y) = -i\langle\Phi_0|T\big(\psi(x)\psi^\dagger(y)\big)|\Phi_0\rangle = -i\langle 0|T\big(\psi(x)\psi^\dagger(y)\big)|0\rangle + i\sum_{k=1}^{N} u_{i_k}(x)u^*_{i_k}(y).$$

As a useful example, we consider the interaction with an external time-dependent potential $v(x)$ so that $\mathcal{A}^{\mathrm{int}} = \int \mathrm{d}x\psi^\dagger(x)v(x)\psi(x)$. The generating function becomes $Z = \mathrm{e}^P\mathrm{e}^{W^0}$, where

$$\begin{aligned} P &= -i\int \mathrm{d}x v(x)\frac{\delta^2}{\delta\eta(x)\delta\bar{\eta}(x)}, \\ W^0 &= -i\int \bar{\eta}(x)G^0(x,y)\eta(y)\mathrm{d}x\mathrm{d}y. \end{aligned}$$

Our purpose is now to calculate Z.

6.2 Dependence of Z on η and $\bar{\eta}$

For later convenience, we consider $Z(\lambda) = \mathrm{e}^P \mathrm{e}^{\lambda W^0}$. We first calculate the derivative of $Z(\lambda)$ with respect to $\bar{\eta}(x)$.

$$\frac{\delta Z(\lambda)}{\delta\bar{\eta}(x)} = \mathrm{e}^P\Big(\frac{\delta \mathrm{e}^{\lambda W^0}}{\delta\bar{\eta}(x)}\Big) = \lambda \mathrm{e}^P\Big(\frac{\delta W^0}{\delta\bar{\eta}(x)}\mathrm{e}^{\lambda W^0}\Big) = -i\lambda \mathrm{e}^P\Big(\int G^0(x,y)\eta(y)\mathrm{d}y \mathrm{e}^{\lambda W^0}\Big).$$

We can apply identity (9) with $f = \int G^0(x,y)\eta(y)\mathrm{d}y$, so that $|f| = 1$ and $g = \mathrm{e}^{\lambda W^0}$. We first note that $Pf = 0$ because f does not contain any factor $\bar{\eta}$. Thus $\mathrm{e}^P f = f$ and since $\mathrm{e}^P g = Z(\lambda)$, equation (9) becomes

$$\frac{\delta Z(\lambda)}{\delta\bar{\eta}(x)} = -i\lambda f Z(\lambda) - i\lambda \sum_{n=1}^{\infty}\frac{1}{n!}\sum(-1)^{|P^n_{(2')}|}\big(P^n_{(1')}f\big)\big(P^n_{(2')}Z(\lambda)\big).$$

To proceed, we must calculate the reduced coproduct of P. We first have the coproduct

$$\Delta P = P\otimes 1 + 1\otimes P - i\int \mathrm{d}z v(z)\frac{\delta}{\delta\eta(z)}\otimes\frac{\delta}{\delta\bar{\eta}(z)} + i\int \mathrm{d}z v(z)\frac{\delta}{\delta\bar{\eta}(z)}\otimes\frac{\delta}{\delta\eta(z)},$$

so that

$$\underline{\Delta} P = -i\int \mathrm{d}z v(z)\frac{\delta}{\delta\eta(z)}\otimes\frac{\delta}{\delta\bar{\eta}(z)} + i\int \mathrm{d}z v(z)\frac{\delta}{\delta\bar{\eta}(z)}\otimes\frac{\delta}{\delta\eta(z)}. \tag{10}$$

The term f is of degree 1 in η and 0 in $\bar{\eta}$. Thus, the factor $P^n_{(1')}f$ is non zero only if $n = 1$ and $P_{(1')} = \delta/\delta\eta(z)$. We find

$$\begin{aligned}\frac{\delta Z(\lambda)}{\delta\bar{\eta}(x)} &= -i\lambda f Z(\lambda) - i\lambda(-i)\int \mathrm{d}z v(z)(-1)\frac{\delta f}{\delta\eta(z)}\frac{\delta Z(\lambda)}{\delta\bar{\eta}(z)}\\ &= -i\lambda f Z(\lambda) + \lambda\int \mathrm{d}y v(y) G^0(x,y)\frac{\delta Z(\lambda)}{\delta\bar{\eta}(y)}.\end{aligned}$$

If we write $Z(\lambda) = \mathrm{e}^{W(\lambda)}$ we get

$$\frac{\delta W(\lambda)}{\delta\bar{\eta}(x)} = -i\lambda\int \mathrm{d}y G^0(x,y)\eta(y) + \lambda\int \mathrm{d}y G^0(x,y)v(y)\frac{\delta W(\lambda)}{\delta\bar{\eta}(y)},$$

with the solution

$$\frac{\delta W(\lambda)}{\delta\bar{\eta}(x)} = -i\lambda\int \mathrm{d}y G(x,y)\eta(y), \tag{11}$$

where $G(x,y)$ satisfies the Dyson equation

$$G(x,y) = G^0(x,y) + \lambda\int \mathrm{d}z G^0(x,z)v(z)G(z,y). \tag{12}$$

In other words, $G(x,y)$ is the Green function of the Schrödinger equation obtained by adding λv to the free Hamiltonian. From equation (11), we see that the function $W(\lambda)$ can be written $W(\lambda) = -i\lambda\int \mathrm{d}x\mathrm{d}y\bar{\eta}(x)G(x,y)\eta(y) + g(\eta,\lambda)$. The same calculation for $\delta Z(\lambda)/\delta\eta(y)$ shows that $\delta W(\lambda)/\delta\eta(y) = i\lambda\int \mathrm{d}x\bar{\eta}(x)G(x,y)$. Thus, g does not depend on η and

$$W(\lambda) = -i\lambda\int \mathrm{d}x\mathrm{d}y\bar{\eta}(x)G(x,y)\eta(y) + g(\lambda), \tag{13}$$

where $g(\lambda)$ is independent of $\bar{\eta}$ and η.

6.3 Calculation of $g(\lambda)$

To calculate $g(\lambda)$, we take the derivative of $Z(\lambda)$ with respect to λ.

$$\frac{\partial Z(\lambda)}{\partial \lambda} = \mathrm{e}^P\Big(\frac{\partial \mathrm{e}^{\lambda W^0}}{\partial \lambda}\Big) = \mathrm{e}^P\Big(W^0\mathrm{e}^{\lambda W^0}\Big).$$

We can apply identity (9) with $f = W^0$, so that $|f| = 0$ and $g = \mathrm{e}^{\lambda W^0}$. We now have

$$PW^0 = -i\int \mathrm{d}x v(x)\frac{\delta^2 W^0}{\delta\eta(x)\delta\bar\eta(x)} = -\int v(x)G^0(x,x)\mathrm{d}x = -\mathrm{tr}(vG^0).$$

Thus $\mathrm{e}^P f = f - \mathrm{tr}(vG^0)$ and since $\mathrm{e}^P g = Z(\lambda)$, equation (9) becomes

$$\frac{\partial Z(\lambda)}{\partial \lambda} = W^0 Z(\lambda) - \mathrm{tr}(vG^0)Z(\lambda) + \sum_{n=1}^{\infty}\frac{1}{n!}\sum\big(P^n_{(1')}W^0\big)\big(P^n_{(2')}Z(\lambda)\big).$$

To calculate the term $n = 1$, we use the reduced coproduct of P given in equation (10) and we obtain

$$\begin{aligned}\sum\big(P_{(1')}W^0\big)\big(P_{(2')}Z(\lambda)\big) &= -i\int \mathrm{d}z v(z)\frac{\delta W^0}{\delta\eta(z)}\frac{\delta Z(\lambda)}{\delta\bar\eta(z)} + i\int \mathrm{d}z v(z)\frac{\delta W^0}{\delta\bar\eta(z)}\frac{\delta Z(\lambda)}{\delta\eta(z)}\\ &= \int \mathrm{d}x\mathrm{d}y\bar\eta(x)G^0(x,y)v(y)\frac{\delta Z(\lambda)}{\delta\bar\eta(y)} + \int \mathrm{d}x\mathrm{d}y v(x)G^0(x,y)\eta(y)\frac{\delta Z(\lambda)}{\delta\eta(x)}.\end{aligned}$$

For the term $n = 2$ we first evaluate, using algebra morphism (8)

$$\begin{aligned}(\underline{\Delta}P)^2 &= \Big(-i\int \mathrm{d}x v(x)\frac{\delta}{\delta\eta(x)}\otimes\frac{\delta}{\delta\bar\eta(x)} + i\int \mathrm{d}x v(x)\frac{\delta}{\delta\bar\eta(x)}\otimes\frac{\delta}{\delta\eta(x)}\Big)\\ &\quad\Big(-i\int \mathrm{d}y v(y)\frac{\delta}{\delta\eta(y)}\otimes\frac{\delta}{\delta\bar\eta(y)} + i\int \mathrm{d}y v(y)\frac{\delta}{\delta\bar\eta(y)}\otimes\frac{\delta}{\delta\eta(y)}\Big)\\ &= \int \mathrm{d}x\mathrm{d}y v(x)v(y)\frac{\delta^2}{\delta\eta(x)\delta\eta(y)}\otimes\frac{\delta^2}{\delta\bar\eta(x)\delta\bar\eta(y)}\\ &\quad - \int \mathrm{d}x\mathrm{d}y v(x)v(y)\frac{\delta^2}{\delta\eta(x)\delta\bar\eta(y)}\otimes\frac{\delta^2}{\delta\bar\eta(x)\delta\eta(y)}\\ &\quad - \int \mathrm{d}x\mathrm{d}y v(x)v(y)\frac{\delta^2}{\delta\bar\eta(x)\delta\eta(y)}\otimes\frac{\delta^2}{\delta\eta(x)\delta\bar\eta(y)}\\ &\quad + \int \mathrm{d}x\mathrm{d}y v(x)v(y)\frac{\delta^2}{\delta\bar\eta(x)\delta\bar\eta(y)}\otimes\frac{\delta^2}{\delta\eta(x)\delta\eta(y)}.\end{aligned}$$

W^0 contains one η and one $\bar\eta$. Thus, the only terms of $(\underline{\Delta}P)^2$ that give non-zero contributions are the second and the third, because the left hand side of the tensor product contains functional derivatives with respect to η and $\bar\eta$. If we interchange the variables x and y, we see that these two terms are identical, thus the term $n = 2$ becomes

$$\begin{aligned}\frac{1}{2}\sum\big(P^2_{(1')}W^0\big)\big(P^2_{(2')}Z(\lambda)\big) &= -\int \mathrm{d}x\mathrm{d}y v(x)v(y)\frac{\delta^2 W^0}{\delta\eta(y)\delta\bar\eta(x)}\frac{\delta^2 Z(\lambda)}{\delta\bar\eta(y)\delta\eta(x)}\\ &= i\int \mathrm{d}x\mathrm{d}y v(x)v(y)G^0(x,y)\frac{\delta^2 Z(\lambda)}{\delta\bar\eta(y)\delta\eta(x)}.\end{aligned}$$

There is no term for $n > 2$ because W^0 is of degree 2.

This gives us the equation for $Z(\lambda)$

$$\begin{aligned}\frac{\partial Z(\lambda)}{\partial \lambda} &= W^0 Z(\lambda) - \mathrm{tr}(vG^0)Z(\lambda) + \int \mathrm{d}x\mathrm{d}y\bar\eta(x)G^0(x,y)v(y)\frac{\delta Z(\lambda)}{\delta\bar\eta(y)}\\ &\quad + \int \mathrm{d}x\mathrm{d}y v(x)G^0(x,y)\eta(y)\frac{\delta Z(\lambda)}{\delta\eta(x)} + i\int \mathrm{d}x\mathrm{d}y v(x)v(y)G^0(x,y)\frac{\delta^2 Z(\lambda)}{\delta\bar\eta(y)\delta\eta(x)}.\end{aligned}$$

If we write $Z(\lambda) = \mathrm{e}^{W(\lambda)}$ we obtain the equation for $W(\lambda)$

$$\begin{aligned}\frac{\partial W(\lambda)}{\partial \lambda} &= -i\int \bar{\eta}(x)G^0(x,y)\eta(y)\mathrm{d}x\mathrm{d}y - \mathrm{tr}(vG^0) + \int \mathrm{d}x\mathrm{d}y\bar{\eta}(x)G^0(x,y)v(y)\frac{\delta W(\lambda)}{\delta\bar{\eta}(y)} \\ &+ \int \mathrm{d}x\mathrm{d}y v(x)G^0(x,y)\eta(y)\frac{\delta W(\lambda)}{\delta\eta(x)} + i\int \mathrm{d}x\mathrm{d}y v(x)v(y)G^0(x,y)\frac{\delta W(\lambda)}{\delta\bar{\eta}(y)}\frac{\delta W(\lambda)}{\delta\eta(x)} \\ &+ i\int \mathrm{d}x\mathrm{d}y v(x)v(y)G^0(x,y)\frac{\delta^2 W(\lambda)}{\delta\bar{\eta}(y)\delta\eta(x)}.\end{aligned}$$

The general form of $W(\lambda)$ is given by equation (13). If we introduce it into the last equation we obtain

$$\begin{aligned}-i\bar{\eta}G\eta - i\lambda\bar{\eta}\frac{\partial G}{\partial\lambda}\eta + g'(\lambda) &= -i\bar{\eta}G^0\eta - \mathrm{tr}(vG^0) - i\lambda\bar{\eta}G^0vG\eta - i\lambda\bar{\eta}GvG^0\eta \\ &\quad -i\lambda^2\bar{\eta}GvG^0vG\eta - \lambda\mathrm{tr}(vG^0vG).\end{aligned}$$

This gives us two independent equations:

$$\begin{aligned}G + \lambda\frac{\partial G}{\partial\lambda} &= G^0 + \lambda G^0vG + \lambda GvG^0 + \lambda^2 GvG^0vG, \\ g'(\lambda) &= -\mathrm{tr}(vG^0) - \lambda\mathrm{tr}(vG^0vG).\end{aligned}$$

Equation (12) enables us to simplify this into

$$\begin{aligned}G + \lambda\frac{\partial G}{\partial\lambda} &= G + \lambda GvG, \\ g'(\lambda) &= -\mathrm{tr}(vG).\end{aligned}$$

The first equation is an identity because the Dyson equation (12) yields

$$\frac{\partial G}{\partial\lambda} = G^0vG + \lambda G^0v\frac{\partial G}{\partial\lambda},$$

so that

$$\frac{\partial G}{\partial\lambda} = GvG.$$

The last equation to solve is simply $g'(\lambda) = -\mathrm{tr}(vG) = -i\int v(x)\rho(x;\lambda)\mathrm{d}x$, where $\rho(x;\lambda) = -iG(x,x)$ is the charge density in the presence of the potential λv. The solution of this equation would be $g(\lambda) - g(0) = \int_0^\lambda g'(\mu)\mathrm{d}\mu$. If $\lambda = 0$, $Z(0) = \mathrm{e}^P 1 = 1$. Thus, $W(0) = 0$. Moreover, for $\lambda = 0$, $G = G^0$ and $W = g(0)$. Thus, $g(0) = 0$. Now we prove that

$$g(\lambda) = -\mathrm{tr}\big(\log(1+\lambda vG)\big). \tag{14}$$

By definition, the right hand side of this equation is

$$-\mathrm{tr}\big(\log(1+\lambda vG)\big) = \sum_{n=1}^{\infty}\frac{(-\lambda)^n}{n}\mathrm{tr}\big((vG)^n\big).$$

If we take the derivative with respect to λ we find

$$\begin{aligned}-\frac{\partial\mathrm{tr}\big(\log(1+\lambda vG)\big)}{\partial\lambda} &= -\sum_{n=1}^{\infty}(-\lambda)^{n-1}\mathrm{tr}\big((vG)^n\big) + \sum_{n=1}^{\infty}(-\lambda)^n\mathrm{tr}\Big(v\frac{\partial G}{\partial\lambda}(vG)^{n-1}\Big) \\ &= -\sum_{n=0}^{\infty}(-\lambda)^n\mathrm{tr}\big((vG)^{n+1}\big) + \sum_{n=1}^{\infty}(-\lambda)^n\mathrm{tr}\big((vG)^{n+1}\big) = -\mathrm{tr}(vG).\end{aligned}$$

Therefore, $g(\lambda)$ and $-\mathrm{tr}\big(\log(1+\lambda vG)\big)$ satisfy the same first order differential equation. Moreover, the boundary conditions are the same because $-\mathrm{tr}\big(\log(1)\big) = 0 = g(0)$.

6.4 Alternative expressions

We can give alternative expressions for $g(\lambda)$. Expanding $G = G^0 + \lambda G^0 vG$ we obtain $G = G^0 \sum_{n=0}^{\infty} (\lambda v G^0)^n$ so that

$$g'(\lambda) = -\mathrm{tr}(vG) = -\sum_{n=0}^{\infty} \lambda^n \mathrm{tr}\big((vG^0)^{n+1}\big).$$

Hence,

$$g(\lambda) = \int_0^{\lambda} g'(\mu)\mathrm{d}\mu = -\sum_{n=0}^{\infty} \frac{\lambda^{n+1}}{n+1} \mathrm{tr}\big((vG^0)^{n+1}\big) = \mathrm{tr}\log(1-\lambda v G^0).$$

A similar result was obtained by Sham [18] in the framework of the density functional theory. The relation with equation (14) is obtained from $G = G^0 + \lambda G v G^0$, so that $vG^0 = vG(1-\lambda v G^0)$. Therefore, formally,

$$\begin{aligned} \mathrm{tr}\log(1-\lambda v G^0) &= \mathrm{tr}\log(vG^0) - \mathrm{tr}\log(vG) = \mathrm{tr}\log(vG^0) - \mathrm{tr}\log(vG^0(1+\lambda vG)) \\ &= -\mathrm{tr}\log(1+\lambda vG). \end{aligned}$$

We can manipulate these operators as if they were scalars because vG is a function of vG^0, so that every term is a series in the single variable vG^0.

To give a last form of $g(\lambda)$, we define the Euler operator $A = \int \mathrm{d}x v(x) \frac{\delta}{\delta v(x)}$, that counts the number of times v is present in an expression. In other words, it is easy to check that $A\mathrm{tr}\big((vG^0)^n\big) = n\mathrm{tr}\big((vG^0)^n\big)$. More generally, $A^k \mathrm{tr}\big((vG^0)^n\big) = n^k \mathrm{tr}\big((vG^0)^n\big)$. Thus, we can write the somewhat formal identity

$$g(\lambda) = -\sum_{n=0}^{\infty} \frac{\lambda^{n+1}}{n+1} \mathrm{tr}\big((vG^0)^{n+1}\big) = -A^{-1} \sum_{n=0}^{\infty} \lambda^{n+1} \mathrm{tr}\big((vG^0)^{n+1}\big) = -\lambda A^{-1} \mathrm{tr}(vG).$$

7 Conclusion

The hierarchy of Green functions is one of the building blocks of an extension of the Bethe-Salpeter equation to open shells. The other main ingredient is an expression of the Green functions in terms of 2-particle-irreducible generating functions. This expression is well known for closed shells [19] but not for open shells. In the latter case, the Dyson equation relating the two-point Green function and the self-energy (i.e. one-particle irreducible Green function) is not valid. This is a bad news because the Dyson equation is required to use the Legendre transformation relating the connected Green function and the one- or two-particle irreducible ones. By a diagrammatic tour de force, Hall was able to obtain the equation corresponding to the Dyson equation for open shells [11]. It looks very complex but, by doubling the size of the Green functions, it is possible to give it a form similar to the traditional Dyson equation. This gives some hope that the Bethe-Salpeter equation for open shells can be obtained, opening the way to an effective unification of the ligand field and Green function methods.

In some applications, the operator P in e^P belongs to a noncommutative algebra [20]. This is the case for example when P is a differential operator with non-constant coefficients. It is possible to generalize our main identity to noncommutative algebras. The main problem is to transform $\mathrm{e}^{\Delta P}$ into an operator e^A acting on $1 \otimes \mathrm{e}^P$. In other words, we have to solve the equation $\mathrm{e}^A = \mathrm{e}^{\Delta P} \mathrm{e}^{-1 \otimes P}$. This can be done by using the Baker-Campbell-Hausdorff formula [21].

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