Many-body theory of degenerate systems: A simple example

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The hierarchy of Green functions for (quasi)degenerate systems, presented in cond-mat/0308058,
is calculated in detail for the case of a system with closed shells plus a single electron in a two-fold
degenerate level. The complete hierarchy is derived explicitly, in terms of Green functions and of
Feynman diagrams.

I. INTRODUCTION

In reference\(^1\), hereafter referred to as I, a many-body theory of degenerate or quasidegenerate systems was presented,
using quantum group methods. In particular, a hierarchy of Green function was derived and formulated in terms of
reduced coproducts. In this paper, the general formula is written explicitly in terms of Green functions and Feynman
diagrams. The case we consider is that of a system with closed shells and a two-fold degenerate level occupied by a
single electron. This does not look like a very interesting example, but we shall see that the hierarchy involves
\(n\)-body Green functions with \(n\) up to 5. In the general case of a \(M\)-fold degenerate level, the Green functions involved go up
to \(n = 3M - 1\). In practice, such complicated Green functions are not usable, and the hierarchy is stopped after the
first terms. The hierarchy we give here contains the first terms of the general hierarchy.

Quantum group concepts are not (yet) familiar in solid-state physics, so the pace will be slow and the calculations
will be presented in full detail.

II. CALCULATION OF \(W_\rho^1\)

The simplest case is one electron \((N = 1)\) in a twofold degenerate level \((M = 2)\). The two degenerate levels are
denoted by 1 and 2. The density matrix is

\[
\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix},
\]

with \(\text{tr}(\rho) = \rho_{11} + \rho_{22} = 1\).

The moment generating function \(\rho(\bar{\alpha}, \alpha)\) is defined in equation (28) of I. In our case, \(N = 1\) and \(\rho(\bar{\alpha}, \alpha) = \rho_0(\bar{\alpha}, \alpha) + \rho_1(\bar{\alpha}, \alpha)\). According to equation (29) of I (with \(N = 1\), \(i_1 = 1\) or 2, \(j_1 = 1\) or 2)

\[
\rho_1(\bar{\alpha}, \alpha) = \rho_{11}\bar{\alpha}_1\alpha_1 + \rho_{12}\bar{\alpha}_1\alpha_2 + \rho_{21}\bar{\alpha}_2\alpha_1 + \rho_{22}\bar{\alpha}_2\alpha_2.
\]

Using now equation (30) of I with \(k = 1\) we obtain

\[
\rho_0(\bar{\alpha}, \alpha) = \text{tr}(\rho) = \rho_{11} + \rho_{22} = 1.
\]

According to equation (32) of I, the cumulant generating function \(\rho^c(\bar{\alpha}, \alpha)\) is obtained from

\[
\log(\rho(\bar{\alpha}, \alpha)) = \log(1 + \rho_1(\bar{\alpha}, \alpha)) = \rho_1(\bar{\alpha}, \alpha) + \rho^c(\bar{\alpha}, \alpha),
\]

where

\[
\rho^c(\bar{\alpha}, \alpha) = \rho_2^c(\bar{\alpha}, \alpha) = \frac{-\rho_1(\bar{\alpha}, \alpha)^2}{2} = -\det(\rho)\bar{\alpha}_1\alpha_1\bar{\alpha}_2\alpha_2 = -(\rho_{11}\rho_{22} - \rho_{12}\rho_{21})\bar{\alpha}_1\alpha_1\bar{\alpha}_2\alpha_2.
\]

According to equation (34) of I, this enables us to calculate \(W^0_\rho\). But we saw in section 7.3 of I that \(W^1_\rho = W^0_\rho\), thus

\[
W^1_\rho = -i \int \bar{\eta}(x)G^0_\rho(x, y)\eta(y)dy + \rho^c_2(\bar{\alpha}, \alpha),
\]

with

\[
G^0_\rho(x, y) = G^0_0(x, y) + i\left( \sum_{m=1}^C u_m(x)\bar{u}_m(y) + \sum_{k=1}^2 \sum_{l=1}^{2} \rho_{kl} u_k(x)\bar{u}_l(y) \right) M,
\]

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where

\[ M = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}. \]

The expression for the \(2 \times 2\) matrix \(G_0^0(x, y)\) is given in equation (15) of I.

For later convenience, we define the identities

\[ \frac{\delta^2 \bar{c}_1 \alpha_1 \bar{c}_2 \alpha_2}{\delta \eta_j(y) \delta \eta_k(x)} = \epsilon_j'(u_1(x) \bar{a}_2 - u_2(x) \bar{a}_1)(\bar{u}_1(y) \alpha_2 - \bar{u}_2(y) \alpha_1). \]

\[ \frac{\delta^4 \rho^2_2(\bar{a}, \alpha)}{\delta \eta_i(x_1) \delta \eta_j(x_2) \delta \eta_k(y_1) \delta \eta_l(y_2)} = -\epsilon_1 \epsilon'_2 \epsilon'_3 \epsilon'_4 r(x_1, x_2, y_1, y_2), \]

where

\[ r(x_1, x_2, y_1, y_2) = -\text{det}(\rho)(u_1(x_1)u_2(x_2) - u_2(x_1)u_1(x_2))(\bar{u}_1(y_1)\bar{u}_2(y_2) - \bar{u}_2(y_1)\bar{u}_1(y_2)). \]

III. HIERARCHY

For one electron in a two-fold degenerate state, equation (43) of I stops at \(n = 3\) because \(M = 2\) and we have

\[ \frac{\delta Z_\rho}{\delta \beta} = \frac{\delta W_\rho^1}{\delta \beta} Z_\rho - i \sum (-1)^{D_1^{(i')}} (D_1^{(i')}, \frac{\delta W_\rho^1}{\delta \beta}) (D_2^{(i')}, Z_\rho) - \frac{1}{2} \sum (-1)^{D_1^{(i')}} (D_2^{(i')}, \frac{\delta W_\rho^1}{\delta \beta}) (D_2^{(i')}, Z_\rho) \]

\[ + \frac{i}{6} \sum (-1)^{D_1^{(i')}} (D_3^{(i')}, \frac{\delta W_\rho^1}{\delta \beta}) (D_3^{(i')}, Z_\rho). \]

To obtain the Green function, we put \(\beta = \eta_i(x)\), we make a functional derivative with respect to \(\eta_j(y)\) and we set all fermion sources to zero (in particular, this implies \(Z_\rho = 1\)). We use also the fact that a functional derivative of \(Z_\rho\) or \(W_\rho^1\) with respect to an odd number of fermion sources is zero if the sources are set to zero. This enables us to calculate the signs \((-1)^{D_1^{(i')}}\).

\[ \frac{\delta Z_\rho}{\delta \eta_i(y) \delta \eta_k(x)} = \frac{\delta W_\rho^1}{\delta \eta_i(y) \delta \eta_k(x)} - i \sum (D_1^{(i')}, \frac{\delta W_\rho^1}{\delta \eta_i(y) \delta \eta_k(x)}) (D_2^{(i')}, Z_\rho) - i \sum (D_1^{(i')}, \frac{\delta W_\rho^1}{\delta \eta_i(y) \delta \eta_k(x)}) (D_2^{(i')}, \frac{\delta Z_\rho}{\delta \eta_i(y)}) \]

\[ - \frac{1}{2} \sum (D_2^{(i')}, \frac{\delta W_\rho^1}{\delta \eta_i(y) \delta \eta_k(x)}) (D_2^{(i')}, Z_\rho) - \frac{1}{2} \sum (D_1^{(i')}, \frac{\delta W_\rho^1}{\delta \eta_i(y) \delta \eta_k(x)}) (D_1^{(i')}, \frac{\delta Z_\rho}{\delta \eta_i(y)}), \]

\[ + \frac{i}{6} \sum (D_3^{(i')}, \frac{\delta W_\rho^1}{\delta \eta_i(y) \delta \eta_k(x)}) (D_3^{(i')}, \frac{\delta Z_\rho}{\delta \eta_i(y)}). \]

A. Coproduct

The non-relativistic interacting Hamiltonian is

\[ \int H^\text{int}(t) dt = \frac{\hbar^2}{2} \int \tilde{\psi}(t, \mathbf{r})\tilde{\psi}(t, \mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} \psi(t, \mathbf{r}')\psi(t, \mathbf{r}) dt d\mathbf{r} d\mathbf{r}'. \]

To simplify the notation, we define \(x_1 = (t, \mathbf{r})\), \(x_1' = (t', \mathbf{r}')\) and \(v(x_1 - x_1') = \delta(t - t')e^2/|\mathbf{r} - \mathbf{r}'|\), so that

\[ \int H^\text{int}(t) dt = \frac{1}{2} \int v(x_1 - x_1') \tilde{\psi}(x_1)\tilde{\psi}(x_1')\psi(x_1)\psi(x_1') dx_1 dx_1'. \]

To define the interacting operator \(D\) (i.e. the functional differential form of \(\int H^\text{int}(t) dt\)), we make the substitutions \(\psi(x_1) \rightarrow -i\delta/\delta \eta(x_1)\) and \(\bar{\psi}(x_1) \rightarrow i\delta/\delta \eta(x_1)\) and we use the simplified notation

\[ \delta \bar{c}_\pm \pm = \frac{\delta}{\delta \eta_{\mp}(x_1)}, \delta \bar{c}_\pm' \pm = \frac{\delta}{\delta \eta_{\mp}(x_1')}, \delta \bar{c}_\pm \pm = \frac{\delta}{\delta \eta_{\mp}(x_1')}, \delta \bar{c}_\pm' \pm = \frac{\delta}{\delta \eta_{\mp}(x_1')}. \]
This gives us $D = D_+ - D_-$ with

$$D_\pm = \frac{1}{2} \int v(x_1 - x'_1) \delta_1 \delta_2 \delta_1 \delta_2 \, dx_1 \, dx'_1.$$  

(5)

Thus

$$D = \frac{1}{2} \int dx_1 \, dx'_1 \, v(x_1 - x'_1) \left( \delta_1 \delta_2 \delta_1 - \delta_1 \delta_2 \delta_1 \right),$$

To further simplify the notation, we replace $\delta_1 \delta_2$ by $\delta_1$ and $x_1$ by 1 and $x'_1$ by $1'$. The interacting operator becomes

$$D = \frac{1}{2} \int d1 \, d1' \, v(1 - 1') \sum_{\pm} \delta \delta_1 \delta_1 \delta_1.$$

To calculate the coproduct of $D$, we start from the coproduct of the basic functional derivatives

$$\Delta \delta_1 = \delta_1 \otimes 1 + 1 \otimes \delta_1, \quad \Delta \delta_1' = \delta_1 \otimes 1 + 1 \otimes \delta_1', \quad \Delta \delta_i = \delta_i \otimes 1 + 1 \otimes \delta_i, \quad \Delta \delta_i' = \delta_i \otimes 1 + 1 \otimes \delta_i'.

Then we use equation (21) of I to calculate the coproduct of $\delta_1 \delta_1'$ and $\delta_i \delta_i'$:

$$\Delta \delta_1 \delta_1' = \delta_1 \delta_1' \otimes 1 + \delta_1 \delta_1' \otimes \delta_1 + 1 \otimes \delta_1 \delta_1', \quad \Delta \delta_i \delta_i' = \delta_i \delta_i' \otimes 1 + \delta_i \delta_i' \otimes \delta_i + 1 \otimes \delta_i \delta_i'.

We use equation (21) of I again to obtain

$$\Delta \delta_1 \delta_1' \delta_i \delta_i' = \delta_1 \delta_1' \delta_i \delta_i' \otimes 1 + 1 \otimes \delta_1 \delta_1' \delta_i \delta_i' + \delta_1 \delta_1' \delta_i \delta_i' \otimes \delta_1 - \delta_1 \delta_1' \delta_i \delta_i' \delta_1 - \delta_1 \delta_1' \delta_i \delta_i' \delta_i + \delta_i \delta_1 \delta_1' \delta_i \delta_i' - \delta_1 \delta_1' \delta_i \delta_i' \delta_i - \delta_1 \delta_1' \delta_i \delta_i' \delta_i - \delta_1 \delta_1' \delta_i \delta_i' \delta_i.$$

(6)

The reduced coproduct with respect to $D$ is obtained by its definition $\Delta' D = \Delta D - D \otimes 1 - 1 \otimes D$. Therefore,

$$\Delta' D = \frac{1}{2} \int d1 \, d1' \, v(1 - 1') \sum_{\pm} \left( \delta \delta_1 \delta_1' \delta_i \delta_i' - \delta_1 \delta_1' \delta_i \delta_i' \delta_1 + \delta_1 \delta_1' \delta_i \delta_i' \delta_1 - \delta_1 \delta_1' \delta_i \delta_i' \delta_1 + \delta_i \delta_1 \delta_1' \delta_i \delta_i' + \delta_1 \delta_1' \delta_i \delta_i' \delta_i - \delta_1 \delta_1' \delta_i \delta_i' \delta_i - \delta_1 \delta_1' \delta_i \delta_i' \delta_i - \delta_1 \delta_1' \delta_i \delta_i' \delta_i \right).$$

(7)

Notice that, in $\Delta' D = \sum D_{(1')} \otimes D_{(1')}$, each term $D_{(1')}$ or $D_{(1')}$ contains between one and three functional derivatives.

**B. Expansion of equation (3)**

Now we are going to examine each term of equation (3). We define the $n$-body Green function as

$$G_{\epsilon_1 \ldots \epsilon_n} (x_1, \ldots, x_n, y_1, \ldots, y_n') = (-i)^n \frac{\delta^{2n} Z_p}{\delta \eta_{\epsilon_1} (x_1) \cdots \delta \eta_{\epsilon_n} (x_n) \delta \eta'_{\epsilon_1} (y_1) \cdots \delta \eta'_{\epsilon_n} (y_n)}. \quad (8)$$

The right hand side is taken at zero external sources. To simplify the notation, we write $i$ for $x_i$ and $i'$ for $y_i$, we consider that $\epsilon_i$ goes with the variable $x_i$, $\epsilon'_i$ with $y_i$, so the $\epsilon$ are now implicit and we have

$$G_{(1, \ldots, n, 1', \ldots, n')} = (-i)^n \delta_1 \ldots \delta_n \delta_{1'} \ldots \delta_{n'} Z_p. \quad (9)$$

With this notation, the left hand side of equation (3) is now

$$\frac{\delta^2 Z_p}{\delta \eta_{\epsilon} (y) \delta \eta'_{\epsilon} (x)} = - \frac{\delta^2 Z_p}{\delta \eta_{\epsilon} (x) \delta \eta'_{\epsilon} (y)} = -i G(x, y).$$

More explicitly $G(x, y) = G_{\epsilon \epsilon'} (x, y)$. In the following we shall calculate in detail all the terms of the right hand side of equation (3).
C. First term of equation (3)

The first term of (3) is very simple. From equation (1), we know that \( W^1_\rho \) is the sum of a term of degree two and a term of degree four in the external sources. The first term in the right hand side of equation (3) contains only two derivatives, the first term gives us

\[
\frac{\delta^2W^1_\rho}{\delta\eta_c(y)\delta\bar{\eta}_c(x)} = -iG^0_{\rho\rho}(x, y).
\]

D. Second term of equation (3)

The second term of equation (3) is

\[
-\frac{i}{2}\int dl dl' v(1 - 1') \sum_{\pm} \left( -\delta_1 \delta_{1'} \otimes \delta_1 \delta_{1'} + \delta_1 \delta_{1'} \otimes \delta_1 \delta_{1'} + \delta_1 \delta_{1'} \otimes \delta_1 \delta_{1'} - \delta_1 \delta_{1'} \otimes \delta_1 \delta_{1'} \right).
\]

The second term of equation (3) becomes

\[
-\frac{i}{2}\int dl dl' v(1 - 1') \sum_{\pm} \left( -\delta_1 \delta_{1'} \otimes \delta_1 \delta_{1'} Z_\rho + (\delta_1 \delta_{1'} \otimes \delta_1 \delta_{1'} Z_\rho) + (\delta_1 \delta_{1'} \otimes \delta_1 \delta_{1'} Z_\rho) - (\delta_1 \delta_{1'} \otimes \delta_1 \delta_{1'} Z_\rho) \right).
\]

(9)

Let us now consider the first term of (9). According to (8), \( \delta_1 \delta_{1'} Z_\rho = -iG(1, 1') \). According to (2),

\[
\delta_1 \delta_{1'} \otimes \delta_1 \delta_{1'} W^1_\rho = \delta_1 \delta_{1'} \otimes \delta_1 \delta_{1'} W^1_\rho = -\epsilon\epsilon' r(x, 1', 1, y).
\]

For the second term of (9) we have \( \delta_1 \delta_{1'} Z_\rho = -iG(1', 1') \) and

\[
\delta_1 \delta_{1'} \otimes \delta_1 \delta_{1'} W^1_\rho = \delta_1 \delta_{1'} \otimes \delta_1 \delta_{1'} W^1_\rho = -\epsilon\epsilon' r(x, 1, 1, y).
\]

Interchanging the variables 1 and 1', we see that the third term of (9) is equal to the first one, and the fourth term is equal to the second one. Finally, the second term of (3) becomes the sum of

\[
-\epsilon\epsilon' \int dl dl' v(1 - 1') r(x, 1', 1, y) \sum_{\pm} G(1, 1'),
\]

and

\[
\epsilon\epsilon' \int dl dl' v(1 - 1') r(x, 1, 1, y) \sum_{\pm} G(1', 1').
\]

E. Third term of equation (3)

The third term is

\[
-\frac{i}{2} \sum (D_{\gamma_1} \delta_2 W^1_\rho) (D_{\gamma_1} \delta_2 Z_\rho).
\]
For this term, two kinds of $D_{(i'j')} \otimes D_{(i'j')}$ intervene: with one or three products in $D_{(i'j')}$. For the first kind of terms, the relevant coproducts are $\delta_1 \otimes \delta_1', \delta_1, \delta_1 - \delta_1 \otimes \delta_1, \delta_1'$ and the result is

$$-\frac{i}{2} \int d1d1'v(1 - 1') \sum_{\pm} \pm (\delta_1 \delta_2 W_{\rho}^1(\delta_1 \delta_1', \delta_1, \delta_1, \delta_1' Z_{\rho}) - (\delta_1' \delta_2 W_{\rho}^1(\delta_1 \delta_1', \delta_1, \delta_1' Z_{\rho})) = -i \int d1d1'v(1 - 1') \sum_{\pm} (\delta_1 \delta_2 W_{\rho}^1(\delta_1 \delta_1', \delta_1, \delta_1 Z_{\rho})$$

We have interchanged the variables $1$ and $1'$ to obtain the last line. We use now $\delta_1 \delta_2 W_{\rho}^1 = -iG_{\rho}(x, 1)$ and $\delta_1' \delta_2 W_{\rho}^1 = -\delta_1 \delta_1' \delta_1 \delta_1' Z_{\rho} = G(1, 1', 1, y)$, to get

$$- \int d1d1'v(1 - 1') \sum_{\pm} \pm G_{\rho}(x, 1)G(1, 1', 1, y).$$

For the second kind of terms, the relevant coproducts are $\delta_1 \delta_1' \delta_1 \otimes \delta_1 - \delta_1 \delta_1' \delta_1 \otimes \delta_1$. Again, interchanging $1$ and $1'$ shows that these two terms give the same contribution and the result is

$$i \int d1d1'v(1 - 1') \sum_{\pm} (\delta_1 \delta_1' \delta_1 \delta_2 W_{\rho}^1(\delta_1, \delta_1' Z_{\rho}) = -i \int d1d1'v(1 - 1') \sum_{\pm} (\delta_1 \delta_1' \delta_1 \delta_2 W_{\rho}^1(\delta_1, \delta_1' Z_{\rho})).$$

We calculate

$$\delta_1 \delta_1' \delta_1 \delta_2 W_{\rho}^1 = -\delta_2 \delta_1 \delta_1' \delta_1 W_{\rho}^1 = \pm \epsilon r(x, 1, 1', y),$$

and $\delta_1 \delta_1' Z_{\rho} = iG(1, y)$. The contribution of the second kind of terms becomes

$$-\epsilon \int d1d1'v(1 - 1')r(x, 1, 1, y') \sum_{\pm} G(1', 1).$$

**F. Fourth term of equation (3)**

The fourth term of equation (3) is

$$-\frac{1}{2} \sum_{\pm} (D_{(i'j')}^2 \delta_1 \delta_2 W_{\rho}^1) (D_{(i'j')}^2 Z_{\rho}).$$

Here we meet something new because we must use the reduced coproduct $\Delta'D^2$. According to the general formula (39) of I, this reduced coproduct is obtained by multiplying $\Delta'D$ by itself. The spacetime variables of the first $\Delta'D$ will still be denoted by $1$ and $1'$, while the spacetime variables of the second $\Delta'D$ will be denoted by $2$ and $2'$. Moreover, the $\pm$ variable of the second $\Delta'D$ will be written $\pm'$. Each term $D_{(i'j')}^2$ of $\Delta'D$ is at least of degree 1, so each term of $D_{(i'j')}^2$ is at least of degree 2. Therefore, the only term of $W_{\rho}^1$ that contributes to $D_{(i'j')}^2 \delta_1 \delta_2 W_{\rho}^1$ is $\rho^2(\alpha, \alpha)$. We use again the fact that $\rho^2(\alpha, \alpha)$ is a product of two sources $\eta$ and two sources $\bar{\eta}$ to deduce that $D_{(i'j')}^2$ must be the product of a functional derivative with respect to $\eta$ and a functional derivative with respect to $\bar{\eta}$. The eight terms $D_{(i'j')}^2$ that satisfy this condition are $\delta_1 \delta_2, \delta_1 \delta_2, \delta_1 \delta_2, \delta_1 \delta_2, \delta_1 \delta_2, \delta_1 \delta_2, \delta_1 \delta_2$, and $\delta_1 \delta_2$. This gives us eight terms which are all identical if we interchange $1$ with $1'$ or $2$ with $2'$ or $(1, 1')$ with $(2, 2')$. Thus, the fourth term of equation (3) becomes

$$- \int d1d1'd2d2'v(1 - 1')v(2 - 2') \sum_{\pm \pm'} (\delta_1 \delta_2 \delta_1' \delta_2 W_{\rho}^1(\delta_1, \delta_1' \delta_1 \delta_2' \delta_2, Z_{\rho}).$$

We have just to calculate

$$\delta_1 \delta_2 \delta_1' \delta_2 W_{\rho}^1 = \delta_2 \delta_1' \delta_1 \delta_2 W_{\rho}^1 = -\epsilon' \pm \epsilon r(x, 2, 1, y),$$

and

$$\delta_1 \delta_1' \delta_2 \delta_2' \delta_2' \delta_1' Z_{\rho} = -\delta_2 \delta_1' \delta_1 \delta_1' Z_{\rho} = -iG(2', 1, 1', 2, 2').$$

The final expression for the fourth term is then

$$-i \epsilon' \int d1d1'd2d2'v(1 - 1')v(2 - 2')r(x, 2, 1, y) \sum_{\pm \pm'} G(2', 1, 1', 2, 2').$$
G. Fifth term of equation (3)

The fifth term of equation (3) is

\[-\frac{1}{2} \sum (D^2_{(i)}, \delta_{\vec{\imath}} W_{\rho}^{\prime})(D^2_{(ii)}, \delta_{\rho} Z_{\bar{\eta}}).\]

To give nonzero contributions, \(D^2_{(i')}\) must contain three functional derivatives: one functional derivative with respect to \(\bar{\eta}\) and two with respect to \(\eta\). This gives us three kinds of terms: (i) the argument of \(\bar{\eta}\) does not come from the same \(D\) as the arguments of the two \(\eta\), as in \(D^2_{(i')} = \delta_{\bar{\eta}} \delta_{\bar{\eta}}\) (ii) the argument of \(\bar{\eta}\) is the same as that of one of the two \(\eta\), for example \(D^2_{(i')} = \delta_{\bar{\eta}} \delta_{\bar{\eta}}\) (iii) the argument of \(\bar{\eta}\) comes from the same \(D\) as the argument of one of the two \(\eta\) but they are not identical, for example \(D^2_{(i')} = -\delta_{\bar{\eta}} \delta_{\bar{\eta}}\). In \(\Delta' D^2\) there are four terms of type (i), eight terms of type (ii) and eight terms of type (iii). All the terms of each class give the same contribution. We calculate now the contribution of the three kinds of terms

1. Terms of kind (i)

The sum of the terms of type (i) is

\[-\frac{1}{2} \int d1d1'd2d2'v(1 - 1')v(2 - 2') \sum_{\pm, \pm'} (\delta_{\bar{\eta}} \delta_{\bar{\eta}} \delta_{\bar{\eta}} W_{\rho}^{\prime})(\delta_{\eta} \delta_{\eta} \delta_{\eta} \delta_{\eta} Z_{\rho}).\]

We compute

\[\delta_{\bar{\eta}} \delta_{\bar{\eta}} \delta_{\bar{\eta}} W_{\rho}^{\prime} = -\delta_{\bar{\eta}} \delta_{\bar{\eta}} \delta_{\bar{\eta}} W_{\rho}^{\prime} = \pm e r(x, 1', 2, 2'),\]

and

\[\delta_{\eta} \delta_{\eta} \delta_{\eta} \delta_{\eta} Z_{\rho} = -\delta_{\eta} \delta_{\eta} \delta_{\eta} \delta_{\eta} Z_{\rho} = i G(1, 2, 2', 1, 1', y)\]

to obtain

\[-\frac{i}{2} \int d1d1'd2d2'v(1 - 1')v(2 - 2')r(x, 1', 2, 2') \sum_{\pm, \pm'} G(1, 2, 2', 1, 1', y).\]

2. Terms of kind (ii)

The sum of the terms of type (ii) is

\[-\int d1d1'd2d2'v(1 - 1')v(2 - 2') \sum_{\pm, \pm'} (\delta_{\bar{\eta}} \delta_{\bar{\eta}} \delta_{\bar{\eta}} W_{\rho}^{\prime})(\delta_{\eta} \delta_{\eta} \delta_{\eta} \delta_{\eta} Z_{\rho}).\]

We use

\[\delta_{\bar{\eta}} \delta_{\bar{\eta}} \delta_{\bar{\eta}} W_{\rho}^{\prime} = -\delta_{\bar{\eta}} \delta_{\bar{\eta}} \delta_{\bar{\eta}} W_{\rho}^{\prime} = \pm e r(x, 2', 1, 2'),\]

and

\[\delta_{\eta} \delta_{\eta} \delta_{\eta} \delta_{\eta} Z_{\rho} = -\delta_{\eta} \delta_{\eta} \delta_{\eta} \delta_{\eta} Z_{\rho} = i G(1, 1', 2, 1', 2, y)\]

Therefore, the fifth term of type (ii) becomes

\[-i e \int d1d1'd2d2'v(1 - 1')v(2 - 2')r(x, 2', 1, 2') \sum_{\pm, \pm'} G(1, 1', 2, 1', 2, y).\]
3. Terms of kind (iii)

The sum of the terms of type (iii) is

\[ \int d1d1'd2d2'v(1 - 1')v(2 - 2') \sum_{\pm, \pm'} (\delta_1 \delta_2 \delta_3 W^1_{1'}) (\delta_1 \delta_2 \delta_3 \delta_4 Z). \]

We have

\[ \delta_1 \delta_2 \delta_3 W^1_{1'} = \delta_2 \delta_3 \delta_1 W^1_{1'} = \mp \epsilon r(x, 2', 1, 2), \]

and

\[ \delta_1 \delta_1 \delta_2 \delta_2 \delta_4 Z = -\delta_1 \delta_2 \delta_1 \delta_2 \delta_4 Z = i G(1, 1', 2, 1', 2', y). \]

The fifth term of type (iii) becomes

\[ -i \epsilon \int d1d1'd2d2'v(1 - 1')v(2 - 2')r(x, 2', 1, 2) \sum_{\pm, \pm'} G(1, 1', 2, 1', 2', y). \]

H. Sixth term of equation (3)

The sixth term of equation (3) is

\[ \frac{i}{\theta} \sum (D^3_{el}) \delta_2 \delta_3 W^1_{1'} (D^3_{el}) \delta_4 Z. \]

It looks complicated because we have now \( \Delta' D^3 = (\Delta' D)(\Delta' D)(\Delta' D) \). The third \( \Delta' D \) will have the variables 3, 3' and \( \pm'' \). Again, we need one derivative with respect to \( \eta \) and two derivatives with respect to \( \eta \) in \( D^3_{el} \). There are 24 terms of this kind in \( \Delta' D^3 \), and they all give the same contribution as \( \delta_1 \delta_2 \delta_3 \delta_4 \delta_5 \delta_6 \delta_7 \delta_8 \delta_9 \delta_{10} \delta_{11} \delta_{12} \delta_{13} \delta_{14} \delta_{15} \delta_{16} \delta_{17} \delta_{18} \delta_{19} \delta_{20} \delta_{21} \delta_{22} \delta_{23} \delta_{24} \). Thus, the sixth term is

\[ \frac{i}{2} \int d1d1'd2d2'd3d3'v(1 - 1')v(2 - 2')v(3 - 3') \sum_{\pm, \pm', \pm''} (\delta_1 \delta_2 \delta_3 W^1_{1'}) (\delta_1 \delta_2 \delta_3 \delta_4 \delta_5 \delta_6 \delta_7 \delta_8 \delta_9 \delta_{10} \delta_{11} \delta_{12} \delta_{13} \delta_{14} \delta_{15} \delta_{16} \delta_{17} \delta_{18} \delta_{19} \delta_{20} \delta_{21} \delta_{22} \delta_{23} \delta_{24} \). \]

We compute

\[ \delta_1 \delta_2 \delta_3 W^1_{1'} = -\delta_2 \delta_1 \delta_3 W^1_{1'} = \pm \epsilon \epsilon'' \epsilon r(x, 1, 2, 3), \]

and

\[ \delta_1 \delta_2 \delta_3 \delta_4 \delta_5 \delta_6 \delta_7 \delta_8 \delta_9 \delta_{10} \delta_{11} \delta_{12} \delta_{13} \delta_{14} \delta_{15} \delta_{16} \delta_{17} \delta_{18} \delta_{19} \delta_{20} \delta_{21} \delta_{22} \delta_{23} \delta_{24} \delta_{25} \].

The last term of equation (3) is then

\[ -\frac{1}{2} \epsilon \int d1d1'd2d2'd3d3'v(1 - 1')v(2 - 2')v(3 - 3')r(x, 1, 2, 3) \sum_{\pm, \pm', \pm''} G(1', 2', 3', 1', 2', 3', y). \]
I. The Green function hierarchy

If we gather all the previous results, we obtain the Green function hierarchy

\[
G(x, y) = G_{ee'}(x, y) = G^0_{pee'}(x, y) - i \int d1d1'v(1 - 1') \sum_{\pm} \pm G^0_{\mu}(x, 1)G(1, 1', 1', y)
\]

\[-i \epsilon' \int d1d1'v(1 - 1')r(x, 1', 1, y) \sum_{\pm} G(1, 1') + i \epsilon' \int d1d1'v(1 - 1')r(x, 1, 1, y) \sum_{\pm} G(1', 1')
\]

\[-i \epsilon \int d1d1'v(1 - 1')r(x, 1, 1', y) \sum_{\pm} G(1', y)
\]

\[+ \frac{1}{2} \epsilon \int d1d1'd2d2'v(1 - 1')v(2 - 2')r(x, 1', 2, 2') \sum_{\pm, \pm'} G(1, 1', 2', 1', y)
\]

\[+ \epsilon \int d1d1'd2d2'v(1 - 1')v(2 - 2')r(x, 2', 1, 2) \sum_{\pm, \pm'} G(1', 2', 1', 2', y).
\]

\[+ \epsilon' \int d1d1'd2d2'v(1 - 1')v(2 - 2')r(x, 2, 1, y) \sum_{\pm, \pm'} G(1', 1', 2', 1')
\]

\[+ \epsilon \int d1d1'd2d2'v(1 - 1')v(2 - 2')r(x, 2', 1', 2') \sum_{\pm, \pm'} G(1', 2', 1', 2, y).
\]

\[- \frac{i}{2} \epsilon \int d1d1'd2d2'd3d3'v(1 - 1')v(2 - 2')v(3 - 3')r(x, 1, 2, 3) \sum_{\pm, \pm', \pm''} G(1', 2, 2', 3, 3', 1, 1', 2', 3', y).
\]

In terms of the Feynman diagrams of nonequilibrium quantum field theory\(^2\), these terms can be rewritten as in figure 1. The order of the terms is the same in equation (10) and in figure 1.

IV. CONCLUSION

The hierarchy of Green functions presented here is an important step in the effective calculation of degenerate systems. However, the practical implementation of this hierarchy requires an approximation to close it. The GW approximation\(^3\)–\(^5\) is a well-known and powerful way of closing the hierarchy. It has to be adapted to our more complicated hierarchy. For the calculation of the optical properties of allochromatic crystals, it will also be necessary to adapt the Bethe-Salpeter approach\(^6\) to our setting.
Moreover, a functional derivation of the energy with respect to the density matrix provides equations that enable us to unify the Green-function formalism and the diagonalization method of many-body theory. This will be presented in a forthcoming publication\textsuperscript{7}.

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