The single-particle Green's function in action: a pedagogical example

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A. Introduction

Many of us are familiar with the time-ordered Green's functions as a formal tool in many-particle quantum mechanics. But for practical applications it is very helpful to have a transparent example that illustrates how it works. To that end, this note presents the Green's function algebra going with a simple Hamiltonian. The Hamiltonian contains 4 orbitals and has one- and two-body terms

$$\hat{H} = \hat{H}_1 + \hat{H}_2 \tag{1}$$

where

$$\hat{H}_1 = \sum_{i=1}^{4} \varepsilon_i \hat{n}_i \tag{2}$$

and

$$\hat{H}_2 = v(\hat{a}_3^\dagger \hat{a}_4^\dagger \hat{a}_2 \hat{a}_1 + \text{h.c.}). \tag{3}$$

The single-particle orbital energies in $\hat{H}_1$ are set to

$$\begin{aligned} \varepsilon_i &= -\varepsilon/2, \;\; i = 1,2 \\ &= \varepsilon/2, \;\; i = 3,4. \end{aligned} \tag{4}$$

In this note we focus on the particle-removal Green's function G^h but we also make the connection with the particle-addition Green;s function G^p.

B. General

The Green's function is to be calculated for operator expectation values in the two-particle ground state $|\text{gs}\rangle$. The ground state wave function is obtained by diagonalizing the Hamiltonian

$$\begin{bmatrix} -\varepsilon & v \\ v & \varepsilon \end{bmatrix} \tag{5}$$

The lower-energy eigenfunction is

$$|\text{gs}\rangle = \alpha\ \hat{a}_1^\dagger \hat{a}_2^\dagger |\rangle + \beta\ \hat{a}_3^\dagger \hat{a}_4^\dagger |\rangle \tag{6}$$

where the amplitudes α, β are given by

$$\begin{aligned} \alpha &= \left(\varepsilon + \sqrt{\varepsilon^2 + v^2}\right)\mathcal{N} \\ \beta &= -v\mathcal{N}; \end{aligned} \tag{7}$$

the normalization factor $\mathcal{N}$ is

$$\mathcal{N} = \left((\varepsilon + \sqrt{\varepsilon^2 + v^2})^2 + v^2\right)^{-1/2}. \tag{8}$$

The energy of ground state is

$$E_{\text{gs}} = -\sqrt{\varepsilon^2 + v^2}. \tag{9}$$

The particle-removal Green's function for an orbital k is defined as

$$G^h_{kk}(\tau) = i\langle \text{gs}|\hat{a}_k^\dagger(\tau)\hat{a}_k|\text{gs}\rangle = i\langle \text{gs}|e^{i\hat{H}\tau}\hat{a}_k^\dagger e^{-i\hat{H}\tau} a_k|\text{gs}\rangle \tag{10}$$

for $\tau > 0$. It is set to zero if $\tau < 0$.

To evaluate the Green's function G^h_{11} we make the following substitutions:

$$\begin{aligned} \hat{a}_1|\text{gs}\rangle &\to \alpha\hat{a}_2^\dagger|\rangle \\ e^{-i\hat{H}\tau}\hat{a}_2^\dagger|\rangle &\to e^{-i(-\varepsilon/2)\tau}\hat{a}_2^\dagger|\rangle \\ \langle\text{gs}|e^{i\hat{H}\tau} &\to e^{iE_{\text{gs}}\tau}\langle\text{gs}| \\ \langle\text{gs}|\hat{a}_1^\dagger &\to \alpha\langle|\hat{a}_2^\dagger \end{aligned}$$

The result is

$$G^h_{11}(\tau) = i\alpha^2 e^{i(\varepsilon/2 - \sqrt{\varepsilon^2+v^2})\tau}. \tag{11}$$

The Table below collects the results for several Green's functions, including this one and G^h_{33}, derived in the same way. Other removal Green's functions are $G^h_{22} = G^h_{11}$ and $G^h_{44} = G^h_{33}$, as is obvious from the symmetry of the Hamiltonian.

	$G(\tau)$	$G(\omega)$
G^h_{11}	$i\alpha^2 e^{i(\varepsilon/2-\sqrt{\varepsilon^2+v^2})\tau}$	$-\alpha^2/(\omega + \varepsilon/2 - \sqrt{e^2+v^2} + i0^+)$
G^h_{33}	$i\beta^2 e^{i(-\varepsilon/2-\sqrt{\varepsilon^2+v^2})\tau}$	$-\beta^2/(\omega - \varepsilon/2 - \sqrt{\varepsilon^2+v^2} + i0^+)$
G^p_{11}	$i\beta^2 e^{i(-\varepsilon/2-\sqrt{\varepsilon^2+v^2})\tau}$	$-\beta^2/(\omega - \varepsilon/2 - \sqrt{\varepsilon^2+v^2} + i0^+))$
G^p_{33}	$i\alpha^2 e^{i(\varepsilon/2-\sqrt{\varepsilon^2+v^2})\tau}$	$-\alpha^2/(omegae + \varepsilon/2 - \sqrt{\varepsilon^2+v^2} + i0^+))$

The first property to be noted is that G^h_{kk} at $\tau = 0^+$ gives the occupation probabilities of the orbitals n_k,

$$n_k = -iG^h_{kk}(0^+) = \langle\text{gs}|\hat{a}_k^\dagger\hat{a}_k|\text{gs}\rangle = \langle\text{gs}|\hat{n}_k|\text{gs}\rangle \tag{12}$$

The total particle number N is obtained by summing over k,

$$N = \sum_k \langle\text{gs}|\hat{n}_k|\text{gs}\rangle = -i\sum_k G^h_{kk}(0^+). \tag{13}$$

It is trivial to verify these relations for the Hamilonian in Eq. (1-4) so we skip the details.

A less trivial application of single-particle Green's functions concerns the energy of the system. To derive an energy formula we start with the equation of motion for operators in the Heisenberg representation,

$$\frac{d}{d\tau}\hat{O} = i[\hat{H}, \hat{O}]. \tag{14}$$

Application of this to the Green's function G^h_{kk} yields the equation

$$\frac{d}{d\tau}G^h_{kk}|_{0^+} = -\langle \mathrm{gs}|[\hat{H}, \hat{a}^\dagger_k]\hat{a}_k|\mathrm{gs}\rangle. \tag{15}$$

We now have to distinguish between the one-body and the two-body parts of the Hamiltonian. For the one-body part $\sum_k[\hat{H}_1, \hat{a}^\dagger_k]\hat{a}_k = \hat{H}_1$ but the sum for the two-body part includes each interaction term twice: $\sum_k[\hat{H}_2, \hat{a}^\dagger_k]\hat{a}_k = 2\hat{H}_2$. Thus the derivative of the Green's function at $\tau = 0^+$ is

$$\frac{d}{d\tau}\sum_k G^h_{kk}|_{0^+} = -\langle \mathrm{gs}|\hat{H}_1|\mathrm{gs}\rangle - 2\langle \mathrm{gs}|\hat{H}_2|\mathrm{gs}\rangle. \tag{16}$$

This relationship was originally derived by Galitskii and Migdal [1] and reformulated for nuclear binding energies by Koltun [2]. Note that additional information is needed to get the total energy $E_{\mathrm{gs}} = \langle \mathrm{gs}|\hat{H}_1|\mathrm{gs}\rangle + \langle \mathrm{gs}|\hat{H}_2|\mathrm{gs}\rangle$ from Eq. (16); normally one relies on experiment or microscopic theory to estimate the first term. An example of the application to nuclear physics may be found in Refs. [3, 4] and an application to condensed matter physics in Ref. [5].

Let us now verify that the Green's function Eq. (10) satisfies Eq. (16). The explicit derivative of Eq. (10) gives

$$\frac{d}{d\tau}G^h_{11}\bigg|_{0^+} = -\alpha^2(E_{\mathrm{gs}} + \varepsilon/2). \tag{17}$$

The righthand side of Eq. (16) is

$$\begin{aligned} &-\langle \mathrm{gs}|[\hat{H}_1 + \hat{H}_2, \hat{a}^\dagger_1]\hat{a}_1|\mathrm{gs}\rangle = \\ &-(-\varepsilon)\langle \mathrm{gs}|\hat{a}^\dagger_1\hat{a}_1|\mathrm{gs}\rangle/2 - v\langle \mathrm{gs}|(\hat{a}^\dagger_3\hat{a}^\dagger_4\hat{a}_2\hat{a}_1|\mathrm{gs}\rangle \\ &= -\alpha^2(-\varepsilon)/2 - \alpha\beta v. \end{aligned} \tag{18}$$

It is now just a few steps of algebra using Eq. (7) to verify that the two sides are indeed equal. The corresponding expressions on the right and left for G^h_{33} are

$$\beta^2(E_{\mathrm{gs}} - \varepsilon/2) = \varepsilon\beta^2 + v\alpha\beta. \tag{19}$$

Again, it is simple algebra with Eq. (7) to verify the equality.

The particle-addition Green's function $G^p$is defined

$$G^p_{kk}(\tau) = \Theta(\tau)\langle \mathrm{gs}|\hat{a}_k(\tau)\hat{a}^\dagger_k|\mathrm{gs}\rangle \tag{20}$$

It can be evaluated in the same way we did for G^h. The expressions are given in the Table.

C. Many-body perturbation theory and the Dyson equation

Many-body perturbation theory is usually formulated with Fourier-transformed Green's functions. They are defined

$$G^h_{kk}(\omega) = \int_{-\infty}^{\infty} d\tau\ e^{i\omega\tau}G^h_{kk}(\tau). \tag{21}$$

We will use the same symbol for both Green's function representations as there is no danger of confusion. Note that the range of integration in Eq. (21) can be reduced to $[0, +\infty]$ because $G^h(\tau)$ vanishes for negative τ. As an example, the Green's function in Eq. (11) is transformed to

$$G^h_{11}(\omega) = -\frac{-\alpha^2}{\omega - \sqrt{e^2 + v^2} + \varepsilon/2 + i0^+} \tag{22}$$

Here 0^+ is an infinitesimal positive quantity. It is needed only as an instruction for carrying out the contour integral in the inverse Fourier transform

$$G^h_{kk}(\tau) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\ e^{-i\omega\tau}G^h_{kk}(\omega). \tag{23}$$

For many-body perturbation theory, one starts with non-interacting Green's functions G^0. They are constructed using only the single-particle term in the Hamiltonian. For the H_1 in Eq. (2) one obtains

$$G^{h0}_{11}(\omega) = -\frac{1}{\omega - \varepsilon/2 + i0^+}. \tag{24}$$

Interactions are included by the term $\Sigma(\omega)$ in the Dyson equation,

$$G^h(\omega)^{-1} = G^{h0}(\omega)^{-1} + \Sigma(\omega). \tag{25}$$

Here G^h, G^{h0} and Σ are matrices in the space of orbitals k. The orbitals are usually defined to make G^0 diagonal. The simplest approximation to Σ is a second-order perturbative expression. For the Hamiltonian in the example, it turns out that the Dyson equation gives the exact G^h as one of its terms. The perturbative Σ_{11} for H_2 in the example is

$$\Sigma_{11}(\omega) = \frac{v^2}{\omega + \varepsilon_2 - \varepsilon_3 - \varepsilon_4}. \tag{26}$$

The interaction Green's function from the Dyson equation is

$$G^{h0}_{11} = \frac{1}{(\omega + \varepsilon_1) - \frac{v^2}{\omega + \varepsilon_2 - \varepsilon_3 - \varepsilon_4)} + i0^+} \tag{27}$$

This function has two poles at

$$\omega_\pm = \frac{\varepsilon}{2} \pm \sqrt{\varepsilon^2 + v^2}\,; \tag{28}$$

the one closest to the unperturbed pole is ω_-. This is just the same frequency as in Eq. (11) for G^h_{11}. The residual of the pole can be found in the usual way by expanding Eq. (25) as a sum over the two poles. After some algebra one can show that the residue is equal to α^2, the amplitude of the exponential in Eq. (11). This demonstrates the assertion the Dyson equation provides the exact G^h.

But what about the second pole? It has the same frequency and residue (up to a sign) as the particle-addition Green's function G^p_{11}. This motivates the contruction of the time-order Green's function treating G^h and G^p together in the function.

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