Introduction to the Green's Function

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1 Defining the Green's Function

The "imaginary time, time-ordered" Green's function is defined as

$$G(\tau,\tau') = -\frac{1}{z}\operatorname{Tr}[T_\tau e^{-\beta\hat{H}}C(\tau)C^\dagger(\tau')]$$

The unfamiliar terms inside $G(\tau,\tau')$ are defined as follows:

$$C(\tau) = e^{\tau\hat{H}}ce^{-\tau\hat{H}} \qquad C^\dagger(\tau') = e^{\tau'\hat{H}}c^\dagger e^{-\tau\hat{H}}$$
$$z = \operatorname{Tr} e^{-\beta\hat{H}} \qquad T_\tau A_\tau B_{\tau'} = \theta(\tau-\tau')A_\tau B_{\tau'} - \theta(\tau'-\tau)B_{\tau'}A_\tau \qquad \beta = \frac{1}{k_B T}$$

θ is the heaviside step function, i.e. $\theta(x) = \mathbf{1}_{x>0}$. For now, suppose the hamiltonian is simply $\hat{H} = -\mu c^\dagger c$. Only one particle is being considered, so the only two states are $|0\rangle$ and $|1\rangle$ with energy eigenvalues of $E_0 = 0$ and $E_1 = -\mu$. For this $\hat{H}$

$$z = \operatorname{Tr} e^{-\beta\hat{H}} = \sum_n \langle n|e^{-\beta\hat{H}}|n\rangle = 1 + e^{\beta\mu}$$

Interestingly, Green's function can be simplified signifcantly for this $\hat{H}$ as well. First simplify the expressions for $C(\tau)$ and $C^\dagger(\tau')$:

$$\begin{aligned}
\frac{d}{d\tau}C(\tau) &= e^{\tau\hat{H}}\hat{H}ce^{-\tau\hat{H}} - e^{\tau\hat{H}}c\hat{H}e^{-\tau\hat{H}} \\
&= e^{\tau\hat{H}}[\hat{H},c]e^{-\tau\hat{H}} \\
&= -\mu e^{\tau\hat{H}}[\hat{n},c]e^{-\tau\hat{H}} \\
&= \mu e^{\tau\hat{H}}ce^{-\tau\hat{H}} \\
&= \mu C(\tau) \\
\frac{d}{d\tau'}C^\dagger(\tau') &= -\mu e^{\tau'\hat{H}}[\hat{n},c^\dagger]e^{-\tau'\hat{H}} \quad \text{skipping previous steps} \\
&= -\mu e^{\tau'\hat{H}}c^\dagger c^{-\tau'\hat{H}} \\
&= -\mu C^\dagger(\tau')
\end{aligned}$$

$$\implies C(\tau) = e^{\mu\tau}c \qquad C^\dagger(\tau') = e^{-\mu\tau'}c^\dagger$$

Plugging these into Green's function:

$$\begin{aligned}
G(\tau,\tau') &= -\theta(\tau-\tau')\operatorname{Tr} e^{-\beta\hat{H}}e^{\mu\tau}ce^{-\mu\tau'}c^\dagger\frac{1}{z} + \theta(\tau'-\tau)\operatorname{Tr} e^{-\beta\hat{H}}e^{-\mu\tau'}c^\dagger e^{\mu\tau}c\frac{1}{z} \\
&= -\theta(\tau-\tau')e^{\mu(\tau-\tau')}\frac{1}{z}\operatorname{Tr} e^{-\beta\hat{H}}cc^\dagger + \theta(\tau-\tau')e^{\mu(\tau-\tau')}\frac{1}{z}\operatorname{Tr} e^{-\beta\hat{H}}c^\dagger c \\
&= e^{\mu(\tau-\tau')}\big[-\theta(\tau-\tau')\frac{1}{1+e^{\beta\mu}} + \theta(\tau'-\tau)\frac{e^{\beta\mu}}{1+e^{\beta\mu}}\big] \\
&= e^{\mu(\tau-\tau')}(-\theta(\tau-\tau')f(\mu) + \theta(\tau'-\tau)f(-\mu)) \qquad \text{with } f(\mu) = \frac{1}{1+e^{\beta\mu}} \\
&= e^{\mu(\tau-\tau')}(\theta(\tau'-\tau) - f(\mu)) \qquad \text{since } f(\mu)+f(-\mu) = 1 \text{ and } \theta(x)+\theta(-x) = 1
\end{aligned}$$

2 Two general properties of the Green's function

2.1 Time-translational invariance

Time-translational invariance is the fact that Green's function is really just dependent on one parameter, the difference $\tau - \tau'$.

$$\begin{aligned} G(\tau, \tau') &= -\frac{1}{z} \operatorname{Tr} T_\tau e^{-\beta \hat{H}} e^{\tau \hat{H}} c e^{-\tau \hat{H}} e^{\tau' \hat{H}} c^\dagger e^{-\tau' \hat{H}} \\ &= -\frac{1}{z} \operatorname{Tr} T_\tau e^{-\beta \hat{H}} e^{(\tau-\tau')\hat{H}} c e^{-(\tau-\tau')\hat{H}} c^\dagger \qquad [\hat{H}, \hat{H}] = 0, \text{ and } \operatorname{Tr} T_\tau AB = \operatorname{Tr} T_\tau BA \\ &= -\frac{1}{z} \operatorname{Tr} T_{\tau-\tau'} e^{-\beta \hat{H}} C(\tau - \tau') C^\dagger(0) \\ &= G(\tau - \tau', 0) \\ &:= G(\tau - \tau') \end{aligned}$$

In the second line, the time ordering operator T_τ doesn't appear to really mean anything since the τ's and τ''s are out of order. But, it actually makes sense, after observing that under a trace T_τ really means

$$\operatorname{Tr} T_\tau \text{expr} = (\theta(\tau - \tau') - \theta(\tau' - \tau)) \operatorname{Tr} \text{expr} = \operatorname{Tr} T_{\tau-\tau'} \text{expr}$$

2.2 Antiperiodicity of β

Green's function is antiperiodic in β, that is, $G(\tau) = -G(\tau + \beta)$. To avoid exponential growth, ideally $\beta \geq \tau + \beta$, so for convenience τ can be assumed to be negative. For the same reason $\tau \geq -\beta$, so $\tau + \beta \geq \tau' = 0$ and $T_{\tau+\beta-\tau'} = 1$.

$$\begin{aligned} G(\tau + \beta) &= -\frac{1}{z} \operatorname{Tr} e^{-\beta \hat{H}} C(\tau + \beta) C^\dagger(0) \\ &= -\frac{1}{z} \operatorname{Tr} e^{-\beta \hat{H}} e^{(\tau+\beta)\hat{H}} c e^{-(\tau+\beta)\hat{H}} c^\dagger \\ &= -\frac{1}{z} \operatorname{Tr} e^{-\beta \hat{H}} e^{-\tau \hat{H}} c^\dagger e^{\tau \hat{H}} c \\ &= -\frac{1}{z} \operatorname{Tr} e^{-\beta \hat{H}} c^\dagger e^{\tau \hat{H}} c e^{-\tau \hat{H}} \\ &= -G(\tau) \end{aligned}$$

Keep in mind the assumption that $\tau \leq \tau'$ was used in the last line, for the proper case of T_τ.
The antiperiodicity of G comes in handy because it allows for the Fourier Transform of G. One can verify that the function $e^{\mu\tau}(\theta(\tau) - f(\mu))$ is antiperiodic in β.

3 Introduction to fourier series/transforms

Fourier transforms is based on fourier series, which is based on the orthogonality of the basis $\{\sin(\frac{n\pi x}{L}), \cos(\frac{m\pi}{L})\}_{m,n=0}^{\infty}$. It is true that

$$\int_{-L}^{L} \sin\left(\frac{m\pi x}{L}\right) \sin\left(\frac{n\pi x}{L}\right) dx = \begin{cases} L & \text{if } m = n \\ 0 & \text{if } m \neq n \end{cases} \qquad \int_{-L}^{L} \cos\frac{m\pi x}{L} \cos\frac{n\pi x}{L} dx = \begin{cases} 2L & \text{if } m = n = 0 \\ L & \text{if } m = n \neq 0 \\ 0 & \text{if } m \neq n \end{cases}$$

$$\int_{-L}^{L} \cos\frac{m\pi x}{L} \sin\frac{n\pi x}{L} dx = 0$$

Therefore any continuous periodic function $f(x)$ can be expressed as

$$f(x) = A_0 + \sum_{m=1}^{\infty} A_m \cos\left(\frac{m\pi x}{L}\right) + \sum_{n=1}^{\infty} B_n \sin\left(\frac{n\pi x}{L}\right)$$

Where the coefficients are given by

$$A_0 = \frac{1}{2L} \int_{-L}^{L} f(x) \qquad A_{m\neq 0} = \frac{1}{L} \int_{-L}^{L} f(x) \cos\left(\frac{m\pi x}{L}\right) dx \qquad B_n = \frac{1}{L} \int_{-L}^{L} f(x) \sin\left(\frac{n\pi x}{L}\right) dx$$

Alternatively, $f(x)$ can be expressed as

$$f(x) = \sum_{n=-\infty}^{\infty} C_n e^{\frac{i\pi n x}{L}} \quad \text{where} \quad C_n = \frac{1}{2}(A_{|n|} - i\,\mathrm{sgn}(n) B_{|n|}) = \frac{1}{2L}\int_{-L}^{L} f(x) e^{-i\frac{n\pi x}{L}} dx$$

In the limit as $L \to \infty$, this provides an explanation for the fourier transform.

$$\begin{aligned} f(x) = \lim_{L\to\infty} \sum_{n=-\infty}^{\infty} C_n e^{i\frac{n\pi x}{L}} &= \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} \frac{\pi}{L} e^{i\frac{n\pi x}{L}} \int_{-L}^{L} f(x) e^{-i\frac{n\pi x}{L}} dx \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\left(\int_{-\infty}^{\infty} f(x) e^{-ikx} dx\right) dk \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx} F(k) dk \end{aligned}$$

Where $F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x) e^{-ikx} dx$ is the fourier transform of $f(x)$.

3.1 Matsubara Frequencies

Let us find the fourier series for $G(\tau)$ calculated for the simple $\hat{H} = -\mu c^\dagger c$ earlier (antiperiodic in β means periodic in 2β, although our allowed range is only 2β). That is, assume $G(\tau)$ takes the form

$$G(\tau) = \sum_{n=-\infty}^{\infty} e^{-i\frac{\pi n \tau}{\beta}} G_n$$

Where G_n is to be determined as follows (let $\omega_n = \frac{\pi n}{\beta}$)

$$\begin{aligned} G_n &= \frac{1}{2\beta}\int_{-\beta}^{\beta} e^{i\omega_n \tau} G(\tau) d\tau = \frac{1}{2\beta}\int_{-\beta}^{\beta} e^{i\omega_n\tau} e^{\mu\tau}(\theta(\tau) - f(\mu)) d\tau \\ &= \frac{1}{2\beta}\left[\int_0^\beta e^{(i\omega_n+\mu)\tau} f(-\mu) d\tau - \int_{-\beta}^{0} e^{(i\omega_n+\mu)\tau} f(\mu) d\tau\right] \\ &= \frac{1}{2\beta(i\omega_n+\mu)}\left[e^{(i\omega_n+\mu)\tau} f(-\mu)\Big|_0^\beta - e^{(i\omega_n+\mu)\tau} f(\mu)\Big|_{-\beta}^{0}\right] \\ &= \frac{1}{2\beta(i\omega_n+\mu)}\left[e^{(i\omega_n+\mu)\tau}\Big|_0^\beta - e^{(i\omega_n+\mu)\tau} f(\mu)\Big|_{-\beta}^{\beta}\right] \\ &= \frac{1}{2\beta(i\omega_n+\mu)}\left[(-1)^n e^{\beta\mu} - 1 - ((-1)^n e^{\beta\mu} - (-1)^n e^{-\beta\mu}) f(\mu)\right] \\ &= \frac{1}{2\beta(i\omega_n+\mu)}\left[(-1)^n (e^{\beta\mu} + \frac{e^{-\beta\mu} - e^{\beta\mu}}{1+e^{\beta\mu}}) - 1\right] \end{aligned}$$

I seem to be unable to simplify this expression.

4 Spin, more angular momentum relations

The discovery of an instrinsic angular momentum possessed by particles motivates the introduction of spin angular momentum operators $\hat{\mathbf{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$. Like regular angular momentum:

$$[\hat{S}_i, \hat{S}_j] = i\hbar\epsilon_{ijk}\hat{S}_k \qquad \hat{S}_z |sm_s\rangle = \hbar m_s |sm_s\rangle \qquad \hat{\mathbf{S}}^2 |sm_s\rangle = s(s+1)|sm_s\rangle$$

An important, simple case to consider is spin$-\frac{1}{2}$. Let the basis $|\uparrow\rangle$ and $|\downarrow\rangle$ such that $\hat{S}_z|\uparrow\rangle = \frac{1}{2}\hbar|\uparrow\rangle$ and $\hat{S}_z|\downarrow\rangle = -\frac{1}{2}\hbar|\downarrow\rangle$. Since there are only two states, $\hat{S}_x^2$ and $\hat{S}_y^2$ turn out to be quite nice.

$$\hat{S}_x^2 = \frac{1}{4}(\hat{S}_+ + \hat{S}_-)^2 = \frac{1}{4}(\hat{S}_+^2 + \hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+ + \hat{S}_-^2) = \frac{1}{2}(\hat{\mathbf{S}}^2 - \hat{S}_z^2) = \hat{S}_z^2$$

If there are only two states, raising or lowering twice must annihilate any state so $\hat{S}_+^2 = \hat{S}_-^2 = 0$. Also, I used $\frac{1}{2}(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+) = \mathbf{S}^2 - \hat{S}_z^2$. It goes without saying that similarly $\hat{S}_y^2 = \hat{S}_z^2$. This can be used to derive new relations. For the following, assume that i comes before j in an even permutation, WLOG

$$\begin{aligned}
\hat{S}_i\hat{S}_j + \hat{S}_j\hat{S}_i &= [\hat{S}_j, \hat{S}_k]\hat{S}_j + \hat{S}_j[\hat{S}_j, \hat{S}_k] \\
&= \hat{S}_j\hat{S}_k\hat{S}_j - \hat{S}_k\hat{S}_j\hat{S}_j + \hat{S}_j\hat{S}_j\hat{S}_k - \hat{S}_j\hat{S}_k\hat{S}_j \\
&= \hat{S}_j^2\hat{S}_k - \hat{S}_j^2\hat{S}_k \qquad \text{as } \hat{S}_j^2 \text{ is a multiple of the identity} \\
&= 0
\end{aligned}$$

And in the case of $i = j$ then $2\hat{S}_i^2 = \frac{\hbar^2}{2}\mathbf{1}$ where $\mathbf{1}$ is the identity. Thus,

$$\{\hat{S}_i, \hat{S}_j\}_+ = \delta_{ij}\frac{\hbar^2}{2}\mathbf{1}$$

By remembering the formula

$$\hat{S}_\pm |sm\rangle = \hbar\sqrt{s(s+1) - m(m \pm 1)}\, |s, m \pm 1\rangle = \hbar\sqrt{(s \mp m)(s \pm m + 1)}\, |s, m \pm 1\rangle$$

The matrix representations of $\hat{S}_+$ and $\hat{S}_-$ are calculated as the following:

$$\hat{S}_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \hat{S}_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Then by noting that $\hat{S}_x = \frac{1}{2}(\hat{S}_+ + \hat{S}_-)$ and $\hat{S}_y = \frac{i}{2}(\hat{S}_- - \hat{S}_+)$ the matrix representations for all three spin components pop out:

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

These matrices turn out to be a bit special so they are given the particular name: Pauli matrices, represented by sigma subscript $\frac{\hbar}{2}\sigma_i = \hat{S}_i$. Since

$$\hat{S}_i\hat{S}_j = \frac{1}{2}(\{\hat{S}_i, \hat{S}_j\} + [\hat{S}_i, \hat{S}_j]) = \frac{\hbar^2}{4}\mathbf{1}\delta_{ij} + i\frac{\hbar}{2}\epsilon_{ijk}\hat{S}_k$$

The same essential relationship applies to the Pauli matrices (which are simply scaled $\hat{S}$ matrices)

$$\sigma_i\sigma_j = \mathbf{1}\delta_{ij} + i\epsilon_{ijk}\sigma_k$$

A neat corollary of this is that

$$\sigma_x\sigma_y\sigma_z = i\sigma_z^2 = i\mathbf{1}$$

It is interesting to note that

$$\{\mathbf{1}, \sigma_x, \sigma_y, \sigma_z\}$$

forms an independent set on a vector space of dimension four (the set of 2x2 matrices), so it spans this set. That is, any 2x2 is a weighted combinations of the Pauli matrices and the identity. Here is another useful identity:

$$\begin{aligned}
(\mathbf{a}\cdot\sigma)(\mathbf{b}\cdot\sigma) &= a_i\sigma_i b_j\sigma_j \\
&= a_i b_j(\mathbf{1}\delta_{ij} + i\epsilon_{ijk}\sigma_k) \\
&= \mathbf{a}\cdot\mathbf{b}\mathbf{1} + i\epsilon_{ijk}a_i b_j\sigma_k \\
&= (\mathbf{a}\cdot\mathbf{b})\mathbf{1} + i(\mathbf{a}\times\mathbf{b})\cdot\sigma
\end{aligned}$$