Green's function time evolution

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1 Introduction to the propagator

Consider the classical mechanics problem of two blocks of mass m in a well coupled by springs to the walls and a spring between them (three springs in total). Denoting x_1 and x_2 as the displacement of each block from the equilibrium position, (note there is a unique equilibrium configuration of the masses, since we can set up two equations with two unknowns and solve them) Hooke's law implies that

$$\begin{aligned} \ddot{x}_1 &= -2\frac{k}{m}x_1 + \frac{k}{m}x_2 \\ \ddot{x}_2 &= \frac{k}{m}x_1 - 2\frac{k}{m}x_2 \end{aligned}$$

Written in matrix form, this is

$$\begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{bmatrix} = \begin{bmatrix} \Omega_{11} & \Omega_{12} \\ \Omega_{21} & \Omega_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \begin{matrix} \Omega_{11} = -\frac{2k}{m} & \Omega_{12} = \frac{k}{m} \\ \Omega_{21} = \frac{k}{m} & \Omega_{22} = -\frac{2k}{m} \end{matrix}$$

From which it is apparent that the matrix Ω is hermitian. This can be represented in a more abstract form as

$$|\ddot{x}(t)\rangle = \Omega\, |x(t)\rangle$$

In this representation, the equivalent of $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ is $|1\rangle$, representing displacement of the first mass from its equilibrium position and the equivalent of $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ is $|2\rangle$, representing displacement of the second mass from its equilibrium position. Therefore

$$|x(t)\rangle = x_1\, |1\rangle + x_2\, |2\rangle$$

The abstract vector equation can be put into a form that more closely relates to the original matrix equation by projecting onto $|1\rangle$ and $|2\rangle$, and using the completeness relation $|1\rangle\langle 1| + |2\rangle\langle 2| = I$:

$$\begin{aligned} \ddot{x}_1 = \langle 1|\ddot{x}(t)\rangle &= \langle 1|\,\Omega(|1\rangle\langle 1| + |2\rangle\langle 2|)\,|x(t)\rangle = \langle 1|\Omega|1\rangle\langle 1|x(t)\rangle + \langle 1|\Omega|2\rangle\langle 2|x(t)\rangle = \Omega_{11}x_1 + \Omega_{12}x_2 \\ \ddot{x}_2 = \langle 2|\ddot{x}(t)\rangle &= \langle 2|\,\Omega(|1\rangle\langle 1| + |2\rangle\langle 2|)\,|x(t)\rangle = \langle 2\Omega|1\rangle\langle 1|x(t)\rangle + \langle 2|\Omega|2\rangle\langle 2|x(t)\rangle = \Omega_{21}x_1 + \Omega_{22}x_2 \end{aligned}$$

Due to the coupling of $|1\rangle$ and $|2\rangle$, one can see that this system as written is hard to solve. To get around this, change basis to the eigenvectors of Ω, which by inspection are

$$\begin{aligned} |\mathbf{I}\rangle &= \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}, \qquad -\omega_1^2 = -\frac{k}{m} \\ |\mathbf{II}\rangle &= \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}, \quad -\omega_2^2 = -\frac{3k}{m} \end{aligned}$$

This gives the decoupled equations of motion and corresponding solutions (assume for convenience that the initial velocity is 0):

$$\begin{aligned} \ddot{x}_I = -\omega_1^2 x_I \qquad &\Longleftrightarrow \qquad x_I = x_I(0)\cos(\omega_1 t) \\ \ddot{x}_{II} = -\omega_2^2 x_{II} \qquad &\Longleftrightarrow \qquad x_{II} = x_{II}(0)\cos(\omega_2 t) \end{aligned}$$

It's likely that we are only given $x_1(0)$ and $x_2(0)$, rather than $x_I(0)$ and $x_{II}(0)$. However, this is no real obstacle. Simply project $x(0)$ onto the basis $\{|\mathbf{I}\rangle, |\mathbf{II}\rangle\}$ using the standard $\mathbb{R}^2$ dot product:

$$\begin{aligned} x_I(0) &= \langle \mathbf{I}|x(0)\rangle &= \langle \mathbf{I}|1\rangle\, x_1(0) + \langle \mathbf{I}|2\rangle\, x_2(0) &= \frac{x_1(0)+x_2(0)}{\sqrt{2}} \\ x_{II}(0) &= \langle \mathbf{II}|x(0)\rangle &= \langle \mathbf{II}|1\rangle\, x_1(0) + \langle \mathbf{II}|2\rangle\, x_2(0) &= \frac{x_1(0)-x_2(0)}{\sqrt{2}} \end{aligned}$$

So then the equation of motion can be written as

$$|x(t)\rangle = |\mathbf{I}\rangle \frac{x_1(0)+x_2(0)}{\sqrt{2}} \cos(\omega_1 t) + |\mathbf{II}\rangle \frac{x_1(0)-x_2(0)}{\sqrt{2}} \cos(\omega_2 t) \tag{$\star$}$$

We can go one step further and represent this in the $\{|1\rangle, |2\rangle\}$ basis by, predictably, projecting onto the $\{|1\rangle, |2\rangle\}$ basis. It might be a bit clearer to write this in vector form, though:

$$\begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \frac{x_1(0)+x_2(0)}{\sqrt{2}} \cos(\omega_1 t) + \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \frac{x_1(0)-x_2(0)}{\sqrt{2}} \cos(\omega_2 t)$$

This can be streamlined into the matrix equation

$$\begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \cos(\omega_1 t)+\cos(\omega_2 t) & \cos(\omega_1 t)-\cos(\omega_2 t) \\ \cos(\omega_1 t)-\cos(\omega_2 t) & \cos(\omega_1 t)+\cos(\omega_2 t) \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix}$$

This surprisingly neat formulation shows that the time evolution of the system is simply determined by a matrix multiply on the initial state of the system, and this matrix turned out to be independent of the initial state (and is Hermitian!) Written in the abstract bra-ket notation,

$$|x(t)\rangle = U(t)\, |x(0)\rangle$$

Actually, by the time we reached ($\star$), we already knew this. ($\star$) states that

$$|x(t)\rangle = U(t)\, |\mathbf{I}\rangle \langle \mathbf{I}|x(0)\rangle + U(t)\, |\mathbf{II}\rangle \langle \mathbf{II}|x(0)\rangle = U(t)(|\mathbf{I}\rangle \langle \mathbf{I}| + |\mathbf{II}\rangle \langle \mathbf{II}|)\, |x_0\rangle = U(t)\, |x_0\rangle$$

and one can infer

$$U(t) = |\mathbf{I}\rangle \langle \mathbf{I}| \cos(\omega_1 t) + |\mathbf{II}\rangle \langle \mathbf{II}| \cos(\omega_2 t)$$

This example is quite instructive for quantum mechanics, since the equation that needs to be solved is

$$i\hbar\, |\dot{\psi}\rangle = \hat{H}\, |\psi\rangle$$

and in the same manner, the solution is found by solving the eigenvalue problem of $\hat{H}$ and using the eigenvalues and eigenstates to construct $U(t)$ such that

$$|\psi(t)\rangle = U(t)\, |\psi(0)\rangle$$

2 Green's Function, Equation of Motion

The Schrödinger picture considers the wavefunction time-dependent and the operator time-independent. On the other hand, the Heisenberg picture considers the wavefunction time-independent and the operator time-dependent. These viewpoints are mathematically equivalent, because the Heisenberg time-dependent operator $\hat{o}_{\mathcal{H}}$ is defined in terms of the Schrödinger time independent operator $\hat{o}_{\mathcal{S}}$ as

$$\hat{o}_{\mathcal{H}} = e^{i\hat{H}t} \hat{o}_{\mathcal{S}} e^{-i\hat{H}t}$$

so that the evolution of the expectation of an operator remains the same, as seen in

$$\langle \Psi(t)|\hat{o}_{\mathcal{S}}|\Psi(t)\rangle = \langle e^{-i\hat{H}t}\psi_0|\hat{o}_{\mathcal{S}}|e^{-i\hat{H}t}\psi_0\rangle = \langle \psi_0|e^{i\hat{H}t}\hat{o}_{\mathcal{S}}e^{-i\hat{H}t}|\psi_0\rangle = \langle \psi_0|\hat{o}_{\mathcal{H}}|\psi_0\rangle$$

Heisenberg's equation can be derived using the chain rule as follows:

$$\frac{\partial \hat{o}_{\mathcal{H}}}{\partial t} = (i\hat{H}) e^{i\hat{H}t} \hat{o}_{\mathcal{S}} e^{-i\hat{H}t} + e^{i\hat{H}t} \hat{o}_{\mathcal{S}} e^{-i\hat{H}t} (-i\hat{H}) = i[\hat{H}, \hat{o}_{\mathcal{H}}]$$

This equation may appear without the factor of i attached to the commutator when working with imaginary time. A useful property is that

$$[\hat{a}_{\mathcal{H}}, \hat{b}_{\mathcal{H}}] = [\hat{a}_{\mathcal{S}}, \hat{b}_{\mathcal{S}}]_{\mathcal{H}}$$

Similarly

$$\{\hat{a}_{\mathcal{H}}, \hat{b}_{\mathcal{H}}] = \{\hat{a}_{\mathcal{S}}, \hat{b}_{\mathcal{S}}\}_{\mathcal{H}}$$

The Green's function can be approached using the framework of equation of motion. As a reminder, the Green's function was

$$G(\tau, \tau') = -\frac{1}{z}\,\mathrm{Tr}\left[e^{-\beta\hat{H}} T_\tau C(\tau) C^\dagger(\tau')\right] = -\langle T_\tau C(\tau) C^\dagger(\tau')\rangle \qquad \langle\hat{o}\rangle := \frac{1}{z}\,\mathrm{Tr}\, e^{-\beta\hat{h}}\hat{o}$$

For now, as a notation that may come in handy in the future, let the subscripts ij in $G_{ij}(\tau, \tau')$ denote subscripts of the $C(\tau)$ and $C^\dagger(\tau')$ respectively. Also, for the purpose of taking a derivative, it's helpful to rewrite the function as

$$G_{ij}(\tau, \tau') = -\,\theta(\tau - \tau')\langle C(\tau) C^\dagger(\tau')\rangle + \theta(\tau' - \tau)\langle C^\dagger(\tau') C(\tau)\rangle$$

Since the derivative of the heaviside function is the delta function. Then (using time-translational invariance and an implicit 0 for the second argument of Green's function)

$$\begin{aligned}
\frac{\partial G_{ij}(\tau)}{\partial \tau} &= -\delta(\tau)\langle C_i(\tau) C_j^\dagger(0) + C_j^\dagger(0) C_i(\tau)\rangle - \theta(\tau)\langle[\hat{H}, C_i(\tau)] C_j^\dagger(0)\rangle + \theta(-\tau)\langle C_j^\dagger(0), [\hat{H}, C_i(\tau)]\rangle \\
&= -\delta(\tau)\delta_{ij} - \theta(\tau)\langle\mu C_i(\tau) C_j^\dagger(0)\rangle + \theta(-\tau)\langle C_j^\dagger(0), \mu C_i(\tau)\rangle \\
&= -\delta(\tau)\delta_{ij} + \mu G_{ij}(\tau)
\end{aligned}$$

Rearranging this:

$$\implies (\mu - \frac{\partial}{\partial \tau}) G_{ij} = \delta(\tau)\delta_{ij}$$

If the right side is interpreted to be "unity," then one might interpret the left side as "$G^{-1}G$". Now, what happens when the Hamiltonian is switched from $-\mu c^\dagger c$ to, say,

$$-\mu(c_\uparrow^\dagger c_\uparrow + c_\downarrow^\dagger c_\downarrow) + U\hat{n}_\uparrow\hat{n}_\downarrow$$

The only thing that changes in the above derivation is $[\hat{H}, C(\tau)]$. Recalling some commutator algebra with creation/annihilation operators:

$$\begin{aligned}
[\hat{n}_{i\sigma}, c_{j\sigma'}] &= c_{i\sigma}^\dagger\{c_{i\sigma}, c_{j\sigma'}\} - \{c_{i\sigma}^\dagger, c_{j\sigma}\} c_{i\sigma} \\
&= -\delta_{ij}\delta_{\sigma\sigma'} c_{i\sigma} \\
[\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, c_{j\sigma}] &= \hat{n}_{i\uparrow}[\hat{n}_{i\downarrow}, c_{j\sigma}] + [\hat{n}_{i\uparrow}, c_{j\sigma}]\hat{n}_{i\downarrow} \\
&= -\delta_{ij}(\delta_{\sigma\downarrow}\hat{n}_{i\uparrow} c_{i\downarrow} + \delta_{\sigma\uparrow}\hat{n}_{i\downarrow} c_{i\uparrow})
\end{aligned}$$

Therefore, the final equation of motion doesn't change much. Concluding the derivation

$$\begin{aligned}
\frac{\partial G_{\sigma\sigma'}}{\partial \tau} &= -\delta(\tau) - \theta(\tau)\langle[\hat{H}, C_\sigma(\tau)] C_{\sigma'}^\dagger(0)\rangle + \theta(-\tau)\langle C_{\sigma'}^\dagger(0), [\hat{H}, C_\sigma(\tau)]\rangle \\
&= -\delta(\tau) - \theta(\tau)\langle(\mu C_\sigma(\tau) - U\hat{N}_{\bar{\sigma}} C_\sigma(\tau)) C_{\sigma'}^\dagger(0)\rangle + \theta(\tau)\langle C_{\sigma'}^\dagger(0)(\mu C_\sigma(\tau) - U\hat{N}_{\bar{\sigma}} C_\sigma(\tau))\rangle \\
&= -\delta(\tau) + \mu G_{\sigma\sigma'} + U\,\theta(\tau)\langle\hat{N}_{\bar{\sigma}} C_\sigma(\tau) C_{\sigma'}^\dagger(0)\rangle - U\,\theta(\tau)\langle C_{\sigma'}^\dagger(0)\hat{N}_{\bar{\sigma}} C_\sigma(\tau)\rangle
\end{aligned}$$

If in fact the simplest form of the hamiltonian is present

$$(-\mu + U)c^\dagger c$$

Then the answer is plainly

$$(\mu - U - \frac{\partial}{\partial \tau})G = \delta(\tau)$$

2.1 Time Evolution

What if you introduce a disturbance to your system over a period of time? Say the hamiltonian is

$$\hat{H} = -\mu c^\dagger c$$

and the disturbance is modeled by

$$S(U) = SU(0 \to t_0) e^{-i \int \theta(t)\, \theta(t_0 - t) U c^\dagger(t) c(t) dt} = e^{-i \int_0^{t_0} U c^\dagger(t) c(t) dt}$$

which changes the Green's function (this one is the real time version) to

$$G(t, t') = -i \langle T_t C(t) C^\dagger(t') S(U) \rangle$$

The presence of the $S(U)$ modifies the value of the normalization constant z (so that $S(U)$ really defines a new expectation) to

$$\begin{aligned} z(u) &= \mathrm{Tr}\left[e^{-i \int_0^{t_0} U c^\dagger c dt} e^{\mu \beta c^\dagger c} \right] \\ &= 1 + e^{\mu\beta} e^{-i \int_0^{t_0} U dt} \\ &= 1 + e^{\mu\beta - iUt_0} \end{aligned}$$

Now let's compute this Green's function for a specific order of $0, t_0, t, t'$. There are essentially 12 orders. The order we will compute Green's function for is $t < 0 < t' < t_0$. The first step is to find an expression for $C(t) = e^{i\hat{H}t} c e^{-i\hat{H}t}$ and one for $C^\dagger(t') = e^{i\hat{H}t'} c^\dagger e^{-i\hat{H}t'}$. Using Heisenberg's equation:

$$\begin{aligned} \frac{\partial C(t)}{\partial t} &= i[-\mu c^\dagger c, C(t)] \\ &= i\mu C(t) \\ \Rightarrow C(t) &= e^{i\mu t} c \\ \frac{\partial C^\dagger(t')}{\partial t'} &= i[-\mu c^\dagger c, C^\dagger(t')] \\ &= -i\mu C^\dagger(t') \\ \Rightarrow C^\dagger(t') &= e^{-i\mu t'} c^\dagger \end{aligned}$$

Evaluating Green's function supposing $t < 0 < t' < t_0$:

$$\begin{aligned} G(t, t') &= i\, \theta(t' - t) \langle SU(t' \to t_0) C^\dagger(t') SU(0 \to t') C(t) \rangle \\ &= \frac{i}{z} \mathrm{Tr}\left[e^{-\beta \hat{H}} e^{-i \int_{t'}^{t_0} U c^\dagger c\, dt} e^{-i\mu t'} c^\dagger e^{-i \int_0^{t'} U c^\dagger c\, dt} e^{i\mu t} c \right] \\ &= \frac{i e^{i\mu(t - t')}}{z} \left[e^{\mu\beta} \langle 1 | e^{-i \int_{t'}^{t_0} U c^\dagger c\, dt} c^\dagger e^{-i \int_0^{t'} U c^\dagger c\, dt} c | 1 \rangle \right] \\ &= \frac{i e^{i\mu(t - t')}}{z} \left[e^{\mu\beta - iU(t_0 - t')} \langle 1 | c^\dagger e^{-i \int_0^{t'} U c^\dagger c\, dt} c | 1 \rangle \right] \\ &= \frac{i e^{i\mu(t - t')}}{z} \left[e^{\mu\beta - iU(t_0 - t')} \langle 0 | e^{-i \int_0^{t'} U c^\dagger c\, dt} | 0 \rangle \right] \\ &= \frac{i}{z} (i e^{\mu\beta - i\mu(t' - t) - iU(t_0 - t')}) \end{aligned}$$

Now, evaluating Green's function supposing $0 < t < t' < t_0$:

$$\begin{aligned} G(t, t') &= i\, \theta(t' - t) \langle SU(t' \to t_0) C^\dagger(t') SU(t \to t') C(t) SU(0 \to t) \rangle \\ &= \frac{i}{z} \mathrm{Tr}\left[e^{-\beta \hat{H}} e^{-i \int_{t'}^{t_0} U c^\dagger c\, dt} e^{-i\mu t'} c^\dagger e^{-i \int_t^{t'} U c^\dagger c\, dt} e^{i\mu t} c e^{-i \int_0^{t} U c^\dagger c\, dt} \right] \\ &= \frac{i e^{i\mu(t - t')}}{z} \langle 1 | e^{-\beta \hat{H}} e^{-i \int_{t'}^{t_0} U c^\dagger c\, dt} c^\dagger e^{-i \int_t^{t'} U c^\dagger c\, dt} c e^{-i \int_0^{t} U c^\dagger c\, dt} | 1 \rangle \\ &= \frac{i e^{i\mu(t - t')}}{z} e^{\beta\mu - iU(t_0 - t' + t)} \langle 0 | e^{-i \int_t^{t'} U c^\dagger c\, dt} | 0 \rangle \\ &= \frac{i}{z} e^{\beta\mu - i\mu(t' - t) - iU(t_0 - t' + t)} \end{aligned}$$

Alternatively this answer can be expressed as

$$\frac{i}{z} e^{\beta\mu + it(\mu - U) + it'(U-\mu) - it_0 U}$$

Now evaluating Green's function supposing $t' < 0 < t_0 < t$:

$$\begin{aligned}
G(t,t') &= -i\,\theta(t-t')\langle C(t) SU(0 \to t_0) C^\dagger(t')\rangle \\
&= -\frac{i}{z}\,\mathrm{Tr}\left[e^{-\beta\hat{H}} e^{i\mu t} c e^{-i\int_0^{t_0} U c^\dagger c\, dt} e^{-i\mu t'} c^\dagger\right] \\
&= -\frac{i e^{i\mu(t-t')}}{z}\,\langle 1| e^{-i\int_0^{t_0} U c^\dagger c\, dt} |1\rangle \\
&= -\frac{i}{z} e^{i\mu(t-t') - iUt_0}
\end{aligned}$$

Now evaluating Green's function supposing $0 < t_0 < t' < t$:

$$\begin{aligned}
G(t,t') &= -i\,\theta(t-t')\langle C(t) C^\dagger(t') SU(0 \to t_0)\rangle \\
&= -\frac{i}{z}\,\mathrm{Tr}\left[e^{-\beta\hat{H}} e^{i\mu t} c e^{-i\mu t'} c^\dagger e^{-i\int_0^{t_0} U c^\dagger c\, dt}\right] \\
&= -\frac{i e^{i\mu(t-t')}}{z}\,\langle 1|1\rangle \\
&= -\frac{i}{z} e^{i\mu(t-t')}
\end{aligned}$$