## Chapter 16

# **Propagators and Green's functions**

#### 16.1

For this potential, the wave function vanishes outside the interval  $x \in (0, a)$ , and inside satisfies

$$H \left| \phi \right\rangle = E \left| \phi \right\rangle \ 
ightarrow \ - rac{1}{2m} rac{\mathrm{d}^2 \phi(x)}{\mathrm{d}x^2} = E \phi(x)$$

Defining  $k = \sqrt{2mE}$ , this equation has normalized solutions

$$\phi_n(x) = \sqrt{\frac{2}{a}}\sin(k_n x)$$

where  $k_n$  takes the discrete values  $k_n = \frac{n\pi}{a}$ ,  $n \in \mathbb{Z}^+$ . This yields discrete energy levels

$$E_n = \frac{\pi^2 n^2}{2ma^2}$$

The general form of a momentum-time representation of the retarded Green's function is given by

$$\begin{aligned} G^+(q,t_x;p,t_y) &= \theta(t_x - t_y) \left\langle q | e^{-iH(t_x - t_y)} | p \right\rangle \\ &= \theta(t_x - t_y) e^{-iE_p(t_x - t_y)} \delta(p - q) \\ G^+(p;t_x,t_y) &= \theta(t_x - t_y) e^{-iE_p(t_x - t_y)} \end{aligned}$$

Using the fact that the momentum and energy come in discrete levels, we can write this as

$$G^{+}(n;t_{x},t_{y}) = \theta(t_{x}-t_{y})e^{-i\left(\frac{n^{2}\pi^{2}}{2ma^{2}}\right)(t_{x}-t_{y})}$$

Lastly, we can obtain a momentum-energy representation by performing a Fourier transform in time (shifting the energies infinitesimally into the complex plane for convergence)

$$\begin{aligned} G^+(n,\omega) &= \int_{-\infty}^{\infty} \mathrm{d}t_x \, G^+(n;t_x,t_y) e^{i\omega(t_x-t_y)} \\ &= \int_{t_y}^{\infty} \mathrm{d}t_x \, e^{i\left(\omega - \frac{n^2\pi^2}{2ma^2} + i\epsilon\right)(t_x-t_y)} \\ &= \frac{1}{i\left(\omega - \frac{n^2\pi^2}{2ma^2} + i\epsilon\right)} \, e^{i\left(\omega - \frac{n^2\pi^2}{2ma^2} + i\epsilon\right)(t_x-t_y)} \Big|_{t_y}^{\infty} \\ \hline G^+(n,\omega) &= \frac{i}{\omega - \frac{n^2\pi^2}{2ma^2} + i\epsilon} \end{aligned}$$

16.2

Starting with the position-time representation of the retarded Green's function

$$G_0^+(t_x, x; t_y, y) = \theta(t_x - t_y) \sum_n \phi_n(x) \phi_n^*(y) e^{-iE_n(t_x - t_y)}$$

we can switch to a position-energy representation by performing a Fourier transform in time with a damping factor as follows

$$G_{0}^{+}(x,y;E) = \int_{-\infty}^{\infty} dt_{x} G_{0}^{+}(t_{x},x;t_{y},y) e^{iE(t_{x}-t_{y})} e^{-\epsilon(t_{x}-t_{y})}$$
$$= \sum_{n} \phi_{n}(x)\phi_{n}^{*}(y) \int_{t_{y}}^{\infty} dt_{x} e^{i(E-E_{n}+i\epsilon)(t_{x}-t_{y})}$$
$$= \sum_{n} \phi_{n}(x)\phi_{n}^{*}(y) \frac{1}{i(E-E_{n}+i\epsilon)} e^{i(E-E_{n}+i\epsilon)(t_{x}-t_{y})} \Big|_{t_{y}}^{\infty}$$
$$\boxed{G_{0}^{+}(x,y;E) = \sum_{n} \frac{i\phi_{n}(x)\phi_{n}^{*}(y)}{E-E_{n}+i\epsilon}}$$

However, we can perform similar calculations without the damping factor by using the following representation of the heaviside function

$$\theta(t) = i \int_{-\infty}^{\infty} \frac{\mathrm{d}z}{2\pi} \frac{e^{-izt}}{z + i\epsilon}$$

Starting from the momentum-time representation of the Green's function

$$G_0^+(p,t) = \theta(t)e^{-iE_pt}$$

we can obtain the momentum-energy representation through a Fourier transform in time  $_{e\infty}$ 

$$G_0^+(p,E) = \int_{-\infty}^{\infty} dt \, G_0^+(p,t) e^{iEt}$$
$$= i \int_{-\infty}^{\infty} \frac{dz}{2\pi} \frac{1}{z+i\epsilon} \int_{-\infty}^{\infty} dt \, e^{i(E-E_p-z)t}$$
$$= i \int_{-\infty}^{\infty} dz \, \frac{1}{z+i\epsilon} \delta(E-E_p-z)$$
$$\boxed{G_0^+(p,E) = \frac{i}{E-E_p+i\epsilon}}$$

#### 16.3

For a one-dimension driven harmonic oscillator, the equation of motion is given by

$$m\left(\frac{\partial^2}{\partial t^2} + \omega_0^2\right) A(t-u) = f(t)$$

Considering a driving force of the form  $f(t) = \tilde{F}(\omega)e^{-i\omega(t-u)}$ . The particular solution can be found by inserting the ansatz

$$A(t-u) = \mathcal{A}(\omega)e^{-i\omega(t-u)}$$

With this, we obtain the condition for the amplitude

$$-m(\omega^2 - \omega_0^2)\mathcal{A}(\omega)e^{-i\omega(t-u)} = \tilde{F}(\omega)e^{-i\omega(t-u)}$$
$$\mathcal{A}(\omega) = -\frac{\tilde{F}(\omega)}{m}\frac{1}{\omega^2 - \omega_0^2}$$

Therefore, the general solution is given by

$$A(t-u) = -\frac{\tilde{F}(\omega)}{m} \frac{e^{-i\omega(t-u)}}{\omega^2 - \omega_0^2} + B(t)$$

where B(t) satisfies the homogeneous equation

$$m \bigg( \frac{\partial^2}{\partial t^2} + \omega_0^2 \bigg) B(t) = 0$$

The Green's function for this differential equation is the solution to

$$m\left(\frac{\partial^2}{\partial t^2} + \omega_0^2\right)G(t, u) = \delta(t - u)$$

This resembles the driven differential equation if we represent the delta function as an integral

$$m\left(\frac{\partial^2}{\partial t^2} + \omega_0^2\right)G(t, u) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega(t-u)}$$

We can solve this by first finding the Fourier transform of the Green's function. Doing this, we obtain

$$\begin{split} m\bigg(\frac{\partial^2}{\partial t^2} + \omega_0^2\bigg) \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \tilde{G}(\omega) e^{-i\omega(t-u)} &= \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega(t-u)} \\ \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \Big(m\big(-\omega^2 + \omega_0^2\big)\tilde{G}(\omega)\Big) e^{-i\omega(t-u)} &= \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega(t-u)} \\ \tilde{G}(\omega) &= -\frac{1}{m} \frac{1}{\omega^2 - \omega_0^2} \end{split}$$

Fourier transforming back, we obtain

$$G(t,u) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \tilde{G}(\omega) e^{-i\omega(t-u)}$$
$$\overline{G(t,u)} = -\frac{1}{m} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{e^{-i\omega(t-u)}}{\omega^2 - \omega_0^2}$$

Assuming that  $t \ge 0$  for the dynamics of the problem, the initial conditions  $G(0, u) = \dot{G}(0, u) = 0$  are equivalent to requiring causality in G(t, u). This can be thought of as G(0, u) = 0 enforcing that the function vanish at t = 0, and  $\dot{G}(0, u) = 0$  enforcing that any flow from t < 0 vanish. With this, the expression for  $G^+(t, u)$  is most easily obtained through complex analysis. With the poles of the function at  $\omega = \pm \omega_0$  and t - u > 0, we can close the contour in the lower half of the complex  $\omega$ -plane, and deform the contour up and around the poles so as to include them in the closed contour



Applying Cauchy's residue theorem, we find

$$G^{+}(t,u) = -\frac{1}{m} \oint \frac{d\omega}{2\pi} \frac{e^{-i\omega(t-u)}}{(\omega+\omega_0)(\omega-\omega_0)}$$
$$= \frac{i}{m} \left[ \frac{e^{-i\omega(t-u)}}{\omega-\omega_0} \Big|_{\omega=-\omega_0} + \frac{e^{-i\omega(t-u)}}{\omega+\omega_0} \Big|_{\omega=\omega_0} \right]$$
$$\frac{1}{m\omega_0} \frac{e^{i\omega_0(t-u)} - e^{-i\omega_0(t-u)}}{2i}$$
$$G^{+}(t,u) = \frac{1}{m\omega_0} \sin \omega_0(t-u)$$

Lastly, for a driving force  $f(t) = F_0 \sin \omega_0 t$ , we can obtain the amplitude as a function of time through the relation

$$A(t) = \int_0^t \mathrm{d}u \, G^+(t, u) f(u)$$
$$= \frac{F_0}{m\omega_0} \int_0^t \mathrm{d}u \sin(\omega_0(t-u)) \sin(\omega_0 u)$$
$$A(t) = \frac{F_0}{2m\omega_0^2} \left(\sin(\omega_0 t) - \omega_0 t \cos(\omega_0 t)\right)$$

### 16.4

Considering the Green's function for the Helmholtz differential operator

$$(\nabla^2 + \mathbf{k}^2)G_{\mathbf{k}}(\mathbf{x}) = \delta^{(3)}(\mathbf{x})$$

we can move to momentum space as follows

$$\begin{aligned} \left(\nabla^2 + \mathbf{k}^2\right) \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \tilde{G}_{\mathbf{k}}(\mathbf{q}) e^{-i\mathbf{q}\cdot\mathbf{x}} &= \int \frac{\mathrm{d}^3 q}{(2\pi)^3} e^{-i\mathbf{q}\cdot\mathbf{x}} \\ \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \left(-\mathbf{q}^2 + \mathbf{k}^2\right) \tilde{G}_{\mathbf{k}}(\mathbf{q}) e^{-i\mathbf{q}\cdot\mathbf{x}} &= \int \frac{\mathrm{d}^3 q}{(2\pi)^3} e^{-i\mathbf{q}\cdot\mathbf{x}} \\ \left(-\mathbf{q}^2 + \mathbf{k}^2\right) \tilde{G}_{\mathbf{k}}(\mathbf{q}) &= 1 \\ \tilde{G}_{\mathbf{k}}(\mathbf{q}) &= \frac{1}{\mathbf{k}^2 - \mathbf{q}^2} \end{aligned}$$

In position space, the Green's function for "outgoing" waves is given by

$$G_{\mathbf{k}}^{+}(\mathbf{x}) = -\frac{1}{4\pi} \frac{e^{i|\mathbf{k}||\mathbf{x}|}}{|\mathbf{x}|}$$

This can be confirmed by taking the Fourier transform and making connection with the previous result. Employing a damping factor, we can write the Fourier transform as

$$\begin{split} \tilde{G}_{\mathbf{k}}^{+}(\mathbf{q}) &= \int \mathrm{d}^{3}x \, G_{\mathbf{k}}^{+}(\mathbf{x}) e^{i\mathbf{q}\cdot\mathbf{x}} e^{-\epsilon|\mathbf{x}|} \\ &= -\frac{1}{4\pi} \int \frac{\mathrm{d}^{3}x}{|\mathbf{x}|} e^{i(|\mathbf{k}|+i\epsilon)|\mathbf{x}|} e^{i|\mathbf{q}||\mathbf{x}|\cos\vartheta} \\ &= -\frac{1}{4\pi} \int_{0}^{2\pi} \mathrm{d}\varphi \int_{-1}^{1} \mathrm{d}(\cos\vartheta) \int_{0}^{\infty} \frac{\mathrm{d}x \, x^{2}}{x} e^{i(|\mathbf{k}|+i\epsilon)x} e^{i|\mathbf{q}|x\cos\vartheta} \\ &= -\frac{1}{2} \int_{0}^{\infty} \mathrm{d}x \, x e^{i(|\mathbf{k}|+i\epsilon)x} \frac{1}{i|\mathbf{q}|x} \left( e^{i|\mathbf{q}|x} - e^{-i|\mathbf{q}|x} \right) \\ &= -\frac{1}{|\mathbf{q}|} \int_{0}^{\infty} \mathrm{d}x \, e^{i(|\mathbf{k}|+i\epsilon)x} \sin(|\mathbf{q}|x) \\ \tilde{G}_{\mathbf{k}}^{+}(\mathbf{q}) &= -\frac{1}{|\mathbf{q}|} \frac{|\mathbf{q}|}{|\mathbf{q}|^{2} - (|\mathbf{k}|+i\epsilon)^{2}} \end{split}$$

Since  $\epsilon$  is an infinitesimal and  $r\epsilon = \epsilon \quad \forall r \in \mathbb{R}$ , this can be rewritten as

$$\tilde{G}^+_{\mathbf{k}}(\mathbf{q}) = \frac{1}{\mathbf{k}^2 - \mathbf{q}^2 + i\epsilon}$$

We can indeed go backwards and take the inverse Fourier transform of our result, yielding

$$\begin{split} G_{\mathbf{k}}^{+}(\mathbf{x}) &= \int \frac{\mathrm{d}^{3}q}{(2\pi)^{3}} G_{\mathbf{k}}^{+}(\mathbf{q}) e^{-i\mathbf{q}\cdot\mathbf{x}} \\ &= -\int \frac{\mathrm{d}^{3}q}{(2\pi)^{3}} \frac{e^{-i\mathbf{q}\cdot\mathbf{x}}}{\mathbf{q}^{2} - \mathbf{k}^{2} - i\epsilon} \\ &= \frac{-1}{(2\pi)^{2}} \int_{-1}^{1} \mathrm{d}(\cos\vartheta) \int_{0}^{\infty} \mathrm{d}q \, q^{2} \frac{e^{-iq|\mathbf{x}|\cos\vartheta}}{q^{2} - \mathbf{k}^{2} - i\epsilon} \\ &= \frac{-1}{4\pi^{2}} \int_{0}^{\infty} \mathrm{d}q \, \frac{q^{2}}{-iq|\mathbf{x}|} \frac{1}{q^{2} - \mathbf{k}^{2} - i\epsilon} \left(e^{-iq|\mathbf{x}|} - e^{iq|\mathbf{x}|}\right) \\ G_{\mathbf{k}}^{+}(\mathbf{x}) &= \frac{i}{4\pi^{2}|\mathbf{x}|} \int_{-\infty}^{\infty} \mathrm{d}q \, \frac{qe^{iq|\mathbf{x}|}}{q^{2} - \mathbf{k}^{2} - i\epsilon} \end{split}$$

A natural factorization of the denominator yields

$$G_{\mathbf{k}}^{+}(\mathbf{x}) = \frac{i}{4\pi^{2}|\mathbf{x}|} \int_{-\infty}^{\infty} \mathrm{d}q \, \frac{q e^{iq|\mathbf{x}|}}{(q - (|\mathbf{k}| + i\epsilon))(q + (|\mathbf{k}| - i\epsilon))}$$

Since  $|\mathbf{x}| > 0$ , we can close the contour in the upper half of the complex-q plane as shown below



This yields

$$\begin{split} G_{\mathbf{k}}^{+}(\mathbf{x}) &= \frac{i}{4\pi^{2}|\mathbf{x}|} \oint \mathrm{d}q \, \frac{q e^{iq|\mathbf{x}|}}{(q - (|\mathbf{k}| + i\epsilon))(q + (|\mathbf{k}| - i\epsilon))} \\ &= -\frac{1}{2\pi |\mathbf{x}|} \left. \frac{q e^{iq|\mathbf{x}|}}{q + (|\mathbf{k}| - i\epsilon)} \right|_{q = |\mathbf{k}| + i\epsilon} \\ G_{\mathbf{k}}^{+}(\mathbf{x}) &= -\frac{1}{4\pi} \frac{e^{i|\mathbf{k}||\mathbf{x}|} e^{-\epsilon|\mathbf{x}|}}{|\mathbf{x}|} \left(1 + i\frac{\epsilon}{|\mathbf{k}|}\right) \end{split}$$

Taking the limit  $\epsilon \to 0$ , we recover the Green's function for the Helmholtz operator in position space corresponding to "outgoing" waves

$$G_{\mathbf{k}}^{+}(\mathbf{x}) = -\frac{1}{4\pi} \frac{e^{i|\mathbf{k}||\mathbf{x}|}}{|\mathbf{x}|}$$

Had we considered considered incoming waves, all that would change is the replacement  $|\mathbf{k}| \rightarrow -|\mathbf{k}|$ . This would cause  $\epsilon \rightarrow -\epsilon$  in the denominator of the momentum-space Green's function, and consequently the locations of the poles would switch in terms of which is above and which is below the real q axis. This would ultimately change which residue is calculated and return a position-space Green's function with a negative exponent, perfectly agreeing with the initial change to the direction of the momentum.