1.

$$\int \mathrm{d}^3x e^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}}\phi(x)$$

$$= \int \mathrm{d}\tilde{k}(2\pi)^3[a(\boldsymbol{k})e^{-\mathrm{i}\omega(\boldsymbol{k})t}\delta^3(\boldsymbol{k}-\boldsymbol{q}) + b^\dagger(\boldsymbol{k})e^{\mathrm{i}\omega(\boldsymbol{k})t}\delta^3(\boldsymbol{k}+\boldsymbol{q})]$$

$$= \frac{1}{2\omega(\boldsymbol{q})}[a(\boldsymbol{q})e^{-\mathrm{i}\omega(\boldsymbol{q})t} + b^\dagger(-\boldsymbol{q})e^{\mathrm{i}\omega(\boldsymbol{q})t}], \quad (1)$$

so

$$2\omega \int \mathrm{d}^3x e^{-\mathrm{i}qx}\phi(x) = a(\boldsymbol{q}) + b^\dagger(-\boldsymbol{q})e^{2\mathrm{i}\omega t}. \quad (2)$$

Next,

$$\dot{\phi}(x) = \int \mathrm{d}\tilde{k}[-\mathrm{i}\omega a(\boldsymbol{k})e^{\mathrm{i}kx} + \mathrm{i}\omega b^\dagger(\boldsymbol{k})e^{-\mathrm{i}kx}], \quad (3)$$

so

$$2\mathrm{i}\int \mathrm{d}^3x e^{-\mathrm{i}qx}\dot{\phi}(x) = a(\boldsymbol{q}) - b^\dagger(-\boldsymbol{q})e^{2\mathrm{i}\omega t}. \quad (4)$$

Hence

$$\boxed{a(\boldsymbol{k}) = \int \mathrm{d}^3x e^{-\mathrm{i}kx}[\omega\phi(x) + \mathrm{i}\dot{\phi}(x)].} \quad (5)$$

Similarly,

$$\boxed{b^\dagger(\boldsymbol{k}) = \int \mathrm{d}^3x e^{\mathrm{i}kx}[\omega\phi(x) - \mathrm{i}\dot{\phi}(x)].} \quad (6)$$

Taking complex conjugates gives us

$$\boxed{a^\dagger(\boldsymbol{k}) = \int \mathrm{d}^3x e^{\mathrm{i}kx}[\omega\phi^\dagger(x) - \mathrm{i}\dot{\phi}^\dagger(x)],} \quad (7)$$

$$\boxed{b(\boldsymbol{k}) = \int \mathrm{d}^3x e^{-\mathrm{i}kx}[\omega\phi^\dagger(x) + \mathrm{i}\dot{\phi}^\dagger(x)].} \quad (8)$$

2.

Only the time derivatives care about the time-ordering symbol, so we have

$$(-\partial_\mu\partial^\mu + m^2)G_2(x,y) = \partial_0^2 G_2 + \langle 0| T\{(-\nabla^2 + m^2)\phi(x)\phi(y)\} |0\rangle \quad (9)$$

Let's start with the first term.

$$\partial_0^2 G_2 = \partial_0^2[\theta(x_0 - y_0) \langle 0| \phi(x)\phi(y) |0\rangle + \theta(y_0 - x_0) \langle 0| \phi(y)\phi(x) |0\rangle]. \quad (10)$$

Remember that

$$\partial_0\theta(x_0 - y_0) = \delta(x_0 - y_0), \quad (11)$$

$$\partial_0\theta(x_0 - y_0) = \delta(x_0 - y_0) \quad (12)$$

and take the first derivative:

$$\begin{aligned}\partial_0 G_2 = \delta(x_0 - y_0) \langle 0| \phi(x)\phi(y) |0\rangle + \theta(x_0 - y_0) \langle 0| \partial_0\phi(x)\phi(y) |0\rangle \\ - \delta(x_0 - y_0) \langle 0| \phi(y)\phi(x) |0\rangle + \theta(y_0 - x_0) \langle 0| \phi(y)\partial_0\phi(x) |0\rangle . \quad (13)\end{aligned}$$

The delta functions in the first and third terms allow us to combine them into a commutator evaluated at equal time,

$$\delta(x_0 - y_0) \langle 0| [\phi(x), \phi(y)] |0\rangle = 0, \quad (14)$$

so

$$\partial_0 G_2 = \theta(x_0 - y_0) \langle 0| \partial_0\phi(x)\phi(y) |0\rangle + \theta(y_0 - x_0) \langle 0| \phi(y)\partial_0\phi(x) |0\rangle . \quad (15)$$

Taking the second derivative gives us

$$\begin{aligned}\partial_0^2 G_2 = \delta(x_0 - y_0) \langle 0| \partial_0\phi(x)\phi(y) |0\rangle + \theta(x_0 - y_0) \langle 0| \partial_0^2\phi(x)\phi(y) |0\rangle \\ - \delta(y_0 - x_0) \langle 0| \phi(y)\partial_0\phi(x) |0\rangle + \theta(y_0 - x_0) \langle 0| \phi(y)\partial_0^2\phi(x) |0\rangle . \quad (16)\end{aligned}$$

Once again, the first and third terms combine into an equal time commutator,

$$\delta(x_0 - y_0) \langle 0| [\partial_0\phi(x), \phi(y)] |0\rangle = -\mathrm{i}\delta^4(x - y) \quad (17)$$

and the second and fourth terms can be combined via the time-ordering symbol, so

$$\partial_0^2 G_2 = -\mathrm{i}\delta^4(x - y) + \langle 0| T\{\partial_0^2\phi(x)\phi(y)\} |0\rangle \quad (18)$$

Now let's look at the second term in (9). From the Klein-Gordon equation,

$$(-\nabla^2 + m^2)\phi(x) = -\partial_0^2\phi(x), \quad (19)$$

so

$$\langle 0| T\{(-\nabla^2 + m^2)\phi(x)\phi(y)\} |0\rangle = -\langle 0| T\{\partial_0^2\phi(x)\phi(y)\} |0\rangle . \quad (20)$$

Plugging in (20) and (18) in (9) gives us

$$\boxed{(-\partial_\mu \partial^\mu + m^2) G_2(x, y) = -\mathrm{i}\delta^4(x - y).} \tag{21}$$

There is a subtle point here about taking the derivative of expression (13). If we had done this without combing the first and third terms into the commutator, we would have had terms like this:

$$\partial_0[\delta(x_0 - y_0) \langle 0| \phi(x)\phi(y) |0\rangle - \delta(x_0 - y_0) \langle 0| \phi(x)\phi(y) |0\rangle]. \tag{22}$$

If we naively apply the product rule to this expression, it looks like it will add another $-\mathrm{i}\delta^4(x - y)$ to the right-hand side of (21). This is not correct. The simplest way to see this is to imagine integrating (22) against a smooth function of x_0:

$$\int \mathrm{d}x_0 \partial_0[\delta(x_0 - y_0) \langle 0| \phi(x)\phi(y) |0\rangle - \delta(x_0 - y_0) \langle 0| \phi(x)\phi(y) |0\rangle] f(x_0). \tag{23}$$

We can integrate by parts to get

$$-\int \mathrm{d}x_0[\delta(x_0 - y_0) \langle 0| \phi(x)\phi(y) |0\rangle - \delta(x_0 - y_0) \langle 0| \phi(x)\phi(y) |0\rangle] \partial_0 f(x_0), \tag{24}$$

where the boundary term is zero because we assume the boundaries are not at y_0 (so the delta function is zero there). We can write this in terms of an equal time commutator, and then

$$-\langle 0| [\phi(x), \phi(y)]_{\mathrm{ET}} |0\rangle \, \partial_0 f(x_0) = 0. \tag{25}$$