Bloch's theorem

In a periodic system, the Schrödinger equation is:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r})$$

$$U(\vec{r}) = U(\vec{r}+\vec{R})$$

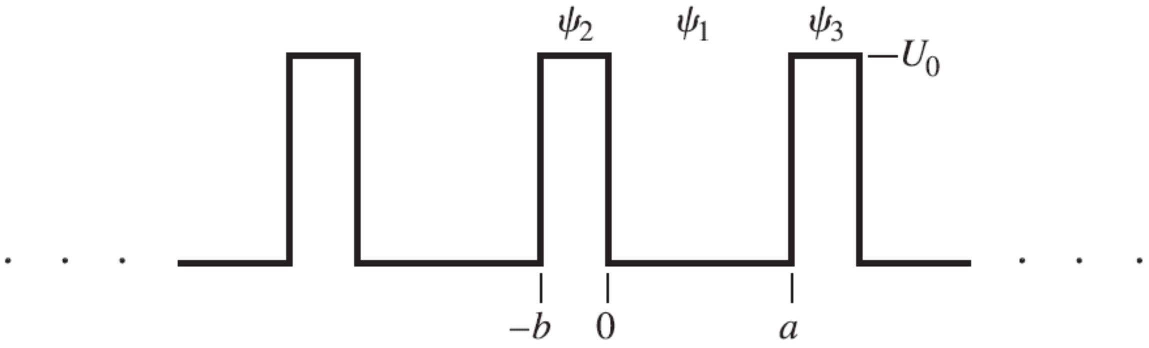
The Bloch's theorem tell us:

$$\psi_{n,\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u_{n,\vec{k}}(\vec{r}) \qquad u_{n,\vec{k}}(\vec{r}+\vec{R}) = u_{n,\vec{k}}(\vec{r})$$

$$\psi_{n,\vec{k}}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\psi_{n,\vec{k}}(\vec{r})$$

The eigenstate can be expressed by a plane wave multiple a periodic function. The difference between $\psi_{n,\vec{k}}(\vec{r}+\vec{R}), \psi_{n,\vec{k}}(\vec{r})$ is $e^{i\vec{k}\cdot\vec{R}}$.

Example one: The Kronig–Penney Model



Consider two region: $\psi_1(x), \psi_2(x)$

We can guess the solution:

$$\psi_1(x) = A_1 e^{iKx} + B_1 e^{-iKx}, 0 < x < a$$

$$\psi_2(x) = A_2 e^{\kappa x} + B_2 e^{-\kappa x}, -b < x < 0$$

According to Bloch theorem, we have

$$\psi_3(x+a+b) = e^{ik\cdot(a+b)}\psi_2(x)$$

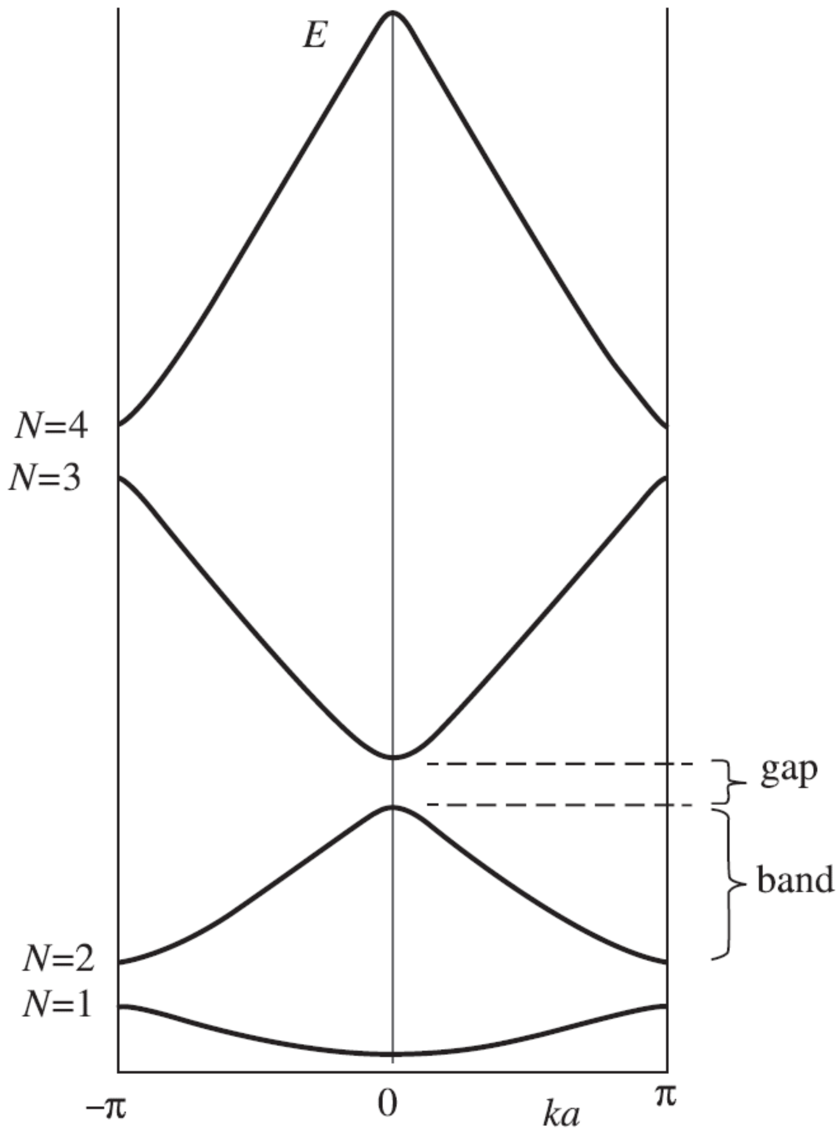
Thus, the boundary condition is:

$$\psi_1(0) = \psi_2(0), \frac{\partial\psi_1}{\partial x}\Big|_{x=0} = \frac{\partial\psi_2}{\partial x}\Big|_{x=0}$$

$$\psi_1(a) = \psi_3(a), \frac{\partial\psi_1}{\partial x}\Big|_{x=a} = \frac{\partial\psi_3}{\partial x}\Big|_{x=a}$$

After some algebra, we can get the A_1,A_2, B_1, B_2 and the system energy $E(k)$, which is dependent on k

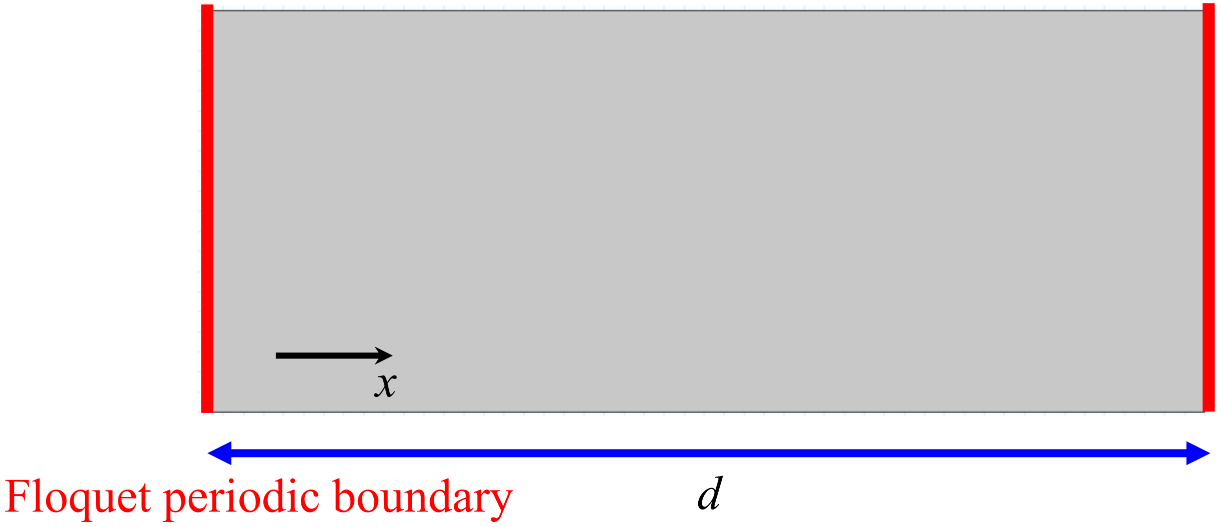
The figure shows the E vs k, when $b \to 0, U_0 \to \infty$

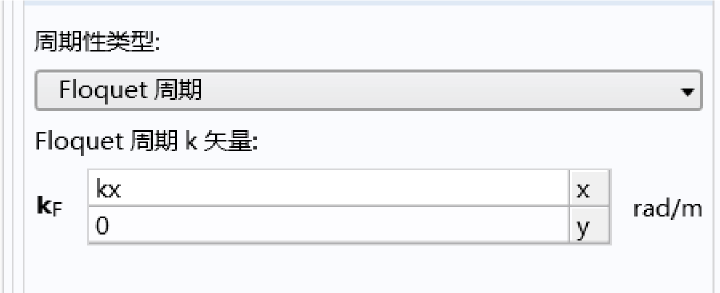


In the pervious page, I said: After 'some' algebra. However, in a crystal(including photonics/phononics crystal) the potential energy U_0 is always very complex. We need some help from Comsol!

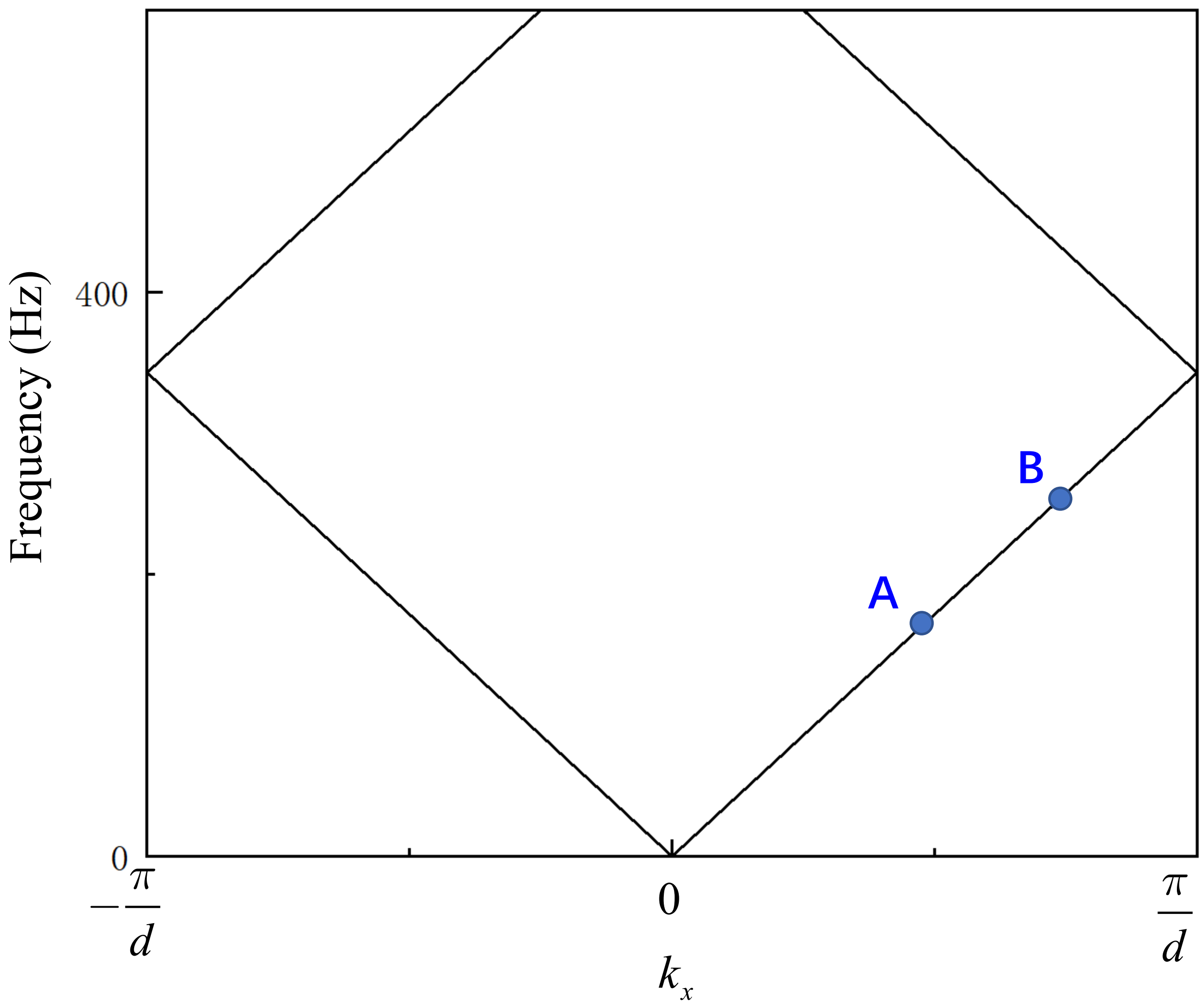
Example two: The infinite length waveguide

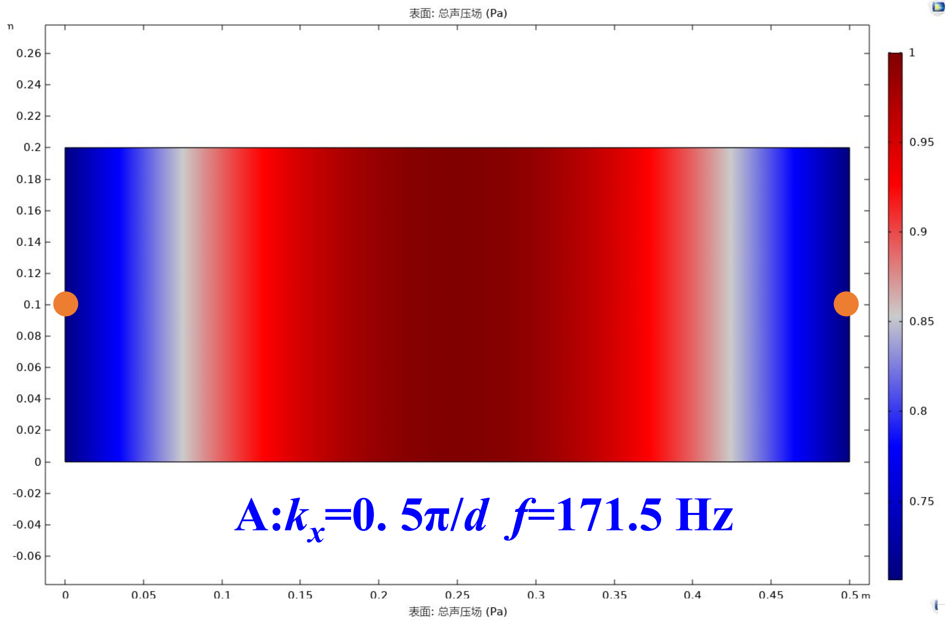
The period is d=0.5m, and the width of the waveguide is set to only support ground state alone y direction

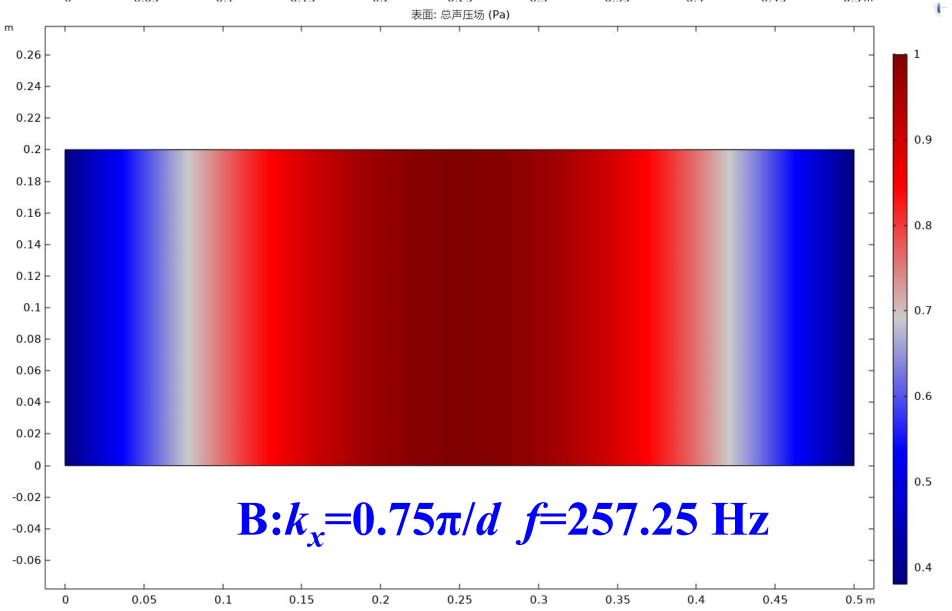




In a acoustic waveguide, there is no dispersion, and everywhere is plane wave. So the frequency is linearly to the wavevector.



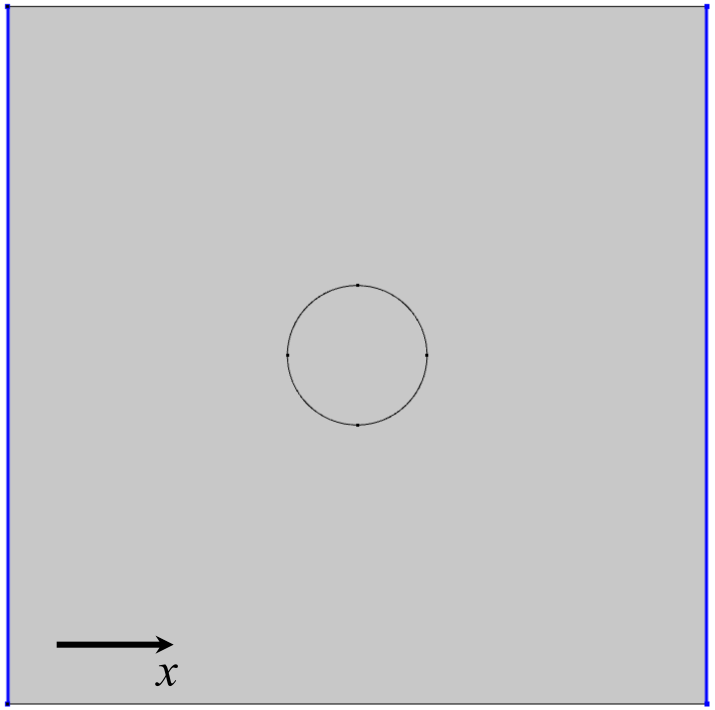




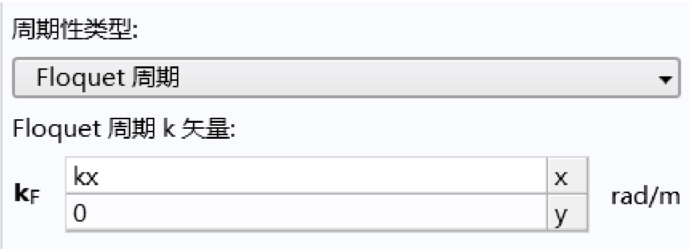
The phase difference between two orange dots satisfies $k_x = kd$ and two orange dots have the same amplitude

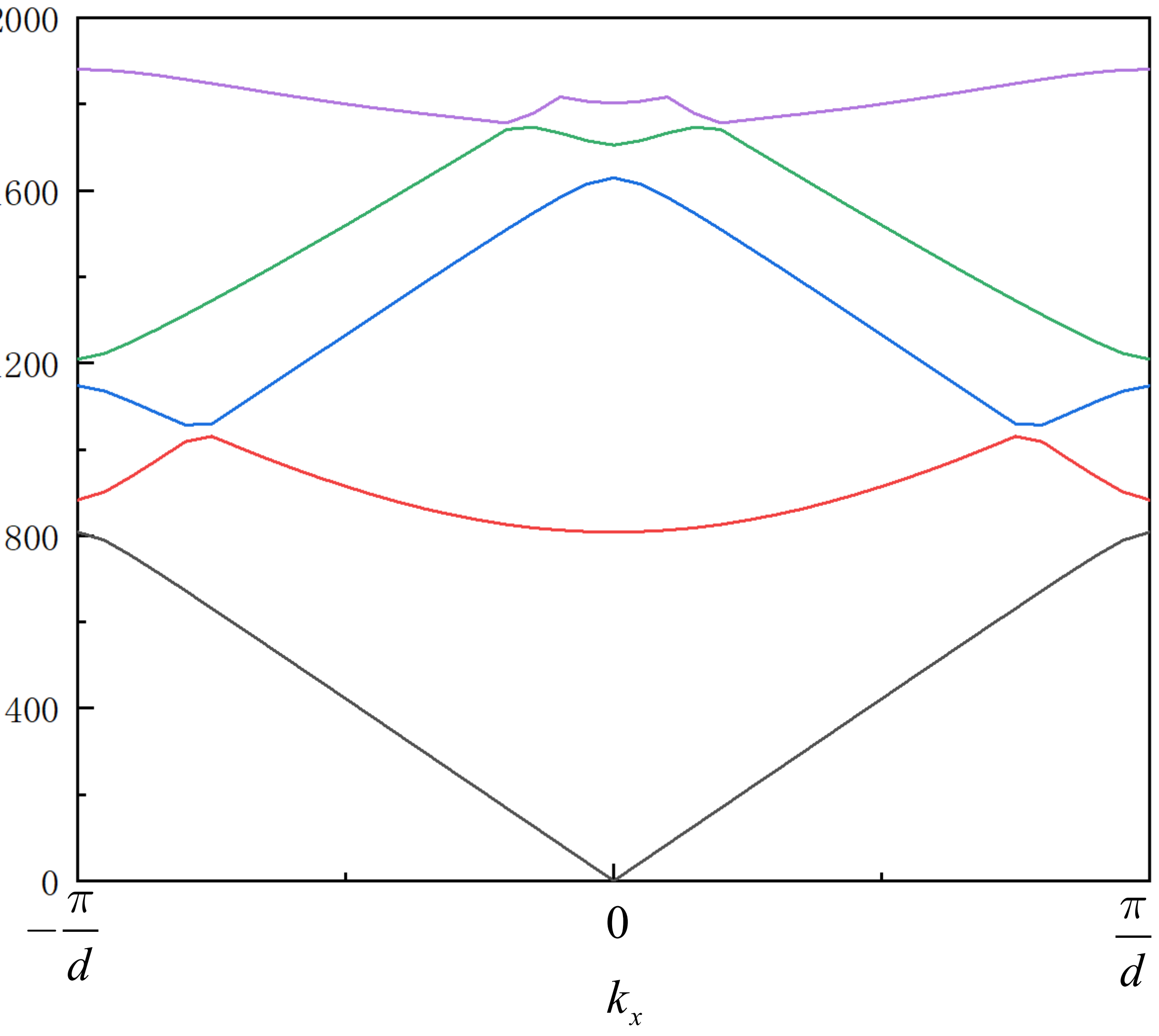
Which implies that the bloch's theory is set up: $\psi(x+d) = e^{ik\cdot d}\psi(x)$

Example three: 1D phononic crystals



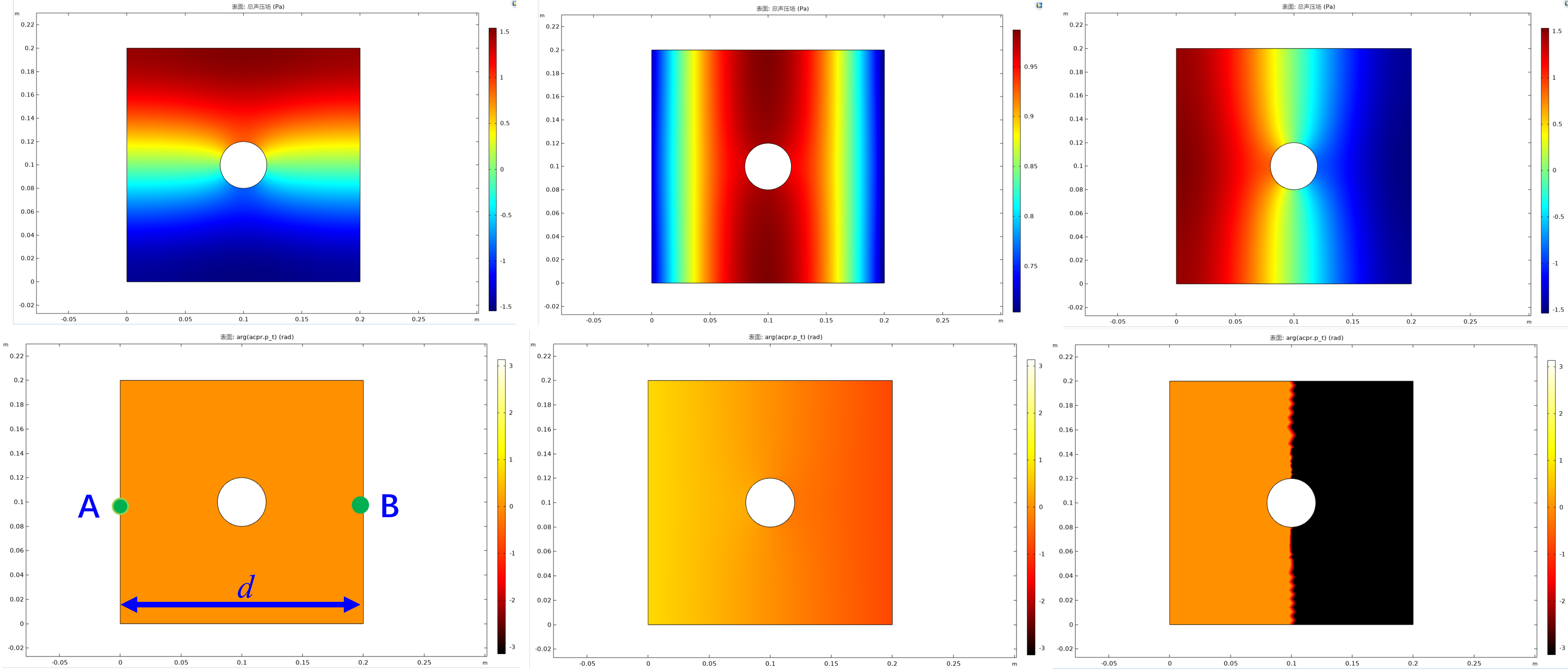
Floquet periodic boundary





Pressure field:

Phase field:



k_x=0

$$\varphi_{AB} = 0 = k_x \cdot d$$

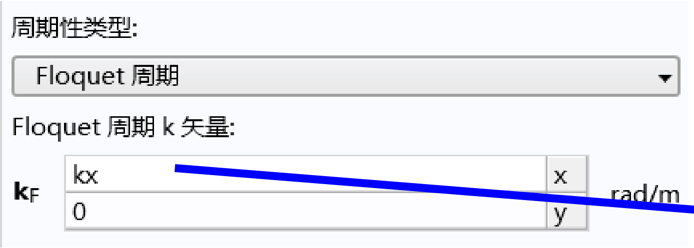
k_x=0. 5π/d

$$\varphi_{AB} = 1.57 = k_x \cdot d$$

k_x=π/d

$$\varphi_{AB} = 3.14 = k_x \cdot d$$

So we know that:



$$\psi(x+d) = e^{ik \cdot d}\psi(x)$$