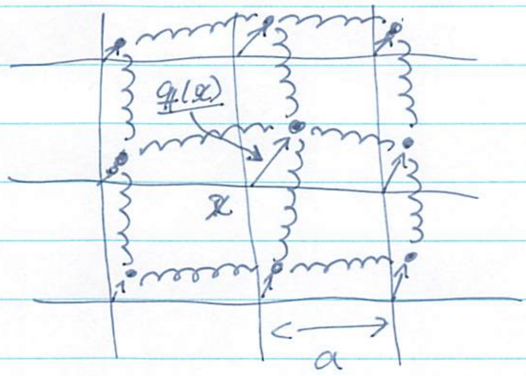
Phonon (Quantization of Lattice Vibration)

- Array of coupled oscillators

• ... atom



$$L = K - U$$

$$K \equiv \frac{m}{2} \sum_{\mathbf{x}} \dot{\mathbf{q}}(\mathbf{x})^2 \quad (m : \text{the mass of an atom})$$

$$U \equiv \frac{m\omega_0^2}{2} \sum_{\mathbf{x},\boldsymbol{\delta}} \left(\mathbf{q}(\mathbf{x}+\boldsymbol{\delta}) - \mathbf{q}(\mathbf{x}) \right)^2$$

$$\sum_{\boldsymbol{\delta}} \equiv \sum_{\boldsymbol{\delta} = \mathbf{e}_x, \mathbf{e}_y, \cdots} = (\text{summation over nearest-neighbor vectors (only positive direction)})$$

$$\mathbf{q}_{\mathbf{k}} \equiv \frac{1}{\sqrt{\Lambda}} \sum_{\mathbf{x}} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathbf{q}(\mathbf{x}) \quad \left(\Lambda \equiv \frac{L^d}{a^d} = (\#\text{ of atoms}) \right)$$

$$K = \frac{m}{2} \frac{1}{\Lambda} \sum_{\mathbf{x}} \sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}} \dot{\mathbf{q}}_{\mathbf{k}'} \cdot \dot{\mathbf{q}}_{\mathbf{k}}$$

$$= \frac{m}{2} \sum_{\mathbf{k}} \dot{\mathbf{q}}_{\bar{\mathbf{k}}} \cdot \dot{\mathbf{q}}_{\mathbf{k}} \quad (\bar{\mathbf{k}} \equiv -\mathbf{k})$$

$$U = \frac{m\omega_0^2}{2} \sum_{\mathbf{x},\boldsymbol{\delta}} \frac{1}{\Lambda} \sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}+\mathbf{k}')\mathbf{x}} (e^{i\mathbf{k}'\cdot\boldsymbol{\delta}} - 1)(e^{i\mathbf{k}\boldsymbol{\delta}} - 1) \times \mathbf{q}_{\mathbf{k}'} \cdot \mathbf{q}_{\mathbf{k}}$$

$$= \frac{m\omega_0^2}{2} \sum_{\mathbf{k}} \sum_{\boldsymbol{\delta}} (e^{-i\mathbf{k}\cdot\boldsymbol{\delta}} - 1)(e^{i\mathbf{k}\boldsymbol{\delta}} - 1) \mathbf{q}_{\bar{\mathbf{k}}} \cdot \mathbf{q}_{\mathbf{k}}$$

○ Continuous Media

To generalize the above discussion, it is convenient to move to the continuous-space description. For the sake of simplicity, we consider only one component of q and denote it as ϕ.

$$L = \frac{m}{2}\sum_{x} \dot{\phi}(x) - \frac{m\omega_0^2}{2}\sum_{x,\delta}\left(\phi(x+\delta)-\phi(x)\right)^2$$

$$\sum_{x} \longrightarrow \int \frac{d^dx}{a^d} \qquad \phi(x+\delta)-\phi(x) = \delta\cdot\frac{\partial\phi}{\partial x}$$

$$L = \frac{\rho}{2}\int dx\, \dot{\phi}^2 - \frac{\rho a^2\omega_0^2}{2}\int dx\,(\nabla\phi)^2$$

$$\pi = \frac{\delta L}{\delta\dot{\phi}} = \rho\dot{\phi} \quad \left(= \frac{m}{a^d}\dot{q} = \frac{p}{a^d}\right)$$

$$\mathcal{H} = \int dx\,(\pi\dot{\phi}) - L$$

$$= \int dx\left(\frac{\pi^2}{2\rho} + \frac{t}{2}(\nabla\phi)^2\right) \quad \left(t \equiv \rho a^2\omega_0^2\right)$$

$$[\pi(x), \phi(x')] = \frac{\hbar}{i}\delta(x-x')$$

$$\left([\frac{1}{a^d}p(x), q(x')] = \frac{\hbar}{i}\frac{1}{a^d}\delta_{x,x'} \rightarrow \frac{\hbar}{i}\delta(x-x')\right)$$

◦ The bosonic creation/annihilation ops.

$$\phi(x) = \frac{1}{\sqrt{L^d}} \sum_{\mathbb{k}} e^{i\mathbb{k}x} A_{\mathbb{k}} \left(b_{\mathbb{k}}^{+} + b_{\mathbb{k}} \right)$$

$$\pi(x) = \frac{1}{\sqrt{L^d}} \sum_{\mathbb{k}} e^{i\mathbb{k}x} i B_{\mathbb{k}} \left(b_{\mathbb{k}}^{+} - b_{\mathbb{k}} \right)$$

with $A_{\mathbb{k}} \equiv \frac{\hbar}{2} \frac{1}{\sqrt{t\rho}\, k}$, $B_{\mathbb{k}} \equiv \frac{\hbar}{2} \sqrt{t\rho}\, k$

Then, $b_{\mathbb{k}}$ and $b_{\mathbb{k}}^{+}$ are dimensionless and

$[b_{\mathbb{k}}, b_{\mathbb{k}'}^{+}] = \delta_{\mathbb{k}\mathbb{k}'}$, so they can be regarded

as bosonic creation/annihilation ops.

◦ With $b_{\mathbb{k}}$ and $b_{\mathbb{k}}^{+}$, the Hamiltonian becomes

$$\mathcal{H} = \sum_{\mathbb{k}} \hbar \omega_{\mathbb{k}} \left(b_{\mathbb{k}}^{+} b_{\mathbb{k}} + \frac{1}{2} \right)$$

where

$$\omega_{\mathbb{k}} = \sqrt{\frac{t}{\rho}}\, k \left(= a\omega_0 k \right)$$

Acoustic Phonons in Isotropic Crystals

- The elastic energy of the isotropic crystals must take the form of the rotationally invariant quantity that is the second order in the deformation gradient tensor

$$F_{\mu\nu} \equiv \frac{\partial q_\mu}{\partial x_\nu}$$

where $q(x)$ is the displacement vector at x. Since the anti-symmetric part of F represents rotation, it doesn't contribute to the strain energy. Therefore we consider only the symmetric part:

$$E_{\mu\nu} \equiv \frac{1}{2}(F_{\mu\nu} + F_{\nu\mu})$$

The scalar fields in second-order in E are

$$E_{\mu\mu} E_{\nu\nu} \quad \text{and} \quad E_{\mu\nu} E_{\mu\nu}$$

Thus we have the strain energy

$$U = \frac{\lambda}{2} \underbrace{\frac{\partial q_\mu}{\partial x_\mu} \frac{\partial q_\nu}{\partial x_\nu}}_{= E_{\mu\mu} E_{\nu\nu}} + \frac{\mu}{2} \underbrace{\left(\frac{\partial q_\mu}{\partial x_\nu} \frac{\partial q_\mu}{\partial x_\nu} + \frac{\partial q_\nu}{\partial x_\mu} \frac{\partial q_\mu}{\partial x_\nu} \right)}_{= 2 E_{\mu\nu} E_{\nu\mu}}$$

where λ and μ are the parameters characterizing the elastic properties of the material (Lamé parameters).

※ As a quadratic form of $E_{11}, E_{22}, E_{33}, E_{23}, E_{31}$ and E_{12}, U must be positive semi-definite (because of the 2nd law of thermodynamics), which leads to $\mu > 0$ and $3\lambda + 2\mu > 0$.

- $\mathcal{H} = \int dx \left\{ \frac{\pi^2}{2\rho} + \frac{\lambda}{2}\left(\frac{\partial q_\mu}{\partial x_\mu}\frac{\partial q_\nu}{\partial x_\nu}\right) + \frac{\mu}{2}\left(\frac{\partial q_\mu}{\partial x_\nu}\frac{\partial q_\mu}{\partial x_\nu} + \frac{\partial q_\mu}{\partial x_\nu}\frac{\partial q_\nu}{\partial x_\mu}\right)\right\}$

- $[\pi_\mu(x), q_\nu(x')] = \frac{\hbar}{i}\delta(x-x')\delta_{\mu\nu}$

- $\begin{cases} \pi(x) = \frac{1}{\sqrt{\Omega}}\sum_{k} e^{-ikx}\,p_k & p_k = \sqrt{\Omega}\int dx\, e^{ikx}\,\pi(x) \\ q(x) = \frac{1}{\sqrt{\Omega}}\sum_{k} e^{ikx}\,q_k & q_k = \sqrt{\Omega}\int dx\, e^{-ikx}\,q(x) \end{cases}$

$$[p^\mu_k, q^\nu_{k'}] = \frac{1}{\Omega}\int dx \int dx'\, e^{ikx-ik'x'}\,[\pi^\mu(x), q^\nu(x')]$$
$$= \frac{1}{\Omega}\int dx\int dx'\, e^{i(kx-k'x')}\,\frac{\hbar}{i}\delta(x-x')\delta_{\mu\nu}$$
$$= \frac{1}{\Omega}\int dx\, e^{i(k-k')x}\,\frac{\hbar}{i}\delta_{\mu\nu}$$
$$= \frac{\hbar}{i}\delta_{kk'}\delta_{\mu\nu}$$

- $K = \int dx\, \frac{1}{2\rho}\frac{1}{\Omega}\sum_{kk'} e^{ikx-ik'x}\, p^{\alpha+}_k p^\alpha_{k'}$
$$= \frac{1}{2\rho}\sum_k p^+_k p_k$$

- Similar calculation yields

$$U = \sum_k \left\{ \frac{\lambda}{2} k_\mu k_\nu q^{\mu+}_k q^\nu_k + \frac{\mu}{2}\left(k_\mu k_\mu q^{\nu+}_k q^\nu_k + k_\mu k_\nu q^{\nu+}_k q^\mu_k\right)\right\}$$
$$= \sum_k \left(\frac{\mu}{2} k_\mu k_\mu q^{\nu+}_k q^\nu_k + \frac{\lambda+\mu}{2} k_\mu k_\nu q^{\mu+}_k q^\nu_k\right)$$

- The longitudinal mode ($\mathbf{k} \parallel \mathbf{q}$; $k_\mu q^\mu_k = k \times q_k$)

$$\sum_k \left(\frac{1}{2\rho} p^\dagger_k p_k + \frac{\lambda+2\mu}{2} k^2 q^\dagger_k q_k \right)$$

$$\longrightarrow \omega^l_k = \sqrt{\frac{\lambda+2\mu}{\rho}}\, k \quad \therefore \quad c_l = \sqrt{\frac{\lambda+2\mu}{\rho}}$$

- The transverse mode ($\mathbf{k} \perp \mathbf{q}$; $k_\mu q^\mu_k = 0$)

$$\longrightarrow \omega^t_k = \sqrt{\frac{\mu}{\rho}}\, k \quad \therefore \quad c_t = \sqrt{\frac{\mu}{\rho}}$$

Because of the remark in 6-7,

$$\rho (c_l^2 - c_t^2) = \lambda + 2\mu - \mu = \lambda + \mu$$

$$> -\frac{2}{3}\mu + \mu = \frac{1}{3}\mu > 0$$

$\Longrightarrow$ $c_l > c_t$ (longitudinal waves are always faster than transverse waves.)

(If we have some isotropic elastic medium that mediates transverse wave faster than longitudinal one, we can construct a perpetual machine !!)

Phonons in Condensed Bosons

- Phonons can be produced not only in crystals.
- Now, we leave lattices and consider phonons in condensed Bose gas:

$$b_0^\dagger b_0 |\Psi\rangle \sim N_0 |\Psi\rangle \quad (b_0 \equiv b_{k=0})$$

We also assume almost all bosons are in $k=0$ state ($N_0 \simeq N$).
(The latter is not the case with liquid ^{4}He. But the argument here is believed to be qualitatively valid.) Then, we can further assume $\quad b_0|\Psi\rangle \sim b_0^\dagger|\Psi\rangle \sim \sqrt{N_0}\,|\Psi\rangle$.

(Obviously, this can't be true in the canonical ensemble, but it is allowed in the grand-canonical ensemble. In other words, it is allowed as a property of a part of the system for which the rest of the system acts as a reservoir.)

- Then we consider the effect of weak interaction among the Bosons represented by

$$V \equiv \frac{1}{2} \sum_{\substack{k_1 k_2 \\ k_1' k_2'}} V(k_1'-k_1)\, \delta_{k_1+k_2,\, k_1'+k_2'} \cdot b_{k_1'}^\dagger b_{k_2'}^\dagger b_{k_1} b_{k_2}$$

(※)

- The total Hamiltonian is

$$\mathcal{H} = K + V$$

$$K = \sum_k \epsilon_k^0 \, b_k^\dagger b_k \quad \left(\epsilon_k^0 = \frac{\hbar^2 k^2}{2M} \right)$$

$$\psi(x) = \frac{1}{\sqrt{\Omega}} \sum_k e^{ikx} b_k$$

$$V = \frac{1}{2} \int dx\,dy\, V(x-y)\, \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(y)\, \psi(y)\, \psi(x)$$

$$= \frac{1}{2} \int dx\,dy\, V(x-y) \frac{1}{\Omega^2} \sum_{k_1 k_2 k_1' k_2'}$$
$$\times\, e^{-ik_1'x - ik_2'y + ik_2 y + ik_1 x}\; b^\dagger_{k_1'} b^\dagger_{k_2'} b_{k_2} b_{k_1}$$

$$= \frac{1}{2} \int dx\,dr\, V(r) \frac{1}{\Omega^2} \sum_{k_1 k_2 k_1' k_2'} \qquad (y = x + r)$$
$$\times\, e^{-i(k_1' + k_2' - k_1 - k_2)x - i(k_2' - k_2) r}\; b^\dagger_{k_1'} b^\dagger_{k_2'} b_{k_2} b_{k_1}$$

$$= \frac{1}{2\Omega} \int dr\, V(r) \sum_{k_1 k_2 k_1' k_2'} \delta_{k_1' + k_2', k_1 + k_2}$$
$$\times\, e^{-i(k_2' - k_2) r}\; b^\dagger_{k_1'} b^\dagger_{k_2'} b_{k_2} b_{k_1}$$

$$= \frac{1}{2} \sum_{k_1 k_2 k_1' k_2'} V(k_2' - k_2)\, b^\dagger_{k_1'} b^\dagger_{k_2'} b_{k_2} b_{k_1}$$

$$= \frac{1}{2} \sum_{k_1 k_2 k_1' k_2'} V(k_1' - k_1)\, b^\dagger_{k_1'} b^\dagger_{k_2'} b_{k_2} b_{k_1}$$

- Since $N_0 (\sim N) \gg 1$, b_0 or b_0^+ generate a larger contribution compared to b_k or b_k^+ $(k \neq 0)$. Therefore among the $b^+ b^+ bb$ terms, the largest contribution would be $b_0^+ b_0^+ b_0 b_0 \sim N_0^2$.
Since terms like $b_k^+ b_0^+ b_0 b_0$ don't exist because of the momentum conservation, the second largest terms are $b_{k_1}^+ b_{k_2}^+ b_0 b_0$, $b_{k_1}^+ b_0^+ b_{k_2} b_0, \cdots$
(i.e. two of the wave numbers are zero).
Therefore, upto this order, our effective Hamiltonian is

$$\mathcal{H} = \frac{1}{2\Omega} N^2 u(0) + \sum_k{}' \overbrace{(\epsilon_k^0 + N V(k))}^{A_k} b_k^+ b_k$$

$(\Omega : \text{volume})$

$$+ \sum_k{}' \frac{1}{2} \underbrace{NV(k)}_{B_k} (b_k^+ b_{\bar{k}}^+ + b_k b_{\bar{k}})$$

$\left(\sum_k{}' \equiv \sum_{k (k \neq 0)} \right)$

$$\mathcal{H} = (\text{const}) + \sum_k{}' \mathcal{H}_k$$

$$\mathcal{H}_k = \frac{1}{2} \left(A_k (b_k^+ b_k + b_{\bar{k}}^+ b_{\bar{k}}) + B_k (b_k^+ b_{\bar{k}}^+ + b_k b_{\bar{k}}) \right)$$

(Here we've assumed $\epsilon_k^0 = \epsilon_{\bar{k}}^0$)

- Bogoliubov transformation $(\bar{k} \equiv -k)$

Let's consider the linear transformation of the creation/annihilation operators (dropping the subscript k),

$$\begin{pmatrix} a \\ \bar{a}^+ \end{pmatrix} = \begin{pmatrix} u & -v \\ -v & u \end{pmatrix} \begin{pmatrix} \alpha \\ \bar{\alpha}^+ \end{pmatrix}$$

$(\bar{a} \equiv a_{\bar{k}})$
(Bogoliubov transformation)

$(\exists \chi \ u = \operatorname{ch} \chi, \ v = \operatorname{sh} \chi)$

If $u^2 - v^2 = 1$, then, α satisfies

$$[\alpha, \alpha^+] = [\bar{\alpha}, \bar{\alpha}^+] = 1 \quad [\alpha, \bar{\alpha}^+] = [\alpha, \bar{\alpha}] = 0$$

Therefore, $\{\alpha_k, \alpha_k^+\}$ can be regarded as a new set of creation/annihilation operators.

- By some arithematics, we can show

$$\mathcal{H}_k = \frac{1}{2}\Big[(A\,\mathrm{ch}\,2\chi - B\,\mathrm{sh}\,2\chi)(\alpha^+\alpha + \bar{\alpha}^+\bar{\alpha})$$
$$+ (-A\,\mathrm{sh}\,2\chi + B\,\mathrm{ch}\,2\chi)(\alpha^+\bar{\alpha}^+ + \alpha\bar{\alpha})$$
$$+ A(\mathrm{ch}\,2\chi - 1) + B\,\mathrm{sh}\,2\chi \Big]$$

Therefore by choosing χ, s.t., $\mathrm{th}\,2\chi_k = \frac{B_k}{A_k}$

$$\left(\mathrm{ch}\,2\chi = \frac{A}{\sqrt{A^2-B^2}}, \quad \mathrm{sh}\,2\chi = \frac{B}{\sqrt{A^2-B^2}} \right)$$

the Hamiltonian $\mathcal{H}_k$ is diagonalized as,

$$\mathcal{H}_k = (\mathrm{const}) + \epsilon_k(\alpha^+\alpha + \bar{\alpha}^+\bar{\alpha})$$

with $\epsilon_k = \sqrt{A^2-B^2}$

$$\epsilon_k^2 = A_k^2 - B_k^2 = (\epsilon_k^0 + N V(k))^2 - (N V(k))^2 \quad \left(n \equiv \frac{N}{\Omega}\right)$$

$$V_0 \equiv V(0)$$

$$= \epsilon_k^0(\epsilon_k^0 + 2NV(k))$$

$$\underset{k\to 0}{\approx} \frac{\hbar^2 k^2}{2M}(2NV_0) = \frac{\hbar^2 N V_0}{M} k^2$$

$$\therefore \boxed{\epsilon_k = \hbar c k} \quad \boxed{c = \sqrt{\frac{NV_0}{M}}}$$

Second Sound (Sound mediated by quantized sound)

- Phonons may behave like regular particles.
  The large thermal conductivity of superfluid ^{4}He is attributed to the density wave of phonons (second sound).

- If the mean-free path of the phonons are shorter than the wave length of the wave that is going to be discussed, the so-called the local equilibrium picture would be valid; we can consider the local distribution function of phonons : $f(\mathbf{k}, \mathbf{x})$, the density of phonons in the $(\mathbf{k}, \mathbf{x})$ space.

- For this quantity, the Boltzmann eq. says

$$\frac{D}{Dt} f \left(\equiv \frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} \right) = g_c(\mathbf{k}, \mathbf{x})$$

where g_c represents the change rate of f caused by the collision among the phonons.
Since $\mathbf{v} = c\,\mathbf{k}/k$,

$$\frac{\partial f}{\partial t} + \frac{c}{k}\mathbf{k} \cdot \nabla f = g_c \qquad \text{— (1)}$$

- At low temperature and for low wave number, we can assume that the collision conserves the momentum and the energy; which yields

$$\left(\frac{\partial \mathbf{P}}{\partial t}\right)_c = \int d\mathbf{k}\ \hbar\mathbf{k}\ g_c(\mathbf{k}, \mathbf{x}) = 0 \qquad \text{— (2)}$$

$$\left(\frac{\partial E}{\partial t}\right)_c = \int d\mathbf{k}\ \hbar c|\mathbf{k}|\ g_c(\mathbf{k}, \mathbf{x}) = 0 \qquad \text{— (3)}$$

∘ ① and ②

$$\longrightarrow \int d\mathbf{k} \left(\hbar k^\alpha \frac{\partial f}{\partial t} + \hbar k^\alpha \frac{c}{k} k^\beta \partial_\beta f \right) = 0$$

$$\frac{\partial p^\alpha}{\partial t} + \partial_\beta \int d\mathbf{k}\ \hbar c \frac{k^\alpha k^\beta}{k} f = 0$$

Generally, $\int d\mathbf{k}\ w(\mathbf{k})\, k^\alpha k^\beta = \frac{\delta^{\alpha\beta}}{3} \int d\mathbf{k}\ w(\mathbf{k})\, \mathbf{k}^2$ for any isotropic function $w(\mathbf{k})$, Therefore,

$$\longrightarrow \frac{\partial p^\alpha}{\partial t} + \partial_\beta \left(\frac{1}{3} \delta_{\alpha\beta} \int d\mathbf{k}\ \hbar c k f \right) = 0$$

$$\longrightarrow \frac{\partial p^\alpha}{\partial t} + \frac{1}{3} \partial_\alpha E = 0 \quad \left(\frac{\partial \mathbf{P}}{\partial t} + \frac{1}{3} \nabla E = 0 \right)$$

② '

∘ ① and ③

$$\longrightarrow \int d\mathbf{k} \left(\hbar c k \cdot \frac{\partial f}{\partial t} + \hbar c^2 k^\alpha \partial_\alpha f \right) = 0$$

$$\longrightarrow \frac{\partial E}{\partial t} + c^2 \nabla \cdot \mathbf{P} = 0 \qquad \text{— ③}'$$

∘ ②' and ③'

$$\longrightarrow \frac{\partial^2 E}{\partial t^2} = - c^2 \nabla \cdot \frac{\partial \mathbf{P}}{\partial t} = \frac{c^2}{3} \nabla \cdot (\nabla E)$$

$$\longrightarrow \frac{\partial^2}{\partial t^2} E = \frac{c^2}{3} \Delta E$$

$$\longrightarrow \boxed{c' = \frac{c}{\sqrt{3}}}$$

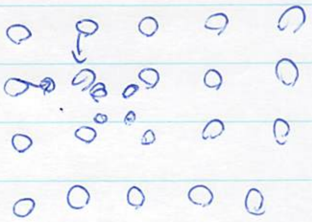
For the "first" and second sounds of liquid ^{4}He, see §3.4 Leggett "quantum liquids"

The energy density wave propergates at the velocity $c/\sqrt{3}$.

Phononはなぜbosonか?

① 直観的説明

Since a phonon is a quantized lattice deformation, we consider two phonons exchanging their position as the continuous change in the lattice configuration.



However, a continuous change in the perturbative lattice deformation do not involve any exchange of the underlying ~~of~~ nucleons.

Therfore, whether the nucleons are bosons or fermions, we will never have the negative sign originationg ~~fom~~ from exchange of particles.

② 形式的説明

$$[p_i\ q_j] = \delta_{ij}\frac{\hbar}{i} \quad \text{を示せばよい。} \quad ①$$

$$p_i = \psi^{\dagger}(x)\frac{\hbar}{i}\partial\psi(x)\Big|_{x\sim x_i}$$

$$q_j = \psi^{\dagger}(x)\,x\,\psi(x)\Big|_{x\sim x_j}$$

phononに限らず一般に粒子数を変化させない演算子は異なる場所では可換.

So, whether $[\psi^{\dagger}(x_i), \psi(x_j)] = 0$ or $\{\psi^{\dagger}(x_i), \psi(x_j)\} = 0$, $[p_i, q_j] = 0$.

そうしないためには

これ~~関係~~は循環論法で、~~形式的には~~ ①を出発点として仮定しないといけない。