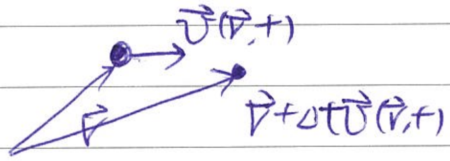
# Phonons in Liquids/gases — the need for second quantization

As we have discussed, classical sound waves also exist in liquids & gases. It is therefore natural to ask what happens to them in quantum mechanics.

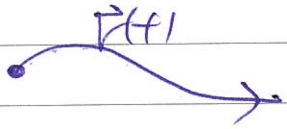
The answer is that they also become phonons. But unlike phonons on crystals, the quantum description is fundamentally different. In crystals, each $\vec{u}_n$ operator describes one atom. In other words, one can still trace the motion of each atom. In liquids or gases, this is not a good description even classically. Quantumechanically, this is not even possible if atoms/ions are identical particles. Classically, we abandon the Lagrangian description and adopt the Euler description: use $\rho(\vec{r},t)$, $\vec{v}(\vec{r},t)$, $p(\vec{r},t)$ to describe.

We no longer distinguish which particle is at $\vec{r}$ at time $t$. For instance, the particle with the velocity $\vec{v}(\vec{r},t)$ will move to $\vec{r}+\Delta t\,\vec{v}(\vec{r},t)$.




Therefore, one has to be careful when using $\vec{v}(\vec{r},t)$ to express the Newton law. The acceleration at $(\vec{r},t)$ is not $\frac{d\vec{v}(\vec{r},t)}{dt}$ $(\neq \vec{a}\ !)$

Instead, one has to follow the same particle by noting that its velocity $\vec{v}(t) = \vec{v}(\vec{r}(t),t)$




$$\therefore\ \vec{a}(r,t) = \frac{d\vec{v}(t)}{dt} = \frac{\partial \vec{v}(\vec{r},t)}{\partial t} + \frac{\partial \vec{v}(\vec{r},t)}{\partial x(t)}\dot{x}(t) + \frac{\partial \vec{v}(\vec{r},t)}{\partial y(t)}\dot{y}(t) + \frac{\partial \vec{v}(\vec{r},t)}{\partial z(t)}\dot{z}(t)$$

i.e. $\vec{a}(r,t) = \frac{\partial v}{\partial t} + (\vec{v}\cdot\vec{\nabla})\,\vec{v}$

This is the basic description that leads to the Navier-Stokes equation that we will discuss it later.

In quantum mechanics, if the liquids are composed by identical particles, we no longer can trace which particle is which particle!

We shall be focused on identical bosons.

In this case, total wave function has to be symmetrized. The experience with phonons in crystals tells us that one may be able to formulate the whole dynamics by expressing $H = \sum_{k\lambda} \hbar\omega_{k\lambda}(a^{+}_{k\lambda} a_{k\lambda} + 1)$ in terms of counting # of some bosonic creation & annihilation operators $[a, a^{+}] = 1$
$[a, a] = 0$, $[a^{+}, a^{+}] = 0$

It turns out that it is sufficient to know #'s of particles in each state. The Hilbert space formed by $|n_1, n_2, \ldots\rangle$ is known as the Fock space.

($n_1$: # of particle in $|1\rangle$; $n_2$: " in $|2\rangle$)

In this new space, operators have different forms; however, calculations of matrix elements of observables (operators) become considerably easy. This method is known as second quantization, first developed by Paul Dirac for treating photons, then extended to fermions by Jordan & Wigner.

# Introduction to second quantization (Bosons)

Let us consider 3 identical bosons as an example

For simplicity, we assume they reside in 2-state space $|\alpha\rangle$, $|\beta\rangle$ (orthonormal) $\dim(V_2 \otimes V_2 \otimes V_2) = 8$

basis : $|\psi_1\rangle = |\alpha\rangle|\alpha\rangle|\alpha\rangle$

$|\psi_2\rangle = |\beta\rangle|\beta\rangle|\beta\rangle$

$|\psi_3\rangle = \frac{\sqrt{2!}}{\sqrt{3!}}\left[|\alpha\rangle|\alpha\rangle|\beta\rangle + |\alpha\rangle|\beta\rangle|\alpha\rangle + |\beta\rangle|\alpha\rangle|\alpha\rangle\right]$

2 1

$|\psi_4\rangle = \frac{\sqrt{2!}}{\sqrt{3!}}\left[|\beta\rangle|\beta\rangle|\alpha\rangle + |\beta\rangle|\alpha\rangle|\beta\rangle + |\alpha\rangle|\beta\rangle|\beta\rangle\right]$

Consider one-body operator : $\hat{F} = f_1 + f_2 + f_3$

indices for particles

e.g. $\hat{F} = \frac{-\hbar^2}{2m}\left[\frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2} + \frac{d^2}{dx_3^2}\right]$

$\langle\psi_1|\hat{F}|\psi_1\rangle = 3\langle\alpha|f|\alpha\rangle \left[= 3\int dx\, \phi_\alpha^*(x) \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\phi_\alpha(x)\right]$

$\langle\psi_2|\hat{F}|\psi_2\rangle = 3\langle\beta|f|\beta\rangle$

$\langle\psi_3|\hat{F}|\psi_3\rangle = 2\langle\alpha|f|\alpha\rangle + 1\langle\beta|f|\beta\rangle$

$\langle\psi_4|\hat{F}|\psi_4\rangle = 1\langle\alpha|f|\alpha\rangle + 2\langle\beta|f|\beta\rangle$

These #s are # of particles appearing in the state involved in the matrix element that $\langle m|f|m\rangle$ follows ! $m = \alpha$ or $\beta$

NO.

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This suggests a rule:

$$\hat{F} \cong \sum_{\ell} a_\ell^\dagger a_\ell \langle \ell | f | \ell \rangle$$

more generally, to include off-diagonal terms, one guesses

$|\psi_1\rangle = |3,0\rangle$
$|\psi_2\rangle = |0,3\rangle$
$|\psi_3\rangle = |2,1\rangle$
$|\psi_4\rangle = |1,2\rangle$

$$\hat{F} = \sum_{\ell m} a_\ell^\dagger a_m \langle \ell | f | m \rangle \quad \text{--- ①}$$

To confirm this, we calculate the off-diagonal terms:

$$\langle \psi_2 | F | \psi_1 \rangle = 3 \langle \beta | f | \alpha \rangle \underline{\langle \beta | \alpha \rangle \langle \beta | \alpha \rangle} = 0$$

$$\langle \psi_1 | F | \psi_2 \rangle = 3 \langle \alpha | f | \beta \rangle \underline{\langle \alpha | \beta \rangle \langle \alpha | \beta \rangle} = 0$$

It appears that the only possible non-vanishing off diagonal terms are

$$\langle \beta | f | \alpha \rangle \, [\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle, \langle \alpha | \alpha \rangle \langle \alpha | \alpha \rangle, \cdots]$$

$$\text{or } \langle \alpha | f | \beta \rangle \cdot [\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle, \langle \alpha | \alpha \rangle \langle \alpha | \alpha \rangle, \cdots]$$

i.e. $\langle \psi_i | \hat{F} | \psi_j \rangle \neq 0$ only when $|\psi_i\rangle$ & $|\psi_j\rangle$ have at least two common states

$\therefore \langle \psi_3 | \hat{F} | \psi_1 \rangle, \langle \psi_1 | \hat{F} | \psi_3 \rangle, \langle \psi_4 | \hat{F} | \psi_2 \rangle$ & $\langle \psi_2 | \hat{F} | \psi_4 \rangle \neq 0$

$$\langle \psi_3 | \hat{F} | \psi_1 \rangle = \left( 3 \cdot \frac{\sqrt{2!}}{\sqrt{3!}} \right) \langle \beta | f | \alpha \rangle$$

each $f_k$ contributes 1

$$\langle \psi_1 | \hat{F} | \psi_3 \rangle = \left( 3 \cdot \frac{\sqrt{2!}}{\sqrt{3!}} \right) \langle \alpha | f | \beta \rangle$$

$$\langle \psi_4 | \hat{F} | \psi_2 \rangle = \left( 3 \frac{\sqrt{2!}}{\sqrt{3!}} \right) \langle \alpha | f | \beta \rangle$$

$$\langle \psi_2 | \hat{F} | \psi_4 \rangle = 3 \frac{\sqrt{2!}}{\sqrt{3!}} \langle \beta | f | \alpha \rangle$$

One can easily check that:

if $a_\alpha^+ |n,m\rangle = \sqrt{n+1}\, |n+1,m\rangle$, $a_\alpha |n,m\rangle = \sqrt{n}\, |n-1,m\rangle$ --- ②

$a_\beta^+ |n,m\rangle = \sqrt{m+1}\, |n,m+1\rangle$, $a_\beta |n,m\rangle = \sqrt{m}\, |n,m-1\rangle$

n particles in $|\alpha\rangle$ ; m particles in $|\beta\rangle$

i.e. $|n,m\rangle = \frac{1}{\sqrt{n!}} (a_\alpha^+)^n \frac{1}{\sqrt{m!}} (a_\beta^+)^m |0,0\rangle$ ← "vacuum"

$$3 \cdot \frac{\sqrt{2!}}{\sqrt{3!}} = \langle 2,1 | a_\beta^+ a_\alpha | 3,0\rangle$$

$$= \langle 3,0 | a_\alpha^+ a_\beta | 2,1\rangle$$

$$= \langle 1,2 | a_\alpha^+ a_\beta | 0,3\rangle = \langle 0,3 | a_\beta^+ a_\alpha | 2,1\rangle$$

∴ ① is correct !! This is what the 2nd quantization is : replace the calculations with $|\Psi_i\rangle$ by calculations with $|n,m\rangle$ & $a_\alpha^+, a_\beta$ !!

Here $\hat{F} = \sum_{\ell m} a_\ell^+ a_m \langle \ell | f | m\rangle$ in the Fock space !!

Now, let's understand the form $\hat{F} = \sum_{\ell m} a_\ell^+ a_m \langle \ell | f | m\rangle$ more closely.

From the above example, we see that in order that $\langle \Psi_i | \hat{F} | \Psi_j\rangle \neq 0$, $|\Psi_i\rangle$ & $|\Psi_j\rangle$ have to be
$= \cdots \langle \alpha | f | \beta\rangle$
the same after removing $|\alpha\rangle$ in $|\Psi_i\rangle$, $|\beta\rangle$ in $|\Psi_j\rangle$

In other words

$|\varphi_i\rangle$ has one extra particle in $|\alpha\rangle$

$|\varphi_j\rangle$ " " " " in $|\beta\rangle$ !

By going from $|\varphi_j\rangle$ to $|\varphi_i\rangle$, it seems that we annihilate one particle in $|\beta\rangle$ while we create one in $|\alpha\rangle$ !

This explains the term $a_\alpha^\dagger a_\beta$ !

Formally, this can be derived as follows:

$$\because \mathbb{1} = \sum_\ell |\ell\rangle\langle\ell|$$

$$\therefore \hat{f} = \sum_{\ell m} |\ell\rangle\langle\ell|\hat{f}|m\rangle\langle m|$$

$$\hat{F} = \sum_k \sum_{\ell m} |\ell\rangle_k \langle\ell|\hat{f}|m\rangle {}_k\langle m|$$

particle index ($k$th particle)

${}_k\langle m|$ annihilates one particle ($k$th) in $|m\rangle$ state

$|\ell\rangle_k$ creates " in $|\ell\rangle$ "

Since we no longer distinguish particles,

we get $\hat{F} = \sum_{\ell m} a_\ell^\dagger a_m \langle\ell|f|m\rangle$

We can generalize the above derivation to "two-body" operators

For instance, $V_{ij} = \frac{e^2}{|r_i - r_j|}$, $V = \sum_{ij} \frac{1}{2} V_{ij}$

for 3 particles, $U = \left( \frac{e^2}{|r_1 - r_2|} + \frac{e^2}{|r_1 - r_3|} + \frac{e^2}{|r_3 - r_2|} \right)$

Since $\hat{U} = \sum_{\substack{kl \\ mn \\ ij}} |kl\rangle_{ij} \langle kl | U_{ij} | mn\rangle_{ij} \langle mn|$

and $|kl\rangle = |k\rangle \otimes |l\rangle \Leftrightarrow a_k^+ a_l^+$

$\langle mn| = (|mn\rangle)^+ \Leftrightarrow (a_m^+ a_n^+)^+ = a_n a_m$,

We have $\hat{U} = \sum_{\substack{kl \\ mn}} \langle kl | V_{ij} | mn\rangle a_k^+ a_l^+ a_n a_m$

Now, $V_{ij} = U(r_i - r_j)$, we can assign $a_n \to i$

$a_m \to j$, then $a_l^+ \to i$, $a_k^+ \to j$ (reverse)

$\therefore \langle kl | U_{ij} | mn \rangle = \int dr_i \int dr_j \, U(r_i - r_j) \phi_l^*(r_1) \phi_k^*(r_2) \phi_n(r_1) \phi_m(r_2)$

Finally, from ②, $[a_\alpha, a_\alpha^+] = 1$, $[a_\beta, a_\beta^+] = 1$

$[a_\alpha, a_\beta] = 0$, $[a_\alpha, a_\beta^+] = 0$, ..

$\therefore$ No restriction of # of particles in $\alpha$ & $\beta$ needs to be imposed. $\Rightarrow$ Bosons

Most general case :

$$|\Psi_1\rangle = |\cdots \overset{\beta}{N_i-1}, \ldots, \overset{\alpha}{N_k}, \cdots\rangle \quad \sqrt{\frac{N_1!N_2!\ldots}{N!}} \quad \sqrt{(N_i-1)!}\sqrt{N_k!}$$

except $N_i-1$, $N_k$

$$|\Psi_2\rangle = | \quad N_i, \ldots, N_k-1, \cdots\rangle \quad \sqrt{\frac{N_1!N_2!}{N!}} \quad \sqrt{N_i!}\sqrt{(N_k-1)!}$$

$$\hat{F} = \sum_n f_n$$

$$I = \langle\Psi_2|\hat{F}|\Psi_1\rangle$$

$$= N\cdot\langle\Psi_2|f_n|\Psi_1\rangle$$

$$= N\cdot\frac{N_1!N_2!\ldots}{N!}\sqrt{(N_i-1)!}\sqrt{N_i!}\sqrt{N_k!}\sqrt{(N_k-1)!}$$

$$\times\int dx\, \phi_\beta^*(x) f(x)\phi_\alpha(x)$$

$\Psi_1$ picks one, after that
$\Psi_2$ " " the remaining is the same

$$\times \frac{(N-1)!}{N_1!N_2!\ldots} \underbrace{\frac{1}{(N_i-1)!(N_k-1)!}}$$

# of ways for permutation of the remaining states
(i.e. # of terms)

$$= \sqrt{N_i}\sqrt{N_k}\int dx\, \phi_\beta^* f\phi_\alpha$$

$$= \int dx\, \phi_\beta^* f\phi_\alpha\langle N_i, N_k-1|a_\beta^\dagger a_\alpha|N_i-1\ N_k\rangle$$

$$\therefore\ \hat{F} = \sum_{\alpha\beta} a_\beta^\dagger a_\alpha\langle\beta|f|\alpha\rangle$$

Why is the name "second quantization"?

Consider $|\alpha\rangle$ & $|\beta\rangle$ as energy eigenkets : $\hat{h}|i\rangle = E_i|i\rangle$

If $H = h_1 + h_2$ (independent particles), after

second quantization : $\hat{H} = \sum_{\ell m} a_\ell^+ a_m \langle \ell|\hat{h}|m\rangle$

$$= \sum_\ell E_\ell a_\ell^+ a_\ell$$

In the Fock space, one can still use

$$\frac{d\hat{a}_i}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{a}_i] = \frac{-i}{\hbar} E_i \hat{a}_i ,$$

Here $\hat{a}_i(t)$ = Heisenburg picture of $\hat{a}_i$

$$\therefore \hat{a}_i(t) = e^{\frac{-i}{\hbar}E_i t}\hat{a}_i(0)$$

$= e^{\frac{i}{\hbar}\hat{H}t} \hat{a}_i(0) e^{-\frac{i}{\hbar}\hat{H}t}$

$\therefore$ If we form the "field operator"

$$\hat{\psi}(x,t) \equiv \sum_i \hat{a}_i(t)\langle x|i\rangle \Leftrightarrow \sum_i \langle x|i\rangle\langle i|\psi\rangle = \psi(x)$$

$\Rightarrow \hat{\psi}(x,t) = e$ $\sim$ transform to different basis

We find $[\hat{\psi}(x,t), \hat{\psi}^+(x',t)]$

$$= \sum_{n,m} \langle x|n\rangle\langle x'|m\rangle^* [\hat{a}_n(0)e^{\frac{-i}{\hbar}E_n t}, \hat{a}_m^+(0)e^{\frac{i}{\hbar}E_m t}]$$

$$= \sum_n \langle x|n\rangle\langle x'|n\rangle^* = \sum_n \langle x|n\rangle\langle n|x'\rangle = \delta(x-x')$$

$\llcorner$-- 3

and $$\frac{d\hat{\psi}(x,t)}{dt} = \sum_n \frac{d\hat{a}_n(t)}{dt}\langle x|n\rangle$$

$$= \sum_n \frac{i}{\hbar}[\hat{H}, \hat{a}_n(t)]\langle x|n\rangle = \frac{i}{\hbar}[\hat{H}, \hat{\psi}(x,t)]$$

$\llcorner$-- 4

Furthermore, $\because \hat{h} = \frac{-\hbar^2}{2m}\nabla^2 + U(x)$.

$$\langle l|\hat{h}|m\rangle = \int d^3x \, \underbrace{\langle l|x\rangle}_{\phi_l^*(x)} \frac{-\hbar^2}{2m}\nabla^2 \underbrace{\langle x|m\rangle}_{\phi_m(x)} + \phi_l^* U(x) \phi_m$$

$$\hat{H} = \sum_l a_l^\dagger a_m \langle l|\hat{h}|m\rangle$$

$$= \int d^3x \left(\sum_l a_l^\dagger \langle l|x\rangle\right) \frac{-\hbar^2}{2m}\nabla^2 \left(\sum_m \langle x|m\rangle a_m\right)$$

$$+ \sum_l a_l^\dagger \langle l|x\rangle U(x) \sum_m \langle x|m\rangle a_m$$

$$= \int d^3x \, \psi^\dagger(x,t) \frac{-\hbar^2}{2m}\nabla^2 \psi(x,t) + \psi^\dagger(x,t) U(x) \psi(x,t)$$

Using eqs. ③ & ④, we find

$$i\hbar \frac{d\hat{\psi}(x,t)}{dt} = \frac{-\hbar^2}{2m}\nabla^2 \hat{\psi}(x,t) + U(x)\hat{\psi}(x,t)$$

$\therefore$ Except to eq. ③, $\hat{\psi}(x,t)$ is similar to the wavefunction $\psi(x,t)$ and satisfies the same equation as $\psi(x,t)$ does!

$\therefore$ The meaning of $\hat{\psi}^\dagger(x,t)$ is clear:

It creates a particle (Boson) localized at $x$, & time $t$

$\hat{\psi}^\dagger(x,t) = e^{\frac{i}{\hbar}\hat{H}t} \hat{\psi}^\dagger(x) e^{-\frac{i}{\hbar}\hat{H}t}$, $\hat{\psi}^\dagger(x)$ creates a particle at $x$ (without specified at $t$)

Except for obeying the same form of equation,

$\hat{\psi}(x,t)$ & $\psi(x,t)$ are similar in many ways

For instance,

$$\int dx\, \psi^*(x,t)\, \psi(x,t) = \text{total probability (one-particle)}$$

$$\int dx\, \hat{\psi}^\dagger(x,t)\, \hat{\psi}(x,t) = \sum_n a_n^\dagger a_n = \text{total \# of particles}$$

(many particle)

$\therefore$ $\hat{\psi}(x,t)$ appears to quantize $\psi$!

This is the field quantization. Since this is the quantization for many-particle systems after we perform quantization for single particle. $\Rightarrow$ second quantization!

When there is no interaction, as we have seen, $\hat{\psi}(x,t)$ & $\psi(x,t)$ obey the same equation. For many particles with interactions, $\psi(x,t)$ no longer plays any role but $\hat{\psi}(x,t)$ seems to be a generalization of $\psi(x,t)$ but the equation is no longer linear!

For general ~~pair wise~~ interaction $V(x-x')$,

$$\to \frac{1}{2}\sum_{\substack{kl\\mn}} \langle kl|V|mn\rangle a_k^\dagger a_l^\dagger a_n a_m$$

$$= \frac{1}{2}\int dx \int dx' \, V(x-x') \sum_{\substack{kl\\mn}} \phi_k^*(x')\phi_l^*(x)\phi_m(x')\phi_n(x) a_k^\dagger a_l^\dagger a_n a_m$$

$$\sum_n \phi_n(x) a_n = \sum_n a_n \langle x|n\rangle = \hat{\psi}(x)$$

$$\sum_m \phi_m(x') a_m = \hat{\psi}(x')$$

$$\sum_k \phi_k^*(x') a_k^\dagger = \sum_k \langle k|x'\rangle a_k^\dagger = \hat{\psi}^\dagger(x')$$

$$\sum_l \phi_l^*(x) a_l^\dagger = \hat{\psi}^\dagger(x)$$

$$\therefore = \int dx \int dx' \frac{1}{2} V(x-x') \hat{\psi}^\dagger(x')\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x')$$

$$= \frac{1}{2}\int dx \int dx' \, \cancel{V(x-x') n(x) n(x')} - \underbrace{\frac{1}{2}\int dx \int dx' \, V(x-x')\rho(x')}_{\propto V_{q=0}\bar{\rho} \text{ can be neglected}}$$

$$\hat{n}(x) = \hat{\psi}^\dagger(x)\hat{\psi}(x)$$

Assuming $V(x-x') = V(x'-x)$, we find $\hat{\psi}(x,t)$ satisfies
(true for identical particles)

$$i\hbar \frac{\partial \hat{\psi}(x,t)}{\partial t} = \frac{-\hbar^2}{2m}\nabla^2 \hat{\psi}(x,t) + V(x)\hat{\psi}(x,t)$$

$$+ \Big(\underbrace{\int_{dx'} V(x-x') \hat{\psi}^\dagger(x',t)\hat{\psi}(x',t)}_{\shortparallel}\Big)\hat{\psi}(x,t). \Rightarrow \text{Nonlinear Schrödinger equation}$$

$V \cdot \hat{\psi}^\dagger(x',t)\hat{\psi}(x',t)$ if $V = V_0\delta(x-x')$

## Phonons in a liquid

To describe phonons in a liquid, one needs to describe density, current ad pressure in terms of quantum mechanics.

In the 2nd quantization language, one has

$\hat{\rho}(\vec{r},t) = m\hat{\psi}^{+}(r,t)\,\hat{\psi}(r,t)$, what are $\vec{v}$ & $p$?
(m= mass of a boson)

We start from the equation of motion

$$i\hbar \frac{d\hat{\psi}(x,t)}{dt} = -\frac{\hbar^2}{2m}\nabla^2\hat{\psi} + U\hat{\psi} + \int dx'\, V(x-x')\,\hat{\psi}^{+}(x')\,\hat{\psi}(x')\,\hat{\psi}(x,t) \quad \text{--- (5)}$$

$$-i\hbar \frac{d\hat{\psi}^{+}(x,t)}{dt} = -\frac{\hbar^2}{2m}\nabla^2\hat{\psi}^{+} + U\hat{\psi}^{+} + \boxed{\int dx'\, V(x-x')\,\hat{\psi}^{+}(x')\,\hat{\psi}(x')}\,\hat{\psi}^{+}(x,t) \quad \text{--- (6)}$$

Forming $\hat{\psi}^{+}$ (5) $-$ (6) $\hat{\psi}$, we find

$$i\hbar \frac{d\hat{\psi}^{+}\psi}{dt} = -\frac{\hbar^2}{2m}\hat{\psi}^{+}\nabla^2\psi + \frac{\hbar^2}{2m}(\nabla^2\psi^{+})\psi$$

$$\therefore \frac{d\hat{\rho}}{dt} = -\nabla\cdot\left[\frac{\hbar}{2i}\left(\hat{\psi}^{+}\nabla\psi - (\nabla\psi^{+})\psi\right)\right]$$

We identify the current operator (momentum flux)

$$\vec{j} = \frac{\hbar}{2i}\left(\hat{\psi}^{+}\nabla\psi - (\nabla\psi^{+})\psi\right)$$

both with t, or without t dependence.

$\hat{\rho}$ & $\vec{j}$ are operators. They don't commute
One needs to find their commutator:

$[\rho(x,t), \vec{j}(x',t)]$

$= \frac{\hbar}{2i}[\rho(x,t), \hat{\varphi}^{+}(x',t)\nabla'\varphi(x',t)]$

$- \frac{\hbar}{2i}[\rho(x,t), (\nabla'\hat{\varphi}^{+}(x',t))\varphi(x',t)]$

Now, $[\rho(x,t), \varphi(x',t)] = m[\varphi^{+}(x,t)\varphi(x,t), \varphi(x',t)]$

using $[AB,C] = A[B,C] + [A,C]B$, we get
$([A,BC] = [A,B]C + B[A,C])$

$[\hat{\rho}(x,t), \hat{\varphi}(x',t)] = -m\delta(x-x')\hat{\varphi}(x',t)$

Similarly, $[\hat{\rho}(x,t), \hat{\varphi}^{+}(x',t)] = \left(-[\hat{\rho}(x,t), \hat{\varphi}(x',t)]\right)^{+}$

$= m\delta(x-x')\hat{\varphi}^{+}(x',t)$

Therefore, $[\hat{\rho}(x,t), \hat{\varphi}^{+}(x',t)\nabla'\varphi(x',t)]$

$= +\delta(x-x')\, m\varphi^{+}(x',t)\nabla'\varphi(x',t)$

$-m\varphi^{+}(x',t)\nabla'[\delta(x-x')\hat{\varphi}(x',t)] = -(\nabla'\delta(x-x'))\hat{\rho}(x',t)$

$[\hat{\rho}(x,t), (\nabla'\hat{\varphi}^{+}(x',t))\hat{\varphi}(x',t)]$

$= m\nabla'(\delta(x-x')\hat{\varphi}^{+}(x',t))\hat{\varphi}(x',t) - m(\nabla'\hat{\varphi}^{+}(x',t))\delta(x-x')\hat{\varphi}(x',t)$

$= +[\nabla'\delta(x-x')]\hat{\rho}(x',t)$

$\therefore [\rho(x,t), \vec{j}(x',t)] = +i\hbar\hat{\rho}(x',t)\nabla'\delta(x-x')$ --- (7)
$= i\hbar\hat{\rho}(x',t)\cdot\nabla'\delta(x'-x)$

To connect with $\vec{v}$, we define

$$\vec{J} = \frac{1}{2}(\hat{\rho}\vec{v} + \vec{v}\hat{\rho}).$$

Then $[\hat{\rho}(x,t), \vec{J}(x',t)] = \frac{1}{2}[\hat{\rho}(x,t), \hat{\rho}(x',t)\vec{v}(x',t)]$

$$+ \frac{1}{2}[\hat{\rho}(x,t), \vec{v}(x',t)\hat{\rho}(x',t)]$$

$\because [\hat{\rho}(x,t), \hat{\rho}(x',t)] = 0 \quad \therefore [\hat{\rho}(x,t), \vec{J}(x',t)]$

$$= \frac{1}{2}\hat{\rho}(x',t)[\hat{\rho}(x,t), \vec{v}(x',t)]$$

$$+ \frac{1}{2}[\hat{\rho}(x,t), \vec{v}(x',t)]\hat{\rho}(x',t)$$

To reproduce eq. (7), we require

$$[\hat{\rho}(x,t), \vec{v}(x',t)] = +i\hbar\nabla'\delta(x'-x) \quad \text{--- (8)}$$

If we put $\vec{v} = \nabla\phi$ (thus define $\phi$), eq (8)

implies $[\hat{\rho}(x,t), \hat{\phi}(x',t)] = i\hbar\delta(x'-x)$ --- (9)

The setting $\vec{v} = \nabla\phi$ would correspond to the potential flow classically. ($\nabla\times\vec{v} = 0$).

In Quantum fields, if we write $\psi = \sqrt{\rho/m}\, e^{\frac{i\phi m}{\hbar}}$,

then $\vec{J} = \frac{\hbar}{2i}(\psi^\dagger\nabla\psi - (\nabla\psi^\dagger)\psi)$

$\sim \rho\nabla\phi$, $\quad \therefore \frac{\phi m}{\hbar} \sim$ phase of $\psi$

$\sqrt{\frac{\rho}{m}} \sim$ amplitude of $\psi$, $\quad \frac{\rho}{m} \sim$ Number of particle $= n$

For a simple harmonic oscillator,

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$$

$$a^\dagger \to a^\dagger e^{-i\phi}, \quad a \to a e^{i\phi}, \quad a^\dagger a \text{ invariant.}$$

but $$|n\rangle \to e^{-in\phi}|n\rangle$$

$$\therefore\ n = i\frac{\partial}{\partial\phi}, \quad [n,\phi] = i\frac{\partial\phi}{\partial\phi} = i$$

Eq. (9) simply reflects this relation: $\underline{\left[\frac{\rho}{m}, \frac{\phi m}{\hbar}\right] = i\delta(x'-x)}$

Using eq. (8), one can construct the Hamiltonian

by requiring $$\frac{\partial\hat{\rho}}{\partial t} = \frac{i}{\hbar}[H,\rho]$$

$$= -\nabla\cdot\vec{j} = -\nabla\cdot\left(\frac{1}{2}\rho\vec{v} + \frac{1}{2}\vec{v}\rho\right)$$

We find $$H = \int \frac{1}{2}\vec{v}\cdot\rho\vec{v} + \underbrace{E(\rho)}_{\substack{\text{some function of } \rho \\ \text{(internal energy, independent} \\ \text{of } \vec{v})}}\ d^3r \quad \text{--- (10)}$$

Check: $$\left[\hat{\rho}(x,t), \int dx' \frac{1}{2}\vec{v}(x',t)\cdot\rho(x',t)\vec{v}(x',t)\right]$$

$$= \int dx' \frac{1}{2}\overbrace{\left[\hat{\rho}(x,t), \vec{v}(x',t)\right]}^{i\hbar\nabla'\delta(x'-x)\ \to\ \text{integration by parts}}\cdot\rho(x',t)\vec{v}(x',t)$$

$$+ \int dx' \frac{1}{2}\vec{v}(x',t)\rho(x',t)\cdot\left[\hat{\rho}(x,t), \vec{v}(x',t)\right]$$

$$= \frac{-i\hbar}{2}\nabla\cdot\left(\rho(x,t)\vec{v}(x,t) + \vec{v}(x,t)\rho(x,t)\right).$$

For density perturbations around $\rho_0$, we can write $\hat{\rho}(r) = \rho_0 + \hat{\rho}_1$ $\quad \hat{\rho}_1 << \rho_0$.

And expand H in $\rho_1$. In the lowest order term, we have

$$\hat{H} = \int E(\rho_0)\, d^3\vec{r} + \frac{1}{2}\int \rho_0 \vec{v}^{\,2}\, d^3\vec{r} + \frac{1}{2}\int v(r,r')\rho_1(r')\rho_1(r)\, d^3\vec{r}\, d^3\vec{r}' \quad \text{---} (11)$$

(we can drop T dependence)

Since the system is translational invariant & homogeneous

, $v(r,r') = v(|\vec{r}-\vec{r}'|)$

As an example, in 2nd quantization, generally one has

$$\hat{H} = \int d^3r\ \psi^\dagger(r)\, \frac{\hbar^2}{2m}\nabla^2 \psi(r) + V(x)\,\psi^\dagger(r)\,\psi(r)$$

$\rightarrow \frac{\hbar^2}{2m}\nabla\psi^\dagger \cdot \nabla\psi$

$$+ \frac{1}{2}\int dr \int dr'\ V(r-r')\,\hat{n}(r)\,\hat{n}(r')$$

$\hat{n}(r) = \hat{\psi}^\dagger(r)\,\psi(r)$.

For translational invariant system, $V(x) = 0$

Setting $\psi = \sqrt{n}\, e^{i\frac{m\phi}{\hbar}}$, one gets

$$\hat{H} = \int dr \left\{ \frac{\hbar^2}{2m}\frac{1}{4}\hat{n}^{-1}(\nabla n)^2 + \frac{\hbar^2}{2m}\hat{n} \times \left(\frac{m}{\hbar}\right)^2 (\nabla\phi)^2 \right.$$

$$+ \frac{1}{2}\int dr \int dr'\ V(r-r')\,\hat{n}(r)\,\hat{n}(r')$$

$$\approx \int dr\ \frac{\hbar^2}{8\rho_0}(\nabla\rho_1)^2 + \frac{1}{2}\rho_0\vec{v}^{\,2} + \frac{1}{2}\int dr \int dr'\ \frac{V(r-r')}{m^2}\,\hat{\rho}_1(r)\,\hat{\rho}_1(r') + \ldots \quad \text{---} (12)$$

$\therefore\ v = \frac{1}{m^2}V(r-r')$ describes two-body interactions in liquids.

Hamiltonian in (11) (or (12)) can be solved by going into k space.

$$\rho_1 = \frac{1}{\sqrt{V}} \sum_k \rho_k e^{i\vec{k}\cdot\vec{r}}$$

$$\vec{v} = \frac{1}{\sqrt{V}} \sum_k \vec{v_k} e^{i\vec{k}\cdot\vec{r}} = \nabla\phi, \quad \vec{v_k} = i\vec{k}\phi_k$$

$$\hat{H} = \int \cancel{E(\rho_0)}\, d^3\vec{r} + \sum_k \frac{1}{2} v_k \rho_k \rho_{-k} + \frac{1}{2}\rho_0 \vec{v_k}\cdot\vec{v_{-k}}$$

const

$$= \sum_k \frac{1}{2}\rho_0 k^2 \phi_k \phi_{-k} + \frac{1}{2} v_k \rho_k \rho_{-k} \quad \cdots (13)$$

Here $v_k = \frac{1}{m^2} U_k \left(\text{or } \frac{1}{m^2} U_k + \frac{\hbar^2 k^2}{4\rho_0}\right) = v_{-k}$

$$[\hat{\rho}_k, \hat{\phi}_{k'}] = \frac{1}{V} \sum_{r,r'} e^{-i\vec{k}\cdot\vec{r}} e^{-i\vec{k}'\cdot\vec{r}'} [\hat{\rho}_1(r), \hat{\phi}(r')]$$

$$= i\hbar \frac{1}{V} \sum_r e^{-i(\vec{k}+\vec{k}')\cdot\vec{r}} = i\hbar\, \delta_{k+k',0}$$

$$\therefore [\hat{\rho}_k, \hat{\phi}_{-k}] = i\hbar\, \delta_{k,k'} \quad \cdots (14)$$

Note that $\because \dot{\rho} + \nabla\cdot(\rho\vec{v}) = 0$

$$\vec{v_k} = \frac{i\dot{\rho}_k}{\rho_0}\frac{\vec{k}}{k^2} \quad \therefore \vec{v_k} \text{ \& } \phi_k \text{ play the}$$

role of $\dot{\rho}_k$.

Hence Eq. (14) is similar to $[\hat{x}_k, \hat{P}_{k'}] = i\hbar\, \delta_{k,k'}$

$\hat{\phi}_k$ is thus called the <u>conjugate momentum</u> to $\rho_k$!

Eq. (13) can be formally put into the same form as that for phonons in crystals.

$$\rho_0 k^2 \equiv \frac{1}{M}, \quad v_k = M\omega_k^2 = \frac{1}{\rho_0 k^2}\omega_k^2$$

$$\therefore \omega_k^2 = \rho_0 k^2 v_k$$

$$\hat{H} = \sum_k \hbar\omega_k (a_k^+ a_k + 1/2) \qquad \omega_k = k\sqrt{\rho_0 v_k}$$

$$\hat{a}_k = \sqrt{\frac{M\omega_k}{2\hbar}}\left(\underset{\updownarrow\, u_k}{\hat{p}_k} + \frac{i\hat{\phi}_k}{M\omega_k}\right) \qquad \hat{\phi}_k \leftrightarrow \hat{p}_k$$

$$= \sqrt{\frac{1}{2\hbar}\sqrt{\frac{v_k}{\rho_0 k^2}}}\left(\hat{p}_k + \frac{i\hat{\phi}_k}{\sqrt{v_k/\rho_0 k^2}}\right)$$

Since $v_0 = \frac{1}{m^2 V}\sum_R V(R) \sim$ const part of $U(R)$

$\therefore$ the speed of sound $c = \sqrt{\rho_0 \cdot V/m^2}$

The above is phonons in liquids, valid for $k \to 0$ (i.e. $\lambda \gg \bar{a}$ = average distance between particles in liquids).

Phonons in liquids do not have umklapp processes but they also suffers anharmonic scattering. By setting $\omega = ck$, one can write $v_k = v_{k=0} = \frac{c^2}{\rho_0}$

then Eq. (11) can be written as

$$\hat{H} = \int E(\rho_0)\, d^3\vec{r} + \int d^3\vec{r}\left(\frac{1}{2}\rho_0 \vec{v}^2 + \frac{c^2}{2\rho_0}\rho_1^2\right).$$

Hence $\frac{c^2}{2\rho_0}\rho_1^2$ is the expansion of $E(\rho)$ in the 2nd order. That is, $\left.\frac{d^2E}{d\rho^2}\right|_{\rho=\rho_0} = \frac{c^2}{\rho_0}$

It's clear that the 3rd order term is then given by $\int \frac{1}{3!}\frac{d}{d\rho_0}\left(\frac{c^2}{\rho_0}\right)\hat{\rho}_1^3\, d^3\vec{r}$

& the 4th order is $\int \frac{1}{4!}\frac{d^2}{d\rho_0^2}\left(\frac{c^2}{\rho_0}\right)\hat{\rho}_1^4\, d^3\vec{r}$.

These terms describe anharmonic scatterings of phonons.

Finally, in the quantum limit, there is also a corresponding fluid equation. This is in terms of the velocity operator $\vec{v}$. Unlike classical fluids, $\hat{v}_\alpha$ doesnot commute with $\hat{v}_\beta$. We shall not go into detailed calculation but just mention that one can use the commutator $[\rho, \vec{v}] = i\hbar \nabla' \delta(x'-x)$ & $\vec{j} = \frac{1}{2}(\rho\vec{v} + \vec{v}\rho)$ to write $\vec{v} = \frac{1}{2}(\rho^{-1}\vec{j} + \vec{j}\rho^{-1})$

From $\vec{v}$ & the commutation between $[\rho, \vec{j}]$,

one finds $[v_\alpha(\vec{r}), v_\beta(\vec{r}\,')] = \frac{\hbar}{i}\delta(\vec{r}-\vec{r}\,')\rho^{-1}(\vec{r})(\nabla\times\vec{v})_{\alpha\beta}(\vec{r})$.

Hence from $\dot{\vec{v}} = \frac{i}{\hbar}[H, \vec{v}]$, one gets

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v}\cdot\nabla)\vec{v} = -\frac{1}{\rho}\nabla P$$

With $P = \rho^2 \frac{d}{d\rho}\left(\frac{E(\rho)}{\rho}\right)$ is the quantum version of pressure!