## Chapter 4

# Linear Response and Sum Rules

## 4.1 Linear Response Theory

In this section, we present basic tools to investigate the excitation spectrum of a many-body system. All results obtained in this section are applicable to both bosons and fermions.

### 4.1.1 *Linear response of density fluctuations*

The excitation spectrum of quasiparticles can be probed through the interaction of a test particle with the system of interest. Let $U(\mathbf{r}, t)$ be a time-dependent external potential that couples to the system at position $\mathbf{r}$. In second-quantized language, the corresponding Hamiltonian is given by

$$\hat{H}_{\mathrm{ext}}(t) = \int d\mathbf{r}\ U(\mathbf{r}, t)\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}), \tag{4.1}$$

where $\hat{\psi}(\mathbf{r})$ is the field operator of the system. Substituting Fourier transforms

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} e^{i\mathbf{kr}}, \tag{4.2}$$

$$U(\mathbf{r}, t) = \sum_{\mathbf{k}} \int \frac{d\omega}{2\pi} U(\mathbf{k}, \omega) e^{i\mathbf{kr}} e^{-i\omega t}, \tag{4.3}$$

into Eq. (4.1) gives

$$\hat{H}_{\mathrm{ext}}(t) = \sum_{\mathbf{k}} \int \frac{d\omega}{2\pi} U(\mathbf{k}, \omega)\hat{\rho}_{-\mathbf{k}} e^{-i\omega t}. \tag{4.4}$$

Here,

$$\hat{\rho}_{\mathbf{k}} \equiv \int d\mathbf{r}\ \hat{n}(\mathbf{r}) e^{-i\mathbf{kr}} = \sum_{\mathbf{p}} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}+\mathbf{k}} = \hat{\rho}^\dagger_{-\mathbf{k}} \tag{4.5}$$

is the Fourier transform of the number-density operator $\hat{n}(\mathbf{r}) \equiv \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$.

Let us consider a situation in which the external potential has a single wave vector $\mathbf{k}$ and single frequency $\omega$. Then,

$$\hat{H}_{\rm ext}(t) = U(\mathbf{k},\omega)\hat{\rho}_{-\mathbf{k}}e^{-i\omega t} + U^*(\mathbf{k},\omega)\hat{\rho}^\dagger_{-\mathbf{k}}e^{i\omega t}. \tag{4.6}$$

The state of the system evolves with time according to the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \left(\hat{H} + \hat{H}_{\rm ext}(t)e^{\epsilon t}\right)|\psi(t)\rangle, \tag{4.7}$$

where $\hat{H}$ is the Hamiltonian of the system and $\epsilon$, an infinitesimal positive number. The factor $e^{\epsilon t}$ is introduced to ensure that the external potential is adiabatically switched off in the remote past. The initial condition is assumed to be

$$|\psi(-\infty)\rangle = |0\rangle, \tag{4.8}$$

where $|0\rangle$ is the ground state of $\hat{H}$.

In linear response theory, we solve Eq. (4.7) up to first order in $U(\mathbf{k},\omega)$. We expand the state vector in terms of a complete set of eigenstates $\{|n\rangle\}$ of $\hat{H}$:

$$|\psi(t)\rangle = \sum_n c_n(t)e^{-\frac{i}{\hbar}E_n t}|n\rangle, \tag{4.9}$$

where

$$\hat{H}|n\rangle = E_n|n\rangle \quad (n = 0, 1, 2, \cdots). \tag{4.10}$$

The initial condition (4.8) is satisfied if the following condition is met:

$$c_n(-\infty) = \delta_{n0}. \tag{4.11}$$

Substituting Eq. (4.9) in Eq. (4.7), we obtain

$$\begin{aligned}\dot{c}_m(t) &= -\frac{i}{\hbar}\sum_n c_n(t)e^{(i\omega_{mn}+\epsilon)t}\langle m|\hat{H}_{\rm ext}(t)|n\rangle \\ &= -\frac{i}{\hbar}\sum_n c_n(t)\Big[U(\mathbf{k},\omega)\langle m|\hat{\rho}_{-\mathbf{k}}|n\rangle e^{i(\omega_{mn}-\omega-i\epsilon)t} \\ &\quad + U^*(\mathbf{k},\omega)\langle m|\hat{\rho}^\dagger_{-\mathbf{k}}|n\rangle e^{i(\omega_{mn}+\omega-i\epsilon)t}\Big],\end{aligned} \tag{4.12}$$

where $\omega_{mn} \equiv (E_m - E_n)/\hbar$ and Eq. (4.6) is substituted in the last equation.

Integrating Eq. (4.12) with respect to $t$ from $-\infty$ to $t$ up to the first order in $U$ gives

$$c_m(t) = \delta_{m0} + (1-\delta_{m0})\left[\frac{U(\mathbf{k},\omega)\langle m|\hat{\rho}_{-\mathbf{k}}|0\rangle}{\hbar(\omega-\omega_{m0}+i\epsilon)}e^{i(\omega_{m0}-\omega-i\epsilon)t} - \frac{U^*(\mathbf{k},\omega)\langle m|\hat{\rho}^\dagger_{-\mathbf{k}}|0\rangle}{\hbar(\omega+\omega_{m0}-i\epsilon)}e^{i(\omega_{m0}+\omega-i\epsilon)t}\right]. \tag{4.13}$$

The change in density due to $\hat{H}_{\rm ext}$ is given as

$$\delta\langle\hat{\rho}_{\mathbf{k}}(t)\rangle \equiv \langle\psi(t)|\hat{\rho}_{\mathbf{k}}|\psi(t)\rangle - \langle 0|\hat{\rho}_{\mathbf{k}}|0\rangle. \tag{4.14}$$

Substituting Eq. (4.9) for $|\psi(t)\rangle$ gives

$$\delta\langle(\hat{\rho}_{\mathbf{k}}(t)\rangle = {\sum_n}' \left(c_n(t)e^{-i\omega_{n0}t}\langle 0|\hat{\rho}_{\mathbf{k}}|n\rangle + c_n^*(t)e^{i\omega_{n0}t}\langle n|\hat{\rho}_{\mathbf{k}}|0\rangle\right), \tag{4.15}$$

where ${\sum_n}'$ denotes the summation over $n$ except $n=0$. Substituting Eq. (4.13) in Eq. (4.15) and simplifying the result using[1]

$$\langle n|\hat{\rho}_{\mathbf{k}}|0\rangle\langle n|\hat{\rho}_{-\mathbf{k}}|0\rangle = \langle 0|\hat{\rho}_{\mathbf{k}}|n\rangle\langle n|\hat{\rho}^\dagger_{-\mathbf{k}}|0\rangle = 0 \tag{4.16}$$

leads to

$$\delta\langle\hat{\rho}_{\mathbf{k}}(t)\rangle = \frac{1}{\hbar}U(\mathbf{k},\omega)e^{-(i\omega-\epsilon)t}{\sum_n}'\left(\frac{|\langle 0|\hat{\rho}_{\mathbf{k}}|n\rangle|^2}{\omega-\omega_{n0}+i\epsilon} - \frac{|\langle n|\hat{\rho}_{\mathbf{k}}|0\rangle|^2}{\omega+\omega_{n0}+i\epsilon}\right). \tag{4.17}$$

We assume that the system possesses the space-inversion symmetry ($\hat{\rho}_{\mathbf{k}} = \hat{\rho}_{-\mathbf{k}}$), so that

$$\langle n|\hat{\rho}_{\mathbf{k}}|0\rangle = \langle n|\hat{\rho}_{-\mathbf{k}}|0\rangle = \langle n|\hat{\rho}^\dagger_{\mathbf{k}}|0\rangle = \langle 0|\hat{\rho}_{\mathbf{k}}|n\rangle^*. \tag{4.18}$$

Then, Eq. (4.17) reduces to

$$\delta\langle\hat{\rho}_{\mathbf{k}}(t)\rangle = \frac{1}{\hbar}U(\mathbf{k},\omega)e^{-(i\omega-\epsilon)t}{\sum_n}'|\langle n|\hat{\rho}^\dagger_{\mathbf{k}}|0\rangle|^2\frac{2\omega_{n0}}{(\omega+i\epsilon)^2-\omega_{n0}^2}. \tag{4.19}$$

Applying the Fourier transform to this equation gives

$$\delta\langle\hat{\rho}(\mathbf{k},\omega)\rangle = U(\mathbf{k},\omega)D^{\rm ret}(\mathbf{k},\omega), \tag{4.20}$$

where

$$D^{\rm ret}(\mathbf{k},\omega) = \frac{1}{\hbar}{\sum_n}'|\langle n|\hat{\rho}^\dagger_{\mathbf{k}}|0\rangle|^2\frac{2\omega_{n0}}{(\omega+i\epsilon)^2-\omega_{n0}^2}. \tag{4.21}$$

Equation (4.20) gives the linear response of density against the external perturbation $U(\mathbf{k},\omega)$, and the ratio

$$\chi_\rho(\mathbf{k},\omega) \equiv \frac{\delta\langle\hat{\rho}(\mathbf{k},\omega)\rangle}{U(\mathbf{k},\omega)} = D^{\rm ret}(\mathbf{k},\omega) \tag{4.22}$$

defines the linear susceptibility of density fluctuations.

[1]Since $\hat{\rho}_{\mathbf{k}} = \sum_{\mathbf{p}}\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}+\mathbf{k}}$ annihilates the net momentum $\mathbf{k}$ from the system, $\langle n|\hat{\rho}_{\mathbf{k}}|0\rangle \neq 0$ only if the total momentum of $|n\rangle$ is $-\mathbf{k}$. Thus, $\langle n|\hat{\rho}_{\mathbf{k}}|0\rangle\langle n|\hat{\rho}_{-\mathbf{k}}|0\rangle = 0$. Similarly, we obtain the second equation using Eq. (4.5).

### 4.1.2 *Retarded response function*

The function $D^{\rm ret}(\mathbf{k},\omega)$ defined in Eq. (4.21) is referred to as the retarded response function or the retarded Green's function of the density. Taking the imaginary part of Eq. (4.21) and using

$$\frac{1}{x+i\epsilon} = P\left(\frac{1}{x}\right) - i\pi\delta(x), \tag{4.23}$$

where $P\left(\frac{1}{x}\right)$ denotes the principal value of $\frac{1}{x}$, we obtain the dynamic structure factor

$$S(\mathbf{k},\omega) \equiv -\frac{\hbar}{\pi}{\rm Im}D^{\rm ret}(\mathbf{k},\omega) = \sum_n{}' |\langle n|\hat{\rho}^\dagger_{\mathbf{k}}|0\rangle|^2[\delta(\omega-\omega_{n0}) - \delta(\omega+\omega_{n0})], \tag{4.24}$$

which gives the excitation spectrum of density, in which the perturbation transfers energy $\hbar\omega$ and momentum $\hbar\mathbf{k}$ to the system.

The inverse Fourier transform of $D^{\rm ret}(\mathbf{k},\omega)$ is given by

$$\begin{aligned} D^{\rm ret}(\mathbf{k},t) &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}D^{\rm ret}(\mathbf{k},\omega)e^{-i\omega t} \\ &= \frac{1}{\hbar}\sum_n{}'|\langle n|\hat{\rho}^\dagger_{\mathbf{k}}|0\rangle|^2\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\left(\frac{1}{\omega+i\epsilon-\omega_{n0}} - \frac{1}{\omega+i\epsilon+\omega_{n0}}\right)e^{-i\omega t}. \end{aligned} \tag{4.25}$$

Because of the factor $e^{-i\omega t}$, the integration contour in Eq. (4.25) must be taken in the lower (or upper) half of the complex $\omega$-plane if $t>0$ (or if $t<0$). Since the poles $\omega = \pm\omega_{n0} - i\epsilon$ lie in the lower-half plane, the integral is nonzero only for $t>0$. Hence,

$$D^{\rm ret}(\mathbf{k},t) = -\frac{i}{\hbar}\theta(t)\sum_n{}'|\langle n|\hat{\rho}^\dagger_{\mathbf{k}}|0\rangle|^2\left(e^{-i\omega_{n0}t} - e^{i\omega_{n0}t}\right), \tag{4.26}$$

where $\theta(t)$ is the unit step function. Comparing this with Eq. (4.24), we find that

$$D^{\rm ret}(\mathbf{k},t) = -\frac{i}{\hbar}\theta(t)\int_{-\infty}^{\infty}d\omega S(\mathbf{k},\omega)e^{-i\omega t}. \tag{4.27}$$

Applying the Fourier transform to this equation with respect to time gives

$$D^{\rm ret}(\mathbf{k},\omega) = \frac{1}{\hbar}\int_{-\infty}^{\infty}\frac{S(\mathbf{k},\omega')}{\omega+i\epsilon-\omega'}d\omega'. \tag{4.28}$$

We may use Eq. (4.18) and the completeness relation to eliminate the sum over $n$ in Eq. (4.26); in fact,

$$\begin{aligned}
{\sum_n}' |\langle n|\hat{\rho}_{\mathbf{k}}^\dagger|0\rangle|^2 e^{-i\omega_{n0}t} &= \sum_n \langle 0|e^{\frac{i}{\hbar}\hat{H}t}\hat{\rho}_{\mathbf{k}}e^{-\frac{i}{\hbar}\hat{H}t}|n\rangle\langle n|\hat{\rho}_{\mathbf{k}}^\dagger|0\rangle = \langle 0|\hat{\rho}_{\mathbf{k}}(t)\hat{\rho}_{\mathbf{k}}^\dagger|0\rangle, \\
{\sum_n}' |\langle n|\hat{\rho}_{\mathbf{k}}^\dagger|0\rangle|^2 e^{i\omega_{n0}t} &= \sum_n |\langle n|\hat{\rho}_{\mathbf{k}}|0\rangle|^2 e^{i\omega_{n0}t} \\
&= \sum_n \langle 0|\hat{\rho}_{\mathbf{k}}^\dagger|n\rangle\langle n|e^{\frac{i}{\hbar}\hat{H}t}\hat{\rho}_{\mathbf{k}}e^{-\frac{i}{\hbar}\hat{H}t}|0\rangle = \langle 0|\hat{\rho}_{\mathbf{k}}^\dagger\hat{\rho}_{\mathbf{k}}(t)|0\rangle,
\end{aligned}$$

where ${\sum_n}'$ is replaced by $\sum_n$ because $\langle 0|\hat{\rho}_{\mathbf{k}}^\dagger|0\rangle = 0$. We thus find that

$$D^{\mathrm{ret}}(\mathbf{k},t) = -\frac{i}{\hbar}\theta(t)\left\langle 0\right|\left[\hat{\rho}_{\mathbf{k}}(t),\hat{\rho}_{\mathbf{k}}^\dagger(0)\right]\left|0\right\rangle, \tag{4.29}$$

where

$$\hat{\rho}_{\mathbf{k}}(t) \equiv e^{\frac{i}{\hbar}\hat{H}t}\hat{\rho}_{\mathbf{k}}e^{-\frac{i}{\hbar}\hat{H}t}. \tag{4.30}$$

In a special case in which $S(\mathbf{k},\omega)$ has a single peak of the form

$$S(\mathbf{k},\omega) = S(\mathbf{k})\delta(\omega-\omega_{\mathbf{k}}), \tag{4.31}$$

we obtain

$$D^{\mathrm{ret}}(\mathbf{k},t) = -\frac{i}{\hbar}\theta(t)S(\mathbf{k})e^{-i\omega_{\mathbf{k}}t} \tag{4.32}$$

from Eq. (4.27) and Eq. (4.28). Applying the Fourier transform to this equation with respect to time gives

$$D^{\mathrm{ret}}(\mathbf{k},\omega) = \frac{S(\mathbf{k})}{\hbar(\omega-\omega_{\mathbf{k}}+i\epsilon)}. \tag{4.33}$$

Equation (4.33) implies that the pole of the retarded Green's function of the density gives the frequency of the collective mode.

## 4.2 Sum Rules

When the system is translationally invariant in space, the excitation spectrum satisfies some exact relations known as sum rules.

### 4.2.1 *Longitudinal f-sum rule*

When the system possesses space-translation invariance, the single-particle Hamiltonian can be diagonalized with respect to the wave vector $\mathbf{k}$:

$$\hat{H}_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}}, \quad \epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}. \tag{4.34}$$

The interaction Hamiltonian is expressed in the second-quantized form as

$$\hat{V} = \frac{1}{2}\int d\mathbf{r} \int d\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}). \tag{4.35}$$

Substituting Eq. (4.2) and

$$V(\mathbf{r}) = \sum_{\mathbf{k}} V_{\mathbf{k}} e^{i\mathbf{kr}} \tag{4.36}$$

into Eq. (4.30), we obtain

$$\hat{V} = \frac{1}{2}\sum_{\mathbf{p},\mathbf{q},\mathbf{k}} V_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{p}} \hat{a}^\dagger_{\mathbf{q}} \hat{a}_{\mathbf{q}+\mathbf{k}} \hat{a}_{\mathbf{p}-\mathbf{k}} = \frac{1}{2}\sum_{\mathbf{k}} V_{\mathbf{k}} \left(\hat{\rho}_{-\mathbf{k}}\hat{\rho}_{\mathbf{k}} - \hat{N}\right), \tag{4.37}$$

where $\hat{\rho}_{\mathbf{k}}$ is given in Eq. (4.5) and

$$\hat{N} = \sum_{\mathbf{p}} \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}} \tag{4.38}$$

is the total number operator. The total Hamiltonian is given by

$$\hat{H} = \hat{H}_0 + \hat{V}. \tag{4.39}$$

A straightforward calculation gives

$$\left[\hat{\rho}_{-\mathbf{k}}, \left[\hat{\rho}_{\mathbf{k}}, \hat{H}\right]\right] = -\sum_{\mathbf{p}} (\epsilon_{\mathbf{p}+\mathbf{k}} + \epsilon_{\mathbf{p}-\mathbf{k}} - 2\epsilon_{\mathbf{p}}) \hat{a}^\dagger_{\mathbf{p}} \hat{a}_{\mathbf{p}}. \tag{4.40}$$

Since $\epsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$,

$$\epsilon_{\mathbf{p}+\mathbf{k}} + \epsilon_{\mathbf{p}-\mathbf{k}} - 2\epsilon_{\mathbf{p}} = \frac{\hbar^2\mathbf{k}^2}{m} = 2\epsilon_{\mathbf{k}},$$

and thus,

$$\left[\hat{\rho}_{-\mathbf{k}}, [\hat{\rho}_{\mathbf{k}}, \hat{H}]\right] = -2\epsilon_{\mathbf{k}}\hat{N}. \tag{4.41}$$

Taking the expectation value of the left-hand side of Eq. (4.41) over $|0\rangle$ and inserting the completeness relation, we have

$$\left\langle 0 \right| \left[\hat{\rho}_{-\mathbf{k}}, \left[\hat{\rho}_{\mathbf{k}}, \hat{H}\right]\right] \left| 0 \right\rangle = -\sum_n \hbar\omega_{n0} \left(|\langle n|\hat{\rho}_{\mathbf{k}}|0\rangle|^2 + |\langle n|\hat{\rho}_{-\mathbf{k}}|0\rangle|^2\right), \tag{4.42}$$

where $\hbar\omega_{n0} = E_n - E_0$. Substituting Eq. (4.41) in Eq. (4.42), we obtain

$$\sum_n \hbar\omega_{n0} \left(|\langle n|\hat{\rho}_{\mathbf{k}}|0\rangle|^2 + |\langle n|\hat{\rho}_{-\mathbf{k}}|0\rangle|^2\right) = 2\epsilon_{\mathbf{k}} N. \tag{4.43}$$

Equation (4.43) is referred to as the longitudinal $f$-sum rule. When the system possesses space-inversion symmetry, the relation $|\langle n|\hat{\rho}_{-\mathbf{k}}|0\rangle| = |\langle n|\hat{\rho}_{\mathbf{k}}|0\rangle|$ holds, and thus Eq. (4.43) reduces to

$$\sum_n f_{n0} = N, \tag{4.44}$$

where

$$f_{n0} \equiv \frac{\hbar\omega_{n0}}{\epsilon_{\mathbf{k}}} |\langle n|\hat{\rho}_{\mathbf{k}}|0\rangle|^2 \tag{4.45}$$

is called the oscillator strength. As Eq. (4.44) suggests, the $f$-sum rule reflects the conservation of the particle number. Equation (4.44) may be regarded as a generalization of the Thomas–Reiche–Kuhn sum rule: for a single particle,

$$\sum_n (E_0 - E_n)|\langle n|\hat{x}|0\rangle|^2 = \frac{\hbar^2}{2M}, \tag{4.46}$$

where $\hat{H}|n\rangle = E_n|n\rangle$.

In terms of the dynamic structure factor $S(\mathbf{k}, \omega)$ in Eq. (4.24), the longitudinal $f$-sum rule is expressed as

$$\int_0^\infty d\omega \hbar\omega S(\mathbf{k}, \omega) = \epsilon_{\mathbf{k}} N. \tag{4.47}$$

For the special case of $S(\mathbf{k}, \omega) = NS(\mathbf{k})\delta(\omega - \omega_{\mathbf{k}})$, Eq. (4.47) gives the energy of an elementary excitation as [Bijl (1940); Feynman (1954)]

$$\hbar\omega_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2mS(\mathbf{k})}, \tag{4.48}$$

where the static structure factor $S(\mathbf{k})$ determines the dispersion relation, *i.e.*, the relation between $\omega_{\mathbf{k}}$ and $\mathbf{k}$.

An extension to finite temperature is straightforward. Multiplying both sides of Eq. (4.41) by

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{Z}, \tag{4.49}$$

where $Z = \mathrm{Tr}\, e^{-\beta\hat{H}}$, we obtain Eq. (4.47) with

$$S(\mathbf{k}, \omega) = \frac{1}{Z} \sum_{m,n} e^{-\beta E_m} (|\langle m|\hat{\rho}_{\mathbf{k}}^\dagger|n\rangle|^2 + |\langle m|\hat{\rho}_{\mathbf{k}}|n\rangle|^2)\delta(\omega - \omega_{nm}), \tag{4.50}$$

where $\omega_{nm} \equiv (E_n - E_m)/\hbar$. In the presense of space-inversion symmetry, Eq. (4.50) reduces to

$$S(\mathbf{k},\omega) = \frac{2}{Z}\sum_{m,n} e^{-\beta E_m} |\langle m|\hat{\rho}_{\mathbf{k}}|n\rangle|^2 \delta(\omega - \omega_{nm}). \tag{4.51}$$

Under the same assumption, we obtain the detailed balance of the dynamic structure factor:

$$S(\mathbf{k},-\omega) = e^{-\beta\hbar\omega} S(\mathbf{k},\omega). \tag{4.52}$$

### 4.2.2 *Compressibility sum rule*

The compressibility $\kappa$ measures the degree of volume reduction against an increase in pressure at a fixed number of particles.

$$\kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_N. \tag{4.53}$$

The pressure $P$ is defined as the derivative of energy with respect to volume,

$$P = -\left(\frac{\partial E}{\partial V}\right)_N. \tag{4.54}$$

Substituting this in Eq. (4.53) gives

$$\kappa^{-1} = V\left(\frac{\partial^2 E}{\partial V^2}\right)_N. \tag{4.55}$$

Noting that $V$ is related to the particle density $n$ through $V = N/n$, we have

$$\frac{\partial}{\partial V} = \frac{\partial n}{\partial V}\frac{\partial}{\partial n} = -\frac{n^2}{N}\frac{\partial}{\partial n}. \tag{4.56}$$

Substituting $E = N\epsilon_g$, where $\epsilon_g$ is the ground-state energy per particle, we obtain

$$\kappa^{-1} = n\frac{d}{dn}\left(n^2\frac{d\epsilon_g}{dn}\right) = n^2\frac{d^2}{dn^2}(n\epsilon_g). \tag{4.57}$$

On the other hand, the chemical potential $\mu$ is given by

$$\mu = \left(\frac{\partial E}{\partial N}\right)_V = \left(\frac{\partial(E/V)}{\partial(N/V)}\right)_V = \frac{d}{dn}(n\epsilon_g). \tag{4.58}$$

Comparing Eqs. (4.57) and (4.58), we obtain

$$\kappa^{-1} = n^2\frac{d\mu}{dn}. \tag{4.59}$$

A microscopic expression of the compressibility can be found from Eqs. (4.22) and (4.28):

$$\frac{\delta\langle\hat{\rho}(\mathbf{k},\omega)\rangle}{U(\mathbf{k},\omega)} = D^{\rm ret}(\mathbf{k},\omega) = \frac{1}{\hbar}\int_{-\infty}^{\infty}\frac{S(\mathbf{k},\omega')}{\omega+i\epsilon-\omega'}d\omega'. \tag{4.60}$$

Suppose that we first take the limit $\mathbf{k}\to\mathbf{0}$ and then take the limit $\omega\to 0$. Then, the denominator on the left-hand side of Eq. (4.60) provides a uniform scalar potential $U(\mathbf{k}=0,\omega=0)$ which may be interpreted as a minus shift in the chemical potential. On the other hand, the numerator gives the concomitant change in the number of particles. Thus, we obtain

$$-\left(\frac{\partial N}{\partial\mu}\right)_V = \lim_{\omega\to 0}\lim_{\mathbf{k}\to 0} D^{\rm ret}(\mathbf{k},\omega) = -\frac{1}{\hbar}\int_{-\infty}^{\infty}\frac{S(\mathbf{k}=\mathbf{0},\omega)}{\omega}d\omega. \tag{4.61}$$

It follows from Eqs. (4.59) and (4.61) that

$$\int_{-\infty}^{\infty}\frac{S(\mathbf{k}=\mathbf{0},\omega)}{\hbar\omega}d\omega = \kappa n^2 V. \tag{4.62}$$

This relation is known as the compressibility sum rule.

The compressibility gives the isothermal and adiabatic sound velocity $c$. In fact, defining the mass density as $\rho\equiv mn$ , we have

$$c = \sqrt{\frac{\partial P}{\partial\rho}} = \sqrt{\frac{1}{m}\frac{dP}{dn}}. \tag{4.63}$$

Since

$$P = -\left(\frac{\partial E}{\partial V}\right)_N = n^2\frac{d\epsilon_g}{dn}, \tag{4.64}$$

from Eq. (4.57), we find that

$$\frac{dP}{dn} = \frac{d}{dn}\left(n^2\frac{d\epsilon_g}{dn}\right) = \frac{1}{n\kappa}. \tag{4.65}$$

Thus,

$$c = \frac{1}{\sqrt{mn\kappa}}. \tag{4.66}$$

We may use this relation to obtain another expression for the compressibility sum rule.

$$\int_{-\infty}^{\infty}\frac{S(\mathbf{k}=\mathbf{0},\omega)}{\hbar\omega}d\omega = \frac{N}{mc^2}. \tag{4.67}$$

The combination of the *f*-sum rule and the compressibility sum rule gives an upper bound for the static structure factor. The Schwartz inequality gives

$$S(\mathbf{k}) \equiv \int_{-\infty}^{\infty} S(\mathbf{k},\omega)d\omega \leq \sqrt{\int_{-\infty}^{\infty} \hbar\omega S(\mathbf{k},\omega)d\omega \int_{-\infty}^{\infty} \frac{S(\mathbf{k},\omega)}{\hbar\omega}d\omega}. \quad (4.68)$$

Substituting Eq. (4.47), we have (note that the range of integration is doubled here)

$$S(\mathbf{k}) \leq \sqrt{2\epsilon_k N \int_{-\infty}^{\infty} \frac{S(\mathbf{k},\omega)}{\hbar\omega}d\omega}. \quad (4.69)$$

Taking the limit of $k \to 0$ and using Eq. (4.67), we obtain

$$S(\mathbf{k}) \leq \frac{\hbar k}{mc}N \quad (k \to 0). \quad (4.70)$$

This inequality implies that the density fluctuations of the system with a finite compressibility become negligible in the long-wavelength limit.

### 4.2.3 *Zero energy gap theorem*

The zero energy gap theorem holds for translationally invariant systems with positive compressibility.

*Theorem.* If a system is translationally invariant in space, the excitation spectrum has zero energy gap in the long-wavelength limit as long as the compressibility is positive.

*Proof.* Let us assume that the excitation spectrum has an energy gap $\Delta$ in the limit $\mathbf{k} \to 0$. Then, $S(\mathbf{k}=0,\omega)=0$ for $\hbar\omega < \Delta$, and therefore, the compressibility sum rule (4.62) gives

$$\frac{1}{2}\kappa n^2 V = \int_{\Delta/\hbar}^{\infty} \frac{S(\mathbf{k}=\mathbf{0},\omega)}{\hbar\omega}d\omega \leq \frac{1}{\Delta}\int_{\Delta/\hbar}^{\infty} S(\mathbf{k}=\mathbf{0},\omega)d\omega. \quad (4.71)$$

On the other hand, the $f$-sum rule (4.47) leads to

$$\frac{\hbar^2\mathbf{k}^2}{2m}N = \int_{\Delta/\hbar}^{\infty} d\omega\ \hbar\omega\ S(\mathbf{k},\omega) \geq \Delta \int_{\Delta/\hbar}^{\infty} S(\mathbf{k},\omega)d\omega. \quad (4.72)$$

Combining Eq. (4.71) and Eq. (4.72), we find

$$\lim_{\mathbf{k}\to 0} \frac{\hbar^2\mathbf{k}^2}{2m}N \geq \frac{\Delta^2}{2}\kappa n^2 V. \quad (4.73)$$

This inequality implies that as long as $\kappa > 0$, $\Delta$ must vanish in the long-wavelength limit.

As a special application of this theorem, we find that a spatially uniform Bose system with repulsive interaction is gapless in the long-wavelength limit.

### 4.2.4 *Josephson sum rule*

The condensate density is defined in terms of the eigenfunction of the single-particle density matrix corresponding to a macroscopic (*i.e.*, extensive) eigenvalue and it is a thermodynamic quantity. The superfluid density, on the other hand, is defined in terms of linear response theory and it is a transport quantity. These two quantities therefore belong to different notions despite their apparent similarity. However, Josephson reported an interesting relation between them that is referred to as the Josephson sum rule [Josephson (1966)].

We consider a situation in which a superfluid is flowing with velocity $\mathbf{v}_\mathrm{s}$ through a long container that is at rest with respect to the laboratory frame. Then, the mass current density operator $\hat{\mathbf{j}}$ is given by

$$\hat{\mathbf{j}}(\mathbf{r}) = \frac{1}{2i}\left[\hat{\psi}^\dagger(\mathbf{r})\nabla\hat{\psi}(\mathbf{r}) - (\nabla\hat{\psi}^\dagger(\mathbf{r}))\hat{\psi}(\mathbf{r})\right]. \tag{4.74}$$

The quantum-statistical average of $\hat{\mathbf{j}}$ defines the superfluid mass density $\rho_\mathrm{s}$ through the relation

$$\langle\hat{\mathbf{j}}\rangle = \rho_\mathrm{s}\mathbf{v}_\mathrm{s}. \tag{4.75}$$

The condensate density $|\psi_0|^2$ is defined in terms of the eigenfunction $\psi_0$ corresponding to a macroscopic eigenvalue of the single-particle density matrix. Because $\psi_0$ is complex, we may decompose it into the amplitude and the phase

$$\psi_0(\mathbf{r}) = A(\mathbf{r})e^{i\phi(\mathbf{r})}. \tag{4.76}$$

When the amplitude $A$ may be considered as a constant, a variation in the wave function is related to a change in the phase through

$$\delta\psi_0 = i\psi_0\delta\phi. \tag{4.77}$$

Since the spatial variation in $\phi$ is related to the superfluid velocity $\mathbf{v}_\mathrm{s}$ through

$$\mathbf{v}_\mathrm{s} = \frac{\hbar}{m}\nabla\phi, \tag{4.78}$$

one may expect to find a relationship between $\rho_\mathrm{s}$ and $|\psi_0|^2$ by examining the responses $\langle\mathbf{j}\rangle$ and $\psi_0$ to a common external perturbation.

A variation in $\psi_0$ is caused by a Hamiltonian that includes a term conjugate to $\hat{\psi}$. Here, we consider the response of the system to the following Hamiltonian:

$$\hat{H}_\mathrm{ext}(t) = \int d\mathbf{r}\left(\xi(\mathbf{k},\omega)e^{i(\mathbf{kr}-\omega t)}\hat{\psi}^\dagger(\mathbf{r}) + \xi^*(\mathbf{k},\omega)e^{-i(\mathbf{kr}-\omega t)}\hat{\psi}(\mathbf{r})\right). \tag{4.79}$$

The state evolution due to $\hat{H}_{\rm ext}(t)$ can be found by following a procedure similar to the one in Sec. 4.1.1. We expand the state vector in tems of the eigenstates $\{|n\rangle\}$ of $\hat{H}$ as in Eq. (4.9), where the expansion coefficients can be calculated up to the first order in $\hat{H}_{\rm ext}$ as

$$c_n(t) = \delta_{n0} + (1-\delta_{n0})\int d\mathbf{r}\left[\frac{\xi(\mathbf{k},\omega)\langle n|\hat{\psi}^\dagger(\mathbf{r})|0\rangle}{\hbar(\omega-\omega_{n0}+i\epsilon)}e^{i\mathbf{kr}}e^{i(\omega_{n0}-\omega-i\epsilon)t}\right.$$
$$\left.-\frac{\xi^*(\mathbf{k},\omega)\langle n|\hat{\psi}(\mathbf{r})|0\rangle}{\hbar(\omega+\omega_{n0}-i\epsilon)}e^{-i\mathbf{kr}}e^{i(\omega_{n0}+\omega-i\epsilon)t}\right]. \tag{4.80}$$

The response of $\hat{\psi}$ is given by

$$\begin{aligned}\delta\langle\hat{\psi}(\mathbf{r},t)\rangle &\equiv \langle\psi(t)|\hat{\psi}(\mathbf{r})|\psi(t)\rangle - \langle 0|\hat{\psi}(\mathbf{r})|0\rangle \\ &= {\sum_n}' \left(c_n(t)e^{-i\omega_{n0}t}\langle 0|\hat{\psi}(\mathbf{r})|n\rangle + c_n^*(t)e^{i\omega_{n0}t}\langle n|\hat{\psi}(\mathbf{r})|0\rangle\right).\end{aligned} \tag{4.81}$$

We assume that each state $|n\rangle$ has a fixed number of particles, so that

$$\langle 0|\hat{\psi}(\mathbf{r})|n\rangle\langle n|\hat{\psi}(\mathbf{r}')|0\rangle = \langle n|\hat{\psi}(\mathbf{r})|0\rangle\langle n|\hat{\psi}^\dagger(\mathbf{r}')|0\rangle = 0. \tag{4.82}$$

Substituting $c_n(t)$ in Eq. (4.80) into Eq. (4.81) and using Eq. (4.82), we obtain

$$\begin{aligned}\delta\langle\hat{\psi}(\mathbf{r},t)\rangle &= \frac{1}{\hbar}\xi(\mathbf{k},\omega)e^{-i\omega t+\epsilon t}{\sum_n}'\int d\mathbf{r}'\left(\frac{\langle 0|\hat{\psi}(\mathbf{r})|n\rangle\langle n|\hat{\psi}^\dagger(\mathbf{r}')|0\rangle}{\omega-\omega_{n0}+i\epsilon}\right. \\ &\quad \left.-\frac{\langle n|\hat{\psi}(\mathbf{r}')|0\rangle^*\langle n|\hat{\psi}(\mathbf{r})|0\rangle}{\omega+\omega_{n0}+i\epsilon}\right)e^{i\mathbf{kr}'} \\ &= -\frac{i}{\hbar}\xi(\mathbf{k},\omega)e^{-i\omega t+\epsilon t}{\sum_n}'\int d\mathbf{r}'\int_0^\infty dt'\left(\langle 0|\hat{\psi}(\mathbf{r},t')|n\rangle\langle n|\hat{\psi}^\dagger(\mathbf{r}',0)|0\rangle\right. \\ &\quad \left.-\langle 0|\hat{\psi}^\dagger(\mathbf{r}',0)|n\rangle\langle n|\hat{\psi}(\mathbf{r},t)|0\rangle\right)e^{i(\omega+i\epsilon)t'}e^{i\mathbf{kr}'},\end{aligned} \tag{4.83}$$

where

$$\hat{\psi}(\mathbf{r},t) \equiv e^{\frac{i}{\hbar}\hat{H}t}\hat{\psi}(\mathbf{r})e^{-\frac{i}{\hbar}\hat{H}t}. \tag{4.84}$$

Since $\langle 0|\hat{\psi}(\mathbf{r},t)|0\rangle = 0$, we may replace the restricted sum ${\sum_n}'$ in Eq. (4.83) with the unrestricted one $\sum_n$. Then, it follows from the completeness relation

$$\sum_n |n\rangle\langle n| = \hat{1} \tag{4.85}$$

that Eq. (4.83) reduces to

$$\delta\langle\hat{\psi}(\mathbf{r},t)\rangle = \xi(\mathbf{k},\omega)e^{-i\omega t+\epsilon t}\int d\mathbf{r}'\int_0^\infty dt' G^{\text{ret}}(\mathbf{r},t';\mathbf{r}',0)e^{i\mathbf{k}\mathbf{r}'}e^{i(\omega+i\epsilon)t'}, \quad (4.86)$$

where we introduced the single-particle retarded Green's function

$$G^{\text{ret}}(\mathbf{r},t;\mathbf{r}',t') \equiv -\frac{i}{\hbar}\theta(t-t')\Big\langle 0\Big|\left[\hat{\psi}(\mathbf{r},t),\hat{\psi}^\dagger(\mathbf{r}',t')\right]\Big|0\Big\rangle. \quad (4.87)$$

For convenience in later discussions, let us introduce the spectral density function $A(\mathbf{k},\omega)$:

$$A(\mathbf{k},\omega) \equiv i\hbar\int d(\mathbf{r}-\mathbf{r}')e^{-i\mathbf{k}(\mathbf{r}-\mathbf{r}')}\int_{-\infty}^{\infty} d(t-t')e^{i\omega(t-t')}G^{\text{ret}}(\mathbf{r},t;\mathbf{r}',t'), \quad (4.88)$$

$$G^{\text{ret}}(\mathbf{r},t;\mathbf{r}',t') = -\frac{i}{\hbar}\int\frac{d\mathbf{k}}{(2\pi)^3}e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega(t-t')}A(\mathbf{k},\omega), \quad (4.89)$$

where $A(\mathbf{k},\omega)$ satisfies

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A(\mathbf{k},\omega) = 1. \quad (4.90)$$

Substituting Eq. (4.89) in Eq. (4.86) gives

$$\delta\langle\hat{\psi}(\mathbf{r},t)\rangle = \frac{1}{\hbar}\xi(\mathbf{k},\omega)e^{i(\mathbf{k}\mathbf{r}-\omega t)+\epsilon t}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A(\mathbf{k},\omega')}{\omega+i\epsilon-\omega'}. \quad (4.91)$$

Taking the limit of $\omega\to 0$ and $\epsilon\to 0$, we obtain

$$\delta\langle\hat{\psi}(\mathbf{r})\rangle = -\frac{1}{\hbar}\xi(\mathbf{k},0)e^{i\mathbf{k}\mathbf{r}}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{A(\mathbf{k},\omega)}{\omega}. \quad (4.92)$$

In a similar manner, the response of the mass current density is given by

$$\delta\langle\hat{\mathbf{j}}(\mathbf{r},t)\rangle = -\frac{i}{\hbar}\xi(\mathbf{k},\omega)e^{-i\omega t+\epsilon t}\int d\mathbf{r}'\int_0^\infty dt' \times\Big\langle 0\Big|\left[\hat{\mathbf{j}}(\mathbf{r},t'),\hat{\psi}^\dagger(\mathbf{r}',0)\right]\Big|0\Big\rangle e^{i\mathbf{k}\mathbf{r}'}e^{i(\omega+i\epsilon)t'}. \quad (4.93)$$

We introduce another spectral density function $B(\mathbf{k},\omega)$ of the correlation function

$$\Big\langle 0\Big|\left[\hat{\mathbf{j}}(\mathbf{r},t'),\hat{\psi}^\dagger(\mathbf{r},0)\right]\Big|0\Big\rangle = \int\frac{d\mathbf{k}'}{(2\pi)^3}\int\frac{d\omega'}{2\pi}B(\mathbf{k}',\omega')e^{i\mathbf{k}'(\mathbf{r}-\mathbf{r}')-i\omega't'}, \quad (4.94)$$

$$B(\mathbf{k},\omega) = \int d\mathbf{r}\int dt\Big\langle\left[\hat{\mathbf{j}}(\mathbf{r},t),\hat{\psi}^\dagger(\mathbf{r}',t')\right]\Big\rangle e^{-i\mathbf{k}(\mathbf{r}-\mathbf{r}')+i\omega(t-t')}. \quad (4.95)$$

Substituting this in Eq. (4.93) gives

$$\delta\langle\hat{\mathbf{j}}(\mathbf{r},t)\rangle = \frac{1}{\hbar}\xi(\mathbf{k},\omega)e^{i(\mathbf{kr}-\omega t)+\epsilon t}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{B(\mathbf{k},\omega')}{\omega+i\epsilon-\omega'}. \tag{4.96}$$

Taking the limit of $\omega \to 0$ and $\epsilon \to 0$, we obtain

$$\delta\langle\hat{\mathbf{j}}(\mathbf{r})\rangle = -\frac{1}{\hbar}\xi(\mathbf{k},0)e^{i\mathbf{kr}}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{B(\mathbf{k},\omega)}{\omega}. \tag{4.97}$$

The right-hand side is proportional to $\delta\langle\hat{\psi}(\mathbf{r})\rangle$, since the Fourier transformation of the continuity equation

$$\nabla\hat{\mathbf{j}}(\mathbf{r},t) + m\frac{\partial\hat{\rho}(\mathbf{r},t)}{\partial t} = 0 \tag{4.98}$$

gives

$$i\mathbf{k}\cdot\hat{\mathbf{j}}(\mathbf{k},t) + m\frac{\partial\hat{\rho}(\mathbf{k},t)}{\partial t} = 0. \tag{4.99}$$

Assuming that $\hat{\mathbf{j}}(\mathbf{k},t)$ is proportional to $\mathbf{k}$, we obtain

$$\hat{\mathbf{j}}(\mathbf{k},t) = \frac{im\mathbf{k}}{\hbar^2}\frac{\partial\hat{\rho}(\mathbf{k},t)}{\partial t}. \tag{4.100}$$

Hence,

$$\begin{aligned}\hat{\mathbf{j}}(\mathbf{r},t) &= \int\frac{d\mathbf{k}}{(2\pi)^3}e^{i\mathbf{kr}}\frac{im\mathbf{k}}{k^2}\frac{\partial\hat{\rho}(\mathbf{k},t)}{\partial t}\\ &= im\frac{\partial}{\partial t}\int d\mathbf{r}'\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{\mathbf{k}}{k^2}e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')}\hat{\rho}(\mathbf{r}',t).\end{aligned} \tag{4.101}$$

Substituting Eq. (4.101) in Eq. (4.95), we have

$$\begin{aligned}B(\mathbf{k},\omega) &= im\int d\mathbf{r}\int dt\ e^{-i\mathbf{k}(\mathbf{r}-\mathbf{r}')+i\omega(t-t')}\frac{\partial}{\partial t}\int d\mathbf{r}''\\ &\quad\times\int\frac{d\mathbf{k}'}{(2\pi)^3}\frac{\mathbf{k}'}{k'^2}e^{i\mathbf{k}'(\mathbf{r}-\mathbf{r}'')}\left\langle\left[\hat{\rho}(\mathbf{r}'',t),\hat{\psi}^\dagger(\mathbf{r}',t')\right]\right\rangle\\ &= \frac{m\omega\mathbf{k}}{k^2}\int dt\ e^{i\omega(t-t')}\int d\mathbf{r}''e^{-i\mathbf{k}(\mathbf{r}''-\mathbf{r}')}\left\langle\left[\hat{\rho}(\mathbf{r}'',t),\hat{\psi}^\dagger(\mathbf{r}',t')\right]\right\rangle.\end{aligned} \tag{4.102}$$

Substituting this in Eq. (4.97), we obtain

$$\delta\langle\hat{\mathbf{j}}(\mathbf{r})\rangle = -\frac{m\mathbf{k}}{\hbar k^2}\xi(\mathbf{k},0)e^{i\mathbf{kr}}\int d\mathbf{r}\ e^{-i\mathbf{k}(\mathbf{r}-\mathbf{r}')}\left\langle\left[\hat{\rho}(\mathbf{r},t),\hat{\psi}^\dagger(\mathbf{r}',t)\right]\right\rangle. \tag{4.103}$$

Using

$$\begin{aligned}\left\langle\left[\hat{\rho}(\mathbf{r},t),\hat{\psi}^\dagger(\mathbf{r}',t)\right]\right\rangle &= \left\langle\left[\hat{\rho}(\mathbf{r}),\hat{\psi}^\dagger(\mathbf{r}')\right]\right\rangle = \left\langle\hat{\psi}^\dagger(\mathbf{r})\left[\hat{\psi}(\mathbf{r}),\hat{\psi}^\dagger(\mathbf{r}')\right]\right\rangle\\ &= \langle\hat{\psi}^\dagger(\mathbf{r})\rangle\delta(\mathbf{r}-\mathbf{r}'),\end{aligned} \tag{4.104}$$

we obtain

$$\delta\langle\hat{\mathbf{j}}(\mathbf{r})\rangle = -\frac{m\mathbf{k}}{\hbar k^2}\xi(\mathbf{k},0)e^{i\mathbf{kr}}\langle\hat{\psi}^\dagger(\mathbf{r})\rangle. \tag{4.105}$$

Comparing Eqs. (4.92) and (4.105), we find that the desired relation between $\delta\langle\hat{\mathbf{j}}\rangle$ and $\delta\langle\hat{\psi}\rangle$ is given by

$$\delta\langle\hat{\mathbf{j}}(\mathbf{r})\rangle = m\frac{\mathbf{k}}{k^2}\left[\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{A(\mathbf{k},\omega)}{\omega}\right]^{-1}\langle\hat{\psi}^\dagger(\mathbf{r})\rangle\delta\langle\hat{\psi}(\mathbf{r})\rangle, \tag{4.106}$$

where we substitute $\psi_0(\mathbf{r}) = \langle\hat{\psi}(\mathbf{r})\rangle$ and use Eq. (4.77) to obtain

$$\delta\langle\hat{\psi}(\mathbf{r})\rangle = \delta\psi_0(\mathbf{r}) = i\psi_0(\mathbf{r})\delta\phi(\mathbf{r}). \tag{4.107}$$

Then, Eq. (4.106) may be rewritten as

$$\begin{aligned}\delta\langle\hat{\mathbf{j}}(\mathbf{r})\rangle &= im\frac{\mathbf{k}}{k^2}\left[\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{A(\mathbf{k},\omega)}{\omega}\right]^{-1}|\psi_0(\mathbf{r})|^2\delta\phi(\mathbf{r}).\\ &= \frac{m}{k^2}\left[\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{A(\mathbf{k},\omega)}{\omega}\right]^{-1}|\psi_0(\mathbf{r})|^2\nabla\delta\phi(\mathbf{r}),\end{aligned} \tag{4.108}$$

since $\delta\phi \propto e^{i\mathbf{kr}}$. From Eqs. (4.75) and (4.78), on the other hand, we have

$$\delta\langle\mathbf{j}(\mathbf{r})\rangle = \frac{\hbar}{m}\rho_{\rm s}\nabla\delta\phi(\mathbf{r}). \tag{4.109}$$

Equating Eqs. (4.108) and (4.109), we finally obtain the relation among the superfluid density $\rho_{\rm s}$, condensate density $|\psi_0|^2$, and spectral density function $A(\mathbf{k},\omega)$ as

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{A(\mathbf{k},\omega)}{\omega} = \frac{m^2|\psi_0|^2}{\hbar k^2\rho_s}. \tag{4.110}$$

This relation may be interpreted as a sum rule obeyed by the single-particle spectral density function $A(\mathbf{k},\omega)$, and is referred to as the Josephson sum rule.

Another sum rule obeyed by $A(\mathbf{k},\omega)$ is

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A(\mathbf{k},\omega) = 1, \tag{4.111}$$

which can be shown directly from Eq. (4.88).

## 4.3 Sum-Rule Approach to Collective Modes

We investigate the collective mode of a system described by Hamiltonian $\hat{H}$. Let $\{|n\rangle\}$ and $\{E_n\}$ be a complete set of exact eigenstates and that of the corresponding eigenvalues:

$$\hat{H}|n\rangle = E_n|n\rangle,$$

where we assume that $E_0 \le E_1 \le E_2 \le \cdots$. In general, a system will exhibit various types of collective modes characterized by symmetries and excitation energies. Let $\hat{F}$ be an excitation operator of the system. When $\hat{F}$ acts on the ground state $|0\rangle$, various states $|F_1\rangle, |F_2\rangle, \cdots$ can, in general, be excited, where $|F_i\rangle$ belongs to the set $\{|n\rangle\}$ and satisfies

$$\hat{H}|F_i\rangle = E_{F_i}|F_i\rangle \quad (i = 1, 2, 3, \cdots) \tag{4.112}$$

with $E_{F_1} \le E_{F_2} \le \cdots$. The following theorem is useful for finding an upper bound of a collective mode.

*Theorem.* An upper bound $\hbar\omega^{\text{upper}}$ to the minimum excitation energy $\hbar\omega^{\min} \equiv E_{F_1} - E_0$ of the states excited by $\hat{F}$ is given by

$$\hbar\omega^{\text{upper}} = \sqrt{\frac{m_3}{m_1}}, \tag{4.113}$$

where $E_0$ is the ground state energy and

$$m_p \equiv \sum_i |\langle F_i|\hat{F}|0\rangle|^2 (E_{F_i} - E_0)^p \tag{4.114}$$

is the $p$-th energy-weighted moment of the excitation.

*Proof.* A straightforward calculation shows that

$$\frac{\left(\hbar\omega^{\text{upper}}\right)^2 - \left(\hbar\omega^{\min}\right)^2}{(F_{F_1} - E_0)^3} = \frac{\sum_i |\langle F_i|\hat{F}|0\rangle|^2 \left[\left(\frac{E_{F_i}-E_0}{E_{F_1}-E_0}\right)^3 - \frac{E_{F_i}-E_0}{E_{F_1}-E_0}\right]}{\sum_i |\langle F_i|\hat{F}|0\rangle|^2 (E_{F_i} - E_0)}.$$

Since $(E_{F_i} - E_0)/(E_{F_i} - E_0) \ge 1$, we have $\hbar\omega^{\min} \le \hbar\omega^{\text{upper}}$.

When $\hat{F}$ is Hermitian, $m_1$ and $m_3$ can be rewritten as

$$m_1 = \frac{1}{2}\left\langle 0\right| \left[\hat{F}^\dagger, \left[\hat{H}, \hat{F}\right]\right] \left|0\right\rangle, \tag{4.115}$$

$$m_3 = \frac{1}{2}\left\langle 0\right| \left[\left[\hat{F}^\dagger, \hat{H}\right], \left[\hat{H}, \left[\hat{H}, \hat{F}\right]\right]\right] \left|0\right\rangle. \tag{4.116}$$

Equations (4.115) and (4.116) can be shown by inserting the completeness relation $\sum_n |n\rangle\langle n| = 1$ and noting that only states $\{|F_i\rangle\}$ are connected to the ground state $|0\rangle$ via $\hat{F}$. In fact, calculating the right-hand sides of Eqs. (4.115) and (4.116), we have

$$\frac{1}{2}\left\langle 0\right| \left[\hat{F}^\dagger, \left[\hat{H}, \hat{F}\right]\right] \left|0\right\rangle = \frac{1}{2}\sum_i \left[|\langle F_i|\hat{F}|0\rangle|^2 + |\langle F_i|\hat{F}^\dagger|0\rangle|^2\right](E_{F_i} - E_0), \tag{4.117}$$

$$\frac{1}{2}\left\langle 0\right| \left[\left[\hat{F}^\dagger, \hat{H}\right], \left[\hat{H}, \left[\hat{H}, \hat{F}\right]\right]\right] \left|0\right\rangle = \frac{1}{2}\sum_i \left[|\langle F_i|\hat{F}|0\rangle|^2 + |\langle F_i|\hat{F}^\dagger|0\rangle|^2\right](E_{F_i} - E_0)^3. \tag{4.118}$$

When $\hat{F}$ is Hermitian ($\hat{F} = \hat{F}^\dagger$), Eqs. (4.117) and (4.118) respectively give $m_1$ and $m_3$, as defined in Eq. (4.114). When $\hat{F}$ is not Hermitian, as in Eq. (4.140), only one among $\langle F_i|\hat{F}|0\rangle$ and $\langle F_i|\hat{F}_i^\dagger|0\rangle$ can be nonzero. In this case, Eqs. (4.117) and (4.118) give $m_1/2$ and $m_3/2$, respectively. In forming the ratio, the factor of 1/2 is canceled out, and thus, Eq. (4.113) still holds.

The advantage of the sum-rule approach is that no information concerning the excited states is required to find the excitation energies. In particular, given a correct excitation operator $\hat{F}$ and the exact ground state, $\hbar\omega^{\rm upper}$ gives the exact excitation energy.

### 4.3.1 *Excitation operators*

Consider an excitation operator

$$\hat{F}(n, l, m) = \sum_{i=1}^{N} r_i^{2n+l} Y_{lm}(\theta_i, \phi_i) \tag{4.119}$$

that excites a state characterized by radial quantum number $n$, angular-momentum quantum number $l$, and magnetic quantum number $m$, where $N$ is the number of atoms, and $r_i$, $\theta_i$, and $\phi_i$ are polar coordinates of the $i$-th atom, that is,

$$x_i = r_i \sin\theta_i \cos\phi_i,\ \ y_i = r_i \sin\theta_i \sin\phi_i,\ \ z_i = r_i \cos\theta_i. \tag{4.120}$$

The spherical harmonic function $Y_{lm}(\theta_i, \phi_i)$ is given by

$$Y_{lm}(\theta, \phi) = e^{im\phi} P_l^{-m}(\cos\theta) = (-1)^m \frac{(l-m)!}{(l+m)!} e^{im\phi} P_l^m(\cos\theta), \tag{4.121}$$

where $P_l^m$ is the associated Laguerre polynomial defined as

$$P_l^m(x) = \frac{(1-x^2)^{\frac{m}{2}}}{2^l l!} \frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l. \tag{4.122}$$

The excitation with $n = 1$ and $l = m = 0$ is called the monopole mode. In this case, $Y_{00} = 1$ and the corresponding excitation operator is given from Eq. (4.119) as

$$\hat{F} = \sum_i r_i^2 = \sum_i \left(x_i^2 + y_i^2 + z_i^2\right). \tag{4.123}$$

The excitations with $n = 0$ and $l = 1$ are called dipole modes that are classified into three types depending on the value of $m$. In this case, the corresponding excitation operator is given from Eq. (4.119) as

$$\hat{F} = \sum_i r_i Y_{lm}(\theta_i, \phi_i) = \begin{cases} \sum_i (x_i + iy_i) & \text{for } m = 1, \\ \sum_i z_i & \text{for } m = 0, \\ \sum_i (x_i - iy_i) & \text{for } m = -1. \end{cases} \tag{4.124}$$

The excitations with $n = 0$ and $l = 2$ are called quadrupole modes that are classified into five types depending on the value of $m$. The corresponding excitation operators are given by

$$\hat{F} = \sum_i r_i^2 Y_{2m}(\theta_i, \phi_i) = \begin{cases} \sum_i (x_i \pm iy_i)^2 & \text{for } m = \pm 2, \\ \sum_i (x_i \pm iy_i)\, z_i & \text{for } m = \pm 1, \\ \sum_i \left(x_i^2 + y_i^2 - 2z_i^2\right) & \text{for } m = 0. \end{cases} \tag{4.125}$$

### 4.3.2 *Virial theorem*

In the following discussions, we shall restrict ourselves to a situation in which $N$ particles are confined in a harmonic potential and undergo contact interactions described by a delta function. The Hamiltonian of our system is then given by

$$\hat{H} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_i \frac{m}{2}\left(\omega_x^2 x_i^2 + \omega_y^2 y_i^2 + \omega_z^2 z_i^2\right) + \frac{U_0}{2} \sum_{i \neq j} \delta(\mathbf{r}_i - \mathbf{r}_j). \tag{4.126}$$

We assume that the state of our system is stationary. Then, the expectation value of $\sum_i x_i p_{ix}$ is constant in time:

$$\frac{d}{dt}\left\langle \sum_i x_i p_{ix} \right\rangle = 0, \tag{4.127}$$

where $p_{ix}$ is the $x$-component of the momentum of the $i$-th particle. On the other hand, Heisenberg's equation of motion gives

$$\frac{d}{dt} \sum_i x_i p_{ix} = \frac{i}{\hbar}\left[H, \sum_i x_i p_{ix}\right]. \tag{4.128}$$

Substituting Eq. (4.126) in Eq. (4.127) gives

$$\frac{d}{dt}\sum_i x_i p_{ix} = 2\sum_i \frac{p_{ix}^2}{2m} - 2\sum_i \frac{m\omega_x^2}{2}x_i^2 - U_0 \sum_{i\neq j} x_i \frac{\partial\delta(\mathbf{r}_i - \mathbf{r}_j)}{\partial x_i}. \quad (4.129)$$

Hence, we have

$$2\langle T_x\rangle - 2\langle U_x\rangle - U_0\Big\langle \sum_{i\neq j} x_i \frac{\partial\delta(\mathbf{r}_i - \mathbf{r}_j)}{\partial x_i}\Big\rangle = 0, \quad (4.130)$$

where $T_x$ and $U_x$ are the $x$-component of the kinetic energy and the potential energy, respectively. The last term in Eq. (4.130) may be rewritten as

$$\begin{aligned}\Big\langle \sum_{i\neq j} x_i \frac{\partial\delta(\mathbf{r}_i - \mathbf{r}_j)}{\partial x_i}\Big\rangle &= \int d\mathbf{r}_i d\mathbf{r}_j x_i \frac{\partial\delta(\mathbf{r}_i - \mathbf{r}_j)}{\partial x_i}\psi^2(\mathbf{r}_i)\psi^2(\mathbf{r}_j) \\ &= -\int d\mathbf{r}_i \frac{\partial\left(x_i\psi^2(\mathbf{r}_i)\right)}{\partial x_i}\psi^2(\mathbf{r}_i) \\ &= -\int d\mathbf{r}_i \left[\psi^4(\mathbf{r}_i) + \frac{x_i}{2}\frac{\partial\psi^4(\mathbf{r}_i)}{\partial x_i}\right] = -\frac{1}{2}\int d\mathbf{r}_i \psi^4(\mathbf{r}_i) \\ &= -\frac{1}{2}\Big\langle \sum_{i\neq j}\delta(\mathbf{r}_i - \mathbf{r}_j)\Big\rangle. \end{aligned} \quad (4.131)$$

We thus obtain

$$2\langle T_x\rangle - 2\langle U_x\rangle + \langle V\rangle = 0, \quad (4.132)$$

where

$$V = \frac{U_0}{2}\sum_{i\neq j}\delta(\mathbf{r}_i - \mathbf{r}_j). \quad (4.133)$$

We can obtain equations similar to Eq. (4.132) for the $y$- and $z$-components. Summing up the $x$-, $y$-, $z$-components, we obtain

$$2\langle T\rangle - 2\langle U\rangle + 3\langle V\rangle = 0. \quad (4.134)$$

The relations (4.132) and (4.134) are known as the virial theorem.

### 4.3.3 *Kohn theorem*

The collective-mode frequency of the dipole mode ($n = 0$, $l = 1$) is independent of interactions and equal to the frequencies of the trapping potential. This fact is known as the Kohn theorem. To show this, we consider some cases of the axisymmetric harmonic potential

$$U = \sum_i \frac{m}{2}\left[\omega_\perp^2\left(x_i^2 + y_i^2\right) + \omega_z^2 z_i^2\right]. \quad (4.135)$$

#### 4.3.3.1 *Case of* $m = 0$

The excitation operator with $m = 0$ is given by

$$\hat{F} = \sum_i z_i. \tag{4.136}$$

Straightforward calculations give

$$\left[\hat{F}^\dagger, \left[\hat{H}, \hat{F}\right]\right] = \frac{\hbar^2}{m} N, \tag{4.137}$$

$$\left[\left[\hat{F}^\dagger, \hat{H}\right], \left[\hat{H}, \left[\hat{H}, \hat{F}\right]\right]\right] = \frac{\hbar^4 \omega_z^2}{m} N. \tag{4.138}$$

We note that the right-hand sides of Eqs. (4.137) and (4.138) are constants, and independent of the state of the system. Substituting Eqs. (4.137) and (4.138) in Eq. (4.113) gives

$$\hbar\omega^{\text{upper}} = \hbar\omega_z. \tag{4.139}$$

#### 4.3.3.2 *Case of* $m = \pm 1$

The excitation operators with $m = \pm 1$ are given by

$$\hat{F} = \sum_i (x_i \pm i y_i). \tag{4.140}$$

Straightforward calculations give

$$\left[\hat{F}^\dagger, \left[\hat{H}, \hat{F}\right]\right] = \frac{2\hbar^2}{m} N, \tag{4.141}$$

$$\left[\left[\hat{F}^\dagger, \hat{H}\right], \left[\hat{H}, \left[\hat{H}, \hat{F}\right]\right]\right] = \frac{2\hbar^4 \omega_\perp^2}{m} N. \tag{4.142}$$

The right-hand sides of Eqs. (4.141) and (4.142) are again independent of the state of the system. Substituting Eqs. (4.141) and (4.142) in Eq. (4.113) gives

$$\hbar\omega^{\text{upper}} = \hbar\omega_\perp. \tag{4.143}$$

Equations (4.139) and (4.143), in fact, give the exact frequencies of the dipole modes.

### 4.3.4 *Isotropic trap*

When the trap is isotropic, the Hamiltonian is given by

$$\hat{H} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_i \frac{m\omega^2}{2} \mathbf{r}_i^2 + \frac{U_0}{2} \sum_{i \neq j} \delta(\mathbf{r}_i - \mathbf{r}_j). \tag{4.144}$$

We discuss two important collective modes.

#### 4.3.4.1 *Monopole mode*

The excitation operator of the monopole (or breathing) mode with $n = 1$ and $l = 0$ is given by

$$\hat{F} = \sum_i \mathbf{r}_i^2 = \sum_i \left(x_i^2 + y_i^2 + z_i^2\right). \tag{4.145}$$

Calculating the commutation relations for $m_1$ gives

$$\left[\hat{F}^\dagger, \left[\hat{H}, \hat{F}\right]\right] = \frac{4\hbar^2}{m} \sum_i \mathbf{r}_i^2. \tag{4.146}$$

Hence,

$$m_1 = \frac{4\hbar^2}{m^2\omega^2} \langle U \rangle. \tag{4.147}$$

Calculating the commutation relations for $m_3$ is slightly complicated. We first note that

$$\left[\hat{F}^\dagger, \hat{H}\right] = \frac{2i\hbar}{m} \sum_i \left(\mathbf{p}_i \mathbf{r}_i + \frac{3}{2} i\hbar\right), \tag{4.148}$$

$$\left[\hat{H}, \left[\hat{H}, \hat{F}\right]\right] = -\frac{4\hbar^2}{m} \left(\sum_i \frac{\mathbf{p}_i^2}{2m} - \sum_i \frac{m\omega^2}{2} \mathbf{r}_i^2 - \frac{U_0}{2} \sum_{i \neq j} \mathbf{r}_i \frac{\partial \delta(\mathbf{r}_i - \mathbf{r}_j)}{\partial \mathbf{r}_i}\right). \tag{4.149}$$

Hence,

$$\left[\left[\hat{F}^\dagger, \hat{H}\right], \left[\hat{H}, \left[\hat{H}, \hat{F}\right]\right]\right] = \frac{16\hbar^4}{m^2} \left\{ \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_i \frac{m\omega^2}{2} \mathbf{r}_i^2 \right.$$
$$\left. + \frac{U_0}{4} \sum_{i \neq j} \left(\mathbf{r}_i \cdot \nabla_i + \mathbf{r}_j \cdot \nabla_j\right) \mathbf{r}_i \cdot \nabla_i \delta\left(\mathbf{r}_i - \mathbf{r}_j\right) \right\}. \tag{4.150}$$

The expectation value of the last term can be evaluated as

$$\begin{aligned} A &= \langle \sum_{i \neq j} \left(\mathbf{r}_i \cdot \nabla_i + \mathbf{r}_j \cdot \nabla_j\right) \mathbf{r}_i \cdot \nabla_i \delta\left(\mathbf{r}_i - \mathbf{r}_j\right) \rangle \\ &= \int d\mathbf{r} d\mathbf{r}' \psi^2(\mathbf{r}) \psi^2(\mathbf{r}') \left(x_i \partial_i + x'_i \partial'_i\right) x_j \partial_j \delta(\mathbf{r} - \mathbf{r}'), \end{aligned}$$

where $x_1 = x$, $x_2 = y$, $x_3 = z$, etc. Integration by parts gives

$$\begin{aligned}
A &= -\int d\mathbf{r}d\mathbf{r}' \left\{\psi^2(\mathbf{r}') \left[\partial i \left(x_i\psi^2(\mathbf{r})\right)\right] x_j\partial_j\delta(\mathbf{r}-\mathbf{r}') \right.\\
&\quad \left. +\psi^2(\mathbf{r}) \left[\partial'_i \left(x'_i\psi^2(\mathbf{r}')\right)\right] x_j\partial_j\delta(\mathbf{r}-\mathbf{r}')\right\}\\
&= \int d\mathbf{r} \left\{\psi^2\partial_j x_j \left[\partial_i \left(x_i\psi^2\right)\right] + \left[\partial_j \left(x_j\psi^2\right)\right]\left[\partial_i \left(x_i\psi^2\right)\right]\right\}\\
&= \int d\mathbf{r} \left\{-\left(\partial_j\psi^2\right) x_j \left[\partial_i \left(x_i\psi^2\right)\right] + \left[\left(\partial_j x_j\right)\psi^2 + x_j\left(\partial_j\psi^2\right)\right]\left[\partial_i \left(x_i\psi^2\right)\right]\right\}\\
&= 3\int d\mathbf{r}\psi^2\partial_i\left(x_i\psi^2\right) = 3\int d\mathbf{r}\left[\psi^4\left(\partial_i x_i\right) + x_i\psi^2\left(\partial_i\psi^2\right)\right\}\\
&= 3\int d\mathbf{r}\left(3\psi^4 + \frac{1}{2}x_i\partial_i\psi^4\right) = \frac{9}{2}\int d\mathbf{r}\psi^4 = \frac{9}{2}\Big\langle \sum_{i\neq j}\delta(\mathbf{r}_i - \mathbf{r}_j)\Big\rangle\\
&= \frac{9}{U_0}\langle V\rangle.
\end{aligned}$$

Hence, we have

$$m_3 = \frac{8\hbar^2}{m^2}\langle T + U + \frac{9}{4}V\rangle. \tag{4.151}$$

We may use the virial theorem (4.134) to eliminate $\langle V\rangle$ in Eq. (4.151), thus obtaining

$$m_3 = \frac{4\hbar^2}{m^2}\langle 5U - T\rangle. \tag{4.152}$$

Substituting Eqs. (4.146) and (4.152) in Eq. (4.113) gives

$$\hbar\omega^{\text{upper}} = \hbar\omega\sqrt{5 - \frac{\langle T\rangle}{\langle U\rangle}}. \tag{4.153}$$

In the absence of interactions, the vitial theorem gives $\langle T\rangle = \langle U\rangle$, and hence, we have $\hbar\omega^{\text{upper}} = 2\hbar\omega$. In the Thomas–Fermi limit, where $\langle T\rangle = 0$, we have $\hbar\omega^{\text{upper}} = \sqrt{5}\hbar\omega$.

#### 4.3.4.2 *Quadrupole mode*

The excitations with $n = 0$ and $l = 2$ are called quadrupole modes. In the case of an isotropic trap, the excitation frequency is independent of $m$. It is therefore sufficient to consider the case of $m = 0$, where the excitation operator is given by

$$F = \sum_i \left(x_i^2 + y_i^2 - 2z_i^2\right). \tag{4.154}$$

Straightforward calculations give

$$m_1 = \frac{8\hbar^2}{m^2\omega^2}\langle U\rangle, \tag{4.155}$$

$$m_3 = \frac{16\hbar^4}{m^2}\langle T+U\rangle. \tag{4.156}$$

Hence, we obtain

$$\hbar\omega^{\text{upper}} = \hbar\omega\sqrt{2\left(1+\frac{\langle T\rangle}{\langle U\rangle}\right)}. \tag{4.157}$$

In the absence of interactions, $\hbar\omega^{\text{upper}} = \sqrt{3}\hbar\omega$, while in the Thomas–Fermi limit, $\hbar\omega^{\text{upper}} = \sqrt{2}\omega$.

### 4.3.5 *Axisymmetric trap*

When the trap is axisymmetric, the Hamiltonian is given by

$$\hat{H} = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_i \frac{m}{2}\left[\omega_\perp^2\left(x_i^2+y_i^2\right)+\omega_z^2 z_i^2\right] + \frac{U_0}{2}\sum_{i\neq j}\delta\left(\mathbf{r}_i-\mathbf{r}_j\right). \tag{4.158}$$

In this case, the frequency of the quadrupole mode depends on the value of $m$. When $n=0$, $l=2$, and $m=\pm 2$, the excitation operators are given by

$$\hat{F} = \sum_i \left(x_i \pm iy_i\right)^2. \tag{4.159}$$

In this case,

$$m_1 = \frac{4\hbar^2}{m}\left\langle \sum_i \left(x_i^2+y_i^2\right)\right\rangle \equiv \frac{16\hbar^2}{m^2\omega^2}\left\langle U_\perp\right\rangle, \tag{4.160}$$

$$m_3 = \frac{16\hbar^4}{m^2}\left\langle \sum_i \frac{p_{ix}^2+p_{iy}^2}{2m} + \sum_i \frac{m\omega^2}{2}\left(x_i^2+y_i^2\right)\right\rangle \equiv \frac{32\hbar^2}{m^2}\langle T_\perp + U_\perp\rangle. \tag{4.161}$$

Hence, we have

$$\hbar\omega^{\text{upper}} = \hbar\omega_\perp\sqrt{2\left(1+\frac{\langle T_\perp\rangle}{\langle U_\perp\rangle}\right)}. \tag{4.162}$$

The mode with $m=0$ is called the radial breathing mode. When $\omega_\perp \neq \omega_z$, the angular momentum is no longer a good quantum number, and the mode with $n=1$, $l=m=0$ $\left(\hat{F}=\sum_i r_i^2\right)$ couples with the mode with $n=0$,

$l = 2$, $m = 0$ $\left(\hat{F} = \sum_i \left(x_i^2 + y_i^2 - 2z_i^2\right)\right)$. The excitation operator for the coupled mode is, in general, given by

$$\hat{F} = \sum_i \left(x_i^2 + y_i^2 - \alpha z_i^2\right), \tag{4.163}$$

where $\alpha$ is a variational parameter to be determined later. Calculations of the commutation relations give

$$m_1 = \frac{4\hbar^2}{m^2\omega_\perp^2}\left[2\langle U_\perp\rangle + \frac{\alpha^2}{\lambda^2}\langle U_z\rangle\right], \tag{4.164}$$

$$m_3 = \frac{8\hbar^4}{m^2}\left[2(\langle T_\perp\rangle + \langle U_\perp\rangle) + \alpha^2(\langle T_\perp\rangle + \langle U_z\rangle) + \left(1 - \frac{\alpha}{2}\right)^2\langle V\rangle\right], \tag{4.165}$$

where $\lambda \equiv \omega_z/\omega_\perp$. Hence, we have

$$\hbar\omega^{\text{upper}} = \sqrt{2}\hbar\omega_\perp\left[\frac{2(\langle T_\perp\rangle + \langle U_\perp\rangle) + \alpha^2(\langle T_z\rangle + \langle U_z\rangle) + \left(1 - \frac{\alpha}{2}\right)^2\langle V\rangle}{2\langle U_\perp\rangle + \frac{\alpha^2}{\lambda^2}\langle U_z\rangle}\right]^{\frac{1}{2}}. \tag{4.166}$$

In the Thomas–Fermi limit, we have $\langle T_\perp\rangle = \langle T_z\rangle = 0$. It can also be shown that $\langle U_\perp\rangle = \langle U_z\rangle$. On the other hand, according to the virial theorem, we obtain $\langle V\rangle = \frac{2}{3}\langle U\rangle = 2\langle U_\perp\rangle$. Hence, we have

$$\hbar\omega^{\text{upper}} = \hbar\omega_z\sqrt{\frac{3\alpha^2 - 4\alpha + 8}{\alpha^2 + 2\lambda^2}}. \tag{4.167}$$

Minimizing this with respect to $\alpha$ gives

$$\omega^{\text{upper}} = \omega_\perp\left[2 + \frac{3}{2}\lambda^2 \pm \sqrt{\frac{9}{4}\lambda^4 - 4\lambda^2 + 4}\right]^{\frac{1}{2}}. \tag{4.168}$$