CHAPTER III

REDUCED DENSITY MATRICES

In this chapter we will study properties of the reduced density matrices and show its usefulness for solving the many-body problem having "off-diagonal long-range order"(ODLRO). For bosons and fermions it is shown how ODLRO can be introduced into the reduced density matrices. The use of ODLRO has been applied in the treatment of superfluid helium.

3.1 N^{th} Order Reduced Density Matrices

For a system in a pure state, these pure system can be described by the means of the density matrix D,

$$D(\vec{x}_1',\ldots,\vec{x}_N',t;\vec{x}_1'',\ldots,\vec{x}_N'',t) = \psi(\vec{x}_1',\ldots\vec{x}_N',t)\ \psi^*(\vec{x}_1'',\ldots,\vec{x}_N'',t) \quad (3\text{-}1)$$

In the usual case, the system is in a mixed state, a state which is impossible to describe by a single wave function. We assume that the Schrödinger equation, $\hbar\frac{\partial\psi_i}{\partial t} = H\psi_i$, can be solved exactly to obtain the eigenfunction $\psi_i,\psi_j,\ldots,$ corresponding to energy eigenvalue $E_i,E_j,\ldots,$ respectively. There will be an uncertainty as to whether the system is in the state $\psi_i,\psi_j,\ldots;$ and so the mixed state will be regarded as an incoherent mixture of pure state ψ_i with the statistical "weights" W_i, i.e, in thermal equilibrium.

$$W_i = \frac{\exp(-E_i/k_BT)}{\sum_{j=1}^{\nu}\exp(-E_j/k_BT)}$$

and $\sum_{i=1}^{\nu} W_i = 1$

where ν is the number of states in the system. The density matrix which can describe the system in mixed state is a weight average of the D(i)

$$D(\vec{x}_1^{'},\ldots,\vec{x}_N^{'},t;\vec{x}_1^{''},\ldots,\vec{x}_N^{''},t) \doteq \sum_{i=1}^{\nu} W_i \psi_i(\vec{x}_1^{'},\ldots,\vec{x}_N^{'},t)\psi_i^{*}(\vec{x}_1^{''},\ldots,\vec{x}_N^{''},t) \tag{3-2}$$

The density matrix was first introduced by Landau(16)

A Hamitonian operator H of an N-body system of identical particles is

$$H = (-\frac{\hbar^2}{2m})\sum_{i=1}^{N}\nabla_i^2 + \frac{1}{2}\sum_{i\neq j} V(\vec{x}_i - \vec{x}_j) \tag{3-3}$$

where the particles interact in pair via the spherically symmetrical two body potential $V(\vec{r})$. The Hamiltonian operator H must be invariant under the interchange of all the coordinate of any two particles. The complete properties of the system can be described by the N-particles wave function $\psi(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_i,\ldots,\vec{x}_N,t)$, which is either symmetric or antisymmetric under the interchange of two coordinates.

$$\psi(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_i,\ldots,\vec{x}_N,t) = \pm\,\psi(\vec{x}_2,\vec{x}_1,\ldots,\vec{x}_i,\ldots,\vec{x}_N.t) \tag{3-4}$$

where x_i denote the collection of all the coordinates of the i th particles, including the position coordinates, and the spin. The plus sign refers to bosons, and minus sign refers to fermions. The particles of integer spin obey Bose statis ics and are called bosons and the particles of half spin obey Fermi statistics and are called fermions. The N-particles wave function are thus assumed here to obey the Schrödinger equation.

$$i\hbar\frac{\partial\psi}{\partial t} = \left(\frac{-\hbar^2}{2m}\right)\sum_{\ell=1}^{N}\nabla_1^2\psi + \frac{1}{2}\sum_{\ell\neq m}V(\vec{x}_\ell - \vec{x}_m)\ \psi(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_\ell,\ldots,\vec{x}_N,t) \quad (3\text{-}5)$$

this equation could be solved under using various approximations

The combined quantum and statistical expectation of an observable, such as the average density $<\rho(\vec{x})>$ of the system of N points particles, is

$$<\rho(\vec{x})> = \sum_{i=1}^{\nu}W_i\int\ldots\int\psi^*(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_N,t)\sum_{i=1}^{N}\delta(\vec{x}-\vec{x}_1)\psi_i(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_N,t)\, d\vec{x}_1,\ldots,d\vec{x}_N$$

$$= N\sum_{i=1}^{\nu}W_i\int\ldots\int\psi^*(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_N,t)\psi_i(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_N,t)\,d\vec{x}_2,\ldots d\vec{x}_N \quad (3\text{-}6)$$

Even if the N particle wave function ψ could be obtained exactly by solving the Schrödinger equation (3-5), it would contain too many uninteresting detials to be of any use. However, the density matrix will provide all possible information. It is far too difficult to solve explicitly. An elegant method for solving the N-body problem is to introduce the "reduced density matrices and ODLRO". The reduced density matrices, for equal times, are defined as follows:

$$\Omega_1(\vec{x}_1';\vec{x}_1'') = \frac{N}{(N-1)}\int\ldots\int D(\vec{x}_1',\vec{x}_2,\ldots,\vec{x}_N;\vec{x}_1'',\vec{x}_2,\ldots,\vec{x}_N)\,d\vec{x}_2,\ldots,d\vec{x}_N \quad (3\text{-}7)$$

$$\Omega_2(\vec{x}_1',\vec{x}_2';\vec{x}_1'',\vec{x}_2'') = \frac{N}{(N-2)}\int\ldots\int D(\vec{x}_1',\vec{x}_2',\vec{x}_3,\ldots,\vec{x}_N;\vec{x}_1'',\vec{x}_2'',\vec{x}_3,\ldots,\vec{x}_N)\,d\vec{x}_3,\ldots,d\vec{x}_N \quad (3\text{-}8)$$

etc, for Ω_n the n th order reduced density matrix. The reduced density matrices as defined in equation (3-8) satisfy the coupled equation of motion,

$$i\hbar\frac{\partial\Omega_n}{\partial t} = \left(\frac{-\hbar^2}{2m}\right)\sum_{r=1}^{n}(\nabla_r'^2-\nabla_r''^2)\Omega_n + \frac{1}{2}\sum_{r,s}\{V(\vec{x}_r'-\vec{x}_s') - V(\vec{x}_r''-\vec{x}_s'')\}\Omega_n$$
$$+\int\sum_{r=1}^{n}\{V(\vec{x}_r'-\vec{y}) - V(\vec{x}_r''-\vec{y})\}\Omega_{n+1}(\vec{x}_1',\ldots,\vec{x}_n',\vec{y};\vec{x}_1'',\ldots,\vec{x}_n'',\vec{y})\,d\vec{y} \qquad (3-9)$$

for the Hamiltonian of equation (3-3). When Ω_{n+1} vanishes, the equation of motion for Ω_n is equivalent to the Schrödinger equation. In the second quantization representation, Ω_n can also be defined, for equal times, as the trace over the nonrelativistic field operator ψ and $\psi^\dagger$

$$\Omega_n(\vec{x}_1',\ldots,\vec{x}_n';\vec{x}_1'',\ldots,\vec{x}_n'') = \mathrm{Tr}\{\Omega(t)\psi^*(\vec{x}_1''),\ldots,\psi^*(\vec{x}_n'')\psi(\vec{x}_n'),\ldots,\psi(\vec{x}_1')\} \qquad (3-10)$$

Ω_n depends on 2n space points and on time t (for equal times). If N is the mean numbers of particles, and if N is greater than n, then Ω_n satisfies the relation.

$$\int\Omega_n(\vec{x}_1',\ldots,\vec{x}_{n-1}',\vec{x}_n';\vec{x}_1'',\ldots,\vec{x}_{n-1}'',\vec{x}_n'')\,d\vec{x}_n = (N-n+1)\,\Omega_{n-1}(\vec{x}_1',\ldots,\vec{x}_{n-1}',\vec{x}_1'',\ldots,\vec{x}_{n-1}'') \qquad (3-11)$$

and Ω_n follows generally the symmetry relations.

$$\Omega_n(\vec{x}_1',\ldots,\vec{x}_{r-1}',\vec{x}_r',\ldots,\vec{x}_n';\vec{x}_1'',\ldots,\vec{x}_{r-1}'',\vec{x}_r'',\ldots,\vec{x}_n'')$$
$$= \Omega_n(\vec{x}_1',\ldots,\vec{x}_r',\vec{x}_{r-1}',\ldots,\vec{x}_n';\vec{x}_1'',\ldots,\vec{x}_r'',\vec{x}_{r-1}'',\ldots,\vec{x}_n'')$$

$$= \pm\Omega_n(\vec{x}_1',\ldots,\vec{x}_r',\vec{x}_{r-1}',\ldots,\vec{x}_n';\vec{x}_1'',\ldots,\vec{x}_{r-1}'',\vec{x}_r'',\ldots,\vec{x}_n'')$$
$$= \Omega_n^*(\vec{x}_1'',\ldots,\vec{x}_{r-1}'',\vec{x}_r'',\ldots,\vec{x}_n'';\vec{x}_1',\ldots,\vec{x}_{r-1}',\vec{x}_r',\ldots,\vec{x}_n') \quad (3-12)$$

where the plus sign refers to bosons and the minus sign refers to fermions. Comparing equations(3-6) and (3-8), we can see that $\Omega_1(\vec{x},\vec{x}) = \langle \rho(\vec{x}) \rangle$. The reduced density matrix is a Hermitian matrix, i.e,

$$\Omega_1(\vec{x}';\vec{x}'') = \Omega_1^*(\vec{x}'';\vec{x}')$$

and

$$\Omega_2(\vec{x}',\vec{y};\vec{x}'',\vec{y}) = \Omega_2^*(\vec{x}'',\vec{y};\vec{x}',\vec{y})$$

Thus Ω_1 posses a complete set of normalized and orthogonal eigenvector $\psi_{\vec{k}}$

$$\Omega_1(\vec{x}';\vec{x}'') = \sum_k n_k \psi_k^*(\vec{x}'')\psi_k(\vec{x}') \quad (3-13)$$

where $\vec{k}$ denote the various eigenvectors corresponding to the eigenvalues

$$n_{\vec{k}} \int \Omega_1(\vec{x}';\vec{x}'')\psi_{\vec{k}}(\vec{x}'')d\vec{x}'' = n_{\vec{k}}\psi_{\vec{k}}(\vec{x}')$$

where

$$\int \psi_{\vec{k}}^*(\vec{x}'')\psi_{\vec{\ell}}(\vec{x}'')dx = \delta_{\vec{k}\,\vec{\ell}}$$

The eigenvalue $n_{\vec{k}}$ is the occupation numbers of the "single particle" state $\vec{k}$. Integrating equation (3-13) over $\vec{x}'$, and using the completeness relation

$$\sum_k \psi_{\vec{k}}^*(\vec{x}'')\psi_{\vec{k}}(\vec{x}') = \delta(\vec{x}'' - \vec{x}')$$

we obtain $N = \sum_{\vec{k}} n_{\vec{k}}$ when $\vec{x}' = \vec{x}''$ (3-14)

3.2 Off-Diagonal Long-Range Order (ODLRO)

In the many body system of bosons or fermions, Yang(20) has shown that there is an off-diagonal long-range order (ODLRO) of the reduced density matrices in the coordinate space representation. The general characteristics of the gaseous, the liquid, and the solid phase are describable in classical mechanical terms. In quantum mechanics, the long range correlation in the solid is exhibited in the diagonal element of Ω_2 in coordinate space and is quite different from the concept of the off-diagonal long-range order. Since the off-diagonal element have no classical analog, the off-diagonal long-range order is a quantum phenomena not describle in classical mechanical term.

The ODLRO as it was called by Yang(20), is due to the appearance of a factorized part in the reduced density matrix. Penrose(19) first suggested this occurrence for a system of an interacting Bose particles. For the ideal Bose gas, the eigenstate of the Hamiltonian is the simple product of single particle states.

$$\psi_{\vec{k}}(\vec{x}) = \left(\frac{1}{V}\right)^{1/2} \exp(i\vec{k}.\vec{x})$$

and $$\sum_{\vec{k}} \longrightarrow \left(\frac{1}{2\pi}\right)^3 \int dk$$

for a translational-rotational invariant system of the ideal Bose gas, and

$$n_{\vec{k}} = \frac{1}{\exp(\varepsilon_{\vec{k}} - \mu)/k_B T - 1} \quad ; \quad \varepsilon_{\vec{k}} = \frac{h^2 k^2}{2m}$$

Therefore, at temperature, above the transition temperature T_c (3.13 K)

$$\Omega_1(\vec{x}' ; \vec{x}'') \quad \alpha \quad \frac{1}{\lambda^3}\exp(-\pi r^2/\lambda_D^2)$$

where $\vec{r} = \vec{x}' - \vec{x}''$ and $\lambda_D(T) = 2\pi h(2mk_BT)^{1/2}$, the de Broglie thermal wave-length.

Thus $\Omega_1(\vec{x}' ; \vec{x}'')$ approaches zero when $r >> \lambda_D$, and the "size" of a single ideal Bose particles is about $\lambda_D(T)$. This means that there is no probability of finding the same particle simultaneously in far removed region space. Below T_c, a macroscopic number of particles begin to condence out. Then

$$\Omega_1(\vec{x}' ; \vec{x}'') = n_0^{1/2}\psi_0^*(\vec{x}'')\, n_0^{1/2}\psi_0(\vec{x}') + \Lambda_1(\vec{x}' ; \vec{x}'') \tag{3-15}$$

where $\Lambda_1(\vec{x}' ; \vec{x}'') = \sum_{k\neq 0} n_{\vec{k}}\psi_{\vec{k}}^*(\vec{x}'')\psi_{\vec{k}}(\vec{x}')$. For a translational-rotational invariant system (bulk system), $\Lambda_1(\vec{x}' ; \vec{x}'') = \Lambda_1(|\vec{x}' - \vec{x}''|)$ is a function which approaches zero, and vanishes at 0 K. Then all particles are in the coordinate, $n_0 = N/V$, at 0 K. For the Bose system, Penrose suggest that the appearance of the facto-rized part in Ω_1 for the condensation in an interacting Bose system, which $\vec{x}'$ and $\vec{x}''$ are sufficiently distant. Thus for the Bose system

$$\Omega_1(\vec{x}' ; \vec{x}'') = \phi(\vec{x}')\phi^*(\vec{x}'') + \Lambda_1(\vec{x}' ; \vec{x}'') \tag{3-16}$$

must hold, where ϕ_1 is the one point macroscopic wave function and $\Lambda_1(\vec{x}' ; \vec{x}'')$ is negligible only if $|\vec{x}' - \vec{x}''|$ is larger than a characteristic length of the order of interatomic distance. This equation defines a two fluid system with density $\phi(\vec{x})\phi^*(\vec{x})$ for the so-called condensate part and $\Lambda_1(\vec{x}' ; \vec{x}'')$ for the depleting part ϕ_1 as well as Ω_1 are physically meaningful quantities and the ratio $|\phi(\vec{x})|^2 : \Omega_1(\vec{x};\vec{x})$ has been measured; it is of the order of 10 % according to Cummings et al. Thus ϕ_1 should be a basic quantity of a consistent theory of superfluidity.

The factorization (ODLRO) can occur in Ω_1 only for the Bose system, but not for the Fermi system because of the exclusion principle. Yang(20) has shown that the presence of ODLRO in Ω_m leads to its presence in Ω_n for n > m. In the interacting Bose system, Ω_1 shows the presence of ODLRO, thus Ω_2 shows the presence of ODLRO. There are several conditions which Ω_2 must satisfy in any system of identical particles ,

$$\Omega_2(\vec{x}',\vec{y}';\vec{x}'',\vec{y}'') \longrightarrow 0 \qquad (3\text{-}17)$$

for a normal system whenever $\vec{x}'$ is far from $\vec{x}''$ or $\vec{y}'$ is far from $\vec{x}''$ or $\vec{y}''$

$$\int\Omega_2(\vec{x}',\vec{y};\vec{x}'',\vec{y})d\vec{y} = (N-1)\Omega_1(\vec{x}';\vec{x}'') \qquad (3\text{-}18)$$

the symmetry conditions expressed in (3-12)

$$\begin{aligned}\Omega_2(\vec{x}',\vec{y}';\vec{x}'',\vec{y}'') &= \Omega_2^*(\vec{x}'',\vec{y}';\vec{x}',\vec{y}''), \qquad (3\text{-}19)\\ &= \Omega_2(\vec{y}',\vec{x}';\vec{x}'',\vec{y}''),\\ &= \Omega_2(\vec{y}',\vec{x}';\vec{y}'',\vec{x}''), \quad \text{for the Bose system,}\end{aligned}$$

$$\Omega_2(\vec{x}',\vec{y}';\vec{x}'',\vec{y}'') \longrightarrow \Omega_1(\vec{x}';\vec{y}'')\Omega_1(\vec{y}';\vec{x}'') \qquad (3\text{-}20)$$

for $\vec{x}' \cong \vec{y}''$; $\vec{x}'' \cong \vec{y}'$ and $|\vec{x}' - \vec{y}'| \longrightarrow \infty$

$$\Omega_2(\vec{x}',\vec{y}'; \vec{x}'',\vec{y}'') \longrightarrow \Omega_1(\vec{x}'; \vec{x}'')\Omega_1(\vec{y}'; \vec{y}'') \qquad (3\text{-}21)$$

only for $\vec{x}' \cong \vec{x}''$; $\vec{y}' \cong \vec{y}''$ and $|\vec{x}' - \vec{y}'| \longrightarrow \infty$

When $\vec{x}' = \vec{x}'' = \vec{x}$, and $\vec{y}' = \vec{y}$, $\Omega_2(\vec{x},\vec{y};\vec{x},\vec{y})$ is proportional to the joint probability that; given one particle is at point $\vec{x}$, what is the probability of finding the other at $\vec{y}$? When $|\vec{x} - \vec{y}| \to \infty$, it will be equally probable to find the second particle one place as another for a liquid, then $\Omega_2(\vec{x},\vec{y};\vec{x},\vec{y})$ will approach a constant (N^2/V^2) in bulk system ,

$$\Omega_2(\vec{x},\vec{y};\vec{x},\vec{y}) = \rho^2 g(\vec{x},\vec{y}) = \rho^2 g(|\vec{x} - \vec{y}|) \qquad (3\text{-}22)$$

Where $\rho = N/V$ = bulk density of liquid, and $g(\vec{x},\vec{y})$ is called the "pair distribution function" $g(|\vec{x} - \vec{y}|) \longrightarrow 1$, when $|\vec{x} - \vec{y}| \longrightarrow \infty$, thus $\Omega_2(\vec{x},\vec{y};\vec{x},\vec{y})$ nay be called the "pair correlation function"

$$\Omega_2(\vec{x},\vec{y};\vec{x},\vec{y}) = \Omega_2(\vec{x} - \vec{y}) \qquad (3\text{-}23)$$

for a translationally invariant system, and

$$\Omega_2(\vec{x},\vec{y};\vec{x},\vec{y}) = \Omega_2(|\vec{x} - \vec{y}|)$$

for a translation-rotation invariant system (bulk system)

For a system with a hard core interaction (a system like liquid ^4He) the "core" condition is

$$\Omega_2(\vec{x}',\vec{y};\vec{x}',\vec{y}) \longrightarrow 0 \qquad (3\text{-}24)$$

for $|\vec{x} - \vec{y}| < 2r_0$

where r_0 is the radius of the "core" region. This expresses the fact that the atoms are impenetrable

$$\Omega_2(\vec{x}',\vec{y}';\vec{x}'',\vec{y}'') = \phi^*(\vec{x}'')\phi^*(\vec{y}'')\phi(\vec{x}')\phi(\vec{y}') \qquad (4\text{-}25)$$

for all four points apart, when ODLRO occurs in Ω_1

From the equation (3-9), the equation of motion for Ω_1 and Ω_2 can thus be written

$$i\hbar\frac{\partial\Omega_1}{\partial t}(\vec{x}_1',\vec{x}_1'') = \frac{-\hbar^2}{2m}\sum_{r=1}^{n}(\nabla_1'^2 - \nabla_1''^2)\Omega_1(\vec{x}_1';\vec{x}_1'') + \int\{V(\vec{x}_1'-\vec{y})-V(\vec{x}_1''-\vec{y})\}\Omega_2(\vec{x}_1',\vec{y};\vec{x}_1'',\vec{y})\,d\vec{y} \qquad (3\text{-}26)$$

and

$$i\hbar\frac{\partial\Omega_2}{\partial t}(\vec{x}_1',\vec{x}_2';\vec{x}_1'',\vec{x}_2'') = \frac{-\hbar^2}{2m}(\nabla_1'^2+\nabla_2'^2-\nabla_1''^2-\nabla_2''^2)\Omega_2 + \{V(\vec{x}_1'-\vec{x}_2')-V(\vec{x}_1''-\vec{x}_2'')\}\Omega_2 + \int\{V(\vec{x}_1'-\vec{y}) + V(\vec{x}_2'-\vec{y}) - V(\vec{x}_1''-\vec{y}) - V(\vec{x}_1''-\vec{y})\}\,\Omega_3(\vec{x}_1',\vec{x}_2',\vec{y};\vec{x}_1'',\vec{x}_2'',\vec{y})\,d\vec{y} \; . \qquad (3\text{-}27)$$

These last two equations are important for deriving the macroscopic law of mass, momentum and energy conservation.

Fröhlich(17) has derived the Navier-Stokes equation as an exact result from the reduced density matrices, with neither continuum assumptions nor intermediate "master equation" required,

$$\rho\frac{\partial\vec{v}}{\partial t} + \rho(\vec{v}.\nabla)\vec{v} = -\nabla P + \eta_2\nabla^2\vec{v} - \eta_1\nabla \times \nabla \times \vec{v} \qquad (3\text{-}28)$$

where P is the pressure, and η_1 , η_2 are the coefficients of viscosity. For a non—interacting system, a derivation of the Euler equation can be obtained from equation (3-26) immediately