Many-Body Schroedinger Equation in First Quantization

Assume we have a system of N identical particles that interact through a 2-body potential V. The Hamiltonian is

$$\hat{H} = \sum_{k=1}^{N} T(x_k) + \frac{1}{2}\sum_{k\neq l=1}^{N} V(x_k, x_l)$$

where x_k is the "coordinate" of the k^{th} particle:

$$x_k \equiv (\vec{x}_k, z)$$

where z can represent discrete quantities such as $S_z, \ldots$

The N-body Schroedinger Equation is

$$i\frac{\partial \Psi(x_1, \ldots, x_N, t)}{\partial t} = \hat{H}\,\Psi(x_1, \ldots, x_N, t)$$

As always, we expand the many particle wave function Ψ in a complete set of time-independent single-particle wave functions suitable for the application and that incorporate the boundary conditions.

<u>Examples</u>

① a large homogeneous system

- $\psi_{\epsilon_k}(x_k)$ = set of plane waves in a box with periodic boundary conditions

2. interacting electrons in an atom

- $\psi_{\epsilon_k}(x_k)$ = set of single-particle Coulomb wave functions

3. particles moving in a crystal lattice

- $\psi_{\epsilon_k}(x_k)$ = set of Bloch wave functions in the appropriate periodic potential

In the notation

$\psi_{\epsilon_k}(x_k)$

ϵ_k denotes a complete set of single-particle quantum #'s:

- $\epsilon_k = \vec{p}$ for a system of spinless bosons in a box
- $\epsilon_k = E, J, M$ for a system of spinless particles in a central field
- $\epsilon_k = \vec{p}, s_z$ for a homogeneous system of fermions

Putting this all together, we have

$$\Psi(x_1, \ldots, x_N, t) = \sum_{E_1', \ldots, E_N' = \epsilon_1}^{\epsilon_\infty} C(E_1', \ldots, E_N', t)\, \psi_{E_1'}(x_1) \cdots \psi_{E_N'}(x_N)$$

sum over all possible $\{E_N\}$ with $E_i \in \{\epsilon_1, \ldots, \epsilon_\infty\}$

time dependence in here

Insert this into the Schrödinger equation, multiply both sides by $\psi^\dagger_{E_1}(x_1)\cdots\psi^\dagger_{E_N}(x_N)$ and "integrate" over all "coordinates":

(1)
$$i\sum_{E_1'\ldots E_N'}\frac{\partial C}{\partial t}\int d^3x_1\ldots d^3x_N\,\psi^\dagger_{E_1}(x_1)\ldots\psi^\dagger_{E_N}(x_N)\,\psi_{E_1'}(x_1)\ldots\psi_{E_N'}(x_N)$$

$$= i\frac{\partial}{\partial t}C(E_1,\ldots,E_N,t)$$

(2)
$$\sum_k\sum_{E_1'\ldots E_N'}C(E_1',\ldots,E_N',t)\int d^3x_1\ldots d^3x_N\,\psi^\dagger_{E_1}(x_1)\ldots\psi^\dagger_{E_N}(x_N)\,\hat{T}(x_k)\,\psi_{E_1'}(x_1)\ldots\psi_{E_N'}(x_N)$$

$$= \sum_k\sum_{E_k'}C(E_1,\ldots,E_{k-1},E_k',E_{k+1},\ldots E_N)\int d^3x_k\,\psi^\dagger_{E_k}(x_k)\,\hat{T}(x_k)\,\psi_{E_k'}(x_k)$$

(3)
$$\frac{1}{2}\sum_{k\neq l}\sum_{E_1'\ldots E_N'}\int d^3x_1\ldots d^3x_N\,\psi^\dagger_{E_1}(x_1)\ldots\psi^\dagger_{E_N}(x_N)\,\hat{V}(x_k,x_l)\,\psi_{E_1'}(x_1)\ldots\psi_{E_N'}(x_N)$$

$$=\frac{1}{2}\sum_{k\neq l}\sum_{E_k'E_l'}C(E_1,\ldots,E_{k-1},E_k',E_{k+1},\ldots,E_{l-1},E_l',E_{l+1},\ldots,E_N,t)$$

$$\times\int d^3x_k\,d^3x_l\,\psi^\dagger_{E_k}(x_k)\,\psi^\dagger_{E_l}(x_l)\,\hat{V}(x_k,x_l)\,\psi_{E_k'}(x_k)\,\psi_{E_l'}(x_l)$$

The statistics of the particles is incorporated in the coefficients

$$C(E_1,\ldots,E_j,\ldots,E_k,\ldots E_N,t) = \pm\, C(E_1,\ldots,E_k,\ldots,E_j,\ldots E_N,t)$$

Necessary and sufficient for $\Psi(x_1,\ldots,x_j,\ldots,x_k,\ldots x_N) = \pm\Psi(x_1,\ldots,x_k,\ldots,x_j,\ldots x_N)$.

Let's now consider bosons (for which the + sign in the previous expression is appropriate). The symmetry in this case under the interchange of quantum numbers E_i and E_j can be used to our advantage.

Out of the given set of quantum numbers $(E_1, \ldots, E_N)$ suppose that n_1 of our bosons are in state ψ_{ϵ_1}, n_2 in state $\psi_{\epsilon_2}, \ldots$

Then

I will have the same state if I interchange particles 2 and 3.

$$C(1,2,1,3,2,4,\ldots,t) = C(\underbrace{1,1,1,\ldots}_{n_1 \text{ times}},\underbrace{2,2,2,\ldots}_{n_2 \text{ times}},\ldots,t)$$

particle 3 is in state ψ_{ϵ_1} with energy ϵ_1 – i.e., $E_3 = \epsilon_1$

$$\equiv \bar{C}(n_1, n_2, \ldots, n_\infty, t)$$

equal in value but a different function relative to C

but $\sum_{i=1}^{N} n_i = N$ ← total # particles

Of course, we have

$$\sum_{E_1 \ldots E_N = \epsilon_1}^{\epsilon_\infty} |C(E_1, \ldots, E_N, t)|^2 = 1$$

$E_1 \in \{\epsilon_1, \epsilon_2, \ldots, \epsilon_\infty\}$

$E_2 \in \{\quad " \quad\}$

$\vdots$

$E_N \in \{\quad " \quad\}$

sum over all possible energies particle 1 (E_1) through particle N (E_N) can take within the possible energy levels $\{\epsilon_1, \ldots, \epsilon_\infty\}$

For the $\bar{C}(n_1, n_2, \ldots, n_\infty, t)$, this translates to

$$\sum_{\substack{n_1, n_2 \ldots n_\infty = 0 \\ \sum_{i=1}^{N} n_i = N}}^{N} |\bar{C}(n_1, n_2, \ldots, n_\infty, t)|^2 \frac{N!}{n_1! n_2! \ldots n_\infty!} = 1$$

where

$$|\overline{C}(n_1, n_2, \ldots, n_\infty, t)|^2 = \text{probability of having } n_1 \text{ particles in state } \psi_{E_1}, n_2 \text{ particles in state } \psi_{E_2}, \ldots$$

$$N!/n_1!n_2!\ldots n_\infty! = \#\text{ of ways of putting our } N \text{ identical bosons into these states}$$

Define

$$f(n_1, n_2, \ldots, n_\infty, t) \equiv \left[\frac{N!}{n_1!n_2!\ldots n_\infty!}\right]^{1/2} \overline{C}(n_1, n_2, \ldots, n_\infty, t)$$

then

$$\sum_{n_1 n_2 \ldots n_\infty} |f(n_1, n_2, \ldots, n_\infty, t)|^2 = 1$$

$$\Psi(x_1, \ldots, x_N, t) = \sum_{E_1 \ldots E_N} C(E_1, \ldots, E_N, t)\, \psi_{E_1}(x_1) \ldots \psi_{E_N}(x_N)$$

$$= \sum_{E_1 \ldots E_N} \overline{C}(\underbrace{n_1, n_2, \ldots, n_\infty}_{\substack{\text{consistent with} \\ E_1, \ldots, E_N}}, t)\, \psi_{E_1}(x_1) \ldots \psi_{E_N}(x_N)$$

$$= \sum_{n_1 n_2 \ldots n_\infty} f(n_1, n_2, \ldots, n_\infty, t) \left(\frac{N!}{n_1!n_2!\ldots n_\infty!}\right)^{-1/2}$$

$$\times \sum_{\substack{E_1 \ldots E_N \\ (n_1 n_2 \ldots n_\infty)}} \psi_{E_1}(x_1) \ldots \psi_{E_N}(x_N)$$

← sum over all $E_1, \ldots, E_N$ consistent with a given set of occupation numbers $(n_1, n_2, \ldots, n_\infty)$

Example: 2 identical bosons and 3 energy levels/states

ϵ_1	ϵ_2	ϵ_3	$C(E_1,E_2)\psi_{E_1}(x_1)\psi_{E_2}(x_2)$	n_1	n_2	n_3	$\bar{C}(n_1,n_2,n_3)\psi_{E_1}(x_1)\psi_{E_2}(x_2)$
1	2		$C(\epsilon_1,\epsilon_2)\psi_{\epsilon_1}(x_1)\psi_{\epsilon_2}(x_2)$	1	1	0	$\bar{C}(1,1,0)\psi_{\epsilon_1}(x_1)\psi_{\epsilon_2}(x_2)$
1		2	$C(\epsilon_1,\epsilon_3)\psi_{\epsilon_1}(x_1)\psi_{\epsilon_3}(x_2)$	1	0	1	$\bar{C}(1,0,1)\psi_{\epsilon_1}(x_1)\psi_{\epsilon_3}(x_2)$
	1	2	$C(\epsilon_2,\epsilon_3)\psi_{\epsilon_2}(x_1)\psi_{\epsilon_3}(x_2)$	0	1	1	$\bar{C}(0,1,1)\psi_{\epsilon_2}(x_1)\psi_{\epsilon_3}(x_2)$
2	1		$C(\epsilon_2,\epsilon_1)\psi_{\epsilon_2}(x_1)\psi_{\epsilon_1}(x_2)$	1	1	0	$\bar{C}(1,1,0)\psi_{\epsilon_2}(x_1)\psi_{\epsilon_1}(x_2)$
2		1	$C(\epsilon_3,\epsilon_1)\psi_{\epsilon_3}(x_1)\psi_{\epsilon_1}(x_2)$	1	0	1	$\bar{C}(1,0,1)\psi_{\epsilon_3}(x_1)\psi_{\epsilon_1}(x_2)$
	2	1	$C(\epsilon_3,\epsilon_2)\psi_{\epsilon_3}(x_1)\psi_{\epsilon_2}(x_2)$	0	1	1	$\bar{C}(0,1,1)\psi_{\epsilon_3}(x_1)\psi_{\epsilon_2}(x_2)$
12			$C(\epsilon_1,\epsilon_1)\psi_{\epsilon_1}(x_1)\psi_{\epsilon_1}(x_2)$	2	0	0	$\bar{C}(2,0,0)\psi_{\epsilon_1}(x_1)\psi_{\epsilon_1}(x_2)$
	12		$C(\epsilon_2,\epsilon_2)\psi_{\epsilon_2}(x_1)\psi_{\epsilon_2}(x_2)$	0	2	0	$\bar{C}(0,2,0)\psi_{\epsilon_2}(x_1)\psi_{\epsilon_2}(x_2)$
		12	$C(\epsilon_3,\epsilon_3)\psi_{\epsilon_3}(x_1)\psi_{\epsilon_3}(x_2)$	0	0	2	$\bar{C}(0,0,2)\psi_{\epsilon_3}(x_1)\psi_{\epsilon_3}(x_2)$

$\sum_{E_1,E_2} \bar{C}(n_1,n_2,n_3)\psi_{E_1}(x_1)\psi_{E_2}(x_2)$

Summing over the last column, which is equivalent to summing over the fourth column, we have

$\sum_{E_1,E_2} C(E_1,E_2)\psi_{E_1}(x_1)\psi_{E_2}(x_2)$

This regrouping is

$$\sum_{n_1 n_2 n_3} \bar{C}(n_1,n_2,n_3) \sum_{\substack{E_1 E_2 \\ (n_1,n_2,n_3)}} \psi_{E_1}(x_1)\psi_{E_2}(x_2)$$

$$\bar{C}(1,1,0)\left[\psi_{\epsilon_1}(x_1)\psi_{\epsilon_2}(x_2)+\psi_{\epsilon_2}(x_1)\psi_{\epsilon_1}(x_2)\right]$$

$$+\ \bar{C}(1,0,1)\left[\psi_{\epsilon_1}(x_1)\psi_{\epsilon_3}(x_2)+\psi_{\epsilon_3}(x_1)\psi_{\epsilon_1}(x_2)\right]$$

$$+\ \bar{C}(0,1,1)\left[\psi_{\epsilon_2}(x_1)\psi_{\epsilon_3}(x_2)+\psi_{\epsilon_3}(x_1)\psi_{\epsilon_2}(x_2)\right]$$

$$+\ \bar{C}(2,0,0)\psi_{\epsilon_1}(x_1)\psi_{\epsilon_1}(x_2)+\bar{C}(0,2,0)\psi_{\epsilon_2}(x_1)\psi_{\epsilon_2}(x_2)+\bar{C}(0,0,2)\psi_{\epsilon_3}(x_1)\psi_{\epsilon_3}(x_2)$$

$$= \sum_{n_1, n_2, n_3 = 0}^{2} \bar{C}(n_1, n_2, n_3) \underbrace{\sum_{E_1, E_2 = \epsilon_1}^{\epsilon_3}}_{(n_1, n_2, n_3)} \psi_{E_1}(x_1) \psi_{E_2}(x_2)$$

The sum over E_1 and E_2 has to be consistent with the given (n_1, n_2, n_3) from the first sum.

For example, for $\bar{C}(1,1,0)$, the only terms in the second sum that are consistent with $\bar{C}(n_1, n_2, n_3) = \bar{C}(1,1,0)$ are $\psi_{\epsilon_1}(x_1)\psi_{\epsilon_2}(x_2)$ and $\psi_{\epsilon_2}(x_1)\psi_{\epsilon_1}(x_2)$.

For $\bar{C}(n_1, n_2, n_3) = \bar{C}(2,0,0)$, there is only one term from the second sum that is consistent with $\bar{C}(2,0,0)$: $\psi_{\epsilon_1}(x_1)\psi_{\epsilon_1}(x_2)$.

Etc.

$$\sum_{E_1 \ldots E_N} |C(E_1, \ldots, E_N, t)|^2 = 1$$

$$\downarrow$$

$$\underbrace{\sum_{n_1 n_2 \ldots n_\infty} |\bar{C}(n_1, n_2, \ldots, n_\infty, t)|^2}_{\text{sum over all possible values of } n_1, n_2, \ldots} \underbrace{\sum_{\substack{E_1 \ldots E_N \\ (n_1 n_2 \ldots n_\infty)}} 1}_{\text{sum over all values of } E_1 \ldots E_N \text{ consistent with a given set of occupation numbers}} = 1$$

$=$ # of ways N identical objects can be put in the states E_1 through E_N with n_1 objects in state E_1, n_2 objects in state E_2, …

Then

$$\Psi(x_1, \ldots, x_N, t) = \sum_{n_1 n_2 \ldots n_\infty} f(n_1, n_2, \ldots, n_\infty, t)\, \Phi_{n_1 n_2 \ldots n_\infty}(x_1, \ldots, x_N)$$

where

$$\Phi_{n_1 n_2 \ldots n_\infty}(x_1, \ldots, x_N) \equiv \left(\frac{N!}{n_1! n_2! \ldots n_\infty!}\right)^{-1/2} \sum_{\substack{E_1 \ldots E_N \\ (n_1 n_2 \ldots n_\infty)}} \psi_{E_1}(x_1) \ldots \psi_{E_N}(x_N)$$

Let's look at the kinetic energy term 2 :

Define

$$\int d^3x_k \, \psi^{\dagger}_{E_k}(x_k)\hat{T}(x_k)\psi_{E_k'}(x_k) \equiv \langle E_k|\hat{T}|E_k'\rangle$$

Then

$$\sum_k \sum_{E_k'} C(E_1,\dots,E_{k-1},E_k',E_{k+1},\dots,E_N,t)\langle E_k|\hat{T}|E_k'\rangle$$

$$= \sum_k \sum_{E_k'} \bar{C}(n_1,n_2,\dots,n_{E_k}-1,\dots,n_{E_k'}+1,\dots,n_\infty,t)\langle E_k|\hat{T}|E_k'\rangle$$

sum over particles; ← sum over energy levels – i.e., states

$$= \sum_E \sum_{E_k'} \bar{C}(n_1,n_2,\dots,n_{E_k}-1,\dots,n_{E_k'}+1,\dots,n_\infty,t)\,n_E\langle E|\hat{T}|E_k'\rangle$$

sum over all possible energies – i.e., states

In the last sum, we have switched to a sum over states, $\psi_E(x)$, with n_E the number of times $E_k = E$ as we sum over k.

$$= \sum_i \sum_j \bar{C}(n_1,n_2,\dots,n_i-1,\dots,n_j+1,\dots,n_\infty,t)\,n_i\langle i|\hat{T}|j\rangle$$

Just simplifying the notation for later use.

Similarly, term 3 becomes

$$\frac{1}{2}\sum_{k\neq l=1}^{N} \sum_{E_k'}\sum_{E_l'} \bar{C}(n_1,\dots,n_{E_k}-1,\dots n_{E_k'}+1,\dots,n_{E_l}-1,\dots,n_{E_l'}+1,\dots,n_\infty,t)$$

2 particles
3 levels ϵ_i

$$i \frac{\partial c(E_1, E_2, t)}{\partial t} = \sum_{k=1}^{2} \sum_{E_k' = \epsilon_1}^{\epsilon_3} C(E_1, \ldots, E_k', \ldots, E_2) \langle E_k | \hat{T} | E_k' \rangle$$

① $$= \sum_{E_1' = \epsilon_1}^{\epsilon_3} C(E_1', E_2) \langle E_1 | \hat{T} | E_1' \rangle$$

② $$+ \sum_{E_2' = \epsilon_1}^{\epsilon_3} C(E_1, E_2') \langle E_2 | \hat{T} | E_2' \rangle$$

$$= \sum_{E_1' = \epsilon_1}^{\epsilon_3} \bar{C}(n_1, \ldots, n_{E_1} - 1, \ldots, n_{E_1'} + 1, \ldots, n_3) \langle E_1 | \hat{T} | E_1' \rangle$$

$$+ \sum_{E_2' = \epsilon_1}^{\epsilon_3} \bar{C}(n_1, \ldots, n_{E_2} - 1, \ldots, n_{E_2'} + 1, \ldots, n_3) \langle E_2 | \hat{T} | E_2' \rangle$$

E_2 is given

① $$= C(\epsilon_1, E_2) \langle E_1 | \hat{T} | \epsilon_1 \rangle + C(\epsilon_2, E_2) \langle E_1 | \hat{T} | \epsilon_2 \rangle + C(\epsilon_3, E_2) \langle E_1 | \hat{T} | \epsilon_3 \rangle$$

Let $E_1 = \epsilon_1$ and $E_2 = \epsilon_2$

① $$= C(\epsilon_1, \epsilon_2) \langle \epsilon_1 | \hat{T} | \epsilon_1 \rangle + C(\epsilon_2, \epsilon_2) \langle \epsilon_1 | \hat{T} | \epsilon_2 \rangle + C(\epsilon_3, \epsilon_2) \langle \epsilon_1 | \hat{T} | \epsilon_3 \rangle$$

$$\bar{C}(1,1,0) \langle \epsilon_1 | \hat{T} | \epsilon_1 \rangle + \bar{C}(0,2,0) \langle \epsilon_1 | \hat{T} | \epsilon_2 \rangle + \bar{C}(0,1,1) \langle \epsilon_1 | \hat{T} | \epsilon_3 \rangle$$

$$(2) = C(E_1, \epsilon_1) \langle E_2 | \hat{T} | \epsilon_1 \rangle$$
$$+ C(E_1, \epsilon_2) \langle E_2 | \hat{T} | \epsilon_2 \rangle$$
$$+ C(E_1, \epsilon_3) \langle E_2 | \hat{T} | \epsilon_3 \rangle$$

$$= C(\epsilon_1, \epsilon_1) \langle \epsilon_2 | \hat{T} | \epsilon_1 \rangle \qquad \bar{C}(2,0,0) \langle \epsilon_2 | \hat{T} | \epsilon_1 \rangle$$
$$+ C(\epsilon_1, \epsilon_2) \langle \epsilon_2 | \hat{T} | \epsilon_2 \rangle \qquad + \bar{C}(1,1,0) \langle \epsilon_2 | \hat{T} | \epsilon_2 \rangle$$
$$+ C(\epsilon_1, \epsilon_3) \langle \epsilon_2 | \hat{T} | \epsilon_3 \rangle \qquad + \bar{C}(1,0,1) \langle \epsilon_2 | \hat{T} | \epsilon_3 \rangle$$

$$\times \langle E_k E_l | \hat{V} | E'_k E'_l \rangle$$

We can now switch to summing over states rather than particles. Since the sum over particles prevents $k = l$, we have

$n_E n_{\bar{E}}$ for $E \neq \bar{E}$ — $k \neq l$ doesn't affect counting for $E \neq \bar{E}$

$n_E (n_E - 1)$ for $E = \bar{E}$ — E is counted one less time if $E = \bar{E}$

for example for $N = 3$ this is the number of pairs with $k \neq l$:

$n_E = 3$ $\quad n_E(n_E - 1) = 3 \cdot 2 = 6$

12, 13, 23, 32, 31, 21

and ③ becomes

$$\frac{1}{2} \sum_E \sum_{\bar{E}} \sum_{E'_k} \sum_{E'_l}$$

$$\times \bar{C}(n_1, n_2, \ldots, n_E - 1, \ldots, n_{E'_k} + 1, \ldots, n_{\bar{E}} - 1, \ldots, n_{E'_l} + 1, \ldots, n_\infty, t)$$

$$\times n_E (n_{\bar{E}} - \delta_{E\bar{E}}) \langle E \bar{E} | \hat{V} | E'_k E'_l \rangle$$

$$= \frac{1}{2} \sum_i \sum_j \sum_k \sum_l$$

$$\times \bar{C}(n_1, n_2, \ldots, n_i - 1, \ldots, n_k + 1, \ldots, n_j - 1, \ldots, n_l + 1, \ldots, n_\infty, t)$$

$$\times n_i (n_j - \delta_{ij}) \langle i j | \hat{V} | k l \rangle$$

Our original equation for the coefficients $C(E_1, \ldots, E_N, t)$

① = ② + ③

can now be pulled together to yield

$$i\hbar \frac{\partial}{\partial t}\left(\frac{N!}{n_1! n_2! \cdots n_\infty!}\right)^{-1/2} f(n_1, n_2, \ldots, n_\infty, t)$$

$$= \sum_i \sum_j \left(\frac{N!}{n_1! \cdots (n_i - 1)! \cdots (n_j + 1)! \cdots n_\infty!}\right)^{-1/2}$$

$$\times f(n_1, \ldots, n_i - 1, \ldots, n_j + 1, \ldots, n_\infty, t)$$

$$\times\, n_i \langle i | \hat{T} | j \rangle$$

$$+ \frac{1}{2} \sum_i \sum_j \sum_k \sum_l \left(\frac{N!}{n_1! \cdots (n_i - 1)! \cdots (n_k + 1)! \cdots (n_j - 1)! \cdots (n_l + 1)! \cdots n_\infty!}\right)^{-1/2}$$

$$\times f(n_1, \ldots, n_i - 1, \ldots n_k + 1, \ldots, n_j - 1, \ldots, n_k + 1, \ldots, n_\infty, t)$$

$$\times\, n_i (n_j - \delta_{ij}) \langle ij | \hat{V} | kl \rangle$$

Multiplying through by $\left(\frac{N!}{n_1! n_2! \cdots n_\infty!}\right)^{1/2}$, we get

$$i\hbar \frac{\partial}{\partial t} f(n_1, n_2, \ldots, n_\infty, t)$$

$$= \sum_i \sum_j \sqrt{n_i}\sqrt{n_j + 1}\, f(n_1, \ldots, n_i - 1, \ldots, n_j + 1, \ldots, n_\infty, t) \langle i | \hat{T} | j \rangle$$

$$+ \frac{1}{2} \sum_i \sum_j \sum_k \sum_l \sqrt{n_i}\sqrt{n_k + 1}\sqrt{n_j}\sqrt{n_l + 1}$$

$$\times f(n_1, \ldots, n_i - 1, \ldots, n_k + 1, \ldots, n_j - 1, \ldots, n_\ell + 1, \ldots, n_\infty, t)$$

$$\times n_i (n_j - \delta_{ij}) \langle ij | \hat{V} | k\ell \rangle$$

which we solve for $f(n_1, n_2, \ldots, n_\infty, t)$ to get $\Psi(x_1, \ldots, x_N, t)$ on page 6. Is there a better way to handle our N-particle system?

Consider the "N-representation" of the state of the system

$$|\Psi(t)\rangle = \sum_{n_1 n_2 \ldots n_\infty} f(n_1, n_2, \ldots, n_\infty, t) \, |n_1 n_2 \cdots n_\infty\rangle$$

with $f(n_1, n_2, \ldots, n_\infty, t)$ defined as before. Then

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \sum_{n_1 n_2 \ldots n_\infty} i\hbar \frac{\partial}{\partial t} f(n_1, n_2, \ldots, n_\infty, t) \, |n_1 n_2 \ldots n_\infty\rangle$$

Consider the kinetic energy term in our equation for

$$\frac{\partial}{\partial t} f(n_1, n_2, \ldots, n_\infty, t)$$

which gives

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle \Big|_{KE}$$

$$= \sum_{n_1 n_2 \cdots n_\infty} \sum_i \sum_j f(n_1, \ldots, n_i - 1, \ldots, n_j + 1, \ldots, n_\infty, t) \langle i | \hat{T} | j \rangle$$
$$\times \sqrt{n_i} \sqrt{n_j + 1} \, |n_1 n_2 \cdots n_\infty\rangle$$

$$\underbrace{\sqrt{n_i}\,\sqrt{n_j+1}}_{\sqrt{n_i'+1}\,\sqrt{n_j'}}\,|n_1 n_2 \ldots \infty\rangle \qquad \text{so we can start } n_i' \text{ sum } \cancel{\text{at}}\ 0$$

$$\sum_{n_i=0}^{N} \to \sum_{n_i'=-1}^{N-1} = \sum_{n_i'=0}^{N-1} \simeq \sum_{n_i'=0}^{N}$$

Define

$n_i' \equiv n_i - 1$ $\qquad n_i = 0,\ldots \qquad n_i' = -1,\ldots$ $\qquad$ but $\sqrt{n_i'+1} = 0$ when $n_i' = -1$

$n_j' \equiv n_j + 1$ $\qquad n_j = 0,\ldots \qquad n_j' = 1,\ldots$ $\qquad$ not 0, but this is okay since $\sqrt{n_j'} = 0$ when $n_j' = 0$

$n_k' = n_k \qquad k \neq i$ or j

with $\sum_k n_k' = \sum_k n_k = N$

so we can start n_j' sum $\cancel{\text{at}}$ 0

$\Rightarrow$ we can extend the sum $\sum_{n_1 n_2 \ldots n_\infty}$ to $\sum_{n_1' n_2' \ldots n_\infty'}$ without difficulty

Then

$i\hbar \dfrac{\partial |\Psi\rangle}{\partial t}$

$$= \sum_{n_1' n_2' \ldots n_\infty'} \sum_i \sum_j$$

$$\times f(n_1', \ldots, n_i', \ldots, n_j', \ldots, n_\infty', t)\ \langle i|\hat{T}|j\rangle$$

$$\times \underbrace{\sqrt{n_i'+1}\,\sqrt{n_j'}\ |n_1' \ldots n_i'+1 \ldots n_j'-1 \ldots n_\infty'\rangle}_{} + \ldots$$

$$= \hat{a}_i^\dagger \hat{a}_j\,|n_1' \ldots n_i' \ldots n_j' \ldots n_\infty'\rangle$$

That is, in the N-representation

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = \ldots + \sum_i \sum_j \langle i|\hat{T}|j\rangle \hat{a}_i^\dagger \hat{a}_j |\Psi(t)\rangle + \ldots$$

One can go through the same analysis for the potential term, and the Schroedinger equation becomes

$$i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = \sum_{ij} \langle i|\hat{T}|j\rangle \hat{a}_i^\dagger \hat{a}_j |\Psi(t)\rangle$$

$$+ \sum_{ijkl} \langle ij|\hat{V}|kl\rangle \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k |\Psi(t)\rangle$$

$$= \hat{H}|\Psi(t)\rangle$$

Note the order, which applies to both bosons and fermions. For bosons, the order does not matter.

Now introduce the field operators

$$\hat{\psi}(x) \equiv \sum_k \psi_k(x)\, \hat{a}_k$$

$$\hat{\psi}^\dagger(x) \equiv \sum_k \psi_k^\dagger(x)\, \hat{a}_k^\dagger$$

Instead of creating and annihilating a particle in state $|k\rangle$, these operators (given the superposition over k) create and annihilate particles at x in state $\psi_k(x)$.

Then

$$\int d^3x\, \hat{\psi}^\dagger(x)\, \hat{T}(x)\, \hat{\psi}(x)$$

$$= \int d^3x \sum_i \psi_i^*(x)\hat{a}_i^\dagger \hat{T}(x) \sum_j \psi_j(x)\hat{a}_j$$

$$= \sum_{ij} \hat{a}_i^\dagger \left[\int d^3x \, \psi_i^*(x) \hat{T}(x) \psi_j(x)\right] \hat{a}_j$$

$$= \sum_i \sum_j \hat{a}_i^\dagger \langle i | \hat{T} | j \rangle \hat{a}_j$$

So the whole Hamiltonian operator can be written

$$\hat{H} = \int d^3x \, \hat{\psi}^\dagger(x) \hat{T} \hat{\psi}(x) + \frac{1}{2}\int d^3x \int d^3x' \, \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') \hat{V}(x,x') \hat{\psi}(x') \hat{\psi}(x)$$