2ND QUANTIZATION FORMALISM

6th LECTURE
FROM THE COURSE
QUANTUM PHYSICS OF LOW DIMENSIONAL STRUCTURES

QPLDS

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CONTENTS

OCCUPATION NUMBER REPRESENTATION FOR MANY-BODY PROBLEM

As the issue goes only with the procedure of specification:

1) is the single-particle level occupied or not,
2) what is an occupation number for a given level,

thus, it is the highest time to give up from the clumsy notation

$$\Phi^B(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2,...,\vec{r}_N\sigma_N)=\sum_{L_i}^{N}C_{L_i}\Phi^B_{L_i}$$ for bosons,

$$\Phi^F(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2,...,\vec{r}_N\sigma_N)=\sum_{L_i}^{N}C_{L_i}\Phi^F_{L_i}$$ for fermions

and to apply the following

$$|n_1...n_k...>$$

where n_k is the number of particles at the level (is like a single-particle level) ϕ_k .

Thus:

$$n_k=\begin{cases}0,\\1.\end{cases}$$ for fermions,

n_k - not restricted for bosons,

However

$\sum_i n_i = N$ for systems with well-defined number of particles *N*.

Remark: the notation of $|n_1 \ldots n_k \ldots >$ enables easy description of systems with variable number of particles

CREATION AND ANNIHILATION OPERATORS

BOSONS

$$a_k \,|...,n_k,...>=\sqrt{n_k}\,|...,n_k-1,...>$$

$$a_k^+ \,|...,n_k,...>=\sqrt{n_k+1}\,|...,n_k+1,...>$$

$$a_k a_k^+ \,|\, n_k>=(n_k+1)\,|\, n_k>$$

$$\boxed{a_k^+ a_k \,|\, n_k>=n_k \,|\, n_k>}$$ - this is the occupation number equation in the *k*-state

also:

$$(a_k a_k^+ - a_k^+ a_k)\,|\, n_k>=|\, n_k>$$

$$a_k a_k^+ - a_k^+ a_k \equiv [a_k, a_k^+]=1$$

$$[a_k, a_{k'}^+]=\delta_{kk'}$$

$$[a_k, a_{k'}]=0$$

$$[a_k^+, a_{k'}^+]=0$$

FERMIONS

as

$$n_k = \begin{cases} 0, \\ 1. \end{cases}$$

for fermions, the simplest way to express this fact using the state vector is to write it as

$$a_k \,|.....1... >= (-1)^m \,|\underbrace{.....}_{m}0... >$$

or

$$a_k \,|.....0... >= 0\,.$$

However this notation does not clearly numerates the *k*-state. Thus, it's better to write

$$a_k \,|.....k... >= (-1)^m \,|\underbrace{.....}_{m}k... >$$

and

$$a_k \,|....\not{k}... >= 0\,,$$

$$a_k^+ \,|.....\not{k}... >= (-1)^m \,|\underbrace{....}_{m}k... >\,,$$

$$a_k^+ \,|.....k... >= 0\,.$$

Is that any equivalence for the occupation number operator $a_k^+ a_k$ applied additionally in the boson-like formalism?

Case $k' \neq k$ and creation-destruction sequence in the $a_k^+ a_k$ operator:

$$a_{k'}^+ a_k \,|...k'\underbrace{...}_{m}k... >= (-1)^m \,|...k'\underbrace{...}_{m}k... >$$

If $k'=k$ then

$$a_k^+ a_k \,|...k... >= a_k^+ (-1)^m \,|...k... >= (-1)^m (-1)^m \,|...k... >= 1|\underbrace{...}_{m}k... >$$

and also $a_k^+ a_k \,|...k... >= 0$.

Case $k' \neq k$ and the destruction-creation sequence in the $a_k a_k^+$ operator:

$$a_k a_{k'}^+ \,|...k'\underbrace{...}_{m}k... >= (-1)^{m-1} \,|...k'\underbrace{...}_{m}k... >$$

If $k'=k$ then $a_k a_k^+ \,|... k... >= 0$

and also $a_k a_k^+ \,|...k... >=|...k... >$.

Conclusions:

1) for fermions $a_k^+ a_k$ works as the occupation number of the state k

2) for fermions $a_k a_k^+$ works as the unoccupation number of the state k

Besides, for fermions the anticommutation relations are valid:

$$a_{k'}^+ a_k + a_k a_{k'}^+ = \delta_{k'k} ,$$

$$a_{k'} a_k + a_k a_{k'} = 0 ,$$

$$a_{k'}^+ a_k^+ + a_k^+ a_{k'}^+ = 0$$

NUMBER OPERATOR - summary

Attention!

The operator $a_k^+ a_k = N_k$ is the single state operator – it acts on a given k-state only, thus:

$$\boxed{N_k \mid ...n_k... >= n_k \mid ...n_k... >}.$$

We can define then the total number occupation operator *N:*

$$\boxed{N = \sum_k N_k}$$

constructed from a single states operators.

The N operator is similar to both a_k and a_k^+ acting on bosons states. These similarities are visible in the commutation relations:

$$[N_k, N_{k'}] = 0 \text{ , as } [a_k, a_{k'}] = 0 \text{ or } [a_k^+, a_{k'}^+] = 0 .$$

IMPORTANTLY,
(BOTH FOR BOSONS AND FERMIONS STATISTICS)

Eigen-values of $\boxed{N = \sum_k N_k}$ are equal to $\boxed{n = \sum_k n_k}$

AND ADDITIONALLY
(BOTH FOR BOSONS AND FERMIONS STATISTICS)

$$[N_k, a_k] = -a_k \text{ and } [N_k, a_k^+] = a_k^+$$

These conditions say us that there is no restrictions in number of objects in the occupation number.

VACUUM STATE

Let's imagine that we repeat following operation acting on different states (using different k)

$$a_k \,|...k...>= (-1)^m \,|...\not{k}...>$$

and, after that, finally we get a limit, the vacuum state $|0>$

$$a_k^+ \,|0>=|k>$$

for an arbitrary k

ALSO (for all k)

$$a_k \,|0>= 0 \text{, and } <0|0>=1$$

OPERATORS IN A SECOND QUANTITAZED FORM

$$H = T + V = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j}u(\vec{r}_i,\vec{r}_j) \quad \text{(old formalism)}$$

$\boxed{T = \sum_{\vec{k}}\frac{\hbar^2 k^2}{2m}a_{\vec{k}}^{+}a_{\vec{k}}}$, $E_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$ are single-particle state-energies lying on a diagonal of the $< \vec{k}_i \mid T \mid \vec{k}_j >$ matrix $(i = j)$.

Next,

$$\boxed{V = \frac{1}{2}\sum_{\vec{k}_1\vec{k}_2\vec{k}_1'\vec{k}_2'} < \vec{k}_1\vec{k}_2 \mid u \mid \vec{k}_1'\vec{k}_2' > a_{\vec{k}_1}^{+}a_{\vec{k}_2}^{+}a_{\vec{k}_1'}a_{\vec{k}_2'}}$$

Remark: the $\vec{k}$ subscript is referred to momentum and spin, in general.

It is possible to choose alternative set of single particle states, not $\phi_{\vec{k}}$, but say ϕ_α in such a way, that off diagonal elements in the $< \alpha \mid T \mid \beta >$ matrix will be accessible. Thus,

$$H = \sum < \alpha \mid T \mid \beta > c_\alpha^{+}c_\beta + 1/2\sum < \alpha\beta \mid u \mid \delta\gamma > c_\alpha^{+}c_\beta^{+}c_\gamma c_\delta$$

FIELD OPERATORS (there is no wave $\psi(\vec{r})$, but the operator)

$$\psi(\vec{r}) = \sum_k a_k \phi_k(\vec{r})$$

$$\psi^+(\vec{r}) = \sum_k a_k^+ \phi_k^*(\vec{r})$$

$$[\psi(\vec{r}), \psi^+(\vec{r}')] = \delta(\vec{r} - \vec{r}')$$

$$[\psi(\vec{r}), \psi\ (\vec{r}')] = [\psi^+(\vec{r}), \psi^+(\vec{r}')] = 0$$

$$N = \sum_k N_k = \sum_k a_k^+ a_k \equiv \int \psi^+(\vec{r})\psi(\vec{r})\, d\vec{r} = \int \sum_{kk'} a_k^+ \phi_k^*(\vec{r})\, a_{k'} \phi_{k'}(\vec{r})\, d\vec{r} =$$

$$= < \psi \mid \psi >$$

$$V = \frac{1}{2} \sum_{k_1 k_2 k_1' k_2'} \iint \phi_{k_1}^*(\vec{r}_1)\phi_{k_2}^*(\vec{r}_2) u(\vec{r}_1, \vec{r}_2) \phi_{k_1'}(\vec{r}_1)\phi_{k_2'}(\vec{r}_2) \times a_{k_2}^+ a_{k_1}^+ a_{k_1'} a_{k_2'}\, d\vec{r}_1 d\vec{r}_2 =$$

$$= \frac{1}{2} \iint \psi^+(\vec{r}_2)\psi^+(\vec{r}_1) u(\vec{r}_1, \vec{r}_2) \psi(\vec{r}_1)\psi(\vec{r}_2)\, d\vec{r}_1 d\vec{r}_2 =$$

$$= \frac{1}{2} < \psi_2 \psi_1 \mid u \mid \psi_1 \psi_2 >$$

THE FUNDAMENTAL QUESTION

WHAT IS A DIFFERENCE BETWEEN OPERATORS EXPRESSED IN 1ST-QUANTIZATION FORMALIZM AND 2ND-QUANTIZATION FORMALIZM ?

like in

$$V = \frac{1}{2}\iint \psi^{+}(\vec{r}_2)\psi^{+}(\vec{r}_1)u(\vec{r}_1,\vec{r}_2)\psi(\vec{r}_1)\psi(\vec{r}_2)d\vec{r}_1 d\vec{r}_2 =$$

$$= \frac{1}{2}\underbrace{< \psi_2\psi_1 |\ \overbrace{u(\vec{r}_1,\vec{r}_2)}^{1^{st}\ quantization\ operator}\ | \psi_1\psi_2 >}_{2^{nd}\ quantization\quad operator}$$

However, more details about relation between both types of operators can be explained using the Green function formalism. In order to provide some imaginations let's write down following expressions for the operator expressed in the 2nd-quantization formalism

$$\hat{J} = < \alpha | J | \beta > a_\alpha^{+} a_\beta = \sum_{\alpha,\chi} \psi_\beta^{+}(\vec{r}',t') J_{\beta\alpha}(\vec{r}) \psi_\alpha(\vec{r},t)$$

$$< \hat{J}(\vec{r}) >= \frac{< \Psi_0 \mid \hat{J} \mid \Psi_0 >}{< \Psi_0 \mid \Psi_0 >} = \lim_{t'' \to t^+} \lim_{\vec{r}' \to \vec{r}} \sum_{\alpha,\beta} J_{\beta\alpha}(\vec{r}) \frac{< \Psi_0 \mid \psi_\beta^+(\vec{r}', t')\psi_\alpha(\vec{r}, t) \mid \Psi_0 >}{< \Psi_0 \mid \Psi_0 >} =$$

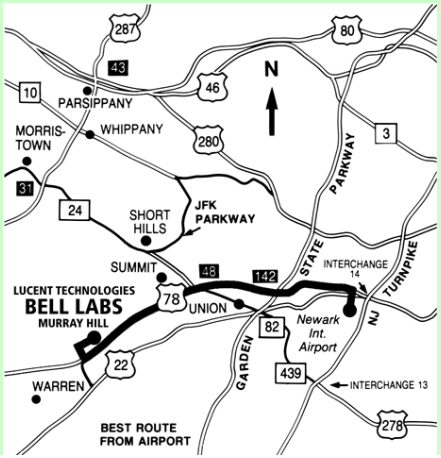
$$= \pm i \lim_{t'' \to t^+} \lim_{\vec{r}' \to \vec{r}} \sum_{\alpha,\beta} J_{\beta\alpha}(\vec{r}) G_{\alpha\beta}(\vec{r}t, \vec{r}'t')$$

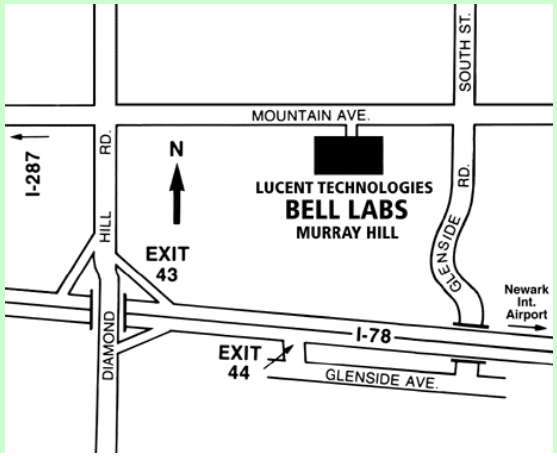
Thus, the average value is expressed by the Green function $G(\vec{r}t, \vec{r}'t')$

$$< \hat{J}(\vec{r}) >= \pm i \lim_{t' \to t^+} \lim_{\vec{r}' \to \vec{r}} tr[J(\vec{r}) G(\vec{r}t, \vec{r}'t')]$$

FIRST EXAMPLE

Bell-Labs, Murray-Hills, New Jersey





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Localized Magnetic States in Metals

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The conditions necessary in metals for the presence or absence of localized moments on solute ions containing inner shell electrons are analyzed. A self-consistent Hartree-Fock treatment shows that there is a sharp transition between the magnetic state and the nonmagnetic state, depending on the density of states of free electrons, the *s-d* admixture matrix elements, and the Coulomb correlation integral in the *d* shell; that in the magnetic state the *d* polarization can be reduced rather severely to nonintegral values, without appreciable free electron polarization because of a compensation effect; and that in the nonmagnetic state the virtual localized *d* level tends to lie near the Fermi surface. It is emphasized that the condition for the magnetic state depends on the Coulomb (i.e., exchange self-energy) integral, and that the usual type of exchange alone is not large enough in *d*-shell ions to allow magnetic moments to be present. We show that the susceptibility and specific heat due to the inner shell electrons show strongly contrasting behavior even in the nonmagnetic state. A calculation including degenerate *d* orbitals and *d-d* exchange shows that the orbital angular momentum can be quenched, even when localized spin moments exist, and even on an isolated magnetic atom, by kinetic energy effects.

THE THEORY OF MAGNETIC METALLIC IMPURITIES DISSOLVED IN NONMAGNETIC METALLIC PHASE

Hamiltonian: $H_{tot} = H_{0f} + H_{0d} + H_{corr} + H_{sd}$, where:

unperturbed energy of the free-electron system (being in the s state)

$$H_{0f} = \sum_{k,\sigma} E_{k\sigma} c^{+}_{k\sigma} c_{k\sigma}$$

unperturbed energy of the “d” electron-state of the impurity atom

$$H_{0d} = E(n_{d+} + n_{d-}) = E\sum_{\sigma} d^{+}_{\sigma} d_{\sigma}$$

The repulsive energy between d-states (within the impurity atom)

$$H_{corr} = U \cdot n_{d\uparrow} n_{d\downarrow} = < \phi_d(1)\phi_d(1) | \frac{e^2}{r_{12}} | \phi_d(2)\phi_d(2) > \cdot n_{d\uparrow} n_{d\downarrow} =$$

$$= U \cdot d^{+}_{\uparrow} d_{\uparrow} d^{+}_{\downarrow} d_{\downarrow}$$

The energy of interaction between *s* free-electrons and the impurity *d* states

$$H_{sd} = \sum_{k,\sigma} V_{dk} (c^{+}_{k\sigma} d_{\sigma} + d^{+}_{\sigma} c_{k\sigma})$$