II. QUANTUM FIELD THEORY, GREEN'S FUNCTION, AND PERTURBATION THEORY: SOME ADDITIONAL NOTES

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A. Perturbation series, time ordering

In the interaction representation, operators become a formal "time" dependence

$$O(\tau) = e^{\tau(H_0-\mu N)} O e^{-\tau(H_0-\mu N} \tag{1}$$

and the evaluation of the partition function at imaginary time $\beta = 1/k_B T$ is pushed into a matrix $\mathcal{A}(\tau)$ defined via

$$\begin{aligned} e^{-\tau(H-\mu N)} &= e^{-\tau(H_0-\mu N)}\mathcal{A}(\tau) \\ e^{\tau(H-\mu N)} &= \mathcal{A}^{-1}(\tau) e^{\tau(H_0-\mu N)} \end{aligned} \tag{2}$$

which plays the role of the S-matrix. We can obtain an explicit representation of $\mathcal{A}$ differentiating the first equation with respect to τ leading to

$$\frac{d\mathcal{A}(\tau)}{d\tau} = -V(\tau)\mathcal{A}(\tau) \tag{3}$$

The formal solution of this differential equation satisfying the initial value $A(\tau = 0) = 1$ has the form

$$\mathcal{A}(\tau) = 1 - \int_0^\tau d\tau_1 V(\tau_1) + \int_0^\tau d\tau_1 V(\tau_1) \int_0^{\tau_1} d\tau_2 V(\tau_2) - \int_0^\tau d\tau_1 V(\tau_1) \int_0^{\tau_1} d\tau_2 V(\tau_2) \int_0^{\tau_2} d\tau_3 V(\tau_3) + \dots \tag{4}$$

$$= 1 + \sum_{n=1}^{\infty} (-1)^n \int_0^\tau d\tau_1 V(\tau_1) \int_0^{\tau_1} d\tau_2 V(\tau_2) \cdots \int_0^{\tau_{n-1}} d\tau_n V(\tau_n) \tag{5}$$

We can verify this solution by direct differentiation. Note that the integration which goes up to τ must always be on the most left place, since V is an operator. In order to formally sum up all the terms of the series one is tempted to use the symmetry of the integrands with respect to the τ_i's and use the symmetrized expression, e.g. in the nth order term

$$\int_0^\tau d\tau_1 V(\tau_1) \int_0^{\tau_1} d\tau_2 V(\tau_2) \cdots \int_0^{\tau_{n-1}} d\tau_n V(\tau_n) = \frac{1}{n!} \int_0^\tau d\tau_1 V(\tau_1) \int_0^\tau d\tau_2 V(\tau_2) \cdots \int_0^\tau d\tau_n V(\tau_n) \quad \textbf{(Not True!)} \tag{6}$$

Such a symmetrization is valid for usual functions, however, it is in general not true for operators since $V(\tau)$ does not necessarily commute with $V(\tau' \neq \tau)$. Introducing the "time-ordering" operator T_τ defined by

$$T_\tau \left[V(\tau)V(\tau') \right] = \begin{cases} V(\tau)V(\tau') \text{for } \tau > \tau' \\ \pm V(\tau')V(\tau) \text{for } \tau < \tau' \end{cases} \tag{7}$$

where the $\pm$ sign has to be used for bosonic/fermionic operators V. Note that our interaction operator is in general a bosonic operator, since the Hamiltonian is invariant against any permutations of particle labels. The generalization for fermionic operators is convienient in later calculations involving intermediate steps; as long as V is bosonic, this definition does not affect any final results.

Extending the time-ordering operator to general products, we can now correct Eq. (6) formally to

$$\int_0^\tau d\tau_1 V(\tau_1) \int_0^{\tau_1} d\tau_2 V(\tau_2) \cdots \int_0^{\tau_{n-1}} d\tau_n V(\tau_n) = T_\tau \left[\frac{1}{n!} \int_0^\tau d\tau_1 V(\tau_1) \int_0^\tau d\tau_2 V(\tau_2) \cdots \int_0^\tau d\tau_n V(\tau_n) \right] \tag{8}$$

and thus resum the series to obtain the formally exact expression

$$\mathcal{A}(\tau) = T_\tau \exp\left\{ -\int_0^\tau V(\tau')\, d\tau' \right\} \tag{9}$$

where T_τ now takes care to arrange the operators from the left to the right in order of decreasing τ.

The partition function then writes

$$Z = \mathrm{Tr}\left\{ e^{-\beta(H_0-\mu N)} T_\tau \exp\left[-\int_0^\beta V(\tau')\, d\tau' \right] \right\} \tag{10}$$

Expanding the exponential on the rhs we obtain the perturbation series in power of V

$$\frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \cdots \int_0^\beta d\tau_n \left\langle T_\tau \left[V(\tau_1) V(\tau_2) \ldots V(\tau_n) \right] \right\rangle_0 \tag{11}$$

where $\langle \ldots \rangle_0$ is the average corresponding to the reference

B. Wick's..

Let us illustrate now how to perform the first terms in the perturbation expansion specializing to the usual translational invariant Hamiltonian

$$H_0 - \mu N = \int d\mathbf{r} \Psi^\dagger \left[-\frac{\hbar^2}{2m} \nabla^2 - \mu \right] \Psi(\mathbf{r}) \tag{12}$$

and

$$V = \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \Psi^\dagger(\mathbf{r}) \Psi^\dagger(\mathbf{r}') v(|\mathbf{r}-\mathbf{r}'|) \Psi(\mathbf{r}') \Psi(\mathbf{r}) \tag{13}$$

in second quantized form, where $\Psi^\dagger(\mathbf{r})$ and $\Psi(\mathbf{r})$ are creation and annihilation operators of the bosonic/fermionic field at $\mathbf{r}$. When the imaginary time variable is not explicitly indicated, we refer to a fixed time, e.g. $\tau = 0$. The (anti-) commutation for bosonic (fermionic) fields write

$$[\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')]_\mp = \delta(\mathbf{r}-\mathbf{r}') \tag{14}$$

Let us now introduce the following extension of the interaction representation of the operators given in Eq. (1) to field operators using the convention that

$$\Psi(\mathbf{r}\tau) \equiv e^{\tau(H_0-\mu N)} \Psi(\mathbf{r}) r^{-\tau(H_0-\mu N)} \tag{15}$$

$$\Psi^\dagger(\mathbf{r}\tau) \equiv e^{\tau(H_0-\mu N)} \Psi^\dagger(\mathbf{r}) r^{-\tau(H_0-\mu N)} \tag{16}$$

so that $\Psi^\dagger(\mathbf{r}\tau)$ is not the hermitian operator of $\Psi(\mathbf{r}\tau)$ (however, the analytic continuations of the operators, $\Psi(\mathbf{r}t)$ and $\Psi^\dagger(\mathbf{r}t)$, to "real time" t, $\tau \to it$, are hermitian). We further extend our time-ordering introduced above for the interaction operator for the field operators

$$T_\tau \left[\Psi(\mathbf{r},\tau) \Psi^\dagger(\mathbf{r}'\tau') \right] = \begin{cases} \Psi(\mathbf{r},\tau)\Psi^\dagger(\mathbf{r}'\tau') \text{for } \tau > \tau' \\ \pm\Psi^\dagger(\mathbf{r}',\tau')\Psi(\mathbf{r}\tau) \text{for } \tau < \tau' \end{cases} \tag{17}$$

where now the negative sign for fermionic fields will come into play.

Our reference Hamiltonian, H_0, is in general chosen such that it can be solved exactly, e.g. we can diagonalize Eq. (12) in Fourier space with the mode decomposition of the field opertor

$$\Psi(\mathbf{r}) = \frac{1}{V^{1/2}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}} \tag{18}$$

where $a_{\mathbf{k}}$ is the annihilation of a particle of wave vector $\mathbf{k}$ (momentum up to $\hbar$) and similar

$$\Psi^\dagger(\mathbf{r}) = \frac{1}{V^{1/2}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} a^\dagger_{\mathbf{k}} \tag{19}$$

for the field creation operator.

Plugging into Eq. (12) we get

$$H_0 - \mu N = \sum_{\mathbf{k}} \varepsilon_k a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \tag{20}$$

with $\varepsilon_k = \hbar^2 k^2/2m - \mu$ and the (anti-)commutation relations, Eq. (14), imply

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}^\dagger]_\mp = \delta_{\mathbf{k},\mathbf{k}'} \tag{21}$$

We can now work out the imaginary time dependence of the field operators using

$$a_{\mathbf{q}}(\tau) = e^{\tau H_0} a_{\mathbf{q}} e^{-\tau H_0} \tag{22}$$

$$= e^{\varepsilon_{\mathbf{q}}\tau a_{\mathbf{q}}^\dagger a_{\mathbf{q}}} a_{\mathbf{q}} e^{-\varepsilon_{\mathbf{q}}\tau a_{\mathbf{q}}^\dagger a_{\mathbf{q}}} \tag{23}$$

where we have used the commutation of operators with different momenta, e.q. $\exp[\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \tau a_{\mathbf{k}}^\dagger a_{\mathbf{k}}] = \prod_k \exp[\varepsilon_{\mathbf{k}} \tau a_{\mathbf{k}}^\dagger a_{\mathbf{k}}]$ Differentiation with respect to τ gives

$$\frac{d}{d\tau} a_{\mathbf{q}}(\tau) = e^{\varepsilon_{\mathbf{q}}\tau a_{\mathbf{q}}^\dagger a_{\mathbf{q}}} \varepsilon_q [a_{\mathbf{q}}^\dagger a_{\mathbf{q}}, a_{\mathbf{q}}]_- e^{-\varepsilon_{\mathbf{q}}\tau a_{\mathbf{q}}^\dagger a_{\mathbf{q}}} = \varepsilon_q a_{\mathbf{q}}(\tau) \tag{24}$$

(For fermions, one has to use that $a_{\mathbf{q}} a_{\mathbf{q}} = a_{\mathbf{q}}^\dagger a_{\mathbf{q}}^\dagger = 0$ due to the anticommuation (Pauli principle: maximal one fermion per state!). We can now integrate together with $a_{\mathbf{q}}(0) \equiv a_{\mathbf{q}}$ to give

$$a_{\mathbf{q}}(\tau) = e^{-\varepsilon_q \tau} a_{\mathbf{q}} \tag{25}$$

and similar

$$a_{\mathbf{q}}^\dagger(\tau) = e^{\varepsilon_q \tau} a_{\mathbf{q}}^\dagger \tag{26}$$

Note that we have managed to replace a time-dependence involving an operator in the exponantial to an exponential containing only numbers.

Since any second quatized operator can be expressed in terms of field operators, using the eigen-mode decompositions in terms of $a_{\mathbf{k}}$s, we can thus simplify the time dependence of the interaction operator in general expressions as Eq. (5) using

$$a_{\mathbf{k}_l}(\tau_l) \ldots a_{\mathbf{k}_m}^\dagger(\tau_m) \cdots a_{\mathbf{k}_n}^\dagger(\tau_n) \cdots = e^{-\tau_l \varepsilon_{\mathbf{k}_l} + \tau_m \varepsilon_{\mathbf{k}_m} + \tau_n \varepsilon_{\mathbf{k}_n}} a_{\mathbf{k}_l} \cdots a_{\mathbf{k}_m}^\dagger \cdots a_{\mathbf{k}_n}^\dagger \cdots \tag{27}$$

Note that the non-interacting reference Hamiltonian will not contain any time-dependence as

$$e^{\tau(H_0-\mu)} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} e^{-\tau(H_0-\mu)} = a_{\mathbf{k}}^\dagger(\tau) a_{\mathbf{k}}(\tau) = a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \tag{28}$$

The calculation of the partition function then necessitates that we have to calculate the expectation value of such a generic expression with respect to the non-interacting system, e.g.

$$\langle a_{\mathbf{k}_l} \cdots a_{\mathbf{k}_m}^\dagger \cdots a_{\mathbf{k}_n}^\dagger \cdots \rangle_0 = \frac{1}{Z_0} \mathrm{Tr} \left[e^{-\beta(H_0 - \mu N)} a_{\mathbf{k}_l} \cdots a_{\mathbf{k}_m}^\dagger \cdots a_{\mathbf{k}_n}^\dagger \cdots \right] \tag{29}$$

Such expressions can now be evaluated as $H_0 - \mu N$ is diagonal in $\mathbf{k}$ and $n_{\mathbf{k}} = a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ simply counts the number of particles in mode $\mathbf{k}$ without changing them. Therefore, every time we create (annihilate) a particle, e.g. $a_{\mathbf{k}}^\dagger$, we also have to destroy (create) it again.

Explicitly, let us note that the partition function of the non-interacting system, Z_0, factorizes, $Z = \prod_{\mathbf{q}} z_{\mathbf{q}}$, with

$$z_q^B = \mathrm{Tr} e^{-\beta\varepsilon_q a_{\mathbf{q}}^\dagger a_{\mathbf{q}}} = \sum_{n=0}^{\infty} e^{-\beta n \varepsilon_q} = \frac{1}{1 - e^{\beta\varepsilon_q}} \tag{30}$$

for bosons, and

$$z_q^F = \mathrm{Tr} e^{-\beta\varepsilon_q a_{\mathbf{q}}^\dagger a_{\mathbf{q}}} = 1 + e^{-\beta n \varepsilon_q} \tag{31}$$

for fermions.

We then have

$$
\begin{aligned}
\langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{q}} \rangle_0 &= \delta_{\mathbf{k},\mathbf{q}} \langle n_{\mathbf{q}} \rangle & (32) \\
&= -\delta_{\mathbf{k},\mathbf{q}} - \frac{\partial \log z_{\mathbf{q}}}{\partial(\beta \varepsilon_q)} & (33) \\
&= \delta_{\mathbf{k},\mathbf{q}} \frac{1}{e^{\beta\varepsilon} \mp 1} & (34)
\end{aligned}
$$

which is our well known Bose/Fermi distribution of the mean number of particles in mode $\mathbf{k}$. It is straighforward to extend to the other ordering $\langle a_{\mathbf{q}} a_{\mathbf{q}}^{\dagger} \rangle_0 = 1 \pm \langle a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} \rangle_0$.

Expressions involving three $a_{\mathbf{k}}$s identically vanish, so lets look at four,

$$
\langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} a_{\mathbf{k}} \rangle_0 = \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} \rangle_0 = \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle_0 \langle \mathbf{q}^{\dagger} a_{\mathbf{q}} \rangle_0 \tag{35}
$$

where we assumed $\mathbf{k} \neq \mathbf{q}$ for the moment. Different orders can be again treated straighforwardly using the commutation relations.

Let us discuss $\mathbf{k} = \mathbf{q}$, commuting one term, this can be worked out explicitly using

$$
\langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle_0 = \frac{\partial^2 \log z_k}{\partial(\beta \varepsilon_q)^2} \tag{36}
$$

We can see explicitly, that as long as we have no Bose-Einstein condensations, such a term remain of order or the mean occupation, $\langle n_{\mathbf{q}}^2 \rangle_0 \sim \langle n_{\mathbf{q}} \rangle_0 \sim \mathcal{O}(1)$. However, the expansion of $\Psi(\mathbf{r})$ in terms of $a_{\mathbf{k}}$ contains a factor $V^{-1/2}$ in front of the summation over all $\mathbf{k}$, so that all our expression, taking care of all summations and volume factors, terms involving double occupations (or higher) will be suppressed increasing with system size (usually by V^{-1} or higher. Excluding phenomena like BEC or BCS pairing, we can thus neglect all complications arising from such terms.

The general structure should then be clear

$$
\langle a_{\mathbf{k}}^{\dagger} \cdots a_{\mathbf{q}}^{\dagger} \cdots a_{\mathbf{k}} \cdots a_{\mathbf{q}} \cdots \rangle_0 = s \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle_0 \cdots \langle a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} \rangle_0 \cdots \tag{37}
$$

where s denots a possible sign since we have to commute the operators, say $a_{\mathbf{q}}$ until reaching $a_{\mathbf{q}}^{\dagger}$.

We now have (almost) Wick's theorem. We simply need to extend these considerations for the time-ordering. We have already taken care of the exponential factors involving τ, however the time ordering will affect the order of the creation and annilihation operators involved, in particular we may have $a_{\mathbf{q}}$ anywhere on the left of $a_{\mathbf{q}}^{\dagger}$, which we then commute just to the point where it is just on the left.