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**LETTER TO THE EDITOR**

# Derivation of Boltzmann equation in closed-time-path formalism

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**Abstract.** A systematic derivation of the Boltzmann equation is presented in the framework of closed-time-path formalism. Introducing a new type of probe, the expectation value of number operator is calculated as a functional of source. Then solving for the source by inverting the relation, the equation of motion for number is obtained when the source is removed, and it turns out to be the Boltzmann equation. The inversion formula is used in the course of derivation.

In this letter, we present a new approach to derive the Boltzmann equation (BE). There have been some works on this subject both in the framework of closed-time-path (CTP) formalism [1, 2], and in the framework of thermo-field dynamics [3]. These approaches have an advantage that the time dependence of the number is not introduced by hand. Instead, a counter-term is first introduced into the CTP or thermo-field Lagrangian and the bare propagator is calculated. Then to determine the counter-term, some condition, such as the cancellation of on-shell part of the self-energy [1, 3] or the cancellation of pinch-singularity [2], is adopted, which leads to the BE. Since their primal purpose is to construct the non-equilibrium perturbation theory, the BE appears as a byproduct. It is preferable if we can derive the BE more directly as an equation of motion (EM) of expectation value of the number operator. Moreover, in these approaches, the condition to determine the counter-term is of course not unique, and the approximation made is not so clear. In the following, a more direct approach is studied based on the inversion method [4, 5]. A new type of probe dictated from the counter-term approach is introduced in the course of the derivation.

Let us briefly describe the inversion method which is a systematic procedure to derive the EM in CTP formalism. In CTP formalism [6, 7], we introduce a time-dependent source $J$ to probe some operator of interest, say $Q(\hat{\varphi})$, which is a function of the dynamical variable $\hat{\varphi}$. Then with the Hamiltonian $\hat{H}$ of $\hat{\varphi}$, the CTP generating functional is defined as

$$e^{\frac{i}{\hbar}W[J_1,J_2]} \equiv \mathrm{Tr}\, T e^{-\frac{i}{\hbar}\int_{t_I}^{t_F} dt(\hat{H}-J_1(t)\hat{Q})}\hat{\rho}\,\tilde{T}e^{\frac{i}{\hbar}\int_{t_I}^{t_F} dt(\hat{H}-J_2(t)\hat{Q})} \tag{1}$$

$$\propto \int [d\varphi_1\, d\varphi_2]\langle\varphi_{1I}|\hat{\rho}|\varphi_{2I}\rangle e^{\frac{i}{\hbar}\int_{t_I}^{t_F} dt(L(\varphi_1)-L(\varphi_2)+J_1 Q(\varphi_1)-J_2 Q(\varphi_2))} \tag{2}$$

where $\hat{\rho}$ is the initial distribution and $T$ and $\tilde{T}$ are the time ordering and anti-ordering operators, respectively. The last equality is due to path-integral representation, where $\varphi_1$ and $\varphi_2$ are respectively introduced as integral variables along the forward and backward time branches.

For convenience of later discussion, let us introduce 'physical' representation [7] through $J_C \equiv \frac{1}{2}(J_1+J_2)$, and $J_\Delta \equiv J_1 - J_2$. Then $J_\Delta = 0$ is physical and $J_C$ plays the role of external force. The expectation value of $\hat{Q}$ at time $t$ under physical external source $J_C = J$ can be calculated as

$$Q(t) \equiv \left. \frac{\delta W[J_\Delta, J_C]}{\delta J_\Delta(t)} \right|_{\substack{J_C = J \\ J_\Delta = 0}} = \langle \hat{Q}(t) \rangle_J. \tag{3}$$

This gives us the expectation value $Q$ as a functional of external source $J$.

In order to obtain the EM of $Q$, we solve relation (3) inversely to express $J$ as a functional of $Q$. Then setting the external source $J = 0$, the obtained relation gives the EM of $Q$. (Inversion method, [5].) Formally, the general expression of the EM can be written with the Legendre transformation of $W$. But practically, the process of Legendre transformation is unnecessary and, in this letter, this inversion is carried out in the following perturbative fashion.

Usually $Q$ as a functional of $J$ is obtained as some perturbation series

$$Q(t) = f[t; J] = \sum_n \varepsilon^n f^{(n)}[t; J] \tag{4}$$

where $\varepsilon$ is a small parameter and $f[t; J]$ expresses that $f$ is a function of $t$ and functional of $J$. Then, if we write the inverted relation as

$$J(t) = g[t; Q] = \sum_m \varepsilon^m g^{(m)}[t; q] \tag{5}$$

the following simple identity is obtained:

$$\begin{aligned} Q(t) = f[t; g[Q]] &= f^{(0)}[t; g^{(0)}[Q]] \\ &+\varepsilon\left( \int \mathrm{d}s \frac{\delta f^{(0)}(t)}{\delta g^{(0)}(s)} g^{(1)}[s; Q] + f^{(1)}[t; g^{(0)}[Q]] \right) \\ &+\varepsilon^2 \left( \int \mathrm{d}s \frac{\delta f^{(0)}(t)}{\delta g^{(0)}(s)} g^{(2)}[s; Q] \right. \\ &+ \frac{1}{2} \int \mathrm{d}s\, \mathrm{d}s' \frac{\delta^2 f^{(0)}(t)}{\delta g^{(0)}(s) \delta g^{(0)}(s')} g^{(1)}[s; Q] g^{(1)}[s'; Q] \\ &+ \left. \int \mathrm{d}s \frac{\delta f^{(1)}(t)}{\delta g^{(0)}(s)} g^{(1)}[s; Q] + f^{(2)}[t; g^{(0)}[Q]] \right) + \mathrm{O}(\varepsilon^3) \end{aligned} \tag{6}$$

where, for example, $\delta f^{(0)}[t; J]/\delta J(s)$ evaluated at $J = g^{(0)}[Q]$ is abbreviated as $\delta f^{(0)}(t)/\delta g^{(0)}(s)$. Comparing the lhs and rhs in each order of $\varepsilon$, we obtain the expressions for $g^{(m)}$ in terms of $f^{(n)}$, which we call the 'inversion formulae' [5]:

$$g^{(0)}[t; q] = f^{(0)^{-1}}[t; q] \tag{7}$$

$$g^{(1)}[t; q] = -\int \mathrm{d}t' \left( \frac{\delta f^{(0)}}{\delta g^{(0)}} \right)^{-1} (t, t') f^{(1)}[t'; g^{(0)}] \tag{8}$$

$$\begin{aligned} g^{(2)}[t; q] = -\int \mathrm{d}t' \left( \frac{\delta f^{(0)}}{\delta g^{(0)}} \right)^{-1} (t, t') &\left( \frac{1}{2} \int \mathrm{d}s\, \mathrm{d}s' \frac{\delta^2 f^{(0)}(t')}{\delta g^{(0)}(s) \delta g^{(0)}(s')} g^{(1)}[s; Q] g^{(1)}[s'; Q] \right. \\ &+ \left. \int \mathrm{d}s \frac{\delta f^{(1)}(t')}{\delta g^{(0)}(s)} g^{(1)}[s; Q] + f^{(2)}[t'; g^{(0)}] \right). \end{aligned} \tag{9}$$

First of all, to make this method work, we need a non-trivial lowest-order functional expression $f^{(0)}[t; J]$ which can be inversely solved for $J$. This becomes the key-point for deriving the BE. If we naively apply this method to the number operator, the expectation value does not reveal such non-trivial dependence on $J$.

Let us examine the problem more closely. We consider a non-relativistic Boson field of a homogeneous system described by the Hamiltonian $H = H_0 + H_{\rm int}$ with $H_0 = \sum_k \epsilon_k \hat{\psi}_k^\dagger \hat{\psi}_k$, and $H_{\rm int} = \frac{\lambda}{4} \sum_{k,k',q} \hat{\psi}_{k+q}^\dagger \hat{\psi}_{k'-q}^\dagger \hat{\psi}_k \hat{\psi}_{k'}$, where $\lambda$ is a coupling constant, which is assumed to be small and plays the role of $\varepsilon$ in (4). Extension to other types of interaction is straightforward. For the initial density matrix $\hat{\rho}$, we assume that no initial correlation exists among the different wavenumber components and $\hat{\rho}$ can be written as a product form $\prod_k \hat{\rho}_k$, where $\hat{\rho}_k$ is a density for each wavenumber which gives $n_k(t_{\rm I}) = {\rm Tr}\ \hat{\rho}_k \hat{\psi}_k^\dagger \hat{\psi}_k$.

In order to derive the EM of the expectation value of the number $\hat{n}_k(t) = \hat{\psi}_k^\dagger(t)\hat{\psi}_k(t)$, a naive choice of the source is $\hat{H} - \sum_k J_k(t)\hat{\psi}_k^\dagger(t)\hat{\psi}_k(t)$. Then, in path-integral representation of the CTP generating functional, this source can be built into the free part of the Lagrangian as

$$L_0^J(\psi_1) - L_0^J(\psi_2) = \sum_k \psi_{i,k}^* \mathcal{D}_{ij,k} \psi_{j,k} \tag{10}$$

with the matrix

$$\mathcal{D}_k(t, \partial_t) \equiv \begin{pmatrix} {\rm i}\hbar\partial_t - \epsilon_k + J_k(t) & 0 \\ 0 & -{\rm i}\hbar\partial_t + \epsilon_k - J_k(t) \end{pmatrix}. \tag{11}$$

The bare propagator is essentially the inverse of the matrix in (11), and with this propagator, if we evaluate the expectation value $n_k(t)$ in the absence of interaction, we just obtain the initial value $\langle \hat{n}_k(t)\rangle_J = n_k(t_{\rm I})$, due to the conservation of $\hat{n}_k$ for $\lambda = 0$ even when $J_k \neq 0$. Since no dependence on $J$ appears, we fail to obtain the inversion in lowest order, and hence the inversion formulae cannot be used in this case. A probe of the form (11) is not enough to handle the number operator.

Then why does the counter-term method work? According to [1], the time-local counter-term is constructed so as to keep the following structure of the full propagator in CTP formalism (we suppress the index of wavenumber for a while):

$$\begin{aligned} G(t,s) &\equiv -{\rm Tr}\ \hat{\rho} \begin{pmatrix} T\hat{\psi}(t)\hat{\psi}^\dagger(s) & \hat{\psi}^\dagger(s)\hat{\psi}(t) \\ \hat{\psi}(t)\hat{\psi}^\dagger(s) & \tilde{T}\hat{\psi}(t)\hat{\psi}^\dagger(s) \end{pmatrix}_{\rm c} \\ &= \theta(t-s) \begin{pmatrix} h(t,s) & k(t,s) \\ h(t,s) & k(t,s) \end{pmatrix} + \theta(s-t) \begin{pmatrix} k^*(s,t) & k^*(s,t) \\ h^*(s,t) & h^*(s,t) \end{pmatrix} \end{aligned} \tag{12}$$

where 'c' means the connected part and

$$h(t,s) \equiv -\langle \hat{\psi}(t)\hat{\psi}^\dagger(s)\rangle_{\rm c} \qquad k(t,s) \equiv -\langle \hat{\psi}^\dagger(s)\hat{\psi}(t)\rangle_{\rm c}. \tag{13}$$

Then it turns out that the counter-term $\psi_i^* \mathcal{M}_{ij} \psi_j$ with the matrix

$$\mathcal{M}(t) = \begin{pmatrix} \hbar\Delta\omega(t) - {\rm i}\alpha(t) & -{\rm i}(\hbar\gamma(t) - \alpha(t)) \\ {\rm i}(\hbar\gamma(t) + \alpha(t)) & -\hbar\Delta\omega(t) - {\rm i}\alpha(t) \end{pmatrix} \tag{14}$$

is allowed to be subtracted from the free part of the Lagrangian, where $\Delta\omega$, $\alpha$ and $\gamma$ are all real functions which are determined by appropriate conditions. The bare propagator calculated from $L_0(\psi_1) - L_0(\psi_2) - \psi_i^* \mathcal{M}_{ij} \psi_j$ leads to non-trivial time dependence of the number in the absence of interaction. The existence of the parameters in non-diagonal elements is a crucial point.

Comparing (14) with (11), the parameter we have utilized as a physical external source in (11) corresponds to $\Delta\omega$ in (14). Equation (14), however, suggests that another physical source corresponding to $\alpha$ or $\gamma$ can be introduced as a probe. Our choice here is the source corresponding to $\alpha$. (The source corresponding to $\gamma$ can be treated similarly.) Then the free part of the Lagrangian including the source now has the matrix

$$\mathcal{D}(t, \partial_t) = \begin{pmatrix} {\rm i}\hbar\partial_t - \epsilon + {\rm i}J(t) & -{\rm i}J(t) \\ -{\rm i}J(t) & -{\rm i}\hbar\partial_t + \epsilon + {\rm i}J(t) \end{pmatrix}. \tag{15}$$

Note that although the source $J$ is introduced in this way, what we calculate in the following is just the expectation value of the number; we integrate $\psi_1^*(t+\varepsilon)\psi_1(t)$ under the existence of the probe (15). (Of course other choices, for example, $\psi_2^*(t-\varepsilon)\psi_2(t)$, produce the same results.)

From the matrix (15), the bare propagator $G_0$ is calculated by

$$\mathcal{D}(t,\partial_t)G_0(t,s) = G_0(t,s)\mathcal{D}(s,-\overleftarrow{\partial}_s) \tag{16}$$

$$= -\mathrm{i}\hbar\delta(t-s). \tag{17}$$

Since $\mathcal{D}$ has been chosen so as to keep the structure (12) unchanged, $G_0$ has the same structure in which $h$ and $k$ are replaced by $h_0$ and $k_0$, respectively. Then (17) leads to the equations

$$(\mathrm{i}\hbar\partial_t - \epsilon)h_0(t,s) = 0 \tag{18}$$

$$(\mathrm{i}\hbar\partial_t - \epsilon)k_0(t,s) = 0 \tag{19}$$

for $t > s$, and

$$(\mathrm{i}\hbar\partial_t - \epsilon + \mathrm{i}J(t))k_0^*(s,t) = \mathrm{i}J(t)h_0^*(s,t) \tag{20}$$

$$(\mathrm{i}\hbar\partial_t - \epsilon - \mathrm{i}J(t))h_0^*(s,t) = -\mathrm{i}J(t)k_0^*(s,t) \tag{21}$$

for $s > t$. The boundary conditions at $t = s$ are given as

$$h_0(s,s) - k_0^*(s,s) = -1 \qquad k_0(s,s) - h_0^*(s,s) = 1 \tag{22}$$

$$h_0(s,s) - h_0^*(s,s) = 0 \qquad k_0(s,s) - k_0^*(s,s) = 0. \tag{23}$$

From (23), $h_0(s,s)$ and $k_0(s,s)$ are real functions. Then the two conditions in (22) are identical and simply express the fact that the expectation value of the equal-time commutator $[\hat{\psi},\hat{\psi}^\dagger]$ is unity. Note that from definition (13), $k_0(t,t)$ gives the expectation value of the number operator (multiplied by $-1$) in the absence of interaction, which we denote as $n^{(0)}(t)$.

From (18) and (19), we obtain for $t > s$

$$k_0(t,s) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\epsilon(t-s)}k_0(s,s) = -n^{(0)}(s)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\epsilon(t-s)} \tag{24}$$

$$h_0(t,s) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\epsilon(t-s)}h_0(s,s) = -(n^{(0)}(s)+1)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\epsilon(t-s)}. \tag{25}$$

Then, exchanging $t$ and $s$ in (24) and (25) and taking the complex conjugation, $h_0^*(s,t)$ and $k_0^*(s,t)$ are obtained for $s > t$. Substituting them into (20) or (21), both equations turn out to give an identical result, and we find that $n^{(0)}$ must satisfy the condition

$$J(t) = \hbar\partial_t n^{(0)}(t) \tag{26}$$

which gives the EM for $n^{(0)}$ and is integrated as

$$n^{(0)}[t;J] = n^{(0)}(t_1) + \int_{t_1}^{t}\mathrm{d}s\,\frac{J(s)}{\hbar}. \tag{27}$$

Equations (24), (25) and (27) determine the bare propagator $G_0$ with the structure (12) in which $h$ and $g$ are replaced by $h_0$ and $g_0$, respectively.

As already seen from (27) or (26), we succeeded in making the expectation value of the number depend on $J$ in the lowest order, i.e. $\mathrm{O}(\lambda^0)$. This makes the inversion formula applicable. The rhs of equation (27) corresponds to the desired lowest-order functional $f^{(0)}$ in (4), and (26) is the inverted relation, the rhs of which corresponds to $g^{(0)}$ of (5). So our next task is to calculate the perturbative correction to $n$, and then to derive the correction to the EM (26) with the aid of the inversion formulae.

With the propagator calculated above, the non-zero perturbative correction to $n_{\boldsymbol{k}}(t)$ first comes from a diagram shown in figure 1, which is of $\mathrm{O}(\lambda^2)$. The contributions of $\mathrm{O}(\lambda)$ from a tadpole-type self-energy insertion vanishes due to the cancellation of terms from the vertices

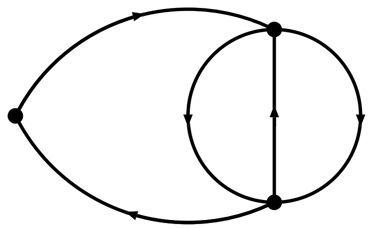

**Figure 1.** Diagram for $O(\lambda^2)$ correction to $n_k$.

on forward and backward time branches. Similarly, the diagram with the two tadpoles insertion vanishes, and only the diagram of figure 1 retains in $O(\lambda^2)$. As a result,

$$n_k[t, J] = n_k^{(0)}(t) + \left(\frac{\lambda}{\hbar}\right)^2 \sum_{q,q'} \int_{t_I}^{t} dt' \int_{t_I}^{t'} ds' \cos(\omega_{k,q,q'}(t'-s'))$$
$$\times \{(n_k^{(0)}+1)(n_{q+q'-k}^{(0)}+1)n_q^{(0)}n_{q'}^{(0)} - n_k^{(0)}n_{q+q'-k}^{(0)}(n_q^{(0)}+1)(n_{q'}^{(0)}+1)\}(s') \qquad (28)$$

where $\omega_{k,q,q'} \equiv \frac{1}{\hbar}(\epsilon_q + \epsilon_{q'} - \epsilon_{q+q'-k} - \epsilon_k)$. Recall that all $n_k^{(0)}$ are functionals of $J_k$ given in (27). Equation (28) corresponds to $f^{(0)} + \varepsilon f^{(1)} + \varepsilon^2 f^{(2)}$ of (4), where $f^{(1)}$ vanishes as mentioned above.

Applying the inversion formulae, we obtain the correction to (26) as

$$J_k(t) = \hbar \partial_t n_k(t) - \frac{\lambda^2}{\hbar} \sum_{q,q'} \int_{t_I}^{t} ds \cos(\omega_{k,q,q'}(t-s))$$
$$\times \{(n_k+1)(n_{q+q'-k}+1)n_q n_{q'} - n_k n_{q+q'-k}(n_q+1)(n_{q'}+1)\}(s). \qquad (29)$$

Note that, in course of the inversion, all the functionals of $J$ are evaluated at $J_k = \hbar \dot{n}_k$ and that $n_k^{(0)}[t; J]$ contained therein becomes $n_k(t)$. If we set the external source $J = 0$, the EM for the number is obtained. The correction term is similar to the collision terms of the BE, but it has non-Markovian form and contains an energy non-conserving process.

The ordinary Markovian BE is obtained by the adiabatic expansion. Setting the initial time $t_I = -\infty$, we abbreviate the products of $n$ and $n+1$ in the integrand of (29) as $N^{(2)}$ and expand it around the time $t$ as $N^{(2)}(s) = N^{(2)}(t) + (s-t)\dot{N}^{(2)}(t) + \cdots$, regarding the time differentiations to be small. Then the integral becomes

$$\int_{-\infty}^{t} ds \cos\omega(t-s) N^{(2)}(s) = \pi\delta(\omega)N^{(2)}(t) + \frac{\wp}{\omega^2}\dot{N}^{(2)}(t) + \cdots. \qquad (30)$$

The second term is proportional to $\dot{n}$ and gives a perturbative correction to the coefficient of the first term in the rhs of (29), which can be neglected. Regarding all higher time derivatives to be small, we take into account up to the first term of (30), and obtain the ordinary time-local BE with energy conserving process

$$\hbar \partial_t n_k(t) = \pi\lambda^2 \sum_{q,q'} \delta(\epsilon_q + \epsilon_{q'} - \epsilon_{q+q'-k} - \epsilon_k)$$
$$\times \{(n_k+1)(n_{q+q'-k}+1)n_q n_{q'} - n_k n_{q+q'-k}(n_q+1)(n_{q'}+1)\}(t). \qquad (31)$$

The key-point of our derivation is the new type of probe introduced in (15). After that, the application of inversion formula is straightforward. Of course with the usage of higher-order inversion formulae [5], we can calculate higher-order corrections to the EM quite systematically. This will be presented elsewhere.

The physical content of (15) becomes somewhat clearer if we consider the effective action of $\psi$. From the CTP generating functional $W$ with $\psi$ itself as the order parameter $Q$, the effective action $\Gamma[\psi_\Delta, \psi_C]$ is calculated through the Legendre transformation of $W$, where $\psi_\Delta \equiv \delta W/\delta J_C$ and $\psi_C \equiv \delta W/\delta J_\Delta$. Roughly speaking, $\psi_\Delta = \psi_1 - \psi_2$, $\psi_C = \frac{1}{2}(\psi_1 + \psi_2)$ and $\mathcal{D}$ is the tree part of second derivative of $\Gamma$. Then the source of the form (15) couples to $\psi_\Delta^* \psi_\Delta$ and corresponds to the quantity $\delta^2\Gamma/\delta\psi_\Delta^*\delta\psi_\Delta$ which is the one-particle-irreducible amputated part of the correlation function $\langle\{\hat{\psi}^\dagger, \hat{\psi}\}\rangle$. This may be the reason why we can handle the number with this source. Another choice of the source corresponding to $\gamma$ in (14) also produces non-trivial time dependence in the lowest order and the EM can be derived. Although the result has somewhat complicated expression, it agrees with (31) after adiabatic expansion.

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