

Numerical Simulation of Quantum Transport Equation for Bose-Einstein Condensate system of Cold gases in One Dimensional Optical Lattice

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1 Introduction

The system of cold neutral atomic gas has attracted attentions since Bose-Einstein condensates were realized. The time scales of the thermal processes are sufficiently slow to observe various nonequilibrium phenomena. We apply the nonequilibrium Thermo Field Dynamics (TFD) [1] to the system, and derive the non-Markovian quantum transport equations [2, 3].

In our previous work [3], we considered the one dimensional system of cold neutral atomic Bose gas confined by combined harmonic and optical lattice potentials. We investigated the thermal process for the system after a sudden displacement of the former potential by solving the quantum transport equation numerically, but assumed there was no condensate. In this work, we extend the previous one to the case where the system has a condensate, and derive the coupled equations consisting of the quantum transport equation, the time-dependent Gross-Pitaevskii (TDGP) one and the time-dependent Bogoliubov-de Gennes (TDBdG) one.

2 Model Hamiltonian

We consider the following Bose-Hubbard Hamiltonian [4] which describes the one dimensional system of cold neutral atomic Bose gas confined by a combined harmonic and optical lattice potentials:

$$H(t) = \sum_{i=1}^{I_s} \left[-J\psi_i^\dagger(t)(\psi_{i+1}(t) + \psi_{i-1}(t)) + \{\nu_i(t) - \mu\}\psi_i^\dagger(t)\psi_i(t) + \frac{U}{2}\psi_i^\dagger(t)\psi_i^\dagger(t)\psi_i(t)\psi_i(t) \right], \quad (1)$$

$$\nu_i(t) = (i - I_c + \theta(-t)d)^2V, \quad (2)$$

where the field operator ψ_i satisfies the following canonical commutation relations:

$$[\psi_i(t), \psi_j^\dagger(t)] = \delta_{ij}, \quad [\psi_i(t), \psi_j(t)] = [\psi_i^\dagger(t), \psi_j^\dagger(t)] = 0. \quad (3)$$

The parameters J , V , μ , U , i , I_s , I_c , and d represent the inter-site hopping, the strength of the harmonic potential, the chemical potential, the on-site coupling, the site index, the total number of sites, the center site index, and the harmonic potential displacement, respectively. The step function $\theta(-t)$ indicates a sudden displacement of the harmonic potential at $t = 0$.

Considering the existence of the condensate, we divide the field operator $\psi_i(t)$ into a classical part $\zeta_i(t)$ and a quantum one $\varphi_i(t)$ by the criterion $\langle 0|\varphi_i(t)|0\rangle = 0$. The order parameter $\zeta_i(t) = \langle 0|\psi_i(t)|0\rangle$ is an arbitrary time-dependent function at this stage because the vacuum has been not specified yet and will be done self-consistently later. We note that due to the time-dependence of $\zeta_i(t)$ the unperturbed Hamiltonians for $\psi_i(t)$ and $\varphi_i(t)$ in the interaction picture are different from each other. We choose the unperturbed Hamiltonian for $\psi_i(t)$ as follows:

$$H_0 = \sum_{ij} \left[\frac{1}{2}\bar{\varphi}_i^\alpha \left(T_{0,ij}^{\alpha\beta} + \delta T_{ij}^{\alpha\beta} \right) \varphi_j^\beta + \varphi_i^\dagger (h_{0,ij}\zeta_j + \delta_{ij}\delta C_i) + \varphi_i (h_{0,ij}\zeta_j^* + \delta_{ij}\delta C_i^*) \right], \quad (4)$$

where

$$\varphi_i^\alpha(t) = \begin{pmatrix} \varphi_i(t) \\ \varphi_i^\dagger(t) \end{pmatrix}^\alpha, \quad \bar{\varphi}_i^\alpha(t) = \begin{pmatrix} \varphi_i^\dagger(t) & -\varphi_i(t) \end{pmatrix}^\alpha, \quad (5)$$

$$T_{0,ij}^{\alpha\beta}(t) = \begin{pmatrix} \mathcal{L}_{0,ij}(t) & \mathcal{M}_{0,ij}(t) \\ -\mathcal{M}_{0,ij}^*(t) & -\mathcal{L}_{0,ij}(t) \end{pmatrix}^{\alpha\beta}, \quad (6)$$

$$\mathcal{L}_{0,ij}(t) = -J(\delta_{i,j+1} + \delta_{i,j-1}) + \delta_{ij}(\nu_i(t) - \mu + 2U|\zeta_i(t)|^2), \quad (7)$$

$$\mathcal{M}_{0,ij}(t) = U\delta_{ij}\zeta_i^2(t), \quad (8)$$

$$h_{0,ij}(t) = -J(\delta_{i,j+1} + \delta_{i,j-1}) + \delta_{ij}(\nu_i(t) - \mu + U|\zeta_i(t)|^2). \quad (9)$$

The counter terms $\delta T_{ij}^{\alpha\beta}(t)$ and $\delta C_i(t)$ are to be determined self-consistently. The criterion $\langle 0|\varphi_i(t)|0\rangle = 0$ at any t leads

$$\delta C_i = i\dot{\zeta}_i - \sum_{ij} h_{0,ij}\zeta_j, \quad (10)$$

and the unperturbed Hamiltonian for $\varphi_i(t)$, denoted by $H_0^\varphi(t)$, becomes

$$H_0^\varphi = \sum_{ij} \frac{1}{2} \bar{\varphi}_i^\alpha \left(T_{0,ij}^{\alpha\beta} + \delta T_{ij}^{\alpha\beta} \right) \varphi_j^\beta. \quad (11)$$

Because the matrix $T_{0,ij}^{\alpha\beta}(t) + \delta T_{ij}^{\alpha\beta}(t)$ is time-dependent, the field operator $\varphi_i(t)$ should be expanded in terms of the 2×2 -matrix time-dependent orthonormal complete set $\{W_{i\ell}(t)\}$ [5] each of which obeys the TDBdG equation:

$$\varphi_i^\alpha(t) = \sum_{\ell} W_{i\ell}^{-1,\alpha\beta}(t) a_\ell^\beta, \quad \bar{\varphi}_i^\beta(t) = \sum_{\ell} \bar{a}_\ell^\alpha W_{i\ell}^{\alpha\beta}(t), \quad (12)$$

$$a_\ell^\alpha = \begin{pmatrix} a_\ell \\ a_\ell^\dagger \end{pmatrix}^\alpha, \quad \bar{a}_\ell^\alpha = \begin{pmatrix} a_\ell^\dagger & -a_\ell \end{pmatrix}^\alpha, \quad (13)$$

$$\sum_i W_{i\ell_1}(t) W_{i\ell_2}^{-1}(t) = \delta_{\ell_1\ell_2}, \quad \sum_{\ell} W_{i_1\ell}^{-1}(t) W_{i_2\ell}(t) = \delta_{i_1i_2}, \quad (14)$$

$$i\dot{W}_{i\ell}^{-1}(t) = \sum_{ij} (T_{0,ij}(t) + \delta T_{ij}(t)) W_{j\ell}^{-1}(t). \quad (15)$$

3 Applying nonequilibrium TFD

In this section, we apply nonequilibrium TFD to the condensed system above. The time-dependent number distribution function $n_\ell(t)$ is introduced as an unknown parameter [1], then the parameter $n_\ell(t)$, the counter term $\delta T_{ij}^{\alpha\beta}(t)$ and the order parameter $\zeta_i(t)$ are simultaneously determined by the self-consistent renormalization conditions. Calculating the self-energy at one-loop level in Feynman diagram method and according to the renormalization conditions on the time-dependent on-shell self-energy which we have proposed recently [6], the quantum transport equation and the counter term $\delta T_{ij}^{\alpha\beta}(t)$ are fixed as

$$\begin{aligned} \dot{n}_\ell(t) = 4U^2 \text{Re} \sum_{\ell_1\ell_2} \int_0^t ds & [C_1[\zeta, W; t] C_1^*[\zeta, W; s] \{n_{\ell_1} n_{\ell_2} (1+n_\ell) - (1+n_{\ell_1})(1+n_{\ell_2}) n_\ell\}_s \\ & + C_2[\zeta, W; t] C_2^*[\zeta, W; s] \{n_{\ell_1} (1+n_{\ell_2})(1+n_\ell) - (1+n_{\ell_1}) n_{\ell_2} n_\ell\}_s \\ & + C_3[\zeta, W; t] C_3^*[\zeta, W; s] \{(1+n_{\ell_1}) n_{\ell_2} (1+n_\ell) - n_{\ell_1} (1+n_{\ell_2}) n_\ell\}_s \\ & + C_4[\zeta, W; t] C_4^*[\zeta, W; s] \{(1+n_{\ell_1})(1+n_{\ell_2})(1+n_\ell) - n_{\ell_1} n_{\ell_2} n_\ell\}_s], \end{aligned} \quad (16)$$

$$\delta T_{ij}^{\alpha\beta}(t) = \delta_{ij} U \begin{pmatrix} 2\tilde{n}_i(t) & \tilde{m}_i(t) \\ -\tilde{m}_i^*(t) & -2\tilde{n}_i(t) \end{pmatrix}^{\alpha\beta}. \quad (17)$$

The subscript s of the braces in Eq. (16) denotes the time argument of n , and the coefficients $C_k[\zeta, W; t]$ ($k = 1, \dots, 4$) depend on both the order parameter $\zeta_i(t)$ and the eigenfunctions $\{W_{i\ell}(t)\}$,

though their explicit expressions are suppressed for simplicity here. The elements in the matrix of Eq. (17) are

$$\tilde{n}_i = \langle 0 | \varphi_i^\dagger \varphi_i | 0 \rangle = \sum_{\ell} \left[n_{\ell} \left(W_{i\ell}^{11} W_{i\ell}^{-1,11} - W_{i\ell}^{21} W_{i\ell}^{-1,12} \right) - W_{i\ell}^{21} W_{i\ell}^{-1,12} \right], \quad (18)$$

$$\tilde{m}_i = \langle 0 | \varphi_i \varphi_i | 0 \rangle = \sum_{\ell} \left[n_{\ell} \left(W_{i\ell}^{22} W_{i\ell}^{-1,12} - W_{i\ell}^{12} W_{i\ell}^{-1,11} \right) + W_{i\ell}^{22} W_{i\ell}^{-1,12} \right]. \quad (19)$$

On the other hand, the order parameter $\zeta_i(t)$ is restricted by the criterion of $\langle 0 | \varphi_i(t) | 0 \rangle = 0$, from which follows the TDGP equation,

$$i\dot{\zeta}_i(t) = \sum_j (h_{0,ij}(t) + \delta_{ij} 2U\tilde{n}_i(t)) \zeta_j(t) + U\tilde{m}_i(t)\zeta_i^*(t) - i\gamma(t)\zeta_i(t), \quad (20)$$

$$\gamma = \frac{1}{2 \sum_i |\zeta_i|^2} \sum_{\ell} \dot{n}_{\ell} \left(W_{i\ell}^{11} W_{i\ell}^{-1,11} - W_{i\ell}^{21} W_{i\ell}^{-1,12} \right). \quad (21)$$

Here we have included the contributions to $\delta C_i(t)$ up to two-loop order, and the last term in Eq. (20) comes from the two-loop order and is necessary to conserve the total particle number.

Thus we have derived a set of the coupled equations, i.e., the quantum transport equation (16), the TDBdG one (15), and the TDGP one (20). The interactions between the condensate and non-condensed excitation modes are taken account of properly. The crucial point in our derivation is that the coupled equations have been derived systematically from the single concept of the self-consistent renormalization. It is remarked that the quantum transport equation derived in our approach has an additional term which is absent in the other methods, namely the last term on the right side of Eq. (16), which we call the triple production term. The term corresponds to the process where three quasiparticles are created or annihilated. The process prevents the system from the thermal relaxation because the collision term is always non-zero $(1 + n_{\ell_1})(1 + n_{\ell_2})(1 + n_{\ell}) - n_{\ell_1}n_{\ell_2}n_{\ell} > 0$. If the negative energy mode does not exist in the system, the process is forbidden because of the energy conservation, but once the negative energy mode appears, the triple production term induces the decay of the condensate. This corresponds to the scenario of the Landau instability.

As a future task, we will perform numerical calculations of the set of the coupled equations. It will be an interesting subject then to trace temporal behaviors of the system with the Landau instability in detail.

References

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