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PROOF OF THE BLOCH-MESSIAH THEOREM IN THE THFB THEORY

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It is shown that application of the thermo field dynamics to the thermal Hartree-Fock-Bogoliubov (THFB) approximation leads to the extended form of the Bloch-Messiah theorem for the finite temperature formalism. The generalized Bogoliubov transformation is brought to the canonical form on the enlarged operator space including tilded operators, and newly defined single-particle density matrix and pair tensor take into account the thermal fluctuation effect of Fermion number.

§1. The thermal Hartree-Fock-Bogoliubov (THFB) approximation

Variational parameters $A_{k\mu}$, $B_{k\mu}$, $A^*_{k\mu}$, $B^*_{k\mu}$ and E_μ are introduced through the generalized Bogoliubov transformation

$$\begin{pmatrix} c_k \\ c_k^\dagger \end{pmatrix} = \sum_\mu W_{k\mu} \begin{pmatrix} \alpha_\mu \\ \alpha_\mu^\dagger \end{pmatrix}, \quad W_{k\mu} = \begin{pmatrix} A_{k\mu} & B^*_{k\mu} \\ B_{k\mu} & A^*_{k\mu} \end{pmatrix} \tag{1}$$

conditioned by

$$W^\dagger W = W W^\dagger = I \tag{2}$$

and the trial density matrix

$$\hat{w} = \frac{\exp(-\beta \sum_\mu E_\mu \alpha_\mu^\dagger \alpha_\mu)}{\mathrm{Tr}[\exp(-\beta \sum_\mu \alpha_\mu^\dagger \alpha_\mu)]}. \tag{3}$$

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The THFB equation is derived from the variational principle applied to the grand potential,[1,2] i.e.

$$\delta F = \delta(\langle \hat{H} - \lambda_p \hat{Z} - \lambda_n \hat{N} - \omega \hat{J}_X \rangle - ST) = 0,\ S = -k\,\mathrm{Tr}(\hat{w}\ln\hat{w}), \tag{4}$$

where $\hat{H}$ is the microscopic Hamiltonian; and ensemble averages of proton (neutron) number operator $\hat{Z}$ ($\hat{N}$) and angular momentum operator $\hat{J}_X$ are constrained by

$$\langle \hat{Z} \rangle = Z, \langle \hat{N} \rangle = N, \langle \hat{J}_X \rangle = I, \text{ or } \sqrt{I(I+1)}. \tag{5}$$

Then, the single-particle density and pair tensor are expressed as

$$\rho_{kl} \equiv \langle c_l^\dagger c_k \rangle = [B^*(1-f)B^{tr} + AfA^\dagger]_{kl}, \tag{6a}$$

$$\kappa_{kl} \equiv \langle c_l c_k \rangle = [B^*(1-f)A^{tr} + AfB^\dagger]_{kl}, \tag{6b}$$

where

$$f_\mu \equiv \langle \alpha_\mu^\dagger \alpha_\mu \rangle = \frac{1}{\exp(\beta E_\mu) + 1} \tag{7}$$

is the quasiparticle distribution function.

The generalized density matrix defined in the same manner as the zero-temperature case (i.e. the HFB approximation),

$$R = \begin{pmatrix} \rho & \kappa \\ \kappa^\dagger & 1-\rho^* \end{pmatrix}, \tag{8}$$

is not a projection, but $R - R^2$ remains finite at $T \neq 0$, i.e.

$$R - R^2 = W f(1-f) W^\dagger. \tag{9}$$

Note

$$R \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} A \\ B \end{pmatrix} f,\ R \begin{pmatrix} B^* \\ A^* \end{pmatrix} = \begin{pmatrix} B^* \\ A^* \end{pmatrix} (1-f). \tag{10}$$

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Because of (2), trace of (9) becomes

$$\mathrm{Tr}(R - R^2) = \mathrm{Tr}[f(1-f)], \tag{11}$$

which is a quantity nothing but thermal fluctuation of Fermion number. Therefore, the Bloch-Messah theorem[3] proved based on the relation $R - R^2 = 0$ seems not to hold for the THFB scheme.[1,2] This means that the pair tensor κ does not take canonical form and has many non-vanishing elements even in the basis which diagonalizes the density ρ.

§2. Application of the thermo field dynamics (TFD)

The thermo field dynamics (TFD) proposed by Takahashi and Umezawa[4,5] introduces tilded operators $\tilde{\alpha}_\mu$ and $\tilde{\alpha}_\mu^\dagger$ to enlarge operator space as

$$\alpha \otimes \tilde{1} \longrightarrow \alpha,\ 1 \otimes \tilde{\alpha} \longrightarrow \tilde{\alpha},\ |0\rangle \otimes |\tilde{0}\rangle \longrightarrow |0\rangle \tag{12}$$

with

$$\alpha_\mu|0\rangle = \tilde{\alpha}_\mu = 0. \tag{13}$$

The temperature-dependent vacuum is defined by

$$|0(\beta)\rangle = e^{-G}|0\rangle,\ G \equiv \sum_\mu \theta_\mu(\alpha_\mu^\dagger\tilde{\alpha}_\mu^\dagger - \tilde{\alpha}_\mu\alpha_\mu), \tag{14}$$

where

$$\sin\theta_\mu = f_\mu^{1/2} \equiv g_\mu,\ \cos\theta_\mu = (1-f_\mu)^{1/2} \equiv \bar{g}_\mu. \tag{15}$$

On the other hand the quasiparticle operators α_μ and $\tilde{\alpha}_\mu$ are related to new operators β_μ and $\tilde{\beta}_\mu$ by the special Bogoliubov transformation,

$$\alpha_\mu = e^G\beta_\mu e^{-G} = \bar{g}_\mu\beta_\mu + g_\mu\tilde{\beta}_\mu^\dagger, \tag{16a}$$

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$$\tilde{\alpha}_\mu = e^G \tilde{\beta}_\mu e^{-G} = \bar{g}_\mu \tilde{\beta}_\mu - g_\mu \beta^\dagger_\mu. \tag{16b}$$

Note

$$\beta_\mu |0(\beta)\rangle = \tilde{\beta}_\mu |0(\beta)\rangle = 0. \tag{17}$$

An essential feature of the TFD is that the ensemble average of any operator $\hat{O}$ is expressed in terms of the vacuum expectation value, i.e.

$$\langle \hat{O} \rangle \equiv \frac{\mathrm{Tr}(e^{-\beta H}\hat{O})}{\mathrm{Tr}(e^{-\beta H})} = \langle 0(\beta)|\hat{O}|0(\beta)\rangle. \tag{18}$$

Then, the single-particle operators c_k and $\tilde{c}_k$ are related to β_μ and $\tilde{\beta}_\mu$ by

$$\begin{pmatrix} c \\ \tilde{c} \\ c^\dagger \\ \tilde{c}^\dagger \end{pmatrix} = \bar{W} \begin{pmatrix} \beta \\ \tilde{\beta} \\ \beta^\dagger \\ \tilde{\beta}^\dagger \end{pmatrix}, \tag{19}$$

with

$$W = \begin{pmatrix} \bar{A} & \bar{B}^* \\ \bar{B} & \bar{A}^* \end{pmatrix}, \ \bar{A} = \begin{pmatrix} A\bar{g} & B^* g \\ -B*g & \bar{A}\bar{g} \end{pmatrix}, \ \bar{B} = \begin{pmatrix} B\bar{g} & A^* g \\ -B^* g & \bar{A}\bar{g} \end{pmatrix}, \tag{20}$$

$$\bar{W}\bar{W}^\dagger = \bar{W}^\dagger \bar{W} = I. \tag{21}$$

Since the formalisn is developed on the temperature-dependent vacuum $|0(\beta)\rangle$, parallel holds between this extended form of the THFB scheme and the HFB scheme. As such a consequence the extended single-particle density matrix and pair tensor are to be defined by

$$\bar{\rho} = \hat{B}^* \bar{B}^{tr} = \begin{pmatrix} \rho & P \\ -P & \rho \end{pmatrix} = \bar{\rho}^\dagger, \tag{22a}$$

$$\bar{\kappa} = \bar{B}^* A^{tr} = \begin{pmatrix} \kappa & Q \\ -Q & \kappa \end{pmatrix} = -\bar{\kappa}^{tr}, \tag{22b}$$

where ρ and κ are the same as defined by (6). P and Q are new quantities given by

$$P = Ag\bar{g}B^{tr} - B^*\bar{g}gA^\dagger = -P, \tag{23a}$$

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$$Q = Ag\bar{g}A^{tr} - B^{*}g\bar{g}B^{\dagger} = Q^{tr}. \tag{23b}$$

Thus, the generalized density matrix R is extended to be

$$\Lambda = \begin{pmatrix} \bar{\rho} & \bar{\kappa} \\ \bar{\kappa}^{\dagger} & 1-\bar{\rho}^{*} \end{pmatrix}, \tag{24}$$

which satisfies

$$\Lambda - \Lambda^{2} = 0. \tag{25}$$

§3. Extension of the Bloch-Messiah theorem

Applying the unitary transformation,

$$V = \frac{1}{2}\begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix} = V^{tr},\ V^{\dagger} = \frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix} = V^{*}, \tag{26}$$

to $\bar{\rho}$ and $\bar{\kappa}$, we get

$$V^{\dagger}\,\bar{\rho}\,V = \begin{pmatrix} \rho+iP & 0 \\ 0 & \rho-iP \end{pmatrix},\ V^{tr}\,\bar{\kappa}\,V = \begin{pmatrix} 0 & \kappa-iQ \\ -\kappa+iQ & 0 \end{pmatrix}. \tag{27}$$

Hermite matrices $\rho+iP$ and $\rho-iP$ can be diagonalized by two different unitary transformations u and u', but have a common set of eigenvalues, i.e.

$$\begin{pmatrix} u^{\dagger} & 0 \\ 0 & u'^{\dagger} \end{pmatrix}\begin{pmatrix} \rho+iP & 0 \\ 0 & \rho-iP \end{pmatrix}\begin{pmatrix} u & 0 \\ 0 & u' \end{pmatrix} = \begin{pmatrix} \rho_{kk}\delta_{kl} & 0 \\ 0 & \rho_{\bar{k}\bar{k}}\delta_{\bar{k}\bar{l}} \end{pmatrix}, \tag{28}$$

with

$$\rho_{kk} = \rho_{\bar{k}\bar{k}} = \rho^{*}_{kk} = \rho^{*}_{\bar{k}\bar{k}}. \tag{29}$$

From (25) we can show

$$[u^{\dagger}(\kappa-iQ)u'^{*}]_{k\bar{l}}(\rho_{kk}-\rho_{\bar{l}\bar{l}}) = 0, \tag{30a}$$

$$[u'^{\dagger}(\kappa-iQ)u^{*}]_{\bar{k}l}(\rho_{\bar{k}\bar{k}}-\rho_{ll}) = 0. \tag{30b}$$

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Thus, we have seen that all the elements $[u^\dagger(\kappa - iQ)u'^*]_{k\tilde{l}}$ and $[u'^\dagger(\kappa - iQ)u^*]_{\tilde{k}l}$ vanish except for

$$[u^\dagger(\kappa - iQ)u'^*]_{k\tilde{k}} \equiv \kappa_{k\tilde{k}}, [u'^\dagger(-\kappa + iQ)u^*]_{\tilde{k}k} \equiv \kappa_{\tilde{k}k} = -\kappa_{k\tilde{k}}. \qquad (31)$$

This completes the proof of the extended form for the Bloch-Messah theorem. We have also found the THFB approximation is such a scheme that takes into account the effect of thermal fluctuation of particle number. In order to define correct form of the density matrix and the pair tensor, operator space should be doubled by inclusion of tilded operators. This must be one of the supporting evidence of the TFD formalism.

References

1) K. Tanabe and K. Sugawara-Tanabe, Phys. Lett. **97B**(1980),337.

2) K. Tanabe, K. Sugawara-Tanabe and H. J. Mang, Nucl. Phys. **A357** (1981), 20 and 45.

3) C. Bloch and A. Messiah, Nucl. Phys. **39**(1962), 95.

4) Y. Takahashi and H. Umezawa, Collec. Phenom. **2**(1975), 55.

5) H. Umezawa, H. Matsumoto and M. Tachiki, Thermo Field Dynamics and Condensed States (North-Holland, Amsterdam, 1982).

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