Some useful relations to derive the thermodynamic potentials of Fermi and Bose systems using spectral-weight functions

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A relation between the thermodynamic potential and certain spectral-weight functions in mixed singlet-triplet states of a Fermi fluid with weakly attractive interaction is established. The entire thermodynamics of the system can be derived using this relation. A similar relation is also established for an assembly of spinless, interacting bosons in the ordered phase. The latter corresponds to the Kadanoff-Baym relation for the normal phase when the necessary conditions are fulfilled. Crossover scaling forms for the susceptibility and the deviation of pressure from its critical value for the Bose system are calculated using the established relation. These forms are in general agreement with those obtained earlier by renormalization-group approaches to the problem.

I. INTRODUCTION

About three decades ago, Kadanoff and Baym[1] established a formula relating the thermodynamic average of a model Hamiltonian for an interacting Bose system in the normal phase to a spectral-weight function. This function can either be defined[1] in terms of the retarded and the advanced single-particle Green's functions or can be given[2] by a discontinuity across the real axis of a certain function[2] constructed by analytic continuation of the Fourier coefficient corresponding to the temperature Green's function of the system to nonreal $z\,(=i\omega_n$, where ω_n is a Matsubara frequency). A few years ago, relations between spectral-weight functions and the Fourier transforms in space and time of the dynamic correlation functions of order parameter fluctuations were established by the present author for the effective Bose system[3] and also for the singlet-spin-pairing and equal-spin-pairing states of a Fermi fluid[4] with weakly attractive interaction. The present work aims at establishing a relation between the thermodynamic potential per unit volume corresponding to mixed singlet-triplet states[5] of this Fermi system and certain other spectral-weight functions. We also aim at establishing the same for an assembly of spinless, interacting bosons in the ordered phase. The former gives the relations for pure singlet and triplet states as special cases whereas, in suitable limits, the latter reduces to the Kadanoff-Baym (KB) relation[1] for the normal phase. The idea behind establishing these relations is to show the possibility of the derivation of finite-temperature thermodynamics and critical behavior of these two systems using the weight-function method.

An outline of the content of this paper is as follows. A relation between the thermodynamic potential per unit volume, in mixed singlet-triplet states[5] of a Fermi fluid and certain spectral-weight functions is established in Sec. II. A set of coupled equations for various gap functions occurring in this relation are also set up. The KB relation for the normal phase of an interacting Bose system is extended to the ordered phase in Sec. III using the well-known Bogolubov prescription.[6] The usefulness of the relation to derive thermodynamics and critical behavior is demonstrated using an approximate form of the Matsubara propagators in the finite-temperature analogues[2,7] of the Beliaev equations. It is shown that crossover scaling forms for the susceptibility and the deviation of pressure from its critical value, calculated using the present method, are in general agreement with the corresponding ones obtained by previous workers[8,9] by their renormalization-group (RG) approaches to the problem. Finally, Sec. IV contains a discussion related to the work presented in this paper.

II. THERMODYNAMIC POTENTIAL OF A FERMI SYSTEM

The system under consideration is an assembly of interacting fermions contained in a box of volume V. In second quantized notation, the mean-field Hamiltonian[10] of the assembly, in the case of mixed singlet-triplet pairing, reads (in units such that $\hbar=1$)

$$H_F=\sum_k A_k^{\dagger}\varepsilon_k A_k\ , \tag{1}$$

$$A_k=\begin{bmatrix} a_{k\uparrow} \\ a_{k\downarrow} \\ a^{\dagger}_{-k\uparrow} \\ a^{\dagger}_{-k\downarrow} \end{bmatrix}\ , \tag{2}$$

$$\varepsilon_k=\frac{1}{2}\begin{bmatrix} \epsilon_F(k) & 0 & \Delta_{11}(k) & \Delta_{12}(k) \\ 0 & \epsilon_F(k) & \Delta_{21}(k) & \Delta_{22}(k) \\ \Delta^{\dagger}_{11}(k) & \Delta^{\dagger}_{21}(k) & -\epsilon_F(k) & 0 \\ \Delta^{\dagger}_{12}(k) & \Delta^{\dagger}_{22}(k) & 0 & -\epsilon_F(k) \end{bmatrix}\ ,$$

$$\epsilon_F(k)=\left[\frac{k^2}{2m_F}-\mu_F\right]\ , \tag{3}$$

$$\Delta_{ij}(k)=\sum_{k'} V_{kk'}\langle a_{-k'i}a_{k'j}\rangle,\quad i,j=(1,2)\ .$$

Here, m_F and μ_F, respectively, denote the mass and chemical potential of a fermion. $V_{kk'}$ denotes an attractive interaction potential. The subscripts 1 and 2 in (3), respectively, correspond to the two spin states $\uparrow$ and $\downarrow$ and angular brackets $\langle\ \rangle$ to the thermodynamic average calculated with H_F. Fermi statistics implies[5,11] that in this case, whereas $(\Delta_{11},\Delta_{22})$ are odd functions of k, $(\Delta_{12},\Delta_{21})$ are neither even nor odd. Equations for these gap functions will be written down towards the end of this section.

Our aim here is to establish a relation between the thermodynamic potential per unit volume

$$\Omega_F=-(\beta V)^{-1}\ln \mathrm{Tr}\exp(-\beta H_F) \tag{4}$$

of the assembly and certain spectral weight functions. Here, β denotes the inverse of the product of temperature T and Boltzmann constant k_B. The specific heat at constant volume will be calculated using this relation also to demonstrate its usefulness.

It is convenient to define a new potential per unit volume $\Omega_F(\lambda)$ in terms of the Hamiltonian $H_F(\lambda)=\lambda H_F$, where λ is a variable, for the purpose stated above. One can write

$$\Omega_F(\lambda)=V^{-1}\int\frac{d\lambda}{\lambda}\langle H_F(\lambda)\rangle_\lambda+\Omega_{0F}\ , \tag{5}$$

where the angular brackets $\langle\ \rangle_\lambda$ denote thermodynamic average calculated with $H_F(\lambda)$ and Ω_{0F} is an integration constant to be specified later [see note below Eq. (28)]. The system under consideration corresponds to $\Omega_F(\lambda=1)$. Obviously, the task now boils down to establishing relations between the average $\langle H_F(\lambda)\rangle_\lambda$ and spectral-weight functions.

We follow the methodology pioneered by Kadanoff and Baym,[1] by and large, to accomplish the task. The first step is to set up equations of motion for the operators $a_{k\sigma}(t)$, $a^\dagger_{k\sigma}(t)$ $(\sigma=\uparrow,\downarrow)$, etc., where

$$a_{k\sigma}(t)=e^{iH_F(\lambda)t}a_{k\sigma}e^{-iH_F(\lambda)t}\ . \tag{6}$$

The next step is to write down equations of motion for the averages $\sum_k\langle a^\dagger_{k\sigma}(t')a_{k'\sigma'}(t)\rangle_\lambda$. These equations yield

$$\langle H_F(\lambda)\rangle_\lambda=\tfrac{1}{4}\lim_{t'\to t}\sum_{k\sigma}\left[i\frac{\partial}{\partial t}-i\frac{\partial}{\partial t'}\right]\times\{\langle a^\dagger_{k\sigma}(t')a_{k\sigma}(t)\rangle_\lambda+\langle a^\dagger_{-k\sigma}(t')a_{-k\sigma}(t)\rangle_\lambda\}\ . \tag{7}$$

The thermodynamic averages in (7) will now be expressed in terms of the spectral-weight functions $A^\lambda_F(\pm k\sigma,\omega)$ given by

$$A^\lambda_F(k\sigma,\omega)=i[G^\lambda_F(k\sigma,k\sigma,\omega_n)|_{i\omega_n=\omega+i0^+}-G^\lambda_F(k\sigma,k\sigma,\omega_n)|_{i\omega_n=\omega-i0^+}]\ , \tag{8}$$

where $G^\lambda_F(k\sigma,k'\sigma',\omega_n)$ are the Fourier coefficients of the temperature Green's functions

$$G^\lambda_F(k\sigma\tau,k'\sigma'\tau')=-\langle T_\tau\{a_{k\sigma}(\tau)a^\dagger_{k'\sigma'}(\tau')\}\rangle_\lambda\ . \tag{9}$$

Here, $\omega_n=(2n+1)\pi/\beta$ with $n=0,\pm1,\pm2,\ldots$, T_τ denotes the time-ordering operator and

$$a_{k\sigma}(\tau)=e^{H_F(\lambda)\tau}a_{k\sigma}e^{-H_F(\lambda)\tau}\ . \tag{10}$$

The Lehmann representations[12] (LR) of $A^\lambda_F(\pm k\sigma,\omega)$ are easy to write. With the help of these representations one obtains

$$A^\lambda_F(\pm k\sigma,\omega)=-2(e^{\beta\omega}+1)\mathrm{Im}f^\lambda_F(\pm k\sigma,\omega)\ , \tag{11}$$

where

$$f^\lambda_F(\pm k\sigma,\omega)=-i\int\int dt\,dt' e^{i\omega(t-t')}\times\langle a^\dagger_{\pm k\sigma}(t')a_{\pm k\sigma}(t)\rangle_\lambda\theta(t-t')\ . \tag{12}$$

In view of (11) and (12), it is easy to see that

$$\langle a^\dagger_{\pm k\sigma}(t')a_{\pm k\sigma}(t)\rangle_\lambda=\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\frac{A^\lambda_F(\pm k\sigma,\omega)}{(e^{\beta\omega}+1)}e^{-i\omega(t-t')}\ . \tag{13}$$

Upon substituting (13) in (7) one finally obtains the relation

$$\langle H_F(\lambda)\rangle_\lambda=\sum_{k\sigma}\int_{-\infty}^{+\infty}\frac{d\omega}{4\pi}\frac{d\omega}{(e^{\beta\omega}+1)}\times[A^\lambda_F(k\sigma,\omega)+A^\lambda_F(-k\sigma,\omega)]\ . \tag{14}$$

This is the relation sought. As for uses, this type of relation serves as the starting point to investigate the thermodynamics of models that include the possibility of both singlet and triplet pairings, such as the Klemm-Liu model[13] for layered, high-T_c superconductors.

The weight functions in (14) can be calculated setting up equations of motion for the temperature Green's functions in (9) and transforming these equations to the ones for the corresponding Fourier coefficients. The latter constitute a system of homogeneous, linear equations. One obtains

$$\sum_\sigma[A^\lambda_F(k\sigma,\omega)+A^\lambda_F(-k\sigma,\omega)]=\sum_{i=1,2}\{C_i(k)\delta(\omega+\lambda E^{(i)}_k)+D_i(k)\delta(\omega-\lambda E^{(i)}_k)\}\ , \tag{15}$$

where

$$C_i(k)=1+\frac{(-1)^{i-1}\epsilon_F(k)[|\Delta_{11}(k)|^2+|\Delta'_{21}(k)|^2]}{E^{(i)}_k\sqrt{\zeta(k)}}\ , \tag{16}$$

$$\Delta'_{21}(k)=\tfrac{1}{2}[\Delta_{12}(k)-\Delta_{21}(k)]\ , \tag{17}$$

$$E^{(i)}_k=[\epsilon^2_F(k)+\eta^2_i(k)]^{1/2}\ , \tag{18}$$

$$\eta_i(k)=\frac{1}{\sqrt{2}}[|\Delta_{11}|^2+|\Delta_{22}|^2+|\Delta_{12}|^2+|\Delta'_{21}|^2+(-1)^{i-1}\sqrt{\zeta(k)}]^{1/2}\ , \tag{19}$$

$$\zeta(k)=\{(|\Delta_{11}|^2-|\Delta_{22}|^2)^2+(|\Delta_{12}|^2-|\Delta'_{21}|^2)^2 +2(\Delta^\dagger_{11}\Delta_{12}-\Delta_{22}\Delta'_{21})^2+2(\Delta_{11}\Delta'^\dagger_{21}-\Delta^\dagger_{22}\Delta_{12})^2\} \tag{20}$$

and the coefficients $D_i(k)$ are obtained replacing $(-1)^{i-1}$ with $(-1)^i$ in (16). In view of (15)–(20), it may be remarked that the introduction of mixed singlet-triplet pairing, within the BCS approximation scheme, has merely complicated the notation without much qualitative change in expressions of quantities, such as that for excitation energy E_k. In fact, as is expected, we have an expression for E_k which gives both the spin singlet ($\Delta_{jj}=0=\Delta'_{21}$) and the spin triplet ($\Delta'_{21}=0$) excitation energies as special cases.

The gap functions (GF) occurring in the sum in (14) are not yet known. These functions can be expressed in terms of appropriate temperature Green's functions. As in the case of $A_F(\pm k\sigma,\omega)$, GF's can then be obtained solving equations for Fourier coefficients corresponding to these temperature functions. Without showing any of the details, we write down here the self-consistent equations for GF's obtained by the above procedure:

$$\Delta_{ij}(k)=\sum_{k'} V_{kk'}\left[A_{ij}(k')\tanh\frac{\beta E^{(1)}_{k'}}{2} +B_{ij}(k')\tanh\frac{\beta E^{(2)}_{k'}}{2}\right], \tag{21}$$

where $i,j=1,2$ and

$$A_{ij}(k)=-\frac{|G^{(1)}_{ij}(k)|}{2E^{(1)}_k(E^{(1)2}_k-E^{(2)2}_k)}\,,$$

$$B_{ij}(k)=\frac{|G^{(2)}_{ij}(k)|}{2E^{(2)}_k(E^{(1)2}_k-E^{(2)2}_k)}\,, \tag{22}$$

$$G^{(1)}_{ii}(k)=\begin{vmatrix}\Delta_{ii}(k) & \Delta^\dagger_{jj}(k)\\ \xi^2(k) & \eta^2_1(k)\end{vmatrix},\quad j\neq i\,,$$

$$G^{(1)}_{12}(k)=\begin{vmatrix}\Delta_{12}(k) & \Delta'^\dagger_{21}(k)\\ \xi^2(k) & \eta^2_1(k)\end{vmatrix}, \tag{23}$$

$$G^{(1)}_{21}(k)=\begin{vmatrix}-\Delta'_{21}(k) & -\Delta^\dagger_{12}(k)\\ \xi^2(k) & \eta^2_1(k)\end{vmatrix},$$

$$\xi^2(k)=\det\begin{vmatrix}\Delta_{11}(k) & \Delta_{12}(k)\\ -\Delta'_{21}(k) & \Delta_{22}(k)\end{vmatrix}.$$

The matrices $G^{(2)}_{ij}(k)$ are obtained replacing $\eta^2_1(k)$ by $\eta^2_2(k)$ in $G^{(1)}_{ij}(k)$. The system of equations given by (21)–(23) gives all the gap elements. The SU(N) representation of these equations is more convenient to deal with. The solutions will be reported in the future. One sees from (21) that in a pure singlet state, $A_{12}=-\Delta/2E_k$ and $B_{12}=0$, where $\Delta=\frac{1}{2}\Delta_{12}$ and $E_k=(\epsilon^2_F+\Delta^2)^{1/2}$. This leads to the familiar gap equation for a BCS superconductor. In the equal-spin-pairing (ESP) states of the system, on the other hand, $\Delta_{12}=0=\Delta_{21}$ and $E^{(i)}_k=(\epsilon^2_F+|\Delta_{ii}|^2)^{1/2}$, $i=(1,2)$. One thus obtains the two independent equations for $\Delta_{ii}(k)$:

$$\Delta_{ii}(k)=-\sum_{k'} V_{kk'}\frac{\Delta_{ii}(k')}{2E^{(i)}_{k'}}\tanh\beta E^{(i)}_{k'}/2\,. \tag{24}$$

One may conclude from here that in an ESP-type triplet superfluid the spin-up and the spin-down particles form two completely independent systems. The small mean-field corrections $\Delta X_{ij}(k,\omega)$ (see Sec. IV also) to the temperature-independent normal-phase values of spin susceptibility components show that this is not entirely true. For example, $\Delta X_{xx}(k,\omega)$ in ESP states is proportional to

$$\frac{(\Delta^\dagger_{11}\Delta_{22}+\Delta_{11}\Delta^\dagger_{22})}{E^{(1)}_{k,\mathrm{ESP}}E^{(2)}_{k,\mathrm{ESP}}}\left[(f_1-f_2)\tanh\frac{\beta E^{(1)}_{k,\mathrm{ESP}}}{2} +(f_1+f_2)\tanh\frac{\beta E^{(2)}_{k,\mathrm{ESP}}}{2}\right], \tag{25}$$

where

$$f_1(k,\omega)=\left[\frac{1}{\omega-\varepsilon_1+i0^+}-\frac{1}{\omega+\varepsilon_1+i0^+}\right],$$

$$f_2(k,\omega)=\left[\frac{1}{\omega-\varepsilon_2+i0^+}-\frac{1}{\omega+\varepsilon_2+i0^+}\right], \tag{26}$$

$$\varepsilon_1(k)=E^{(1)}_{k,\mathrm{ESP}}+E^{(2)}_{k,\mathrm{ESP}},\quad \varepsilon_2(k)=E^{(1)}_{k,\mathrm{ESP}}-E^{(2)}_{k,\mathrm{ESP}}\,, \tag{27}$$

$$E^{(i)}_{k,\mathrm{ESP}}=[\epsilon^2_F(k)+|\Delta_{ii}(k)|^2]^{1/2}\,.$$

The details are to be submitted for publication elsewhere in the future. Obviously, the correction above does not appear as the sum of two separate contributions arising from the spin-up and the spin-down particles. Also the peaks in $\mathrm{Im}\Delta X_{xx}(k,\omega)$ (and the corresponding neutron scattering function) occur at $(\varepsilon_1,\varepsilon_2)$ and not at $(E^{(1)}_{k,\mathrm{ESP}},E^{(2)}_{k,\mathrm{ESP}})$. This can be verified by the inelastic scattering of neutrons in the A-phase of liquid ^{3}He.

We now substitute (15) in (14) to obtain $\langle H_F(\lambda)\rangle_\lambda$. This, on being used in (5), gives

$$\Omega_F(\lambda=1)=\Omega_{0F}-(\beta V)^{-1}\sum_k\sum_{j=1,2}\ln\cosh\beta E^{(i)}_k/2\,. \tag{28}$$

Since, in the present approximation, the normal phase of the system corresponds to an ideal Fermi gas, the integration constant Ω_{0F} must be $[-(\beta V)^{-1}2\ln 2\sum_k 1+(2V)^{-1}\sum_k\sum_j E^{(j)}_k]$, for then the resultant expression of $\Omega_F(\lambda=1)$ will reduce to that for the ideal gas in the normal phase. For pure triplet states, (28) remains the same formwise. However, for pure

singlet states, it reduces to the simple expression

$$\Omega_{FS}=-2(\beta V)^{-1}\sum_k \ln\{1+e^{-\beta E_k}\},\quad E_k=(\epsilon_F^2+\Delta^2)^{1/2}\ . \tag{29}$$

The entropy per unit volume, in view of the note below (28), is given by

$$S_F=\frac{k_B\beta}{2V}\sum_{j=1,2}\sum_k\left\{E_k^{(j)}+\beta\frac{\partial E_k^{(j)}}{\partial\beta}\right\}e^{-\beta E_k^{(j)}/2}\operatorname{sech}\frac{\beta E_k^{(j)}}{2}+\frac{k_B}{V}\sum_{j=1,2}\sum_k\ln\{1+e^{-\beta E_k^{(j)}}\}\ . \tag{30}$$

Then the specific heat at constant volume and μ_F is

$$C_V=\frac{-k_B\beta^2}{2V}\sum_{j=1,2}\sum_k\left[2\frac{\partial E_k^{(j)}}{\partial\beta}+\beta\frac{\partial^2 E_k^{(j)}}{\partial\beta^2}\right]e^{-\beta E_k^{(j)}/2}\operatorname{sech}\frac{\beta E_k^{(j)}}{2}+\frac{k_B\beta^2}{4V}\sum_{j=1,2}\sum_k\left[E_k^{(j)}+\beta\frac{\partial E_k^{(j)}}{\partial\beta}\right]^2\operatorname{sech}^2\frac{\beta E_k^{(j)}}{2}\ . \tag{31}$$

In the case of a BCS superconductor, (30) assumes the simple form

$$S_{FS}=-\frac{k_B\beta}{V}\sum_k\left[E_k+\beta\frac{\partial E_k}{\partial\beta}\right]\left[\tanh\frac{\beta E_k}{2}-1\right]+\frac{k_B}{V}\sum_k 2\ln\{1+e^{-\beta E_k}\}\ . \tag{32}$$

The term

$$\left[-k_B\beta V^{-1}\sum_k\beta(\partial E_k/\partial\beta)(\tanh\beta E_k/2-1)\right]$$

in (32) is a typical consequence of Fermi statistics, for Leggett's expression[5] for S_{FS}, calculated using Planck's formula and the ansatz that the probability of occurrence of ground pair, broken pair, and excited pair states are given by the Boltzmann distribution, does not contain this term. Near the critical temperature of the superconductor, this term may be assumed to be small compared to the other terms in (32) as the gap Δ may be approximated by a constant at criticality. This emphasizes that the statistics does not play a significant role[4] in determining critical behavior of thermodynamic functions.

Other useful relations also exist for calculating thermodynamic potential of a Fermi system, e.g., the relation[14] for pure singlet states involving pair susceptibility. Sofo and Balseiro[15] used this relation to derive the thermodynamics of a two-dimensional electron gas in the low-density limit. However, as remarked by these authors, the correct way of doing the calculation is through the approach of Kadanoff and Baym.[1]

III. THERMODYNAMIC POTENTIAL OF A BOSE SYSTEM

The Hamiltonian of an assembly of spinless, interacting bosons of mass m_B contained in a box of volume V (in units such that $\hbar=1$) is

$$H_B=\sum_q\epsilon_B(q)b_q^\dagger b_q+\frac{u}{V}\sum_{q_1q_2q_3}b_{q_1}^\dagger b_{q_2}^\dagger b_{q_3}b_{q_1+q_2-q_3}\ , \tag{33}$$

where $\epsilon_B(q)=[(q^2/2m_B)-\mu_B]$, b_q denotes a boson annihilation operator for the single-particle state of momentum q and u the two-body interaction constant. μ_B denotes the chemical potential of a boson.

The aim in this section is to establish a relation similar to Sec. II between the thermodynamic potential of the assembly in the ordered phase and certain spectral-weight functions. The usefulness of this relation to derive the thermodynamics and the critical behavior of the system will be discussed towards the end of this section.

For the system of bosons in the ordered phase ($\langle b_0\rangle$, $\langle b_0^\dagger\rangle\neq 0$), an external-field term $[-(hV^{1/2}/2)(b_0+b_0^\dagger)]$ must be added to the Hamiltonian in (33), where h denotes the field conjugate to the real part of $b_0/\sqrt{V}$. Following Bogolubov,[6] we replace $b_0/\sqrt{V}$ everywhere in the Hamiltonian by a real c number M. Consequently H_B in (33), together with the external-field term, can be written in the form

$$H_B'(M)=H_B(M)-hMV\ , \tag{34}$$

where

$$H_B(M)=VE_0(M)+\tfrac{1}{2}{\sum_q}'[\epsilon_B(q)+2U(M)](b_q^\dagger b_q+b_{-q}^\dagger b_{-q})+\tfrac{1}{2}U(M){\sum_q}'(b_q^\dagger b_{-q}^\dagger+b_{-q}b_q)+\frac{u}{V}{\sum_{q_1q_2q_3}}'b_{q_1}^\dagger b_{q_2}^\dagger b_{q_3}b_{q_1+q_2-q_3}\ , \tag{35}$$

$$E_0(M)=[-\mu_BM^2+uM^4],\quad U(M)=2uM^2\ . \tag{36}$$

The primed q summations above exclude the point $q=0$. In writing (35), three-operator terms have not been taken into account, as in the weak-interaction approximation only averages involving two and four operators contribute to various thermodynamic functions. The unknown M is determined by demanding stationarity of the thermodynamic potential per unit volume

$$\Omega_B=-(\beta V)^{-1}\ln\operatorname{Tr}\exp[-\beta H_B'(M)] \tag{37}$$

with respect to variations in M. As in Sec. II, it is con-

venient to define a new thermodynamic potential per unit volume $\Omega_B(\lambda)$ in terms of the Hamiltonian $H'_B(M,\lambda)=\lambda H'_B(M)$. The potential $\Omega_B(\lambda)$ will be then given by a relation similar to (5). Thus, as in the preceding section, the aim boils down to obtaining $\langle H'_B(M,\lambda)\rangle_\lambda$ in terms of weight functions.

To achieve this goal, we first set up equations of motion for the operators $b_q(t)$, $b_q^\dagger(t)$, etc., where

$$b_q(t)=e^{iH'_B(M,\lambda)t}b_q e^{-iH'_B(M,\lambda)t} . \tag{38}$$

Next, we manipulate these equations to obtain

$$\langle H'_B(M,\lambda)\rangle_\lambda=\lambda VE_0(M)-\lambda hMV+\tfrac{1}{8}\sum_q{}' \lim_{t'\to t}\left\{i\frac{\partial}{\partial t}-i\frac{\partial}{\partial t'}+2[\epsilon_B(q)+2U(M)]\right\}\{\langle b_q^\dagger(t')b_q(t)\rangle_\lambda+\langle b^\dagger_{-q}(t')b_{-q}(t)\rangle_\lambda\}$$
$$+\frac{U(M)}{4}\sum_q{}' \lim_{t'\to t}\{\langle b^\dagger_{-q}(t')b_q^\dagger(t)\rangle_\lambda+\langle b_q(t')b_{-q}(t)\rangle_\lambda\} . \tag{39}$$

The averages in (39) can be expressed in terms of the spectral-weight functions $A^\lambda_{jB}(q,\omega)$ $(j=1,2,3,4)$ given by

$$A^\lambda_{jB}(q,\omega)=i[G^\lambda_j(q,\omega)|_{i\omega_n=\omega+i0^+}-G^\lambda_j(q,\omega_n)|_{i\omega_n=\omega-i0^+}] , \tag{40}$$

where $G^\lambda_j(q,\omega_n)$ are the Fourier coefficients of the temperature Green's functions

$$G^\lambda_{1,2}(q\tau,q'\tau')=-\langle T_\tau\{b_{\pm q}(\tau)b^\dagger_{\pm q'}(\tau')\}\rangle_\lambda ,$$
$$G^\lambda_3(q\tau,q'\tau')=-\langle T_\tau\{b_q^\dagger(\tau)b_{q'}^\dagger(\tau')\}\rangle_\lambda , \tag{41}$$
$$G^\lambda_4(q\tau,q'\tau')=-(T_\tau\{b_{-q}(\tau)b_{-q'}(\tau')\}\rangle_\lambda .$$

Here, $\omega_n=2n\pi/\beta$, $n=0,\pm1,\pm2,\ldots$ and

$$b_q(\tau)=e^{H'_B(M,\lambda)\tau}b_q e^{-H'_B(M,\lambda)\tau} . \tag{42}$$

In (41), the subscript 1 corresponds to (q,q') and the subscript 2 to $(-q,-q')$. Now introducing the functions

$$f^\lambda_j(q,\omega)=-i\int\int dt\,dt' e^{i\omega(t-t')}\langle\ \rangle_\lambda\theta(t-t') , \tag{43}$$

where $\langle\ \rangle_\lambda$ is a thermodynamic average appearing in the right-hand side of (39), and substituting LR's (Ref. 12) of $G^\lambda_j(q,\omega_n)$ in (40) one obtains

$$A^\lambda_{jB}(q,\omega)=-2(e^{\beta\omega}-1)\mathrm{Im}f^\lambda_j(q,\omega) . \tag{44}$$

As in Sec. II, (43) and (44) yield

$$\langle b_q^\dagger(t')b_q(t)\rangle_\lambda=\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\frac{A^\lambda_{1B}(q,\omega)}{(e^{\beta\omega}-1)}e^{-i\omega(t-t')} \tag{45}$$

and similar expressions for the rest of the averages in (39). Using these expressions one finally obtains

$$\Omega_B(\lambda)=\Omega_{0B}-\lambda hM+\lambda E_0(M)+\frac{1}{V}\int\frac{d\lambda}{\lambda}\sum_q{}'\int_{-\infty}^{+\infty}\frac{d\omega}{8\pi}\frac{[\omega+\epsilon_B(q)+2U(M)]}{(e^{\beta\omega}-1)}[A^\lambda_{1B}(q,\omega)+A^\lambda_{2B}(q,\omega)]$$
$$+\frac{1}{V}\int\frac{d\lambda}{\lambda}U(M)\sum_q{}'\int_{-\infty}^{+\infty}\frac{d\omega}{8\pi}\frac{[A^\lambda_{3B}(q,\omega)+A^\lambda_{4B}(q,\omega)]}{(e^{\beta\omega}-1)} \tag{46}$$

for the ordered phase ($h\to0$, $M\neq0$, $h/M\to0$), where Ω_{0B} is an integration constant to be specified later [see note below Eq. (57)]. In the normal phase ($h\to0$, $M\to0$, $h/M\neq0$), since $E_0=0=U$, $A^\lambda_{3B}=0=A^\lambda_{4B}$, and $A^\lambda_{1B}=A^\lambda_{2B}$, (46) corresponds to the well-known KB relation.[1]

To demonstrate the usefulness of (46) to derive thermodynamics and critical behavior, the weight functions are to be calculated. We calculate these functions and the thermodynamic potential per unit volume in an approximation scheme[7,16,17] where the momentum and Matsubara frequency dependence of the normal and anomalous self-energies, denoted by $\Sigma^*_{11}(q,\omega_n)$ and $\Sigma^*_{02}(q,\omega_n)$, respectively, occurring in the finite temperature analogues of the Baliaev equations (FTABE) are ignored altogether. The approximate Matsubara propagators in FTABE give the following expressions for the weight functions:

$$A^\lambda_{1B}(q,\omega)=A^\lambda_{2B}(q,\omega)=2\pi[u_q^2\delta(\omega-\lambda\epsilon_q)-v_q^2\delta(\omega+\lambda\epsilon_q)] ,$$
$$A^\lambda_{3B}(q,\omega)=A^\lambda_{4B}(q,\omega)=2\pi u_q v_q[\delta(\omega+\lambda\epsilon_q)-\delta(\omega-\lambda\epsilon_q)] , \tag{47}$$

where

$$u_q^2=\tfrac{1}{2}\left[\frac{\epsilon_B(q)+\Sigma^*_{11}(0,0)}{\epsilon_q}+1\right] ,$$
$$v_q^2=\tfrac{1}{2}\left[\frac{\epsilon_B(q)+\Sigma^*_{11}(0,0)}{\epsilon_q}-1\right] , \tag{48}$$

$$\epsilon_q^2=[\epsilon_B(q)+\Sigma^*_{11}(0,0)-\Sigma^*_{02}(0,0)]\times[\epsilon_B(q)+\Sigma^*_{11}(0,0)+\Sigma^*_{02}(0,0)] , \tag{49}$$

$$\frac{h}{2M}=-\mu_B+\Sigma_{11}^*(0,0)-\Sigma_{02}^*(0,0)\ . \tag{50}$$

Equation (50) is the equation to determine M. This corresponds to the finite temperature analogue[7,16,17] of the Hugenboltz-Pines theorem. The thermodynamic potential per unit volume, on the other hand, is given by

$$\Omega_B(\lambda=1)=\Omega_{0B}-hM+E_0(M) -\frac{1}{2V}\sum_q{}'\left[\frac{q^2}{2m_B}+\frac{h}{2M}\right] +(\beta V)^{-1}\sum_q{}'\ln\sinh\frac{\beta\epsilon_q}{2}\ . \tag{51}$$

In the ordered phase, the equation to determine M and the thermodynamic potential per unit volume are obtained by taking the limits $h\to 0$ and $h/M\to 0$ $(M\neq 0)$ in (50) and (51), respectively. The self-energies, in the approximation scheme of Ref. 16, are given by

$$\Sigma_{11}^*(0,0)=2U(M)+4un'(T,\Sigma_{11}^*,\Sigma_{02}^*)+2uy(T,\Sigma_{11}^*,\Sigma_{02}^*)\ , \tag{52}$$

$$\Sigma_{02}^*(0,0)=U(M)+2uy(T,\Sigma_{11}^*,\Sigma_{02}^*)\ ,$$

where

$$n'=V^{-1}\sum_q{}'\langle b_q^\dagger b_q\rangle =\frac{1}{V}\sum_q{}'\left[\frac{\epsilon_B(q)+\Sigma_{11}^*(0,0)}{\epsilon_{q0}(\exp\beta\epsilon_{q0}-1)} +\frac{\epsilon_B(q)+\Sigma_{11}^*(0,0)-\epsilon_{q0}}{2\epsilon_{q0}}\right], \tag{53}$$

$$y=V^{-1}\sum_q{}'\langle b_q b_{-q}\rangle =-\frac{1}{V}\sum_q{}'\Sigma_{02}^*(0,0)\left[\frac{1}{2\epsilon_{q0}}+\frac{1}{\epsilon_{q0}(\exp\beta\epsilon_{q0}-1)}\right], \tag{54}$$

$$\epsilon_{q0}^2=\left[\frac{q^2}{2m_B}\right]\left[\frac{q^2}{2m_B}+2\Sigma_{02}^*(0,0)\right]\ . \tag{55}$$

The term $E_0(M)$ is given by $[-\mu_B M^2+uM^4-2un'^2-uy^2]$. Equations (52)–(54) are the self-consistent equations for Σ_{11}^*, Σ_{02}^*, n', and y. Starting with Eqs. (51)–(55) the entire thermodynamics of a Bose system in the ordered phase can be derived. We now obtain crossover scaling forms,[8,9] for the susceptibility and the deviation of pressure from its critical value, for the normal phase of the system starting with these equations.

We note that, in the normal phase, the inverse susceptibility $h/2M$ $(\equiv\gamma_n)$ is nonzero. The equation of the λ line is given by $\gamma_n\to 0_+$. From (51) we obtain

$$\Omega_B(T,\gamma_n)=\Omega_{0B}-(2V)^{-1}\sum_q{}'\left[\frac{q^2}{2m_B}+\gamma_n\right] +(\beta V)^{-1}\sum_q{}'\ln\sinh\frac{\beta}{2}\left[\frac{q^2}{2m_B}+\gamma_n\right] -2un'^2(T,\gamma_n)\ , \tag{56}$$

where, in view of (50) and (52)–(54), γ_n is given by self-consistent equations

$$n'(T,\gamma_n)=\frac{1}{V}\sum_q{}'\frac{1}{\left\{\exp\left[\beta\left[\frac{q^2}{2m_B}+\gamma_n\right]-1\right]\right\}}\ , \tag{57}$$

$$\gamma_n=-\mu_B+4un'(T,\gamma_n)\ .$$

Upon choosing $\Omega_{0B}=(\beta V)^{-1}\sum_q{}'\ln 2$ the boson pressure (P) becomes $[P_0(T,\gamma_n)+2un'^2(T,\gamma_n)]$, where P_0 is formwise the same as the ideal gas pressure. The choice is guided by the fact that, on turning off the interaction, $\Omega_B(T,\gamma_n)$ should reduce to the thermodynamic potential of the ideal gas. The deviation in pressure from its λ-line value $P_C(T,\mu_{BC})$, where $\mu_{BC}=4un'(T,0)$ is the value of μ_B on the λ line at a given T, is

$$\beta(P-P_C)=\beta[P_0(T,\gamma_n)-P_0(T,0)] +2\beta u[n'^2(T,\gamma_n)-n'^2(T,0)]\ . \tag{58}$$

We now split n' above into two parts, viz., n_l' and n_h', where the subscripts l and h, respectively, correspond to the momentum ranges $0<|q|<q_0$ and $q_0<|q|<\infty$. Since the γ_n dependence of n' can be ignored for the latter range, we take $q_0=\Gamma\sqrt{\gamma_n}$ with $\Gamma\simeq 10\sqrt{2m_B}$. As regards $P_0(T,\gamma_n)$, we split it also into two parts, viz., P_{0l} and P_{0h}. It is well known[7,16,17] that singularities, in various thermodynamic functions, near the λ line have their origin in the low-momentum $(0<|q|<q_0)$ operators of the system. With all these in view, we write explicitly the part of $\beta(P-P_C)$ which is a function of T and γ_n both and also correspond to low momenta:

$$\{\beta(P-P_C)\}_l=\beta P_{0l}(T,\gamma_n) +2\beta u[n_l'^2(T,\gamma_n) +2n_h'(T,\gamma_n)n_l'(T,\gamma_n)]\ . \tag{59}$$

The high-momentum part, on the other hand, is given by the remaining terms in (58). Close to the λ line one may assume $\beta\gamma_n\ll 1$. For a $(4-\epsilon)$-dimensional system of bosons, one then obtains

$$\{\beta(P-P_C)\}_l=B(T,\gamma_n)(\beta\gamma_n)^{2-\epsilon/2} +B'(T)u(\beta\gamma_n)^{2-\epsilon}+O(u\gamma_n^{3-\epsilon})\ , \tag{60}$$

where, to the leading order in ϵ,

$$B(T,\gamma_n)=\frac{\Gamma^4 f_0}{16\pi^2\beta^2}\left[1+\frac{\beta\gamma_n}{2f_0}\left[\frac{\Gamma^2}{2m_B}+1\right]+O(\beta\gamma_n)^2\right],$$
$$f_j=\int_0^1\frac{x^{5-j}dx}{\left[x^2+\frac{2m_B}{\Gamma^2}\right]},$$
$$B'(T)=\frac{m_B^2\Gamma^4 f_2}{8\pi^4\beta^2}(f_2+2n''), \tag{61}$$
$$n''=\int_1^\infty\frac{(\beta q_0^2/2m_B)x^3dx}{\left[\exp\left[\frac{\beta q_0^2}{2m_B}x^2-1\right]\right]}.$$

To write down $\{\beta(P-P_C)\}$ in the scaling form in Ref. 8, $(\beta\gamma_n)$ in (60) is to be expressed in terms of the scaling variable defined by Eq. (7.33) in Ref. 18 [see also (98) in Ref. 9]. A similar variable defined by (52) in Ref. 9, however, is more suitable for the present task.

As mentioned above, $(\beta\gamma_n)$ can be calculated from Eqs. (57). On considering, in the first approximation, only the low-momentum part of $n'(T,\gamma_n)$ and defining t as the variable $\beta(\mu_B-\mu_{BC})$, it is easy to see from (57) that

$$\beta\gamma_n\simeq -t-Cu(\beta\gamma_n)^{1-\epsilon/2},$$
$$C=\left[\frac{m_B}{\pi\beta^{1/2}}\right]^2\ln\left[1+\frac{\Gamma^2}{2m_B}\right]. \tag{62}$$

Equation (62) implies that the susceptibility $(\beta\gamma_n)^{-1}$ is expressible in the crossover scaling form [cf. Eqs. (75) and (6.24) in Refs. 9 and 18, respectively]

$$(\beta\gamma_n)^{-1}=|t|^{-1}Y(x),\quad x\equiv Cu|t|^{-\epsilon/2}, \tag{63}$$

where the scaling function Y is given by the equation

$$1=Y-xY^{\epsilon/2}. \tag{64}$$

Equation (64) differs from Eq. (76) in Ref. 9, for the latter has been obtained from a renormalized Hamiltonian. It is possible to obtain the latter, within the framework of this method, provided the thermodynamic potential is calculated with the renormalized Hamiltonian in Ref. 9.

Now substituting (63) in (60) and noting that the high-momentum part of $\{\beta(P-P_C)\}$, for a given T, can be expressed in the form $[A(T)|t|+O(|t|^2)]$ close to the λ line, one obtains

$$\beta(P-P_C)=A(T)|t|[1+b(T,x)|t|^{1-\epsilon/2}(1+x)^{-4/5}], \tag{65}$$

where

$$b(T,x)=A^{-1}(T)Y'^{-2}(x)\left[B(T)+\frac{x}{C}B'(T)\right],$$
$$Y'(x)=Y(x)(1+x)^{-2/5}. \tag{66}$$

This is the crossover scaling form of the pressure deviation sought for [cf. Eq. (15) in the second paper in Ref. 8]. It is also possible to obtain a similar result by the mapping[18] of a Bose system onto a classical S^4 spin model. In the weak interaction limit ($x\ll 1$), since $Y'\simeq 1$, $b(T,x)\simeq B(T)/A(T)$. In the opposite limit ($x\gg 1$), $Y'\simeq x^{-3/5+\epsilon/2}$ and, therefore, $b(T,x)\simeq B'(T)x^{-1/5}/A(T)C$. One notices that, whereas (65) agrees with the Walasek's result[8] in the weak interaction limit, in the opposite limit the second term in the former is of order $|t|^{2-\epsilon/2}x^{-1}$ and that in the latter is $|t|^{2-\epsilon/2}x^{-4/5}$. The reason for this disagreement, as mentioned above, can be traced to the fact that the thermodynamic potential has not been calculated here using a renormalized Hamiltonian. The results above show that the weight function technique is quite efficacious even for deriving crossover critical behavior.

IV. DISCUSSION

The main aim behind the work reported in this paper was to show the possibility of deriving the thermodynamics of Fermi and Bose systems using spectral weight functions in (8) and (40). The idea of the work was derived from the Kadanoff-Baym relation[1] [see the note below (46)] published about thirty years ago. In the recent past, too, some investigation[19] has been done in this regard. Apart from thermodynamic potential per unit volume, the weight-function method can also provide explicit expression for Gibb's potential per particle, starting with an appropriate second quantized Hamiltonian, for all quantum-mechanical systems. Thermodynamics and critical behavior exhibited by these systems can then be derived in terms of the experimental variables temperature and pressure. The method, therefore, has a wide scope.

It was shown by Lukierska *et al.*[20] that critical behavior of the correlation length changes from that characteristic of the $(d+1)$-dimensional, classical Ising model to one characterizing the critical behavior of the d-dimensional, classical Ising model. The problem is to examine other thermodynamic functions, to generalize this effect (called "dimensional crossover"), with the help of the weight-function method. If the Gibbs potential per particle of a Fermi fluid (liquid ^{3}He) is calculated by some means (by the weight-function method, for instance) starting with the approriate microscopic basis, hopefully one then obtains appropriate explanation of various features associated with the A and B transitions in liquid ^{3}He.

A Kubo-type formula involving a retarded correlation function of spin-density operators has been used to compute $\Delta X(k,\omega)$ in (25). A similar correction for the static case was obtained by Brinkman[21] several years ago. The procedure adopted, however, was different. To first order in an applied field, self-consistent equations for gap functions were expanded and, substituting these expansions in the expression for magnetization, the susceptibility was obtained.

The scaling form similar to (65) can be obtained for the ordered phase of the system starting with Eqs. (51)–(55). In a forthcoming publication of Singh,[22] this will be derived within the ambit of the RG study in Ref. 9. It will be shown that the normal-phase scaling form of Walasek

is not entirely valid for the ordered phase; in place of $b(1+x)^{-d/5}$ [see Eq. (15) in the second paper in Ref. 8] a structurally different term is present. These terms are, however, approximately equal in the weak interaction limit as well as in the opposite limit.

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