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Quasiparticles and thermodynamical consistency

A. A. Shanenko[1,2], T. S. Biró[2], and V. D. Toneev[1]

[1] BLTP, JINR, 141980 Dubna, Russia,

[2] MTA RMKI, H-1525 Budapest, P.O.Box 49

Abstract. A brief and simple introduction into the problem of the thermodynamical consistency is given. The thermodynamical-consistency relations, which should be taken into account under constructing a quasiparticle model, are found in a general manner from the finite-temperature extension of the Hellmann-Feynman theorem. Restrictions following from these relations are illustrated by simple physical examples.

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1. Introduction

It is well-known that the concept of quasiparticles, proposed by Landau [1] and developed by Bogoliubov [2], is one of the most powerful tools of the present many-body physics. Quasiparticles provide us with understanding of such important phenomena as the superfluidity and superconductivity. Investigations of the Bose and Fermi gases, of the quantum liquids and of the solid state involves quasiparticle aspects, as a rule. At last, the most interesting for the heavy-ion community, the deconfinement problem is unlikely to be understood while ignoring these aspects. The deconfinement problem now is even formulated in terms of quasiparticles. Indeed, investigating the thermodynamics of strong interactions, we meet a dramatic change in properties, called the QCD phase transition, or deconfinement. Approaching the confinement, the characteristic quasiparticles are bound clusters of quarks and gluons. On the other hand, at high temperatures and large chemical potentials, unbound but effective quarks and gluons as quasiparticles play the major role. The intermediate regime is also explored in terms of the quark and gluon quasiparticles (constituent quarks, massive gluons, hadron-like excitations surviving the QCD phase transition etc.). Thus, as a rule, quasiparticle models of deconfinement are of special interest.

A distinctive feature of quasiparticles is that they have medium-dependent properties, for instance, a medium-dependent mass. One should pay attention to this fact, as it has been emphasized by a number of investigators [3]. The matter is as follows. When a quasiparticle picture is exactly derived from first principles, like in the case of the familiar Bogoliubov model of a weakly interacting Bose gas [2], there is no worry with the medium-dependent properties. However, turning to the thermodynamics of strong interactions, we cannot derive the quasiparticle properties exactly from first principles (unless we solve the confinement problem). Here physicists are forced *to construct* a quasiparticle picture, based, more or less, on their intuition with some additional assumptions involved. These assumptions are not easily to be controlled, which leads often to a loss of the thermodynamical consistency (for more details see the papers by Gorenstein and Yang in Ref. [3]). The problem was intensively studied with the result that to escape such a serious trouble, some special constraints called *the thermodynamical-consistency relations* should be applied. There are indeed rather detailed investigations on this problem but with the common shortcoming that a form of these thermodynamical-consistency relations varies from model to model. The absence of a general form of the relations is quite inconvenient, because everybody who tries to develop a quasiparticle approach should explore its thermodynamical correctness from the very beginning by himself, which requires essential experience in thermodynamics. This is why inconsistent models are still met in the literature. So, the main aim of this report is to demonstrate that the thermodynamical-consistency relations can be obtained in a quite general form being elegant and physically sound. Besides, this paper can be considered as a simple but useful introduction into the problem of interest.

2. Thermodynamical-consistency relations

Let us consider a system governed by a Hamiltonian $\hat{H}$ depending on a set of parameters $\xi = \{\xi_1, \xi_2, \ldots\}$. They are not the basic thermodynamical variables but functions of them, and the Hamiltonian depends on the thermodynamical characteristics only through the parameters. This is exactly the most general way of introducing particles with medium-dependent properties, or, in other words, quasiparticles. Below, for the sake of simplicity, we restrict ourselves to the situation of the only parameter ξ, which does not change the final conclusions. Let us assume, for a moment, that we deal with the Grand Canonical Ensemble so that the basic thermodynamical variables are the temperature T, the volume V and the chemical potential μ. Then, according to the prescriptions of the statistical mechanics, the parameter ξ has to lead to a minimum of the thermodynamical potential in equilibrium at any given T, V and μ. For the Grand Canonical Ensemble the thermodynamical potential is given by the following well-known formula:

$$\begin{aligned} \Omega(\xi; T, V, \mu) &= -T \ln \, \mathrm{Tr} \, e^{-\frac{\hat{H}(\xi) - \mu \hat{N}}{T}} = \\ &= -T \ln \sum_i \langle \psi_i(\xi) | e^{-\frac{\hat{H}(\xi) - \mu \hat{N}}{T}} | \psi_i(\xi) \rangle, \end{aligned} \tag{1}$$

where $\psi(\xi)$ stands for the eigenstates of the operator $\hat{H}(\xi)-\mu\hat{N}$. It is important to stress that ξ influences the thermodynamical potential in two ways: directly trough the Hamiltonian, and trough the eigenstates, which depend on this parameter, too. The extremum condition for ξ yields

$$\left.\frac{\partial\Omega}{\partial\xi}\right|_{T,V,\mu=const}=0. \tag{2}$$

So, introducing a parameter, one can hardly set its dependence on the thermodynamical variables in an arbitrary way: it should not contradict Eq. (2). This important but quite simple point is directly related to the question of the thermodynamical consistency of a quasiparticle model.

The generalized Hellmann-Feynman theorem. To make the next step in our consideration, we should take into account the relation

$$\delta\Omega(\xi)=\langle\delta\hat{H}(\xi)\rangle. \tag{3}$$

known from the statistical physics [4]. This relation is a generalization of the Hellmann-Feynman theorem to the finite temperature case. Here $\delta\Omega$ and $\delta\hat{H}$ are the infinitesimal changes of Ω and $\hat{H}$ with respect to ξ at any fixed T, V and μ. And $\langle\ldots\rangle$ means the statistical averaging. It is deductive to give here the proof of this important formula, not so familiar for the heavy-ion community. The proof is close to that of the Hellmann-Feynman theorem and based on the normalization condition of the system eigenstates

$$\langle\psi_i(\xi)|\psi_j(\xi)\rangle=\delta_{ij}, \tag{4}$$

where δ_{ij} is the Kronecker $\delta-$symbol. So, for the infinitesimal change of the product $\langle\psi_i|\psi_j\rangle$ we have

$$\delta\langle\psi_i|\psi_j\rangle=\langle\delta\psi_i|\psi_j\rangle+\langle\psi_i|\delta\psi_j\rangle=0. \tag{5}$$

Equation (5) makes it possible to significantly simplify the expression for $\delta\Omega$ given by

$$\begin{aligned}\delta\Omega &= \\ &= \frac{T}{\sum_i\langle\psi_i|\,e^{-\frac{\hat{H}-\mu\hat{N}}{T}}|\psi_i\rangle}\sum_i\left\{\langle\psi_i|\frac{\delta\hat{H}}{T}\,e^{-\frac{\hat{H}-\mu\hat{N}}{T}}|\psi_i\rangle\right. \\ &\quad\left.-\,\langle\delta\psi_i|\,e^{-\frac{\hat{H}-\mu\hat{N}}{T}}\,|\psi_i\rangle\,-\,\langle\psi_i|\,e^{-\frac{\hat{H}-\mu\hat{N}}{T}}\,|\delta\psi_i\rangle\right\}.\end{aligned} \tag{6}$$

Indeed, as ψ_i represents the set of the eigenstates of the operator $\hat{H}-\mu\hat{N}$ then the last two terms in the sum of the right-hand-side of Eq. (6) are reduced to

$$-\,e^{-\frac{E_i-\mu N_i}{T}}\Big[\langle\delta\psi_i|\psi_i\rangle+\langle\psi_i|\delta\psi_i\rangle\Big]$$

with $\hat{H}|\psi_i\rangle = E_i|\psi_i\rangle$ and $\hat{N}|\psi_i\rangle = N_i|\psi_i\rangle$. According to Eq. (5) the latter expression is equal to zero, and, thus, Eq. (6) turns to

$$\delta\Omega(\xi) = \frac{\sum_i \langle\psi_i(\xi_i)|\delta\hat{H}(\xi)\, e^{-\frac{\hat{H}(\xi)-\mu\hat{N}}{T}}|\psi_i(\xi)\rangle}{\sum_i \langle\psi_i(\xi)|e^{-\frac{\hat{H}(\xi)-\mu\hat{N}}{T}}|\psi_i(\xi)\rangle}, \tag{7}$$

which is nothing more but Eq. (3).

Now, taking Eq. (2) in conjunction with the generalization of the Hellmann-Feynman theorem (3), one can arrive at the important equation

$$\Big\langle \frac{d\hat{H}}{d\xi} \Big\rangle = 0. \tag{8}$$

Though Eq. (8), similar to Eq. (2), is tightly connected with the thermodynamical consistency of a quasiparticle scheme, this equation is not yet the most useful in practice. It is much more convenient to rearrange Eq. (8) in the following manner. As it has been mentioned above, the Hamiltonian depends on the thermodynamical variables only through the parameter ξ. So, for any of them $(a = T, V, \mu)$ one has

$$\Big\langle \frac{\partial\hat{H}}{\partial a} \Big\rangle = \Big\langle \frac{d\hat{H}}{d\xi}\,\frac{\partial\xi}{\partial a} \Big\rangle = \frac{\partial\xi}{\partial a}\,\Big\langle \frac{\partial\hat{H}}{\partial\xi} \Big\rangle = 0.$$

Thus, operating with the Grand Canonical Ensemble we arrive at

$$\Big\langle \frac{\partial\hat{H}}{\partial T} \Big\rangle = \Big\langle \frac{\partial\hat{H}}{\partial V} \Big\rangle = \Big\langle \frac{\partial\hat{H}}{\partial\mu} \Big\rangle = 0. \tag{9}$$

The same procedure can be realized in the Canonical Ensemble with the result

$$\Big\langle \frac{\partial\hat{H}}{\partial T} \Big\rangle = \Big\langle \frac{\partial\hat{H}}{\partial V} \Big\rangle = \Big\langle \frac{\partial\hat{H}}{\partial N} \Big\rangle = 0, \tag{10}$$

where N denotes the number of quasiparticles. Equations (9) and (10) are the most general representations of *the thermodynamical consistency relations*. Though these representations are derived in the Grand Canonical and Canonical Ensembles, they are fulfilled in any situation, beyond a statistical-ensemble context. For homogeneous systems the following variant of the consistency relations is convenient to be used:

$$\Big\langle \frac{\partial\hat{H}}{\partial T} \Big\rangle = \Big\langle \frac{\partial\hat{H}}{\partial n} \Big\rangle = 0 \tag{11}$$

with $n = N/V$. Thus, introducing a quasiparticle Hamiltonian depending on some thermodynamical quantities, one should be careful and fulfill the relations (11). Otherwise, one faces some fault with the thermodynamics. It can, for example, manifest itself in the fact that different ways of calculating the same thermodynamical quantity are able to yield different results. Nonequivalence of the statistical ensembles in spite of the large volume limit is possible, too. At last, violence of the thermodynamical-consistency relations can result in an appearance of derivatives of an order parameter in expressions for the first derivatives of the thermodynamical potential. In this case the second-order phase transition is accompanied by a divergence of the entropy and mean energy at the transition point [5].

It is further interesting to choose a useful sample Hamiltonian, to go in more detail concerning Eq. (11). With this aim we adopt the following expression:

$$\hat{H} = \sum_i \sum_f \varepsilon_{ki}(T,n)\; a^{\dagger}_{fi}\; a_{fi} + V\varphi(T,n), \tag{12}$$

which is often involved in the quaisparticle models of the deconfinement. Here $a^{\dagger}_{fi}$ and a_{fi} are the creation and annihilation operators for quasiparticles of the sort i in the state $f = (\mathbf{k}, \sigma)$, where $\mathbf{k}$ stands for the momentum and σ is for inner degrees of freedom. The quantity $\varepsilon_{ki}(T,n)$ denotes the single-particle spectrum dependent on the thermodynamical variables T and $n = \{n_1, n_2, n_3, ...\}$. Special explanations are needed for the $c-$number term $V\,\varphi(T,n)$ in Eq. (12). This term comes from the difference between the vacuum of the primordial particles $|0\rangle$ and the quasiparticle vacuum $|0,q\rangle$. We have the following structure of the Hamiltonian of interest:

$$\hat{H} = \hat{A}(a^{\dagger}, a) + c, \quad \hat{A}(a^{\dagger}, a)\;|0,q\rangle = 0.$$

Therefore, $\hat{H}|0,q\rangle = c|0,q\rangle$, while $\hat{H}|0\rangle = 0$. So, $c = V\;\varphi(T,n)$ is the system energy in the quasiparticle vacuum which should not be equal to zero in general due the difference between $|0\rangle$ and $|0,q\rangle$. Besides, in what concerns the Hamiltonian (12), it is also worth noting that ε_{ki} has to depend on the quasiparticle densities n_i in the case considered. Indeed, there are two possible situation of dealing with quasiparticles. The first is related to uninteracting quasiparticles. This simplification is justified, in particular, in the low-temperature physics with extremely small densities of quasiparticles in spite of large particle densities when the dependence of the quasiparticle spectra on the quasiparticle densities can be ignored (phonons in the superfluidity problem). The other, more complicated variant corresponds to interacting and, so, correlated quasiparticles. Here the quasiparticle spectra should involve the quasiparticle densities, like in the familiar Hartree-Fock approximation. This variant has to be introduced when dealing with large quasiparticle densities. Exactly such a nontrivial situation takes place in the problem of the QCD phase transition. Now, inserting Eq. (12) in Eq. (11), we can arrive at

$$\left\langle \frac{\partial \hat{H}}{\partial T} \right\rangle = \sum_i \sum_f \frac{\partial \varepsilon_{ki}}{\partial T}\;\langle a^{\dagger}_{fi}\; a_{fi}\rangle + V\,\frac{\partial \varphi(T,n)}{\partial T} = 0,$$

$$\left\langle \frac{\partial \hat{H}}{\partial n_j} \right\rangle = \sum_i \sum_f \frac{\partial \varepsilon_{ki}}{\partial n_j}\;\langle a^{\dagger}_{fi}\; a_{fi}\rangle + V\,\frac{\partial \varphi(T,n)}{\partial n_j} = 0.$$

For the Hamiltonian taken in the form (12) the mean occupation number is given by

$$\nu_{ki} = \langle a^\dagger_{fi} a_{fi} \rangle = \frac{1}{e^{\frac{\varepsilon_{ki}-\mu_i}{T}} + \zeta_i} \tag{13}$$

with the statistical factor $\zeta_i = +1$ or -1. So, in the thermodynamical limit, when

$$\sum_f \to V d_i \int \frac{d^3k}{(2\pi)^3}\ ,$$

the thermodynamical-consistency relations for the system governed by (12) are represented in the following form:

$$\begin{aligned} \sum_i d_i \int \frac{d^3k}{(2\pi)^3}\, \frac{\partial \varepsilon_{ki}}{\partial T}\, \nu_{ki} + \frac{\partial \varphi}{\partial T} &= 0, \\ \sum_i d_i \int \frac{d^3k}{(2\pi)^3}\, \frac{\partial \varepsilon_{ki}}{\partial n_j}\, \nu_{ki} + \frac{\partial \varphi}{\partial n_j} &= 0. \end{aligned} \tag{14}$$

As it is seen, the quasiparticle spectra $\varepsilon_{ki}(T,n)$ are directly involved in the thermodynamical-consistency relations. In order to emphasize importance of this connection, we discuss some physically relevant examples below.

3. Density-dependent mean field

Let the spectrum of the quasiparticles of the i-th sort be approximated as

$$\varepsilon_{ki}(T,n) = \varepsilon^{(0)}_{ki} + u_i(T,n), \tag{15}$$

where $\varepsilon^{(0)}_{ki}$ denotes the energy of the corresponding free particles and $u(T,n)$ stands for a mean-field potential. This approximation can often be met in the literature on properties of the excited nuclear matter, see for example [6]. Inserting Eq. (15) in Eq. (14), one can arrive at

$$\begin{aligned} \sum_i n_i \frac{\partial u_i}{\partial n_j} + \frac{\partial \varphi}{\partial n_j} &= 0, \\ \sum_i n_i \frac{\partial u_i}{\partial T} + \frac{\partial \varphi}{\partial T} &= 0. \end{aligned} \tag{16}$$

The first equation is known since the paper by Olive (see the first reference in [3]). Whereas the second one has first been published in Ref. [7].

There are interesting consequences of Eqs. (16) leading to important constraints on the mean-field potentials u_i. Indeed, the second equation in Eqs. (16) is integrated to

$$f(n) = \sum_i n_i\, u_i + \varphi, \tag{17}$$

where f is some function of the quasiparticle densities only. Equation (17) can be rewritten as

$$\frac{\partial f}{\partial n_j} = u_j + \sum_i n_i \frac{\partial u_i}{\partial n_j} + \frac{\partial \varphi}{\partial n_j},$$

which, taken together with the first relation in Eqs. (16), allows for concluding that u_j and φ are temperature-independent Note that this important point is missed in some papers treating the excluded volume effects through the mean-field approximation [8].

It is worth doing one more remark on the density-dependent mean field approximation. In this case we have a specific crossing relation

$$\frac{\partial u_i}{\partial n_j} = \frac{\partial u_j}{\partial n_i} \tag{18}$$

found by Zimányi et al [9]. This relation follows from Eqs. (16) under the requirement of smooth second derivatives:

$$\frac{\partial^2 u_i}{\partial n_l \partial n_j} = \frac{\partial^2 u_i}{\partial n_j \partial n_l}, \quad \frac{\partial^2 \varphi}{\partial n_l \partial n_j} = \frac{\partial^2 \varphi}{\partial n_j \partial n_l}.$$

Ignorance of (18) results in the loss of the thermodynamical consistency (see, for example, the paper by Kapusta and Olive in Ref. [6]). The physics hidden beyond the crossing relation can easily be understood with the help of the Hartree approximation: $u_i = \sum_j \alpha_{ij} n_j$. In this case Eq. (18) is reduced to $\alpha_{ij} = \alpha_{ji}$, i.e. the interaction of a quasiparticle of the sort i with that of j coincides with the interaction of a quasiparticle of the sort j with that of i, nothing more but the third low of Newton. Equation (18) is very useful in dealing with a system of many particle species because of its simplicity, which makes it possible to immediately realize if some approximation for the mean field u_i is thermodynamically consistent or not. For example, the relation $u_i = \sum_j \beta_{ij} n_j^\gamma$, where γ is some power factor and β_{ij} does not depend on the thermodynamical variables, can be correct from the thermodynamical point of view only when $\gamma = 1$, otherwise one would face the crossing relation $\beta_{ij} n_j^{\gamma-1} = \beta_{ji} n_i^{\gamma-1}$ to be fulfilled at any set of densities n_i and n_j. So, the question arises about general constructions for u_i which would satisfy Eq. (18). An interesting variant was proposed in Ref. [9]:

$$u_i = g_i\, \widetilde{u}(\sum_j g_j n_j), \tag{19}$$

where g_i is a coupling constant and $\widetilde{u}$ stands for an arbitrary function of $\sum_j g_j n_j$.

4. Effective mass

One more interesting and educative example is based on the approximation [10]

$$\varepsilon_{ki}(T,n) = \sqrt{k^2 + m_i^2(T,n)} \tag{20}$$

involving medium-dependent effective masses. Taken together with the thermodynamical-consistency relations, this approximation yields

$$\sum_i n_{s,i}\,\frac{\partial m_i}{\partial n_j}+\frac{\partial\varphi}{\partial n_j}=0,$$
$$\sum_i n_{s,i}\,\frac{\partial m_i}{\partial T}+\frac{\partial\varphi}{\partial T}=0, \tag{21}$$

where $n_{s,i}$, the Lorentz scalar density, is given by

$$n_{s,i}=d_i\int\frac{d^3k}{(2\pi)^3}\,\nu_{ki}\,\frac{m_i}{\sqrt{k^2+m_i^2}}. \tag{22}$$

This elegant form of the thermodynamical-consistency relations for the approximation (20) (compare with the result of the paper by Gorenstein and Yang in Ref. [3]) was recently derived in [11], where it was shown that m_i and φ are likely to depend on the thermodynamical variables only through the scalar densities: $m_i = m_i(n_s)$ and $\varphi = \varphi(n_s)$ with $n_s = \{n_{s,1}, n_{s,2}, \ldots\}$ being the set of the scalar densities. This is exactly proved for the situation of one quasiparticle sort, and there are serious arguments in favor of the same picture for many quasiparticle species. The proof of this statement in the case of a single quasiparticle sort is based on the formula

$$\frac{\partial n_s}{\partial T}\Big/\frac{\partial n_s}{\partial n}=\frac{\partial m}{\partial T}\Big/\frac{\partial m}{\partial n} \tag{23}$$

resulting from the thermodynamical-consistency relations (21). This relation testifies that the gradients of functions $n_s(T,n)$ and $m(T,n)$ are parallel vectors in the (T,n) plane. Hence, m is constant along any line where n_s is constant. And as $n_s(T,n)$ and $m(T,n)$ are differentiable functions of T and n, then the (T,n) plane is densely covered by lines of constant n_s. If m_i and φ are indeed functions of the scalar densities then Eq. (21) can be represented in the following form:

$$\sum_i n_{s,i}\,\frac{\partial m_i}{\partial n_{s,j}}+\frac{\partial\varphi}{\partial n_{s,j}}=0. \tag{24}$$

So, we have the situation very similar to that of the previous section with only exception that now we face the scalar densities rather than the usual ones. In particular, the crossing relation turns to

$$\frac{\partial m_i}{\partial n_{s,j}}=\frac{\partial m_j}{\partial n_{s,i}}, \tag{25}$$

and a solution of Eq. (25) is given by

$$m_i=g_i\,\widetilde{m}(\sum_j g_j n_{s,j}), \tag{26}$$

where $\widetilde{m}$ can, for example, be a constituent quark mass with g_i being the number of quarks in a quasiparticle of the sort i.

5. Conclusion

The problem of the thermodynamical consistency of a quasiparticle picture has briefly been outlined. The thermodynamical-consistency relations have been derived in a general manner on the basis of the finite-temperature extension of the Hellmann-Feynman theorem. Some illuminating physical examples have been considered with a particular emphasis on the restrictions following from the relations.

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