Connection between the real-time technique in thermofield dynamics and the Matsubara approach in quantum statistical physics

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In the calculation of thermodynamic quantities by quantum-field methods the Matsubara integration contour can be deformed in the complex-time plane. The admissible deformations are limited by the singularities of the Hamiltonian as a function of time. They correspond to the change of the parameters of the system as the interaction is switched on. The real-time technique must be constructed over the true thermodynamic vacuum with allowance for the interaction.

The thermodynamic approach to quantum field theory is attracting great attention at the present time. The properties of a quark-gluon plasma are important for an understanding of the physics of the hot universe and of collisions of heavy ions. The theory of superstrings at high temperatures promises to become no less of a "hot spot." It is interesting to understand not only the thermodynamic properties but also the kinetic characteristics such as the viscosity, thermal conductivity, etc. An intermediate stage on the route to this is the real-time formalism (RTF), which permits one to find the thermodynamic functions by means of a Feynman-diagram technique in a specially defined thermal vacuum that takes into account the Gibbs distribution over the energies.[1,2]

In Ref. 2 it was shown that this technique can be related to the standard Matsubara approach. For this, in the complex plane one must deform the contour of integration in the exponent in the functional integral for the thermodynamic generating function (see Fig. 1). This leads to a doubling (familiar in the kinetics of quantum systems) of the number of degrees of freedom: The integral along C_{II} generates the distinctive "ghosts" of the RTF. It is assumed that the integrals along the vertical parts C_{III} and C_{IV} lead, in the limit $T\to\infty$, only to multiplicative renormalization of the generating functional.

In the present paper it is shown that in the complex-time plane the Hamiltonian of a system with an interaction has singularities (t_1^*, t_2^*) that obstruct the passage to the limit $T\to\infty$. Their appearance is related to the adiabatic switching-off of the interaction as $|t|\to\infty$. After the singularities have been taken into account it is found that the RTF must be constructed over the true thermodynamic vacuum of the interacting system, and the vertical parts correspond to the restructuring of the vacuum under the influence of the interaction. In ordinary quantum field theory the question of the adiabatic switching-on of the perturbation is not so important in principle, since the ground state is assumed to be nondegenerate and can be changed only by a phase factor. Statistical physics differs in that, first, the thermal vacuum is not the ground state, and second, there may be no energy gap in the excitation spectrum, making the system sensitive even to slow switching on of the perturbation.

The significance of this is particularly clear when the simple thermodynamic vacuum is unstable against the interaction. For example, in the theory of superconductivity an arbitrarily weak attraction between electrons leads to a change of the spectrum near the Fermi surface and to the formation of Cooper pairs. The starting point for study of the properties of the system should be the true vacuum with allowance for the condensate.

Let us indicate the obstacles that may be encountered upon deformation of the integration contour in the complex plane. The physical characteristics are completely determined by the density matrix $\rho(q,t,q',t')$ of the system, where q are the generalized coordinates and t is the time. Values of the density matrix at different times are connected by the relation

$$\rho(q,t,q',t') = \int dq_1\,dq_2\,S(q,t,q_1,t_1)\rho(q_1,t_1,q_2,t_2)S^{-1}(q',t',q_2,t_2). \quad (1)$$

Here, $S(q,t,q',t')$ is the evolution operator:

$$S(q,t,q',t') = \int\limits_{q\to q'} [Dp][Dq]\exp\left\{i\int\limits_t^{t'}[p\dot{q}-H-V(t)]\,dt\right\}. \quad (2)$$

The evolution occurs in ordinary time, q and q' are the coordinate of the initial and final states, respectively, H is the free Hamiltonian, and $V(t)$ is the terms corresponding to the interaction.

Equation (1) in the limit $t_1 = t_2 \to -\infty$ makes it possible to develop the diagram technique of Ref. 3, which is well known in physical kinetics and works for arbitrary, not necessarily equilibrium initial density matrices $\rho(-\infty)$. Here too the number of degrees of freedom undergoes doubling, associated with the presence of the factor $S^{-1}(t',-\infty)$ in the formula.

The density matrix of the equilibrium thermal distribution can be expressed by a formula analogous to (2), but with a purely imaginary quantity in the role of the time:

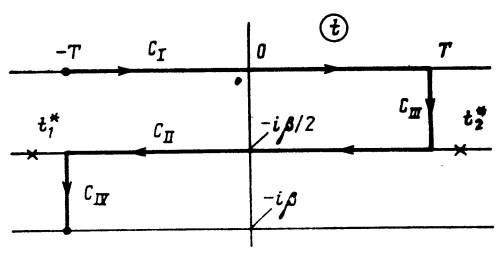

FIG. 1. Integration contour used in the derivation of the real-time technique; t_1^* and t_2^* are singularities bounding the physical region.

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$$\rho_V^M(q_1,q_2,t_r)=\int\limits_{q_1\to q_2}[Dp][Dq]\exp\left\{i\int\limits_0^{-i\beta}[p\dot{p}-H-V(t_r)]\,dt\right\},\tag{3}$$

where β is the inverse temperature and t_r is the real time, which, for now, is simply a parameter of the interaction.

Substituting the expression for ρ^M into the definition (1), we see that the matrix $\rho(q,t,q',t')$ can be expressed in the form of a functional integral, in which the integration contour in the exponent of the exponential runs along the contour C in the complex plane (see Fig. 2). The contour C consists of three pieces, for each of which the procedure of functional integration is well defined. The question arises: Are deformation of the contour C admissible?

We recall that the density matrix $\rho(\ldots)$ given by Eq. (1) is, for real t, a solution of the equations

$$\frac{\partial}{\partial t}\rho(q,t,q',t')=-i[\hat{H}+\hat{V}]\rho,\tag{4a}$$

$$\frac{\partial}{\partial t'}\rho=i\rho[\hat{H}+\hat{V}].\tag{4b}$$

Therefore, if H and V are defined for complex values of t, the matrix ρ can be analytically continued. When the problem of the thermodynamics of a system with a constant Hamiltonian is reformulated in field-theoretical real-time terms it is no longer possible, generally speaking, to regard V as time-independent. However, certain restrictions must be imposed on the operator-valued function V.

First, it is necessary that V be an analytic function, real on the real axis. Under complex conjugation, $V(\bar{t})=\bar{V}(t)$. Second, the standard formulation of the problem in quantum field theory assumes that the interaction is absent at $t=\pm\infty$:

$$V(t=\pm\infty)=0\tag{5}$$

and is switched on adiabatically in the physical region. Then $\rho_0^M(-\infty)$ is the usual thermal density matrix of the free fields.

Finally, in thermal equilibrium we must impose on the function V the Kubo-Martin-Schwinger condition,[1,2] i.e., periodicity in imaginary time:

$$V(t+i\beta)=V(t).\tag{6}$$

Since the equilibrium wave functions of Fermi (Bose) fields are antiperiodic (periodic), (6) implies that the temperatures of the perturbation and of the system coincide.

Although the conditions listed do not fix the dependence $V(t)$, it necessarily follows from them that in the strip $-\beta\leqslant\mathrm{Im}\,t\leqslant 0$ the function V has at least two simple poles (or one second-order pole). In fact, according to (6), the lines $\mathrm{Im}\,t=0$ and $\mathrm{Im}\,t=-\beta$ can be identified, and the domain of definition of V turns out to be topologically equivalent to a sphere with two punctures $t=\pm\infty$, at which its definition can be supplemented by (5).

From the theory of analytic functions on Riemann surfaces it is known that on a sphere the number of zeros coincides with the number of poles, when allowance is made for the multiplicity.[1)] We confine ourselves to the simplest case, when V has two simple poles at the points t_1^* and t_2^*. The quantity $|t_1^*-t_2^*|$ is the characteristic time for switching on the interaction. The physical region lies between the poles: $\mathrm{Re}\,t_1^*\leqslant\mathrm{Re}\,t\leqslant\mathrm{Re}\,t_2^*$. From the periodicity $V(t)=V(t-i\beta)$, since $V(\bar{t})=\bar{V}(t)$, it follows that the poles lie symmetrically about the line $\mathrm{Im}\,t=-\beta/2$. In our case, $\mathrm{Im}\,t_1^*=\mathrm{Im}\,t_2^*=-\beta/2$.

The singular points of the function $V(t)$ are branch points of the solutions of Eqs. (4). Depending on the physical formulation of the problem, one must draw cuts through them and fix the lower branch.

The choice of cuts shown in Fig. 3a makes it possible to find the response of the equilibrium free system to the switching-on of the interaction. We have

$$\rho_a(q,t,q',t')=\int dq_1\,dq_2\,S(q,t,q_1,-\infty)\times\rho_0^M(q_1,q_2,-\infty)S^{-1}(q',t',q_2,-\infty).\tag{7a}$$

The characteristics of the thermodynamic equilibrium system with interaction must be calculated with the cuts drawn as in Fig. 3b, since the initial Matsubara contour lies in the physical region. In Eq. (1) we must substitute the thermal density matrix with interaction

$$\rho_b(q,t,q',t')=\int dq_1\,dq_2\,S(q,t,q_1,t_0)\times\rho_V^M(q_1,t_0,q_2,t_0)S^{-1}(q',t',q_2,t_0),$$

$$\mathrm{Re}\,t_1^*<t_0<\mathrm{Re}\,t_2^*.\tag{7b}$$

If we attempt to deform the integration contour in Eq. (7b), as shown in Fig. 1, in order to obtain the RTF, the poles of the function $V(t)$ prevent one from taking the vertical parts of the contour outside the physical region. Thus, the true vacuum is the thermal vacuum with allowance for the interaction.

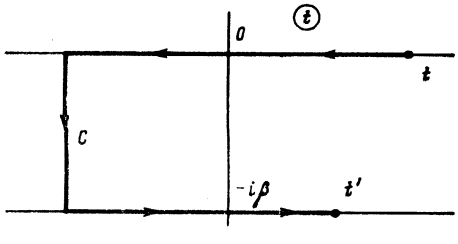

FIG. 2. Contour determining the evolution of the density matrix.

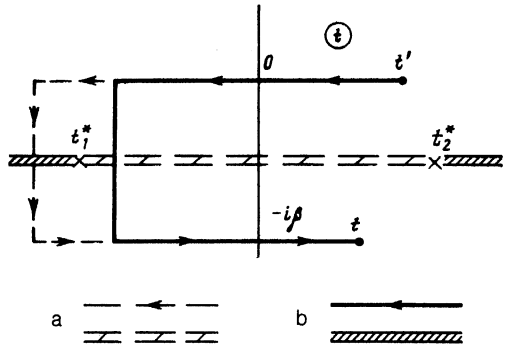

FIG. 3. Two variants of the choice of cuts.

In order to understand the essence of the difference between the two solutions ρ_a and ρ_b, let us calculate the density matrix $\rho_V^M(q,q',t)$ at $t = \mathrm{Re}\, t^* \pm 0$, where ρ_a and ρ_b differ only in the way of going round the pole $t = t^*$. Near the pole the operator function V can be represented in the form

$$V(t) = \frac{W(t^*)}{t-t^*} + o(1), \tag{8}$$

where $W(t^*) = \mathrm{Res}_{t=t^*} V(t)$ is the residue at the point t^*. Therefore, the solutions of Eq. (4a) in this neighborhood look like

$$\rho(t, q, t', q') = (t-t^*)^{-iW(t^*)}\varphi(t, q, t', q'), \tag{9}$$

where φ is a function that is regular at the point t^*. The solutions $\rho_V^M(t^* + 0)$ and $\rho_V^M(t^* - 0)$ differ by a "half-circuit" around the singularity:

$$\rho_V{}^M(t^* \pm 0) = \int [Dp\, Dq] \exp\Big[i \int_{t^*}^{t^*-i\beta/2} (p\dot{q} - H - V)\, dt \Big]$$
$$\times e^{\mp \pi W} \exp\Big[i \int_{t^*+i\beta/2}^{t^*} (p\dot{q} - H - V)\, dt \Big]. \tag{10}$$

It is remarkable that, to within quantities that are small in $\beta/(t_2^* - t_1^*)$, the residues $W(t_k^*)$ can be expressed in terms of the value of V in the physical region:

$$W(t_k^*) = (-1)^k \int_0^{-i\beta} \frac{V(t)\, dt}{2\pi i} = (-1)^{k+1} \frac{\beta V(0)}{2\pi} + o\Big(\frac{\beta}{t_2^* - t_1^*} \Big), \quad k = 1, 2. \tag{11}$$

It is easy to convince oneself of this by integrating $V(t)$ over the contours C_1 and C_2 of Fig. 4. It is obvious that

$$\oint_{C_k} V(t)\, dt = 2\pi i W(t_k^*). \tag{12}$$

By virtue of the periodicity of $V(t)$, the integrals along the straight lines $\mathrm{Im}\, t = 0$ and $\mathrm{Im}\, t = -i\beta$ cancel each other, $V(\pm\infty) = 0$, and a nonzero contribution is given only by the part from 0 to $-i\beta$.[2)] Substituting (11) into Eq. (10), we see that the passage around the pole introduces into ρ_V^M the operator factor $e^{-\beta V}$. Contracting $\rho_V^M(t_1^* + 0)$ with $\rho_V^M(t_1^* - 0)^{-1}$, we obtain

$$\mathrm{Tr}\,[\rho_V{}^M(\mathrm{Re}\, t_1^* + 0)\, (\rho_V{}^M(\mathrm{Re}\, t_1^* - 0))^{-1}] = \mathrm{Tr} \exp(-\beta V). \tag{13}$$

The right-hand side is equal to $e^{-\beta \Delta\Omega}$, where $\Delta\Omega$ is the correction to the thermodynamic potential Ω as a consequence of the switching on of the interaction:[4]

$$\Delta\Omega = -\frac{1}{\beta} \ln \mathrm{Tr} \exp(-\beta V), \tag{14}$$

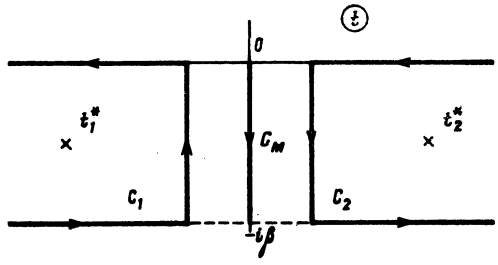

FIG. 4. Calculation of the residues of the function $V(t)$; C_M is the Matsubara contour.

and is a sum of closed loop graphs in the Matsubara technique.

In conclusion, we enumerate again the main results. The path of the functional integration can be deformed within the physical region (bounded by the singular points of the Hamiltonian) in the complex-time plane. The residues at the poles correspond to vacuum loops in the Matsubara technique. In the construction of the real-time technique for the investigation of kinetic properties it is necessary to take into account the true structure of the thermal vacuum. The restructuring of the vacuum is especially important when there is no gap in the energy spectrum or if the unperturbed vacuum is unstable against the switching on of the interaction.

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[1)] The generalization to operator-valued functions appears to be admissible for physical interactions $V(t)$. This is obvious for a homogeneous dependence $V(t) = Vf(t)$ and for matrix elements V_{mn} in any basis. It hardly makes sense to consider specially complicated analytic properties of $V(t)$, since this will lead to a decrease of the radius of convergence of the perturbation-theory series.

[2)] As an example, we may consider the function $V(t) = V(0)\,[1 + \mathrm{ch}(2t^*\pi/\beta)] \cdot [\mathrm{ch}(2\pi t/\beta) + \mathrm{ch}(2\pi t^*/\beta)]^{-1}$, with poles at the points $\pm t^* - i\beta/2$. For this function, (11) is fulfilled to within $o(\exp(-2\pi t^*/\beta))$.

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