Two-level atom at finite temperature

Tomasz Sowiński
Center for Theoretical Physics of the Polish Academy of Sciences

Introduction

The main purpose of this work is to show that a new method of describing qubits within the quantum field theory formalism developed by us in [2] can be also used to describe qubits at finite temperature. The main idea comes from the observation made long time ago by Takeo Matsubara that there exists a close analogy between Feynman propagators and the so called temperature propagators. In this paper we will adopt this formalism to analyze the temperature properties of qubit. To make all our argumentation clear, we restrict ourselves to the problem of a two-level atom (TLA) and its polarizability.

Physical situation

The Hamiltonian of studied system reads

$$\widehat{\mathcal{H}} = \widehat{\mathcal{H}}_0 + \widehat{\mathcal{H}}_{\mathrm{I}} \qquad (1)$$

where

$$\widehat{\mathcal{H}}_0 = m\sigma_z + \int_0^\infty \mathrm{d}k\, k\, a^\dagger(k)a(k),$$
$$\widehat{\mathcal{H}}_{\mathrm{I}} = \sigma_x \int_0^\infty \mathrm{d}k\, g(k)\,\Phi(k).$$

The operators $a^\dagger(k)$ and $a(k)$ create and annihilate photons in the appropriate modes of EM and they form a quantum scalar field

$$\Phi(k) = \frac{a(k) + a^\dagger(k)}{\sqrt{2k}}. \qquad (2)$$

We assume that system is in thermal equilibrium – its state is represented by the following density matrix

$$\hat{\rho} = \frac{1}{\widehat{\mathcal{Z}}}\mathrm{e}^{-\beta\widehat{\mathcal{K}}}, \qquad \widehat{\mathcal{Z}} = \mathrm{tr}\left[\mathrm{e}^{-\beta\widehat{\mathcal{K}}}\right]. \qquad (3)$$

The statistical Hamiltonian $\widehat{\mathcal{K}}$ is given by

$$\widehat{\mathcal{K}} = \widehat{\mathcal{H}} - \mu\mathcal{N}.$$

The operator $\mathcal{N}$ represents the number of photons.
Expectation value of any operator $\mathcal{O}$ in such a quantum state of the system is given by

$$\langle\!\langle \mathcal{O} \rangle\!\rangle = \mathrm{tr}\left[\hat{\rho}\,\mathcal{O}\right] = \frac{\mathrm{tr}\left[\mathrm{e}^{-\beta\widehat{\mathcal{K}}}\mathcal{O}\right]}{\mathrm{tr}\left[\mathrm{e}^{-\beta\widehat{\mathcal{K}}}\right]}. \qquad (4)$$

We are going to find the **linear polarizability** of TLA – the physical measure of the reaction of the system to small external electromagnetic perturbations. It is defined as follows

$$\alpha(t,t') = -i\,\theta(t-t')\,\left\langle\!\!\left\langle\left[\mathrm{e}^{i\widehat{\mathcal{H}}t}\sigma_x\,\mathrm{e}^{-i\widehat{\mathcal{H}}t}, \mathrm{e}^{i\widehat{\mathcal{H}}t'}\sigma_x\,\mathrm{e}^{-i\widehat{\mathcal{H}}t'}\right]\right\rangle\!\!\right\rangle.$$

Second quantization

We introduce, by performing second-quantization, the fermionic field operator representing the states of an electron in the atom. We introduce creation and annihilation operators of the electron: $\psi_\downarrow$ and $\psi_\downarrow^\dagger$ for the ground state, and $\psi_\uparrow$ and $\psi_\uparrow^\dagger$ for the exited state. They form together the fermion field operator

$$\Psi = \begin{pmatrix}\psi_\uparrow \\ \psi_\downarrow\end{pmatrix}, \qquad \Psi^\dagger = \left(\psi_\uparrow^\dagger, \psi_\downarrow^\dagger\right). \qquad (5)$$

The second-quantized form of the Hamiltonian has the form

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\mathrm{I}} \qquad (6)$$

where

$$\mathcal{H}_0 = m\Psi^\dagger\sigma_z\Psi + \int_0^\infty \mathrm{d}k\, k\, a^\dagger(k)a(k),$$
$$\mathcal{H}_{\mathrm{I}} = \Psi^\dagger\sigma_x\Psi \int_0^\infty \mathrm{d}k\, g(k)\,\Phi(k).$$

Notice that the system described by the Hamiltonian $\mathcal{H}$ may have states with different number of fermions. However, the number of fermions operator commutes with $\mathcal{H}$.
Now we introduce a new statistical operator ρ

$$\rho = \frac{1}{\mathcal{Z}}\mathrm{e}^{-\beta\mathcal{K}}, \qquad \mathcal{Z} = \mathrm{tr}\left[\mathrm{e}^{-\beta\mathcal{K}}\right] \qquad (7)$$

where the statistical Hamiltonian $\mathcal{K}$ is given by

$$\mathcal{K} = \mathcal{H} - \mu\mathcal{N}.$$

The expectation value of any operator $\mathcal{O}$ in this state is

$$\langle \mathcal{O} \rangle = \mathrm{tr}\left[\rho\,\mathcal{O}\right] = \frac{\mathrm{tr}\left[\mathrm{e}^{-\beta\mathcal{K}}\mathcal{O}\right]}{\mathrm{tr}\left[\mathrm{e}^{-\beta\mathcal{K}}\right]}. \qquad (8)$$

Notice, that the expectation values (4) and (8), even for the same physical observable $\mathcal{O}$, are different since the statistical Hamiltonians $\mathcal{K}$ and $\widehat{\mathcal{K}}$ act in different Hilbert spaces. Nevertheless, for those qubit operators $\mathcal{O}_1, \ldots, \mathcal{O}_n$ that are represented by traceless 2×2 matrices one can show that following connection holds

$$\langle\!\langle \mathcal{O}_1 \cdots \mathcal{O}_n \rangle\!\rangle = \frac{\mathcal{Z}}{\widehat{\mathcal{Z}}}\langle \Psi^\dagger\mathcal{O}_1\Psi \cdots \Psi^\dagger\mathcal{O}_n\Psi\rangle. \qquad (9)$$

This relation gives a connection between the expectation values of physical quantities and the expectation values of their non-physical second-quantized counterpart.
This all means that a linear polarizability of TLA can be reproduced from its second-quantized counterpart

$$\alpha(t,t') = -i\,\theta(t-t')\,\left\langle\left[\Psi^\dagger(t)\sigma_x\Psi(t), \Psi^\dagger(t')\sigma_x\Psi(t')\right]\right\rangle$$

Note that function $\alpha(t,t')$ has no direct physical sense and we treat $\alpha(t,t')$ only as a very convenient tool to find a physical quantity.

Matsubara imaginaty time formalism

In the Matsubara-Heisenberg picture all operators evolve (in the imaginary-time variable τ) according to the statistical Hamiltonian $\mathcal{K}$

$$\mathcal{O}(\tau) = \mathrm{e}^{\mathcal{K}\tau}\,\mathcal{O}\,\mathrm{e}^{-\mathcal{K}\tau}$$

while in the Matsubara-Dirac picture they evolve according to the free statistical Hamiltonian $\mathcal{K}_0$

$$O(\tau) = \mathrm{e}^{\mathcal{K}_0\tau}\,\mathcal{O}\,\mathrm{e}^{-\mathcal{K}_0\tau}.$$

In this picture the evolution of the field operators (2) and (5) can be found directly.
In the Matsubara formalism we define temperature propagators. The temperature photon propagator and the temperature fermion propagator are defined as follow

$$\widetilde{\mathcal{S}}_{\alpha\beta}(\tau_1-\tau_2) = -\langle \mathbb{T}_\tau\,\Psi_\alpha(\tau_1)\Psi_\beta^\dagger(\tau_2)\rangle, \qquad (10)$$
$$\widetilde{\mathcal{D}}(k,k',\tau_1-\tau_2) = -\langle \mathbb{T}_\tau\,\Phi(k,\tau_1)\Phi(k',\tau_2)\rangle. \qquad (11)$$

They are defined on the finite range of length 2β and they fulfill the symmetric boundary condition $\widetilde{\mathcal{G}}(-\beta) = \widetilde{\mathcal{G}}(\beta)$. Therefore one can represent them as the following Fourier series:

$$\widetilde{\mathcal{G}}(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty}\mathrm{e}^{-i\omega_n\tau}\,\widetilde{\mathcal{G}}(\omega_n), \quad \omega_n = \begin{cases}\frac{2n\pi}{\beta}, & \text{bosons,}\\ \frac{2(n+1)\pi}{\beta}, & \text{fermions.}\end{cases}$$

Matsubara-Feynman rules

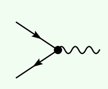
- The free temperature photon propagator

$$= -\widetilde{D}(k,k',\omega_n) = \frac{\delta(k-k')}{\omega_n^2+k^2},$$

- The free temperature fermion propagator

$$= -\widetilde{S}(\omega_n) = \frac{-1}{i\omega_n - m\sigma_z},$$

- Vertex – meeting point of two fermion lines and one photon line



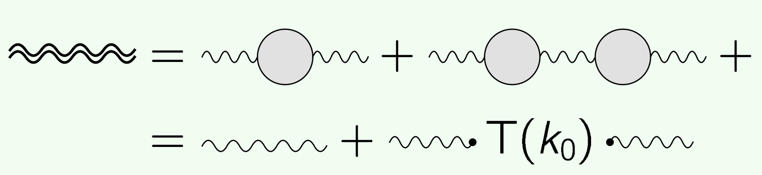
$$= -V(k) = -g(k)\sigma_x.$$

- In each vertex the frequency conservation law holds.
- The fermion propagators are 2×2 matrices – they must be multiplied in the order given by the directions of the lines.
- Each closed fermion loop leads to the trace operation of the matrices and gives a factor -1.

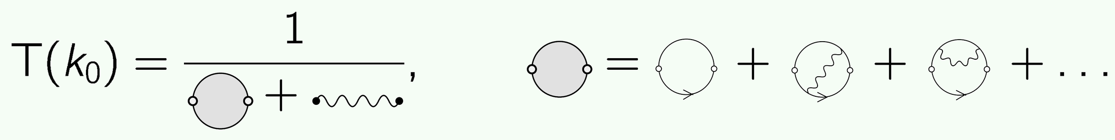
In the end one should integrate such an expression over all internal momenta k and take a sum over all internal frequencies ω_n. Moreover each sum must be divided by β.

Temperature photon propagator

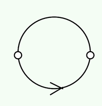
According to the M-F rules the temperature photon propagator (11) in the theory with interactions has the following expansion



where



In the lowest order of perturbation theory one can find that



$$= \frac{4m}{4m^2+\omega_n^2}\tanh\left(\frac{\beta m}{2}\right).$$

and therefore the temperature transition matrix reads

$$\mathrm{T}^{(2)}(\omega_n) = -\frac{4m}{(4m^2+\omega_n^2)\coth\left(\frac{\beta m}{2}\right) - 4m\widetilde{h}(\omega_n)}. \qquad (12)$$

Retarded photon propagator

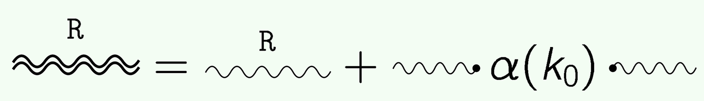
The real-time retarded photon propagator is defined as usual in the Heisenberg

$$\mathcal{D}_{\mathrm{R}}(k,k',t-t') = -i\theta(t-t')\langle[\Phi(t),\Phi(t')]\rangle \qquad (13)$$

and for the free photon field it reads

$$D_{\mathrm{R}}(k,k',t-t') = -i\theta(t-t')\langle[\phi(t),\phi(t')]\rangle_0. \qquad (14)$$

It is known that these propagators are directly connected with function $\alpha(k_0)$



(15)

Moreover, they can be directly extracted, in each order of perturbation theory, from the temperature propagators by performing the analytic continuation in the frequency domain. Therefore, it is self-evident that the linear polarizabilty $\alpha(k_0)$ can be extracted from the temperature transition matrix $\mathrm{T}(k_0)$ by the following rule:

$$\alpha(k_0) = -\mathrm{T}(-ik_0+\epsilon). \qquad (16)$$

Final result

Once we have determined the temperature transition matrix in the second order of perturbation (12), we are able to find the polarizability in this order. First, by making the analytic continuation (16) we find the function $\alpha(k_0)$. Then, by using correspondence formula (9), we find the linear-polarizability. The result is following

$$\boxed{\alpha^{(2)}(\omega) = \frac{4mA_{\mathrm{T}}}{4m^2-\omega^2-4m\left[\Delta_{\mathrm{T}}(\omega)+i\,\mathrm{sign}(\omega)\,\Gamma_{\mathrm{T}}(\omega)\right]}}$$

where we introduced the effective temperature-dependent amplitude of the polarizability, as well as an effective shift and width of the resonance

$$A_{\mathrm{T}} = (1+\delta^{(2)})\tanh(\beta m),$$
$$\frac{\Delta_{\mathrm{T}}(\omega)}{\Delta(\omega)} = \frac{\Gamma_{\mathrm{T}}(\omega)}{\Gamma(\omega)} = \tanh(\beta m/2).$$

Thermal line narrowing

In conclusion, let us concentrate on the problem of the width of the resonance. As was shown above, the resonance width unexpectedly decreases when the temperature grows. Such a behavior is contrary to the natural expectations. In typical situations we expect broadening of the resonance rather than narrowing. The best known examples where the resonance broads with temperature are obviously heated gases where, according to the Doppler effect and the chaotic motion of the molecules, all spectral lines become wider.
Notice that in the studied situation there is only one freezed qubit. Therefore there is no place for any influence of the Doppler effect or of any interaction with other qubits. We call this phenomenon as **motionless narrowing**, since it is clear that freezing of spatial degrees of freedom is a main source of the narrowing of the resonance.

References

[1] T. Sowiński, quant-ph/0901.3268
[2] I. Bialynicki-Birula, T. Sowiński, Phys. Rev. A **76**, 062106 (2007)