BOLTZMANN STATISTICS OF QUANTUM FRICTION

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In this paper we investigate the thermodynamic properties of simple quantum-mechanical systems in the presence of friction. Using the propagators for these simple models we calculate the response functions in Boltzmann statics. In the low temperature region the response functions exhibit singular behaviour.

As is well known, from the propagator of a quantum system it is possible to obtain the Boltzmann statistics of the system [1]. Recently many authors [2–7] have studied the problem of quantum friction through the solution of the Schrödinger equation for the Caldirola–Kanai hamiltonian. The same result can be obtained from the classical action S_c via the van Vleck–Pauli formula [8,9]

$$K(x_2,t_2;x_1,t_1)=\left(\frac{\mathrm{i}}{2\pi\hbar}\frac{\partial^2 S_c}{\partial x_1\,\partial x_2}\right)^{1/2}\exp[(\mathrm{i}/\hbar)S_c(x_2,t_2;x_1,t_1)]\,. \tag{1}$$

Using a global transformation of "space" and "time", Junker and Inomata [10] succeeded in finding the propagator of the most general quadratic lagrangian.

The statistical mechanics of quantum friction has been investigated by Jannussis, Papatheou and Vlachos [11] for the case of imaginary coefficient of friction. They obtained real and regular response functions.

In the following, a free particle, a harmonic oscillator and a harmonic oscillator in a uniform magnetic field are examined in the presence of friction.

(a) *Free particle*. The equation of motion for a classical particle in three-dimensional space, in the presence of friction, is written as

$$\ddot{\boldsymbol{r}}+\gamma\dot{\boldsymbol{r}}=0\,, \tag{2}$$

and according to ref. [12] the corresponding propagator for a quantum particle is written as

$$K(\boldsymbol{r}_2,t_2;\boldsymbol{r}_1,t_1)=\left(\frac{\gamma m}{2\pi\mathrm{i}\hbar}\right)^{1/2}(\mathrm{e}^{-\gamma t_1}-\mathrm{e}^{-\gamma t_2})^{-1/2}\exp\left(\frac{\mathrm{i}\gamma m}{2\hbar}\frac{(\boldsymbol{r}_2-\boldsymbol{r}_1)^2}{\mathrm{e}^{-\gamma t_1}-\mathrm{e}^{-\gamma t_2}}\right). \tag{3}$$

Using the substitutions $t_1\to 0$ and $t_2\to -\mathrm{i}\hbar\beta$ where $\beta=1/k_BT$ we obtain the density matrix

$$K(\boldsymbol{r};\boldsymbol{r},\beta)=(\gamma m/2\pi\mathrm{i}\hbar)^{1/2}(1-\mathrm{e}^{\mathrm{i}\gamma\hbar\beta})^{-1/2}\,, \tag{4}$$

from which we can find the partition function

$$Z(\beta)=\int_V K(\boldsymbol{r};\boldsymbol{r},\beta)\,\mathrm{d}\boldsymbol{r}=V\mathrm{e}^{-3\mathrm{i}\hbar\beta/4}\left(\frac{\gamma m}{4\pi\hbar\sin(\frac{1}{2}\gamma\hbar\beta)}\right)^{3/2}\,. \tag{5}$$

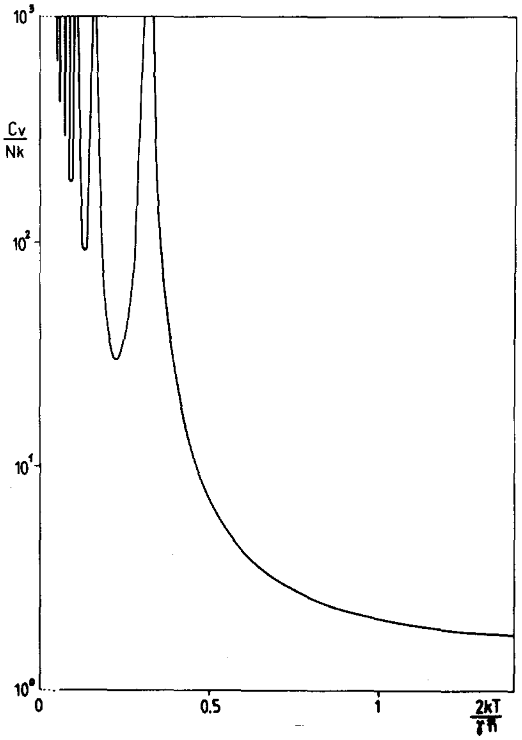

Fig. 1. The specific heat of a free particle in a frictional medium.

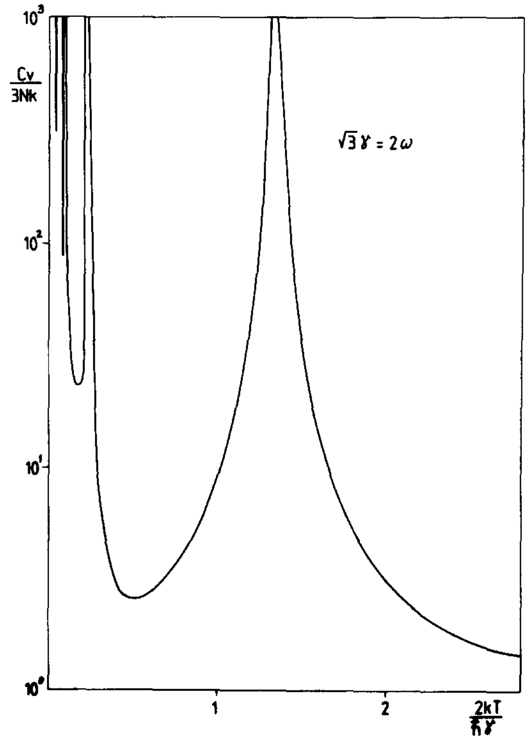

Fig. 2. The specific heat of a damped harmonic oscillator in the case $\sqrt{3}\,\gamma=2\omega$.

This partition function is a complex one. The same happens for the free energy

$$F(\beta)=-\frac{3}{2\beta}\ln\left(\frac{\gamma m V^2}{4\pi\hbar\sin(\frac{1}{2}\gamma\hbar\beta)}\right)+\tfrac{3}{4}\mathrm{i}\gamma\hbar\,. \tag{6}$$

The specific heat

$$C_v/k_\mathrm{B}=\tfrac{3}{2}(\tfrac{1}{2}\gamma\hbar\beta)^2/[\sin(\tfrac{1}{2}\gamma\hbar\beta)]^2 \tag{7}$$

is a real function and for $\gamma\hbar\beta/2=n\pi$ ($n=1, 2, ...$) tends to infinity (fig. 1). At the limit of high temperatures eq. (7) takes the classical value 3/2.

(b) *Harmonic oscillator*. Similarly, for a harmonic oscillator in the presence of friction, the equation of motion is

$$\ddot{\boldsymbol{r}}+\gamma\dot{\boldsymbol{r}}+\omega^2\boldsymbol{r}=0\,. \tag{8}$$

According to ref. [7] the propagator is given by

$$K(\boldsymbol{r}_2,t_2;\boldsymbol{r}_1,t_1)=\frac{\mathrm{e}^{3\gamma(t_2+t_1)/4}}{\{(2\pi\mathrm{i}\hbar/m\Omega)\sin[\Omega(t_2-t_1)]\}^{3/2}}$$

$$\times\exp\left[\frac{\mathrm{i}m\Omega}{2\hbar}\left(\cot[\Omega(t_2-t_1)](\mathrm{e}^{\gamma t_2}r_2^2+\mathrm{e}^{\gamma t_1}r_1^2)-\frac{2\boldsymbol{r}_1\cdot\boldsymbol{r}_2\mathrm{e}^{\gamma(t_2+t_1)/2}}{\sin[\Omega(t_2-t_1)]}\right)+\frac{\mathrm{i}\gamma m}{4\hbar}(\mathrm{e}^{\gamma t_2}r_2^2-\mathrm{e}^{\gamma t_1}r_1^2)\right], \tag{9}$$

where $\Omega^2=\omega^2+\gamma^2/4$. Therefore the density matrix is

$$K(\boldsymbol{r};\boldsymbol{r},\beta)=\left(\frac{m\Omega}{2\pi\hbar\,\mathrm{sh}(\Omega\hbar\beta)}\right)^{3/2}\mathrm{e}^{-3\mathrm{i}\hbar\gamma\beta/2}$$

$$\times\exp\left\{-\left[\frac{m\Omega}{\hbar}\left(\mathrm{cth}(\Omega\hbar\beta)\cos(\tfrac{1}{2}\gamma\hbar\beta)-\frac{1}{\mathrm{sh}(\Omega\hbar\beta)}\right)-\frac{\gamma m}{2\hbar}\sin(\tfrac{1}{2}\gamma\hbar\beta)\right]\mathrm{e}^{-\mathrm{i}\gamma\hbar\beta/2}r^2\right\}. \tag{10}$$

By integrating eq. (10) we obtain the partition function

$$Z(\beta)=\{2[\mathrm{ch}(\Omega\hbar\beta)\cos(\tfrac{1}{2}\gamma\hbar\beta)-1]-(\gamma/\Omega)\,\mathrm{sh}(\Omega\hbar\beta)\sin(\tfrac{1}{2}\gamma\hbar\beta)\}^{-3/2}, \tag{11}$$

which for $\gamma=0$ coincides with the well-known partition function of the harmonic oscillator. Finally, for the specific heat we obtain

$$\frac{C_v}{k_\mathrm{B}}=\frac{3}{2}\left(\frac{(\gamma/\Omega)\,\mathrm{ch}(\Omega\hbar\beta)\sin(\tfrac{1}{2}\gamma\hbar\beta)+(\gamma^2/4\Omega^2-1)\,\mathrm{sh}(\Omega\hbar\beta)\cos(\tfrac{1}{2}\gamma\hbar\beta)}{(1/\Omega\hbar\beta)[\mathrm{ch}(\Omega\hbar\beta)\cos(\tfrac{1}{2}\gamma\hbar\beta)-1-(\gamma/2\Omega)\,\mathrm{sh}(\Omega\hbar\beta)\sin(\tfrac{1}{2}\gamma\hbar\beta)]}\right)^2$$

$$-\frac{3}{2}\frac{(\gamma/2\Omega)(\gamma^2/4\Omega^2-3)\,\mathrm{sh}(\Omega\hbar\beta)\sin(\tfrac{1}{2}\gamma\hbar\beta)+(1-3\gamma^2/4\Omega^2)\,\mathrm{ch}(\Omega\hbar\beta)\cos(\tfrac{1}{2}\gamma\hbar\beta)}{(1/\Omega^2\hbar^2\beta^2)[\mathrm{ch}(\Omega\hbar\beta)\cos(\tfrac{1}{2}\gamma\hbar\beta)-1-(\gamma/2\Omega)\,\mathrm{sh}(\Omega\hbar\beta)\sin(\tfrac{1}{2}\gamma\hbar\beta)]}. \tag{12}$$

If $\gamma=0$, then eq. (12) is reduced to the specific heat on an ordinary quantum oscillator

$$C_v/k_\mathrm{B}=3(\tfrac{1}{2}\omega\hbar\beta)^2/[\mathrm{sh}(\tfrac{1}{2}\omega\hbar\beta)]^2. \tag{13}$$

In the region of low temperatures the specific heat which is given by eq. (12) exhibits (see fig. 2) an infinite number of singularities, while $\lim_{T\to\infty} C_v/k_\mathrm{B}=3$.

(c) *Uniform magnetic field and damped oscillator.* The hamiltonian of a damped harmonic oscillator in a uniform magnetic field is written as

$$\mathscr{H}=(1/2m)[\boldsymbol{p}+(e/c)\boldsymbol{H}\mathrm{e}^{\gamma t}\times\boldsymbol{r}]^2\mathrm{e}^{-\gamma t}+\tfrac{1}{2}\mathrm{e}^{\gamma t}m\omega^2r^2. \tag{14}$$

For this case, according to ref. [7], the propagator is given by the relation

$$K(\boldsymbol{r}_2,t_2;\boldsymbol{r}_1,t_1)=\left(\frac{m\Omega_3}{2\pi\mathrm{i}\hbar\sin[\Omega_3(t_2-t_1)]}\right)^{1/2}\frac{m\Omega\mathrm{e}^{3\gamma(t_2-t_1)/4}}{2\pi\mathrm{i}\hbar\sin[\Omega(t_2-t_1)]}\exp\Bigg(-\frac{\mathrm{i}m\gamma}{4\hbar}(\mathrm{e}^{\gamma t_1}r_1^2-\mathrm{e}^{\gamma t_2}r_2^2)$$

$$+\frac{\mathrm{i}m\Omega_3}{2\hbar\sin[\Omega_3(t_2-t_1)]}\{\cos[\Omega_3(t_2-t_1)](\mathrm{e}^{\gamma t_2}z_2^2+\mathrm{e}^{\gamma t_1}z_1^2)-2z_1z_2\mathrm{e}^{\gamma(t_2+t_1)/2}\}$$

$$+\frac{\mathrm{i}m\Omega}{2\hbar\sin[\Omega(t_2-t_1)]}\{\cos[\Omega(t_2-t_1)][\mathrm{e}^{\gamma t_2}(x_2^2+y_2^2)+\mathrm{e}^{\gamma t_1}(x_1^2+y_1^2)]$$

$$-2\cos[\omega_\mathrm{L}(t_2-t_1)]\mathrm{e}^{\gamma(t_2+t_1)/2}(x_1x_2+y_1y_2)-2\sin[\omega_\mathrm{L}(t_2-t_1)]\mathrm{e}^{\gamma(t_2+t_1)/2}(x_1y_2-x_2y_1)\}\Bigg), \tag{15}$$

where $\Omega^2=\omega_\mathrm{L}^2+\Omega_3^2$, $\omega_\mathrm{L}=eH/2mc$ and $\Omega_3^2=\omega^2+\gamma^2/4$. Using eq. (15) we obtain the following density matrix

$$K(\boldsymbol{r};\boldsymbol{r},\beta)=\left(\frac{m\Omega_3}{2\pi\hbar\,\mathrm{sh}(\Omega_3\hbar\beta)}\right)^{1/2}\frac{m\Omega\mathrm{e}^{-3\mathrm{i}\hbar\gamma\beta/4}}{2\pi\hbar\,\mathrm{sh}(\Omega\hbar\beta)}\exp[-\alpha(x^2+y^2)\delta z^2], \tag{16}$$

where α and δ are given by

$$\alpha=\frac{m\Omega}{2\hbar}\frac{\mathrm{e}^{-\mathrm{i}\hbar\gamma\beta/2}}{\mathrm{sh}(\Omega\hbar\beta)}[2\,\mathrm{ch}(\Omega\hbar\beta)\cos(\tfrac{1}{2}\gamma\hbar\beta)-2\,\mathrm{ch}(\omega_\mathrm{L}\hbar\beta)-(\gamma/\Omega)\,\mathrm{sh}(\Omega\hbar\beta)\sin(\tfrac{1}{2}\gamma\hbar\beta)], \tag{17}$$

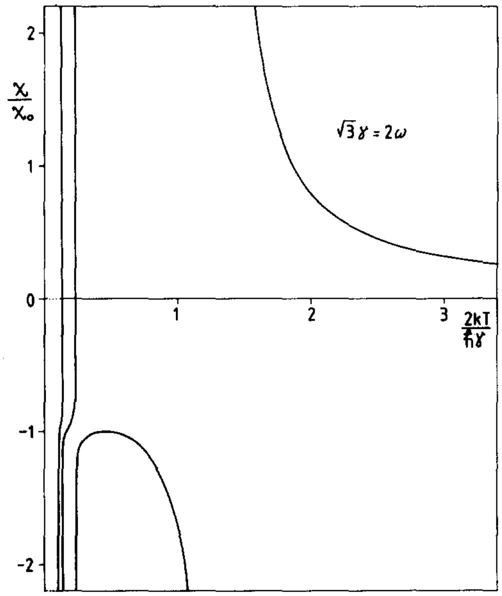

Fig. 3. The initial susceptibility of a damped harmonic oscillator in a uniform magnetic field in the case $\sqrt{3}\,\gamma=2\omega$.

$$\delta=\frac{m\Omega_3}{2\hbar}\frac{e^{-i\hbar\gamma\beta/2}}{\mathrm{sh}(\Omega\hbar\beta)}\,[2\,\mathrm{ch}(\Omega_3\hbar\beta)\cos(\tfrac{1}{2}\gamma\hbar\beta)-1-(\gamma/\Omega_3)\mathrm{sh}(\Omega_3\hbar\beta)\sin(\tfrac{1}{2}\gamma\hbar\beta)]\ .$$

For the partition function we obtain

$$Z(\beta)=\{2[\mathrm{ch}(\Omega_3\hbar\beta)\cos(\tfrac{1}{2}\gamma\hbar\beta)-(\gamma/2\Omega_3)\,\mathrm{sh}(\Omega_3\hbar\beta)\sin(\tfrac{1}{2}\gamma\hbar\beta)-1]\}^{1/2}$$

$$\times\{2[\mathrm{ch}(\Omega\hbar\beta)\cos(\tfrac{1}{2}\gamma\hbar\beta)-(\gamma/2\Omega)\,\mathrm{sh}(\Omega\hbar\beta)\sin(\tfrac{1}{2}\gamma\hbar\beta)-\mathrm{ch}(\omega_{\mathrm{L}}\hbar\beta)]\}^{-1}\ . \qquad (18)$$

The initial (for $H=0$) magnetic susceptibility is

$$\chi=\chi_0[\mathrm{ch}(\Omega\hbar\beta)\cos(\tfrac{1}{2}\gamma\hbar\beta)-(\gamma/2\Omega)\,\mathrm{sh}(\Omega\hbar\beta)\sin(\tfrac{1}{2}\gamma\hbar\beta)-\mathrm{ch}(\omega_{\mathrm{L}}\hbar\beta)]^{-1}$$

$$\times[(\gamma/2\Omega)\,\mathrm{ch}(\Omega\hbar\beta)\sin(\tfrac{1}{2}\gamma\hbar\beta)+(\Omega/\omega_{\mathrm{L}})\,\mathrm{sh}(\omega_{\mathrm{L}}\hbar\beta)-\mathrm{sh}(\Omega\hbar\beta)\cos(\tfrac{1}{2}\gamma\hbar\beta)$$

$$-(\gamma/2\Omega^2\hbar\beta)\,\mathrm{sh}(\Omega\hbar\beta)\sin(\tfrac{1}{2}\gamma\hbar\beta)]\ , \qquad (19)$$

where $\chi_0=e^2\hbar/4m^2c^2\Omega$. If $\gamma=0$, then eq. (19) becomes

$$\chi=\chi_0[\omega\hbar\beta-\mathrm{sh}(\omega\hbar\beta)]/[\mathrm{ch}(\omega\hbar\beta)-1]\ . \qquad (20)$$

Fig. 3 shows the behaviour of the initial susceptibility as a function of temperature. The singularities in the magnetic susceptibility are at the same points as the singularities in the specific heat which is given by eq. (12).

In conclusiion we see that the extension of the Boltzmann statistics to damped systems with real damped coefficients leads to interesting properties of thermodynamic functions. In a forthcoming paper we shall apply the Fermi–Dirac statistics to the above problems.

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