Brownian motion of quantum particles

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A quantum theory of interaction of particles, moving in a one-dimensional potential with a thermostat in the form of a viscous medium, is constructed. The equilibrium density distribution and the particle lifetime in a potential well of finite depth in the presence of tunneling and dissipation are determined.

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One-dimensional motion of a classical particle with mass m in a potential $U(x)$ in the presence of a viscous medium can be described by the Langevin equation $\ddot{x} = -\gamma \dot{x} - m^{-1} U''(x) + \eta(t)$, where $\eta(t)$ is the random force and γ is the coefficient of friction, which is the only characteristic of the interaction with the thermostat.

To examine the quantum situation, we shall explicitly introduce the thermostate in the form of an infinite string, attached to the particle and tightened perpendicular to the axis of particle motion. In the classical limit, the action of the string on the particle is equivalent to the presence of a viscous medium with a coefficient of friction $\gamma = \rho s/m$, where ρ is the linear density of the string, and s is the velocity of traveling waves along the string[1]; in the quantum case, there can be only this combination of ρ and s. The number of degrees of freedom then increases; on the other hand, we obtain a nondissipative dynamic system, which can be quantized in the usual manner. We note that the approach presented here is applicable to any medium with linear response.

We shall first find the equilibrium coordinate distribution of quantum Brownian particles in the potential $U(x)$ at temperature $T \equiv \beta^{-1}$. The state of the system particle + string is completely determined by the displacement of the string along the axis of motion of the particle $x(z)$ [z is the distance along the string and the coordinate of the particle is $x \equiv x(0)$]. The equilibrium coordinate distribution of particles $N(x)$ is given by the Feynman integral over the periodic trajectories $x(z,t)$ with imaginary time

$$N(x) = \int \exp(-S/\hbar) D[x(z,t)], \qquad (1)$$

$$x(z, \hbar\beta) = x(z, 0), \; x(0, 0) = x(0, \hbar\beta) = x$$

with the action

$$S = \int_0^{\hbar\beta} \frac{1}{2} \{ m\dot{x}^2(0) + 2U(x(0)) + \int_0^{\infty} [\rho \dot{x}^2(z) + \rho s^2 (\frac{\partial x(z)}{\partial z})^2] dz \} dt. \qquad (2)$$

If the temperature is small compared to the characteristic drop in the potential, in calculating integral (1) we can assume that the potential U is quadratic near the point

x, i.e., we can drop the third and higher-order terms in the Taylor expansion of the potential near this point. [In the case of a harmonic oscillator, the expression obtained below for $N(x)$ is exact.] Expanding the coordinate of the particle in a Fourier series with respect to the Matsubara frequencies

$$x(0, t) = x + a_0 + \sum_{n=1}^{\infty} (a_n \cos \omega_n t + b_n \sin \omega_n t), \quad \omega_n \equiv 2\pi n/\beta\hbar$$

and minimizing action (2) with respect to configurations of the string, we obtain

$$S = \beta\hbar \{U(x) + U'(x) a_0$$

$$+ \frac{m}{2} [m^{-1} U''(x) a_0^2 + \frac{1}{2} \sum_{n=1}^{\infty} (\omega_n^2 + \gamma\omega_n + m^{-1} U''(x))(a_n^2 + b_n^2)]\}.$$

Substituting this expression into (1) and integrating with respect to a_n and b_n with the condition $\Sigma_{n=0}^{\infty} a_n = 0$, we find to within a factor independent of the coordinate

$$N(x) = \phi^{1/2}(x) \Gamma(1 - \beta\hbar\lambda^+(x)/2\pi) \Gamma(1 - \beta\hbar\lambda^-(x)/2\pi) \cdot \exp\{-\beta[U(x)$$

$$-(1 - \phi(x))(U'(x))^2/2U''(x)]\}, \tag{3}$$

where

$$\phi(x) \equiv [m^{-1} U''(x) \sum_{n=-\infty}^{\infty} (\omega_n^2 + \gamma|\omega_n| + m^{-1} U''(x))^{-1}]^{-1}, \tag{4}$$

λ^+ and λ^- are roots of the equation [1)]

$$\lambda^2 + \gamma\lambda + m^{-1} U''(x) = 0. \tag{5}$$

Expression (3) is applicable in regions of x where $U''(x)$ exceeds some (negative) boundary value U''_b, corresponding to the right-most pole of ϕ as a function of U''. As the region, where $U'' \leqslant U''_b$, is approached $N(x)$ is determined by trajectories that are increasingly more distant from x, so that the quadratic approximation finally becomes inapplicable. At $\gamma = 0$, we have

$$\phi(x) = [\beta\hbar(U''(x)/m)^{1/2}/2]^{-1} \operatorname{th}(\beta\hbar(U''(x)/m)^{1/2}/2) \text{ and } U''_{\text{rp}} = -m(\pi/\beta\hbar)^2.$$

We shall now examine the problem of Brownian particles leaving the one-dimensional potential well through the barrier. We shall assume that the depth of the well $U_0 \gg T$ and we shall use the quasistationary approximation, i.e., we shall assume that the distribution of particles in the well is an equilibrium distribution, while the flow through the barrier is a steady-state flow. The classical problem in this formulation was solved by Kramers,[2] and Affleck[3] obtained the solution in the quantum case for particles that do not interact with the thermostat. Quantum tunneling was studied with exponential accuracy by I. Lifshitz and Yu. Kagan[4] (at a finite temperature without dissipation), Caldeira and Leggett[5] (with dissipation at zero temperature), and Larkin and Ovchinnikov[6] (with dissipation at finite temperature).

Since the flow is weak, the particle distribution differs from the equilibrium distribution only in the region near the top of the barrier, where the barrier can be assumed to be quadratic $U(x) = -m\omega^2x^2/2$, ω is the frequency of the corresponding inverted oscillator. We shall first write the Wigner function for the distribution of particles over the coordinate x and momentum p (see, for example, Ref. 7) at $\gamma = 0$ corresponding to steady-state flow. The equilibrium distribution functions for the inverted quantum oscillator differs from the classical oscillator by the fact that the temperature T is replaced by $(\hbar\omega/2)\mathrm{ctg}(\hbar\omega/2T)$. Steady-state flow through the barrier (from left to right) corresponds to the distribution function

$$f(p,x) = \text{const}\ \theta(p - m\omega x) \exp[-(2/\hbar\omega)\mathrm{tg}(\beta\hbar\omega/2)(p^2/2m - m\omega^2x^2/2). \qquad (6)$$

It is easy to verify that this function is stationary, transforming into an equilibrium function in the limit $x \to -\infty$, while in the limit $x \to +\infty$ the number density of particles $\int f(p,x)dp$ approaches zero.

To determine $f(p,x)$ with $\gamma \neq 0$, we shall transform to normal oscillations of the particle + string system. Aside from stable, oscillator-type modes, there is a single unstable mode, corresponding to an inverted oscillator with frequency λ^+, which is the positive root of Eq. (5) at the point $x = 0$. It is evident that for a steady-state flow, the coordinate and momentum distribution function of each of the stable modes will be the equilibrium function, while for the unstable mode, we have (6) with λ^+, instead of ω. After the particle distribution function is determined by integrating over the coordinates and momenta of all modes and calculating the flux through the barrier $J = m^{-1}\int pf(p,x)dp$, we find

$$J = \lambda^+ (2\pi\beta m\omega^2 \phi(0))^{-1/2} N(0), \qquad (7)$$

where $N(0)$ is the equilibrium particle density at the top of the barrier. Relation (7) from the classical relation only by the factor $\phi^{-1/2}(0)$.

It is usually interesting to know the lifetime of the particle in the well, i.e., the ratio of the number of particles in the well (in the region $x < 0$) to the flux (7). At $T \ll U_0$, the particles are concentrated near the bottom of the well, where the well may be assumed to be an oscillator with frequency Ω. Calculating in this approximation the number of particles in the well according to (3), we obtain

$$\tau^{-1} = \frac{\lambda^+ \Omega \Gamma(1 - \beta\hbar\lambda^+/2\pi)\Gamma(1 - \beta\hbar\lambda^-/2\pi)}{2\pi\omega\Gamma(1 - \beta\hbar\Lambda^+/2\pi)\Gamma(1 - \beta\hbar\Lambda^-/2\pi)} e^{-\beta U_0}, \qquad (8)$$

where

$$\lambda^{\pm} = -\gamma/2 \pm (\gamma^2/4 + \omega^2)^{1/2} \quad \text{and} \quad \Lambda^{\pm} = -\gamma/2 \pm (\gamma^2/4 - \Omega^2)^{1/2}.$$

Since expression (8) does not contain $\phi(0)$, when the temperature decreases, the singularity in τ^{-1} arises only when $\Gamma(1 - \beta\hbar\lambda^+/2\pi)$ becomes infinite, so that the region of applicability of (8) $T > T_c = \hbar\lambda^+/2\pi$ is wider than that of expressions (3) and (7) To calculate the flux at temperatures close to T_c and below, the deviation of the barrier shape from the parabolic shape must be taken into account (see also Refs. 3, 4, and 6).

At high temperatures, the expression obtained for τ^{-1} becomes the Kramers expression[2] (all Γ functions are equal to 1), while in the limit $\gamma \ll \omega, \Omega$ [using relation

$\Gamma(1+z)\Gamma(1-z) = \pi z/\sin\pi z$] gives Affleck's result.[1),3] Thus our result is a direct generalization of Refs. 2 and 3 to the case when both the quantum effects and viscosity are present.

[1)]We point out that the equilibrium distribution remains unaffected by viscosity only in the classical limit.
[2)]To be rigorous, we point out that when the viscosity is too low (when $\gamma/\Omega \lesssim T/U_0$), the quasistationary approximation is not applicable.[2]

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