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Kubo–Einstein Relation for Quantum Brownian Motion in a Periodic Potential

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Using a previously derived general formalism for a dissipative quantum particle in a boson bath, we prove that when the damping is Ohmic, the Kubo–Einstein relation between the diffusion constant and the linear mobility $D = kTM$ holds to all orders in V_0 for a periodic potential $V(x) = V_0 \cos(k_0 x)$.

KEY WORDS: Quantum Brownian motion; Wigner distribution; Kubo–Einstein relation.

1. INTRODUCTION

Because of its direct relation to a realistic physical system—the well-known Josephson junctions between two superconductors—the dynamics of a dissipative quantum particle in a periodic cosine potential has attracted a great deal of recent theoretical interest.(1-4) In a previous work,(5) we developed for this system a very general real-time description in terms of the so-called Wigner distribution. Various physically interesting quantities can be calculated in this formalism. Included among these is the mobility of the particle under an external force that corresponds directly to the I–V characteristic of a current-biased Josepson junction.(4)

In this paper, we shall focus our attention on the Einstein relation which links the linear mobility M and the diffusion constant D via $D = kTM$. Although Kubo(6) has given a rather formal derivation of the linear-response theory to which the Einstein relation belongs, there are some problems here with the definition of M arising from the fact that the stationary state in which the particle moves with a constant velocity is not normalizable. To get over these problems in the classical system one has to

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define the measure on the environment as seen by the particle (the so-called Palm measure[7]), which is stationary whenever the medium in which the particle moves is translationally invariant, e.g., a homogeneous random environment (this includes the periodic case). Alternatively, one can use, for the periodic potential, a finite box with the same periodicity and compute the stationary distribution of the particle in that box. This will then give the same answer for the velocity distributions as the infinite system. Unfortunately, neither of these prescriptions works for quantum systems, because we cannot define appropriately the Palm measure and the equivalence for a periodic potential between an infinite system and a finite periodic box does not hold due to the requirement of periodicity of the wave functions in the latter case. We are therefore forced to consider an initial state in which the particle is localized near the origin and then define the mean velocity $v(F)$ in the presence of an external force F as

$$v(F)=\lim_{t\to\infty}\langle\hat{p}/m\rangle(t,F)=\lim_{t\to\infty}\langle\hat{x}\rangle(t,F)/t$$

assuming that the limit in fact exists. The linear mobility M is given by $M=[v(F)/F]|_{F\to 0}$. One can likewise define the diffusion constant as $D=[\langle x^2\rangle/2t]|_{t\to\infty}$.

The advantage and disadvantage of this definition of M is that we neither require nor obtain any information about the stationary distribution in the presence of the force F—except for the assumption of the existence of the two limits. There is, however, also a question now about the applicability of the general derivation of linear-response theory, so it is important to investigate the Einstein relation explicitly for the quantum case. Here it is not obvious *a priori* whether $D\to 0$ or $M\to\infty$ (or both) as $T\to 0$. In refs. 1, 3, and 4 the relation has been proved to the lowest order in V_0 (cf. below) as well as to all orders of V_0 under some approximations.[3]

The strategy used in refs. 1 and 4 is now generalized to arbitrary orders in V_0. In what follows, we shall first review briefly in Section 2 the derivation of the general expressions for M and D. Then the proof of the Kubo–Einstein relation is presented in Section 3. Finally, some discussions are given in Section 4.

2. THE LINEAR MOBILITY AND DIFFUSION CONSTANT

We consider a system consisting of a particle of mass m moving in a potential $V(x)=V_0\cos(k_0x)$ and a "heat bath" representing its environment. The total Hamiltonian is

$$\hat{H}=\hat{H}_p+\hat{H}_c+\hat{H}_e \tag{1}$$

with

$$\hat{H}_p = \frac{\hat{p}^2}{2m} + V(x) \tag{2a}$$

$$H_e = \sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k \tag{2b}$$

the Hamiltonian of the particle and environment, respectively, and

$$\hat{H}_c = \hat{x} \sum_k C_k(\hat{a}_k^\dagger + \hat{a}_k) + \sum_k \frac{C_k^2}{\hbar\omega_k} x^2 \tag{2c}$$

the coupling interaction [the second term in (2c) cancels the adiabatic potential shift induced by the first term]. $\{\hat{a}_k^\dagger, \hat{a}_k\}$ is the set of creation and annihilation operators of the boson bath and the carets indicate that the objects are operators. It is convenient to introduce the dissipation spectrum[1-5] defined as

$$J(\omega) = \pi \sum_k C_k^2[\delta(\omega - \omega_k) - \delta(\omega + \omega_k)] \tag{3}$$

which will be taken, in the thermodynamic limit, to be a smooth function of ω. In particular, for the Ohmic damping $J(\omega) = \eta\omega$.

Given a density matrix $\hat{d}(0)$ at time 0, we call $\hat{\rho}(t) = \mathrm{Tr}_e[\hat{d}(t)]$ the reduced density matrix for the particle (where the subscript "e" indicates the "environment") and write its position representation in terms of the symmetric, $Q = (x + x')/2$, and antisymmetric, $r = (x - x')$, coordinates,

$$\rho(Q, r, t) = \langle Q + r/2 |\, \hat{\rho}(t)\, | Q - r/2 \rangle \tag{4}$$

The Wigner distribution (see, e.g., ref. 8) is then given by

$$w(Q, P, t) = \int \frac{dr}{2\pi\hbar} \rho(Q, r, t) \exp\left(-\frac{i}{\hbar} Pr\right) \tag{5}$$

For simplicity we shall consider the following kind of product initial states

$$\hat{d}(0) = \hat{\rho}(0) \exp(-\beta \hat{H}_e)/\mathrm{Tr}_e[\exp(-\beta \hat{H}_e)] \tag{6}$$

where $\hat{\rho}(0)$ operates on the particle's variables only. Physically the product state assumes a sudden switch-on of the coupling at $t = 0^+$. It was then derived explicitly in ref. 5 that the Wigner distribution at time t is given by

$$w(Q_f, P_f, t) = \Big\langle \delta(Q_f - Q_0(t))\,\delta(P_f - P_0(t))$$

$$+ \sum_{n=1}^{\infty} \left[\frac{V_0}{\hbar}\right]^n \int_0^t dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1 \sum_{\{\sigma_j = \pm 1\}} \delta(Q_f - Q_n(t))$$

$$\times\, \delta(P_f - P_n(t)) \prod_{j=1}^{n} \sigma_j \sin[k_0 Q_n(t_j)] \Big\rangle \tag{7}$$

where the average is with respect to both the initial Wigner distribution of the particle $w(Q_i, P_i, 0)$ and a Gaussian random process introduced in the derivation. The quantities $P_n(t)$ and $Q_n(t)$ are defined through the following modified "classical Langevin process":

$$m\ddot{Q}_n + \int_0^t dt'\, \alpha_1(t-t')\, \dot{Q}_n(t') = \alpha_1(t)\, Q_i + \frac{k_0^2}{2} \sum_{j=1}^{n} \sigma_j (t - t_j) + \xi(t) \tag{8a}$$

$$P_n(t) = m\dot{Q}_n(t), \qquad Q_n(0) = Q_i, \qquad P_n(0) = P_i \tag{8b}$$

where $\xi(t)$ is Gaussian noise with covariance

$$\langle \xi(t)\, \xi(t') \rangle = \alpha_2(t - t') \tag{9}$$

The functions $\alpha_1(t)$ and $\alpha_2(t)$ are in turn determined by

$$\alpha_1(t) = 2 \int_{-\infty}^{+\infty} \frac{J(\omega)}{\omega} \cos(\omega t) \tag{10a}$$

$$\alpha_2 = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} J(\omega)\, \hbar \coth\left(\frac{\beta\hbar\omega}{2}\right) \cos(\omega t) \tag{10b}$$

The solution of (8a) and (8b) can be further decomposed into two parts,

$$Q_n(t) = Q_0(t) + \frac{k_0}{2} \sum_{j=1}^{n} \sigma_j\, g(t - t_j) \tag{11}$$

where $Q_0(t)$ is the solution in the absence of the δ-forces and $g(t)$ is the Green's function of the homogeneous part

$$m\ddot{g}(t) + \int_0^t dt'\, \alpha_1(t - t')\, \dot{g}(t') = \delta(t) \tag{12a}$$

with the initial condition

$$g(t) = \dot{g}(t) = 0 \qquad \text{for} \quad t < 0 \tag{12b}$$

We now derive the general expressions for the mobility and the diffusion constant. To obtain the mobility, we need to add to the system an external force F. But the formalism remains unchanged provided we add F to the $\xi(t)$ in Eq. (8a). In the Ohmic damping limit $J(\omega)=\eta\omega$, the Green's function $g(t)$ has the simple form [$\theta(t)$ is the usual step function]

$$g(t)=\theta(t)[1-\exp(-\eta t/m)]/\eta \tag{13}$$

while the zeroth-order solution is (for $t>0^+$)

$$Q_0(t)=Q_i+(P_i+\eta Q_i)\, g(t)/m+\int_0^t dt'\, [F+\xi(t')]\, g(t-t') \tag{14}$$

Using (7), it is then a straightforward matter to find the expressions for M and D. They are[5]

$$\begin{aligned} M=\frac{1}{\eta}+\frac{k_0^2}{2\eta^2}\sum_{n=1}^{\infty}(-1)^n V_0^{2n}\int_{-\infty}^{0} dt_{2n-1}\cdots\int_{-\infty}^{t_2} dt_1 \\ \times\sum_{\{\mu_j=\pm 1\}}\sum_{k=1}^{2n}\mu_k t_k F_1 F_2\big|_{t_{2n}=\sum_{j=1}^{2n}\mu_j=0} \end{aligned} \tag{15}$$

and

$$\begin{aligned} D=\frac{kT}{\eta}+2kT\left(M-\frac{1}{\eta}\right)-\frac{\hbar k_0^2}{4\eta^2}\sum_{n=1}^{\infty}(-1)^n V_0^{2n}\int_{-\infty}^{0} dt_{2n-1}\cdots\int_{-\infty}^{t_2} dt_1 \\ \times\sum_{\{\mu_j=\pm 1\}}\sum_{k=1}^{2n-1}\operatorname{cotan}\left[\frac{\hbar k_0^2}{2}\sum_{j=k+1}^{2n}\mu_j g(t_j-t_k)\right]F_1\times F_2\big|_{t_{2n}=\sum_{j=1}^{2n}\mu_j=0} \end{aligned} \tag{16}$$

The functions F_1 and F_2 entering (15) and (16) have the form

$$F_1(\{t_j,\mu_j\})=\prod_{k=1}^{2n-1}\frac{1}{\hbar}\sin\left[\frac{\hbar k_0^2}{2}\sum_{j=k+1}^{2n}\mu_j\, g(t_j-t_k)\right] \tag{17}$$

$$F_2(\{t_j,\mu_j\})=\exp\left[\frac{k_0^2}{2}\sum_{j,k=1}^{2n}\mu_j\mu_k C(t_j-t_k)\right] \tag{18}$$

where $C(t)$ is the free particle's "mean-square displacement" after a "long time,"

$$\begin{aligned} C(t)&=\lim_{t'\to\infty}\langle[Q_0(t+t')-Q_0(t')]^2\rangle/2 \\ &=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\eta\omega\hbar\left(\coth\frac{\beta\omega\hbar}{2}\right)\frac{1-\cos(\omega t)}{\omega^2(m^2\omega^2+\eta^2)} \end{aligned} \tag{19}$$

These are formally exact expressions for the mobility and the difussion constant (cf. also refs. 1–3). They serve as the starting point for the proof of the Kubo–Einstein relation.

3. THE KUBO–EINSTEIN RELATION

To proceed, let us rewrite the diffusion constant as

$$D = kTM + \frac{kTk_0^2\hbar}{2\eta} \sum_{n=1}^{\infty} (-1)^n A_n \left(\frac{V_0}{\hbar}\right)^{2n} \tag{20a}$$

where

$$A_n = \sum_{s=1}^{2n-1} \int_{-\infty}^{0} dt_{2n-1} \int_{-\infty}^{t_{2n-1}} dt_{2n-2} \cdots \int_{-\infty}^{t_2} dt_1$$
$$\times \operatorname{Im}[(t_s - i\beta\hbar/2)\, S_s] \prod_{k=1, k\neq s}^{2n-1} \mu_k \operatorname{Im}[S_k]|_{t_{2n}=\sum_{j=1}^{2n} \mu_j = 0} \tag{20b}$$

$$S_k(\{t_j, \mu_j\}) = \exp\left[\mu_k \sum_{j>k}^{2n} \mu_j R(t_j - t_k)\right] \tag{21}$$

and $R(t)$ is given by

$$R(t) = \left[C(t) + \frac{i\hbar g(t)}{2}\right] k_0^2$$
$$= k_0^2 \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\eta\hbar}{\omega(m^2\omega^2 + \eta^2)} \frac{\cosh(\beta\omega\hbar/2) - \cosh(\beta\hbar/2 - it)\,\omega}{\sinh(\beta\omega\hbar/2)} \tag{22}$$

Note that $R(t)$ can be analytically continuated into the striplike regime $-\beta\hbar \leqslant \operatorname{Im} t \leqslant 0$ in the lower half-plane. Moreover, it satisfies

$$R(t - i\beta\hbar) = R^*(t^*) \qquad \text{for} \quad \beta\hbar \geqslant \operatorname{Im} t \geqslant 0 \tag{23a}$$

$$R(-i\tau) = R^*(-i\tau) \qquad \text{for} \quad \operatorname{Im} \tau = 0 \tag{23b}$$

For the lowest order term in (20a),

$$A_1 = 2 \int_{-\infty}^{0} dt_1 \operatorname{Im}\{(t_1 - i\beta\hbar/2) \exp[-R(-t_1)]\} \tag{24}$$

is indeed zero. This is proved by deforming the integral contour over t_1 into $+i\beta\hbar - \infty \to i\beta\hbar \to 0$. We have

$$A_1 = 2\int_{-\infty}^{0} dt_1 \,\mathrm{Im}\{(t_1 - i\beta\hbar/2)\exp[-R(-t_1)]\}^*$$
$$+ 2\,\mathrm{Im}\int_{\beta\hbar}^{0} d\tau_1(-\tau_1 + \beta\hbar/2)\exp[-R(-i\tau_1)]$$
$$= -A_1 \tag{25}$$

where we have used (23) and the contribution at infinity vanishes (see the next section for further discussions).

The above trick was first used in ref. 1. The question now is how to generalize it to arbitrary orders in V_0. Our strategy is essentially to cast the integral over the real axis into an integral over the imaginary axis (from $i\beta\hbar \to 0$) one by one. In the first step, this can be achieved for $t_k < t_s$ [see the right-hand side of (20a) for t_s]. Following the same approach used in Eq. (25), we obtain for the integral over t_1,

$$I_1 = \int_{-\infty}^{t_2} dt_1 \,\mathrm{Im}[\mu_1 S_1(\{t_j, \mu_j\})]$$
$$= \int_{\beta\hbar}^{0} \frac{d\tau_1}{2}\mu_1 \exp\left[\mu_1 \sum_{j=2}^{2n} \mu_j R(t_j - t_2 - i\tau_1)\right] \tag{26}$$

where in the last step the "Re" sign has been removed because the resulting integral is real. This can be checked by substituting $\tau_1 = \beta\hbar - \tilde{\tau}_1$ and using (23). The result of (26) is then incorporated into the integrand for the integral over t_2, which now becomes

$$I_2 = \int_{-\infty}^{t_3} dt_2 \int_{\beta\hbar}^{0} \frac{d\tau_1}{2} \,\mathrm{Im}\left[\sum_{\mu_1,\mu_2} \mu_1\mu_2 \exp(E_2)\right] \tag{27}$$

In (27) we have introduced another expression $E_k(\{\tau_i, t_i, \mu_i\})$ for later convenience:

$$E_1(\{\tau_i, t_i, \mu_i\}) = \mu_1 \sum_{j>1}^{2n} \mu_j R(t_j - t_1) \tag{28a}$$

and for $k > 1$

$$E_k = E_{k-1}|_{t_{k-1}\to t_k + i\tau_{k-1}} + \mu_k \sum_{j>k}^{2n} \mu_j R(t_j - t_k)$$
$$= \sum_{j>i=1}^{k} \mu_i\mu_j R\left(-i\sum_{s=i}^{k-1} \tau_s\right)$$
$$+ \sum_{j>k}^{2n} \mu_j \left[\sum_{i=1}^{k-1} \mu_i R\left(t_j - t_k - i\sum_{s=i}^{k-1} \tau_s\right) + \mu_k R(t_j - t_k)\right] \tag{28b}$$

Moreover, if we define an operation P under which

$$(\mu_1, \mu_2, \ldots, \mu_k) \to (\mu_k, \ldots, \mu_2, \mu_1)$$
$$(\tau_1, \tau_2, \ldots, \tau_{k-1}) \to (\tau_{k-1}, \ldots, \tau_2, \tau_1)$$

then

$$P: \quad E_k|_{t_k \to t_k + i(\beta\hbar - \sum_{i=1}^{k-1} \tau_i)} = E_k^* \tag{29}$$

On the other hand, E_k is now an analytic function within

$$\beta\hbar - \tau_1 - \tau_2 - \cdots - \tau_{k-1} \geqslant \operatorname{Im} t_k \geqslant 0$$

only. Going back to Eq. (27), we now use (29) and deform the contour into $i(\beta\hbar - \tau_1) - \infty \to i(\beta\hbar - \tau_1) + t_3 \to t_3$. It yields [for the same reason as in (26), the result does not contain either the "Im" or "Re" sign]

$$I_2 = \int_{\beta\hbar}^{0} \frac{d\tau_1}{2} \frac{d\tau_2}{2} \theta(\beta\hbar - \tau_1 - \tau_2)$$
$$\times \sum_{\mu_1, \mu_2} \mu_1 \mu_2 \exp(E_2)|_{t_2 \to t_3 + i\tau_2} \tag{30}$$

For a general integral over t_k, the relevant integrand is

$$\operatorname{Im}\left[\sum_{\mu_1, \ldots, \mu_k} \mu_1 \mu_2 \cdots \mu_k \exp(E_k)\right]$$

The corresponding deformed contour is

$$i\left(\beta\hbar - \sum_{j=1}^{k-1} \tau_j\right) - \infty \to i\left(\beta\hbar - \sum_{j=1}^{k-1} \tau_j\right) + t_{k+1} \to t_{k+1}$$

Therefore the property (29) can be applied. Substituting the results back into (20), we obtain

$$A_n = \sum_{s=1}^{2n-1} \int_{-\infty}^{0} dt_{2n-1} \cdots \int_{-\infty}^{t_{s+1}} dt_s \int_{\beta\hbar}^{0} \frac{d\tau_1}{2} \cdots \frac{d\tau_1}{2} \theta\left(\beta\hbar - \sum_{i=1}^{s-1} \tau_i\right)$$
$$\times \sum_{\{\mu_j = \pm 1\}} \left[\prod_{k>s}^{2n-1} \mu_k \operatorname{Im}(S_k)\right]$$
$$\times \operatorname{Im}\left[\left(t_s - \frac{i\beta\hbar}{2}\right) \exp(E_s)\right]\Bigg|_{t_{2n} = \sum_{j=1}^{2n} \mu_j = 0} \tag{31}$$

In the second step we deal with the difficulties arising from the factor $(t_s - i\beta\hbar/2)$. Starting once more from the t_1 integral, we have [again for the same reasons leading to (26)]

$$K_1 = \int_{-\infty}^{t_2} dt_1 \, \mathrm{Im}\left[\left(t_1 - \frac{i\beta\hbar}{2}\right)\exp(E_1)\right]$$
$$= \int_{\beta\hbar}^{0} \frac{d\tau_1}{2}\left[i\left(\tau_1 - \frac{\beta\hbar}{2}\right) + t_2\right]\exp(E_1)|_{t_1 \to t_2 + i\tau_1} \tag{32}$$

To integrate over t_2, we must include the $s=2$ term in (31) so that the integrand has an imaginary part odd under

$$t_2 \to t_2 - i(\beta\hbar - \tau_1) \qquad \text{and} \qquad \mu_1 \leftrightarrow \mu_2$$

In this way the result of

$$K_2 = \mathrm{Im}\int_{-\infty}^{t_3} dt_2 \int_{\beta\hbar}^{0} \frac{d\tau_1}{2} \sum_{\mu_1,\mu_2} \left\{(\mu_1+\mu_2)\left[t_2 - \frac{i(\beta\hbar - \tau_1)}{2}\right]\right.$$
$$\left. + \frac{i}{2}(\mu_2 - \mu_1)\tau_1\right\}\exp(E_2) \tag{33}$$

is simply that: (a) changing $\int_{-\infty}^{t_3} dt_2 \to \frac{1}{2}\int_{\beta\hbar-\tau_1}^{0} d\tau_2$; (b) substituting for the integrand $t_2 \to t_3 + i\tau_2$. Carrying out this procedure, we observe that the integration has the general structure

$$K_s = \mathrm{Im}\int_{-\infty}^{t_{s+1}} dt_s \int_{\beta\hbar}^{0} \frac{d\tau_{s-1}}{2}\cdots\frac{d\tau_1}{2}\,\theta\left(\beta\hbar - \sum_{j=1}^{s-1}\tau_j\right)\sum_{\mu_1,\ldots,\mu_s} Y_s \exp(E_s) \tag{34a}$$

with the preexponential factor in the integrand

$$Y_s(\tau_i, t_i, \mu_i) = \left(\prod_{i=1}^{s}\mu_i\right)\left\{\left(\sum_{j=1}^{s}\mu_j\right)\left[t_s - i\left(\beta\hbar - \sum_{k=1}^{s-1}\tau_k\right)\right]\right.$$
$$\left. + \frac{i}{2}\sum_{j=1}^{s-1}\tau_j\left(\sum_{k=1}^{j}\mu_k - \sum_{k>j}^{s}\mu_k\right)\right\} \tag{34b}$$

which also satisfies the relation

$$P\colon \quad Y_s|_{t_s \to t_s + i(\beta\hbar - \sum_{j=1}^{s-1}\tau_j)} = Y_s^* \tag{34c}$$

Therefore K_s can again be transformed into an integral over the imaginary axis. This yields

$$K_s = \int_{\beta\hbar}^{0} \frac{d\tau_1}{2}\cdots\frac{d\tau_s}{2}\,\theta\left(\beta\hbar - \sum_{j=1}^{s}\mu_j\right)$$
$$\times \sum_{\mu_1,\ldots,\mu_s} Y_s \exp(E_s)|_{t_s \to t_{s+1} + i\tau_s} \tag{35}$$

Adding the result to the next integrand for the integral over t_{s+1} leads to

$$\mu_{s+1} Y_s|_{t_s \to t_{s+1} + i\tau_s} + \left(\prod_{i=1}^{s} \mu_i\right)(t_{s+1} - i\beta\hbar/2) = Y_{s+1} \tag{36}$$

We can in this way continue the program. Eventually we arrive at

$$A_n = \mathrm{Im} \int_{\beta\hbar}^{0} \frac{d\tau_1}{2} \cdots \frac{d\tau_{2n-1}}{2} \theta\left(\beta\hbar - \sum_{i=1}^{2n-1} \tau_i\right)$$
$$\times i \sum_{\{\mu_i = \pm 1\}} Y_{2n-1} \exp(E_{2n-1})|_{t_{2n-1} = i\tau_{2n-1},\, t_{2n} = \sum_{j=1}^{2n} \mu_j = 0} \tag{37}$$

The right-hand side is obviously zero because the integrand is now nowhere imaginary! We therefore arrive at the conclusion that the Kubo–Einstein relation holds to all orders in V_0.

4. DISCUSSION

Until now we have assumed that the integrands are well behaved as $t_i \to -\infty$, so that the integrals converge and the contributions from $t_i = -\infty$ vanish during the contour deformations. For finite-temperature Ohmic damping, this is indeed the case. Note that, going back to Eqs. (13)–(19), for $t \to \infty$, $C(t) \approx k_0^2 kTt/\eta$. For a given integral there let us divide the integral variables $\{t_{2n-1},..., t_1\}$ into two subgroups and let the separations between them be large. One then finds that if the total "spins" in the subgroups are nonzero, the integrand is supressed by the $C(t)$'s; if the "spins" vanish, the suppression comes from the $g(t)$'s. Both of the suppressions have the exponential decay form. It is therefore not difficult to show that for sufficiently small V_0 the series (15) and (16) are absolutely convergent (for this see Appendix C of ref. 5). Therefore the Einstein relation then holds exactly.

The problem of localization arises at zero temperature. In this case $C(t) \approx \hbar k_0^2 \ln |t|/2\pi\eta$ and the coefficient of V_0^{2n} for the velocity $v(F)$ has the structure (for large separations between the t's)

$$B_n(\tilde{F}) \sim \int_{-\infty}^{0} dt_{2n-1} \cdots \int_{-\infty}^{t_2} dt_1 \sum_{\{\mu_j = \pm 1\}} (\cdots)$$
$$\times \mathrm{Im} \exp\left\{ i \sum_{j=1}^{2n} \mu_j \tilde{F} t_j \right.$$
$$\left. + \frac{1}{2\alpha} \sum_{j,k=1}^{2n} \mu_j \mu_k \ln |t_j - t_k| \right\}\Bigg|_{t_{2n} = \sum_{j=1}^{2n} \mu_j = 0} \tag{38}$$

where $\tilde{F} = k_0 F/\eta$ and $\alpha = 2\pi\eta/\hbar k_0^2$. The oscillating phase in (38) is now responsible for the convergence of the integral. Rescaling the time by $\tilde{t} = \tilde{F}t$, we have

$$B_n(F) \sim F^{(1+2n(1-\alpha)/\alpha)} \times (\cdots) \tag{39}$$

Thus it is singular in F. For $\alpha > 1$, the linear mobility cannot be defined via a series in terms of V_0. In fact, it is believed that the system then suffers a localization transition.[1-3]

In summary, we have proved that in the Ohmic damping limit the Kubo–Einstein relation is exact for the cosine potential; thus to a very general extent we have removed the boundary between the classical and the quantum Brownian motion for this problem. Moreover, the mathematical methods may be very useful for other studies on this system. It may be possible to generalize the result to more general cases, for example, to non-Ohmic dampings or non-cosine potentials. These are currently under investigation.

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