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To cite this article: O A Ilinskaya *et al* 2018 *New J. Phys.* **20** 063036

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## OPEN ACCESS

## RECEIVED

6 February 2018

## REVISED

1 May 2018

## ACCEPTED FOR PUBLICATION

23 May 2018

## PUBLISHED

20 June 2018

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**Keywords:** micro- and nano-electromechanical systems (MEMS/NEMS) and devices, magnetoelectronics, spintronics: devices exploiting spin-polarized transport or integrated magnetic fields, electronic transport in mesoscopic systems, nano-electromechanical systems, coulomb blockade, single-electron tunneling

## Abstract

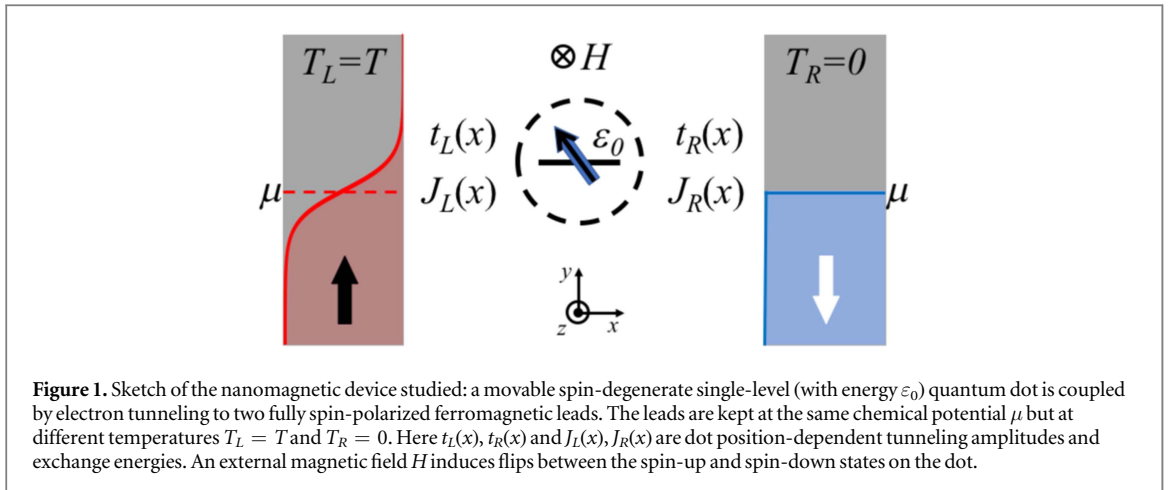
A theory of a thermally induced single-electron ‘shuttling’ instability in a magnetic nano-mechanical device subject to an external magnetic field is presented in the Coulomb blockade regime of electron transport. The model magnetic shuttle device considered comprises a movable metallic grain suspended between two magnetic leads, which are kept at different temperatures and assumed to be fully spin-polarized with anti-parallel magnetizations. For a given temperature difference shuttling is found to occur for a region of external magnetic fields between a lower and an upper critical field strength, which separate the shuttling regime from normal small-amplitude ‘vibronic’ regimes. We find that (i) the upper critical magnetic field saturates to a constant value in the high temperature limit and that the shuttle instability domain expands with a decrease of the temperature; (ii) the lower critical magnetic field depends not only on the temperature-independent phenomenological friction coefficient used in the model but also on intrinsic friction (which vanishes in the high temperature limit) caused by magnetic exchange forces and electron tunneling between the quantum dot and the leads. The feasibility of using thermally driven magnetic shuttle systems to harvest thermal breakdown phenomena is discussed.

## 1. Introduction

Mechanically promoted electric transport, being one of the most interesting features of nanoelectromechanics (NEM), offers a new functionality to devices on the nanometer length scale. Shuttling of electrons, as predicted in [1] and actively studied both theoretically and experimentally, is a prominent example of this statement (see, e.g., the review [2]).

Heat transport in nanostructures is a subject of enhanced interest [3] especially due to the importance of heat removal on a nanometer length scale. Electrically induced mechanical shuttling of electrons results in an exponential decrease of electric resistance (electric breakdown) and this new type of electric conductivity also significantly affects the heat transport through a NEM device. An intriguing question occurring in this context is whether or not the similar shuttle instability can be induced thermally at zero bias voltage applied to the device. In other words—is there a room for mechanically induced thermal breakdown in NEM shuttle devices?

The electric force, which drives a charged movable quantum dot (QD), vanishes in the zero voltage limit, implying that the coupling between mechanical and electronic degrees of freedom of the NEM device disappears. No pumping energy can be extracted from an electrically unbiased device. In what follows we will show that in a magnetic shuttle [4] the magnetic exchange force can provide the necessary work to induce a mechanical instability. Therefore a thermal breakdown in a magnetic unbiased shuttle device can take place.



In a mechanically soft NEM shuttle device, where a QD is coupled by electron tunneling to source and drain electrodes, an onset of a mechanical instability occurs when the bias voltage exceeds a critical value known as the instability threshold. When this happens a limit cycle of mechanical oscillations is reached (self-oscillation regime) and a steady state electrical current, which provides mechanical transportation of charge, is established. This current, which typically exceeds the tunnel current in the absence of a shuttle instability by several orders of magnitude, is called an electrical shuttle current (see [4] and [5]).

In an electric shuttle device both the energy source and the driving force are electrical in nature: the energy source is a bias voltage applied between the leads and the driving force is the Coulomb force between charges in the dot and the leads. In a magnetic shuttle device with spin-polarized electrons in the leads the energy source and the driving force may have a different physical nature: the energy source could still be a bias voltage while the driving force could be the magnetic (exchange) force between electron spins in the dot and the magnetic leads. (For a nanometer size geometry the exchange force may be as strong as the Coulomb force [6].) Therefore, it is in principle possible to employ a thermal rather than an electrical energy source in a magnetic shuttle device, i.e. to apply a temperature difference between leads kept at the same chemical potential. In this paper we show that such thermally induced magnetic shuttling is possible.

The action of the spin force is different from that of the Coulomb force. While the Coulomb force tends to repel electrons transferred to the dot from the lead they were injected from (Coulomb repulsion), the magnetic force, caused by the spin of the injected electron, acts in the opposite direction<sup>5</sup>. Therefore the work done by the magnetic force has the opposite sign compared to the work performed by the Coulomb force. Hence, the exchange force itself can not pump energy into the mechanical subsystem. However, if an external magnetic field  $H$  perpendicular to the magnetization in the leads is applied, this becomes possible. Such a field forces electrons in the dot to flip their spins and the densities of spin-up and spin-down electrons in the dot oscillate with a frequency determined by the magnetic field. Therefore the direction of the magnetic exchange force may change. As a result it becomes possible to trigger a shuttle instability in a magnetic device by applying an external magnetic field.

In what follows we will assume for simplicity that the magnetic leads are fully spin-polarized and that their magnetizations are anti-parallel. Under this condition the electrical current is blocked completely until ‘spin flips’<sup>6</sup> are induced by the external magnetic field (which is assumed to be oriented perpendicularly to the magnetization of the leads). The influence of a partial spin polarization on the shuttle instability was considered in [7] and [8].

The model we use to study a thermally induced magnetic shuttle is sketched in figure 1. It is the standard shuttle device (see, e.g., [4] and [9]), the only difference being that a temperature drop  $\delta T$  is applied to the leads instead of an electrical bias voltage and that one is interested in the heat flow  $J_q$  in response to this temperature drop. The thermal resistance  $R_T$  can be defined in analogy with the electrical resistance as  $R_T = \delta T/J_q$ . An exponential decrease in the thermal resistance (thermal breakdown) is possible due to transduction of thermal energy into the mechanical energy stored in the shuttle vibrations.

<sup>5</sup> Nonzero magnetization of a lead implies spin-split electron energy levels, with majority-spin electrons occupying the lower split level. The transfer of such an electron from the lead to the dot diminishes the magnitude of the energy split and therefore increases the total energy of the electron. Hence, the magnetic force on the dot, which acts to lower the energy of the system, will be oriented towards the magnetic lead that the electron tunneled from. This interaction is ferromagnetic irrespective of the nature of the exchange interaction (ferromagnetic or antiferromagnetic) in the bulk leads.

<sup>6</sup> Here the term ‘spin flips’ does not refer to any spin relaxation mechanism but to spin flips caused by the coherent spin dynamics (spin-up/down oscillations) in a magnetic field. The rate of these spin flips is much higher than those related to spin relaxation processes.

Below we will show that a mechanical shuttle instability occurs within a finite interval of external magnetic fields strengths, ( $H_{c1} < H < H_{c2}$ ). The dependence of the upper,  $H_{c2}$ , and lower,  $H_{c1}$ , threshold magnetic fields (which separate the shuttle and tunnel (outside this interval) regimes of electron transport) on the large temperature difference  $\delta T$  close to the temperature  $T$  of the ‘hot’ lead is the main result of our paper. The lower threshold field  $H_{c1}$  is determined by the dissipation (friction) coefficient in the mechanical subsystem. The friction coefficient  $\gamma_f = \gamma_0 + \gamma_f(T)$  is the sum of a (phenomenological) friction coefficient  $\gamma_0$  (see e.g. [10]) and the intrinsic friction coefficient [11]  $\gamma_f(T)$  induced in our case by magnetic exchange forces and electron tunneling between the dot and the leads at finite temperatures. We will call this coefficient the *magnetic* friction coefficient. We will show that the phenomenological friction coefficient can be neglected for a mechanical system with a high quality factor. The main contribution to magnetic friction is due to the hot electron reservoir (we assume a large temperature difference). We show that magnetic friction exists even in the absence of an external magnetic field and that it is a non-monotonic function of temperature: it is exponentially small at low temperatures, becomes temperature-independent in the region  $T \simeq \Gamma$  (where  $\Gamma$  is the characteristic energy of the dot-lead coupling) and scales as  $1/T$  in the high temperature limit. Since the pumping of energy into the mechanical subsystem in our model is triggered by the external magnetic field (the corresponding rate of increase of the oscillation amplitude in low magnetic fields being proportional to  $H^2$ ) a lower threshold magnetic field  $H_{c1}$  with a nontrivial temperature dependence appears. As we have shown before [4] the mechanical instability disappears in high magnetic fields. This is why an upper threshold field  $H_{c2}$  appears in the temperature driven shuttle as well.

Our calculations do not give any information about the low temperature limit, ( $\delta T \ll \Gamma$ ), since we use an approximation where the thermal energy is large compared to the width of the energy levels on the dot (sequential electron tunneling) and since in our model  $\delta T = T$ . However, our previous results (see, e.g., [12]) allow us to expect that the instability occurs at temperature differences not smaller than a value of the order of  $\hbar\omega$ . Therefore one may expect a non-monotonic dependence of the upper threshold field on the temperature difference with a maximum at  $\delta T \sim \Gamma$ .

This paper is organized as follows. In section 2 the model system we use to discuss thermo-induced single-electron shuttling is introduced; an equation for the reduced density operator of the QD and an equation of motion for the classical coordinate of the dot are obtained. In section 3 the domain where a magnetic shuttle instability occurs in the adiabatic regime of electron transport is characterized. In the concluding section 4 we highlight the main results obtained and discuss possible applications of a temperature induced shuttle instability.

## 2. Thermo-induced single-electron shuttle

The system under consideration (see figure 1) consists of a single-level QD that is coupled by electron tunneling to two ferromagnetic electrodes (leads). The leads are fully spin-polarized with their magnetization pointing in opposite directions. There is an external magnetic field  $\vec{H}$  in the gap between the source and drain leads, which is directed perpendicular to the magnetization in the leads. We assume that the leads are kept at equal chemical potentials ( $\mu_L = \mu_R \equiv \mu$ ) but at different temperatures  $T_L \neq T_R$ , so that a temperature gradient  $\delta T = T_L - T_R$  is applied to the system. The proposed design of the electrodes (suitable for thermal transport measurements as in [13]) allows one to maintain a temperature difference between the leads, while keeping their chemical potentials equal. To simplify calculations in what follows we will assume that  $T_L = T$  and  $T_R = 0$ . It follows that in our system the temperature difference  $\delta T = T$  and the mean temperature  $T_m = T/2$  are not independent quantities.

The Hamiltonian of the system has three terms,

$$\hat{\mathcal{H}} = \hat{H}_l + \hat{H}_d + \hat{H}_t. \quad (1)$$

The Hamiltonian,  $\hat{H}_l$ , describes non-interacting electrons in the electrodes,

$$\hat{H}_l = \sum_{k,\kappa} \varepsilon_{k,\kappa} a_{k,\kappa}^\dagger a_{k,\kappa}, \quad (2)$$

where  $a_{k,\kappa}^\dagger$  ( $a_{k,\kappa}$ ) is the creation (annihilation) operator of electron with momentum  $k$  (energy  $\varepsilon_{k,\kappa}$ ) in the lead  $\kappa = (L, R)$ . The QD Hamiltonian reads ( $\sigma = (\uparrow, \downarrow) = (+, -)$  is the spin projection index),

$$\begin{aligned} \hat{H}_d = & \sum_{\sigma} \varepsilon_{\sigma} c_{\sigma}^{\dagger} c_{\sigma} - \frac{g\mu_B H}{2} (c_{\uparrow}^{\dagger} c_{\downarrow} + c_{\downarrow}^{\dagger} c_{\uparrow}) \\ & + U c_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger} c_{\downarrow} c_{\uparrow} + \hat{H}_v, \quad \hat{H}_v = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}, \end{aligned} \quad (3)$$

where  $\varepsilon_\sigma = \varepsilon_0 - (\sigma/2)J(x)$  is spin- and position-dependent energy of QD split levels ( $\varepsilon_0$  is the level energy),  $J(x) = J_L(x) - J_R(x) \simeq J_0 - \alpha x$  ( $\alpha > 0$  and we consider only small deviations,  $x$ , of the dot center-of-mass coordinate from its equilibrium position) is the coordinate-dependent exchange energy produced by the ferromagnetic coupling between the dot and the leads, the operator  $c_\sigma^\dagger$  ( $c_\sigma$ ) creates (annihilates) an electron with spin projection  $\sigma$  in the dot;  $H$  is the external magnetic field directed along the  $z$ -axis (see figure 1),  $g$  is the gyromagnetic ratio,  $\mu_B$  is the Bohr magneton,  $U$  is the Coulomb repulsion energy in the dot. Vibrations of the dot are described by the harmonic-oscillator Hamiltonian  $\hat{H}_v$  ( $m$  and  $\omega$  are the mass and angular vibration frequency of the dot). In what follows we will consider  $x$  and  $p$  as classical time-dependent variables.

Tunneling of electrons between dot and leads is described by the standard tunneling Hamiltonian

$$\hat{H}_t = t_L(x) \sum_k c_\uparrow^\dagger a_{k,L} + t_R(x) \sum_k c_\downarrow^\dagger a_{k,R} + \text{h.c.}, \quad (4)$$

where  $t_\kappa(x) = t_\kappa \exp[\mp x/(4\lambda)]$  is the tunneling amplitude, which has an exponential dependence on the dot center-of-mass coordinate ( $\lambda > 0$  is the tunneling length, the signs ' $\mp$ ' correspond to the left and right electrodes respectively).

The quantum description of the electron subsystem is based on the assumption that the density matrix of the system can be factorized,

$$\hat{\rho}(t) = \hat{\rho}_d \otimes \hat{\rho}_l, \quad (5)$$

where  $\hat{\rho}_l$  is the equilibrium density matrix (Gibbs distribution function) of the leads. This assumption is always valid for  $T \gg \Gamma$  ( $\Gamma$  is the tunnel coupling energy—level width), when sequential electron tunneling is the main process of electron transport. In equation (5)  $\hat{\rho}_d$  is the density matrix of the QD interacting with the magnetic leads.

In a general case one has to pay attention to the appearance of an implicit time dependence of both the unperturbed Hamiltonian,  $\hat{H}_0 = \hat{H}_l + \hat{H}_d$ , and the tunneling Hamiltonian,  $\hat{H}_t$ , due to the time dependence of the dot coordinate (and momentum),  $x(t)$ ,  $p(t)$ . Therefore the derivation of the kinetic equations in [14] requires some modifications.

The equation for the density operator (in units where  $\hbar = 1$ ),

$$\frac{\partial \hat{\rho}(t)}{\partial t} + i[\hat{H}_0 + \hat{H}_t, \hat{\rho}(t)] = 0, \quad (6)$$

has the formal solution

$$\hat{\rho}(t) = \hat{\rho}(t = -\infty) - i \int_{-\infty}^t dt' \hat{u}(t, t') [\hat{H}_t(t'), \hat{\rho}(t')] \hat{u}^\dagger(t, t'), \quad (7)$$

where  $\hat{u}(t, t')$  is the evolution operator of the unperturbed Hamiltonian,

$$\hat{u}(t, t') = e^{-i\hat{H}_l(t-t')} \hat{u}_d(t, t'), \quad \hat{u}_d(t, t') = 1. \quad (8)$$

In equation (8)  $\hat{u}_d(t, t')$  is a dot evolution operator. After substitution of equations (5) and (7) into equation (6) and tracing out the electronic degrees of freedom in the leads one gets

$$\begin{aligned} \frac{\partial \hat{\rho}_d(t)}{\partial t} + i[\hat{H}_d, \hat{\rho}_d] &= -\text{Tr} \int_{-\infty}^t dt' [\hat{H}_t(t), e^{-i\hat{H}_l(t-t')} \hat{u}_d(t, t') \\ &\times [\hat{H}_t(t'), \hat{\rho}(t')] e^{i\hat{H}_l(t-t')} \hat{u}_d^\dagger(t, t')]. \end{aligned} \quad (9)$$

The term on the rhs of equation (9) has the sense of a collision integral,  $\hat{I} = \hat{I}_L + \hat{I}_R$ , due to the interaction between the dot and the leads. The kernel of this integral is expressed through the function  $K_\kappa(t, t')$  that can be evaluated exactly in the wide-band approximation limit, when one assumes that the density of states in the leads is energy independent,

$$K_\kappa(t, t') = K_\kappa(t - t') \equiv K_\kappa(\tau) = \sum_k e^{-i\varepsilon_{k,\kappa}\tau} f(\varepsilon_{k,\kappa}) = \frac{i\pi\nu_\kappa T_\kappa e^{-i\mu\tau}}{\sinh \pi(T_\kappa\tau + i0)}. \quad (10)$$

In equation (10)  $\nu_\kappa = \text{const}$ ,  $T_\kappa (= \beta_\kappa^{-1})$  are the density of states and the temperature (inverse temperature) in the lead  $\kappa$ ,  $f(\varepsilon)$  is the Fermi–Dirac distribution function,  $\mu$  is the chemical potential. As stated above we restrict ourselves to the case of zero temperature in the right lead,  $T_R = 0$ . Then using the well-known formula from the theory of distribution functions,

$$\frac{e^{i\tau z}}{\tau - i0} = \begin{cases} 2i\pi\delta(\tau), & z \rightarrow \infty, \\ 0, & z \rightarrow -\infty, \end{cases}$$

one readily gets the following expression for the collision integral  $\hat{I}_R$  in the regime of non-resonant tunneling,  $(\varepsilon_0 - \mu)/\Gamma_\kappa \gg 1$ ,

$$\hat{I}_R = \Gamma_R(x) \left[ c_{\downarrow} \hat{\rho}_d(t) c_{\downarrow}^{\dagger} - \frac{1}{2} [\hat{\rho}_d(t), c_{\downarrow}^{\dagger} c_{\downarrow}]_+ \right], \quad (11)$$

where  $[\hat{A}, \hat{B}]_+ = \hat{A}\hat{B} + \hat{B}\hat{A}$  is an anticommutator and  $\Gamma_{\kappa}(x) = 2\pi\nu_{\kappa} t_{\kappa}^2(x)$  is the partial level width.

The reduced density operator  $\hat{\rho}_d(t)$  acts in Fock space, which in our case is the finite dimensional space of a single-electron level on the dot. Matrix elements of the density operator are

$$\rho_0 = \langle 0 | \hat{\rho}_d | 0 \rangle, \quad \rho_{\sigma} = \langle \sigma | \hat{\rho}_d | \sigma \rangle, \quad \rho_{\sigma\sigma'} = \langle \sigma | \hat{\rho}_d | \sigma' \rangle, \quad \rho_2 = \langle 2 | \hat{\rho}_d | 2 \rangle, \quad (12)$$

where  $|\sigma\rangle = c_{\sigma}^{\dagger} | 0 \rangle$ ,  $|2\rangle = c_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger} | 0 \rangle$ ,  $\rho_{\sigma} \equiv \rho_{\sigma\sigma}$ ,  $\sigma \neq \sigma'$ . In what follows we restrict ourselves to the Coulomb blockade regime,  $U \gg T$ . Under this condition the doubly occupied state is forbidden,  $\rho_2 = 0$ .

In a classical description of the vibrational degrees of freedom, equation (3), the Hamilton equations for the dot coordinate and momentum take the form

$$\frac{\partial x}{\partial t} = \text{Tr} \left\{ \hat{\rho}_d(t) \frac{\partial \hat{H}_d}{\partial p} \right\} = \frac{p}{m}, \quad (13)$$

$$\frac{\partial p}{\partial t} = -\text{Tr} \left\{ \hat{\rho}_d(t) \frac{\partial \hat{H}_d}{\partial x} \right\} = -m\omega^2 x - \frac{\alpha}{2} (\rho_{\uparrow} - \rho_{\downarrow}). \quad (14)$$

The oscillator coordinate  $x(t)$  obeys the integro-differential equation

$$\frac{\partial^2 x}{\partial t^2} + \omega^2 x = -\frac{\alpha}{2m} (\rho_{\uparrow} - \rho_{\downarrow}), \quad (15)$$

where  $\rho_{\uparrow, \downarrow}$  are functionals of coordinate,  $\rho_{\uparrow, \downarrow} = \rho_{\uparrow, \downarrow}\{x(t)\}$ .

### 3. Adiabatic regime of dot oscillations

In the adiabatic limit  $\omega \ll \Gamma_{\kappa}$  when evaluating the collision integral  $\hat{I}_L$  one can neglect the dependence of coordinate on time. Then the evolution operator of the dot takes the form,

$$\hat{u}_d(t, t') = \exp[-i\hat{H}_d(t - t')]. \quad (16)$$

After straightforward calculations the collision integral  $\hat{I}_L$  in equation (9) can be represented in the form (we omit the index 'd' in  $\hat{\rho}_d(t)$ ,  $\hat{H}_d$  and index 'L' in  $\beta_L, T_L$ ):

$$\begin{aligned} \hat{I}_L = & \frac{\Gamma_L(x)}{2} [c_{\uparrow}^{\dagger} \hat{\rho}(t) c_{\uparrow} + c_{\downarrow} \hat{\rho}(t) c_{\downarrow}^{\dagger} - \hat{\rho}(t)] + \frac{i\Gamma_L(x)}{4} \\ & \times \left\{ \int_{-\infty}^{\infty} d\tau \frac{e^{i\beta\mu\tau}}{\sinh \pi\tau} c_{\uparrow} e^{-i\beta\hat{H}\tau} [\rho(t - \beta\tau), c_{\uparrow}^{\dagger}]_+ e^{i\beta\hat{H}\tau} \right. \\ & \left. + \int_{-\infty}^{\infty} d\tau \frac{e^{-i\beta\mu\tau}}{\sinh \pi\tau} c_{\downarrow}^{\dagger} e^{-i\beta\hat{H}\tau} [\rho(t - \beta\tau), c_{\downarrow}]_+ e^{i\beta\hat{H}\tau} - \text{h.c.} \right\} \quad (17) \end{aligned}$$

(here  $\tau$  is the dimensionless integration variable). In equation (17) the singular integrals are understood in the sense of the principal value. In the limit of high temperatures,  $\Gamma_L \ll T$ , one can neglect the retardation effects and replace  $\rho(t - \beta\tau) \rightarrow \rho(t)$  in equation (17).

From equations (9), (11), (17) one gets the following system of equations for the matrix elements of the density operator (note, that the Hamiltonian  $\hat{H}_d$  is not diagonal in  $\sigma$ -representation, but it can be easily diagonalized by unitary transformation):

$$\begin{aligned} \frac{\partial \rho_0}{\partial t} = & \Gamma_L(x)(1 - f_+) \rho_{\uparrow} - \Gamma_L(x) f_+ \rho_0 + \Gamma_R(x) \rho_{\downarrow} \\ & - \Upsilon_1(x)(\rho_0 + \rho_{\uparrow}) - \Upsilon_2(x)(\rho_{\uparrow\downarrow} + \rho_{\uparrow\downarrow}^*), \quad (18) \end{aligned}$$

$$\frac{\partial \rho_{\uparrow}}{\partial t} = -\Gamma_L(x)(1 - f_+) \rho_{\uparrow} - i\Omega_H(\rho_{\uparrow\downarrow} - \rho_{\uparrow\downarrow}^*) \quad (19)$$

$$\begin{aligned} & + \Gamma_L(x) f_+ \rho_0 + \Upsilon_1(x)(\rho_0 + \rho_{\uparrow}) + \Upsilon_2(x)(\rho_{\uparrow\downarrow} + \rho_{\uparrow\downarrow}^*), \\ \frac{\partial \rho_{\downarrow}}{\partial t} = & -\Gamma_R(x) \rho_{\downarrow} + i\Omega_H(\rho_{\uparrow\downarrow} - \rho_{\uparrow\downarrow}^*), \quad (20) \end{aligned}$$

$$\begin{aligned} \frac{\partial \rho_{\uparrow\downarrow}}{\partial t} = & iJ(x)\rho_{\uparrow\downarrow} - i\Omega_H(\rho_{\uparrow} - \rho_{\downarrow}) - \frac{\Gamma_L(x)}{2}(1 - f_{\pm})\rho_{\uparrow\downarrow} \\ & - \frac{\Gamma_R(x)}{2}\rho_{\uparrow\downarrow} - \frac{\Upsilon_1(x)}{2}\rho_{\uparrow\downarrow} + \Upsilon_2(x)(\rho_0 + \rho_{\uparrow}), \end{aligned} \quad (21)$$

where  $\Omega_H = g\mu_B H/2$  and

$$\Upsilon_1(x) = f_- \frac{J(x)\Gamma_L(x)}{\sqrt{J^2(x) + 4\Omega_H^2}}, \quad (22)$$

$$\Upsilon_2(x) = f_- \frac{\Omega_H\Gamma_L(x)}{\sqrt{J^2(x) + 4\Omega_H^2}}, \quad (23)$$

$$f_{\pm} = \frac{f(E_-) \pm f(E_+)}{2}, \quad (24)$$

$$E_{\pm} = \varepsilon_0 \pm \frac{\sqrt{J^2(x) + 4\Omega_H^2}}{2}. \quad (25)$$

To simplify the problem we consider the symmetric QD,  $J_0 = 0$ ,  $\Gamma_L(0) = \Gamma_R(0) = \Gamma$ . We are interested in the conditions when the stationary position of the dot ( $x = 0$ ) is not stable. In this case it is sufficient to consider small deviations  $x/\lambda \ll 1$  and to linearize the coordinate dependence of  $\Gamma_n(x) \simeq \Gamma(1 \mp x/2\lambda)$ .

At first we solve the problem in the high temperature limit,  $\beta \rightarrow 0$  ( $f_- = 0$ ,  $f_+ = 1/2$ ). It is convenient to rewrite the system, equations (18)–(21), in new variables,

$$R_{1,2} = \rho_{\uparrow} \pm \rho_{\downarrow}, R_3 = -i(\rho_{\uparrow\downarrow} - \rho_{\uparrow\downarrow}^*), R_4 = \rho_{\uparrow\downarrow} + \rho_{\uparrow\downarrow}^*. \quad (26)$$

In what follows we will assume that the dimensionless parameter  $\tilde{\alpha} = \alpha/(m\lambda\omega^2)$  is small,  $\tilde{\alpha} \ll 1$ . Since we study small vibrations of the dot, one can solve the system, equations (18)–(21) by perturbations,  $|R\rangle = |R^{(0)}\rangle + |R^{(1)}\rangle + \dots$ , where  $|R\rangle = (R_1, R_2, R_3)^T$  (note, that the equation for  $R_4$  is decoupled from the other equations and it is not relevant). In zero order of perturbation theory one gets

$$\begin{aligned} \langle R^{(0)} | = & \frac{1}{2\Delta} \left( \frac{3\Gamma^2}{4} + 4\Omega_H^2, \frac{3\Gamma^2}{4}, -2\Gamma\Omega_H \right), \\ \Delta = & \frac{3\Gamma^2}{4} + 5\Omega_H^2. \end{aligned} \quad (27)$$

In the first order of perturbation theory the equation for  $|R^{(1)}\rangle$  takes the form

$$\frac{\partial |R^{(1)}\rangle}{\partial t} = \hat{A}|R^{(1)}\rangle + \frac{\Gamma}{2\lambda}x(t)|g\rangle, \quad (28)$$

where

$$\hat{A} = -\frac{\Gamma}{4} \begin{pmatrix} 5 & -1 & 0 \\ 1 & 3 & -8\Omega_H/\Gamma \\ 0 & 8\Omega_H/\Gamma & 3 \end{pmatrix}, |g\rangle = \frac{\Omega_H}{4\Delta} \begin{pmatrix} -8\Omega_H \\ 0 \\ \Gamma \end{pmatrix}. \quad (29)$$

Substituting the solution of equation (28) into the rhs of equation (15) we derive the desired equation for single-electron shuttle coordinate

$$\frac{\partial^2 x}{\partial t^2} + \omega^2 x = -\frac{\alpha\Gamma}{4\lambda m} \int_0^\infty d\tau \langle e_0 | e^{\hat{A}\tau} | g \rangle x(t - \tau), \quad (30)$$

where  $\langle e_0 | = (0, 1, 0)$ .

In the adiabatic limit  $\omega \ll \Gamma$  one can expand  $x(t - \tau) \simeq x(t) - \tau\dot{x}(t)$ . We see that the electro-mechanical coupling results in (small) additive renormalization of vibrational frequency  $\omega$  and the appearance of damping (or pumping) term  $\gamma\dot{x}$  in the mechanical equation, where the coefficient  $\gamma(\Gamma, \Omega_H)$  reads

$$\begin{aligned} \gamma(\Gamma, \Omega_H) = & -\frac{\alpha\Gamma}{4\lambda m} \int_0^\infty d\tau \tau \langle e_0 | e^{\hat{A}\tau} | g \rangle \\ = & \frac{\hbar\alpha\Gamma\Omega_H^2}{4\lambda m\Delta^3} \left( \Omega_H^2 - \frac{7\Gamma^2}{4} \right) \end{aligned} \quad (31)$$

(we restored the dimension in the last formula). It is easy to find from equation (31) that in weak magnetic fields,

$$\left| \frac{g\mu_B H}{2} \right| < \frac{g\mu_B H c_2}{2} = \frac{\sqrt{7}}{2}\Gamma, \quad (32)$$

the shuttle instability occurs. Note, that the increment  $r(\Gamma, \Omega_H) = -\gamma(\Gamma, \Omega_H)/2$  of the exponential growth of shuttle oscillations amplitude in the limit  $\omega \ll \Gamma$  does not depend on the dot frequency  $\omega$ .

For finite temperatures the calculations are similar to the previous ones but they are more lengthy. For simplicity we restrict ourselves to the case of relatively large magnetic fields,  $|\Omega_H| \gg \alpha\lambda$ . Under this condition for the damping (pumping) coefficient one gets the expression

$$\gamma_T(\Gamma, \Omega_H) = -\frac{\alpha\Gamma}{8\lambda m} \int_0^\infty d\tau \tau \langle e_1 | e^{\hat{A}_T \tau} | g_1 \rangle, \quad (33)$$

where  $\langle e_1 | = (0, 1, 0, 0)$  and

$$\hat{A}_T = -\frac{\Gamma}{2} \begin{pmatrix} 2 + f_+ & f_+ & 0 & -f_- \\ -f_+ & 2 - f_+ & 2\Omega_H/\Gamma & f_- \\ 0 & -2\Omega_H/\Gamma & 2 - f_+ & 0 \\ f_- & -f_- & 0 & 2 - f_- \end{pmatrix}, \quad (34)$$

$$|g_1\rangle = \frac{4}{\Delta_T} \begin{pmatrix} -4\Omega_H^2[f_+(2 - f_+) + f_-^2] \\ 0 \\ \Gamma\Omega_H[f_+(2 - f_+) + f_-^2]f_+ \\ [\Gamma^2(2 - f_+) + 8\Omega_H^2]f_- \end{pmatrix}, \quad (35)$$

$$\Delta_T = \Gamma^2(2 - f_+)^2 + 4\Omega_H^2(4 - f_+^2 + f_-^2). \quad (36)$$

The shuttle instability condition is given by the inequality

$$C_1(\Omega_H/\Gamma)^4 - C_2(\Omega_H/\Gamma)^2 + C_3 < 0, \quad (37)$$

where

$$C_1 = 2f_+^3(2 - f_+)^3 - f_+f_-^2(2 - f_+)^2(4 - 5f_+) - 4f_-^4(2 - f_+)(1 - f_+) - f_-^4(4 - f_-^2), \quad (38)$$

$$C_2 = \frac{2 - f_+}{2} [f_+^2(2 - f_+)^2(4 - f_+) - f_-^2(2 - f_+)(4 - f_+)(1 - 2f_+) + f_-^4(5 - f_+)], \quad (39)$$

$$C_3 = \frac{(2 - f_+)^3(4 - f_+)f_-^2}{16}. \quad (40)$$

As a consequence, the shuttle instability region is defined by the (transcendental) relation

$$\Omega_{Hc1}^2 < \Omega_H^2 < \Omega_{Hc2}^2, \quad (41)$$

where

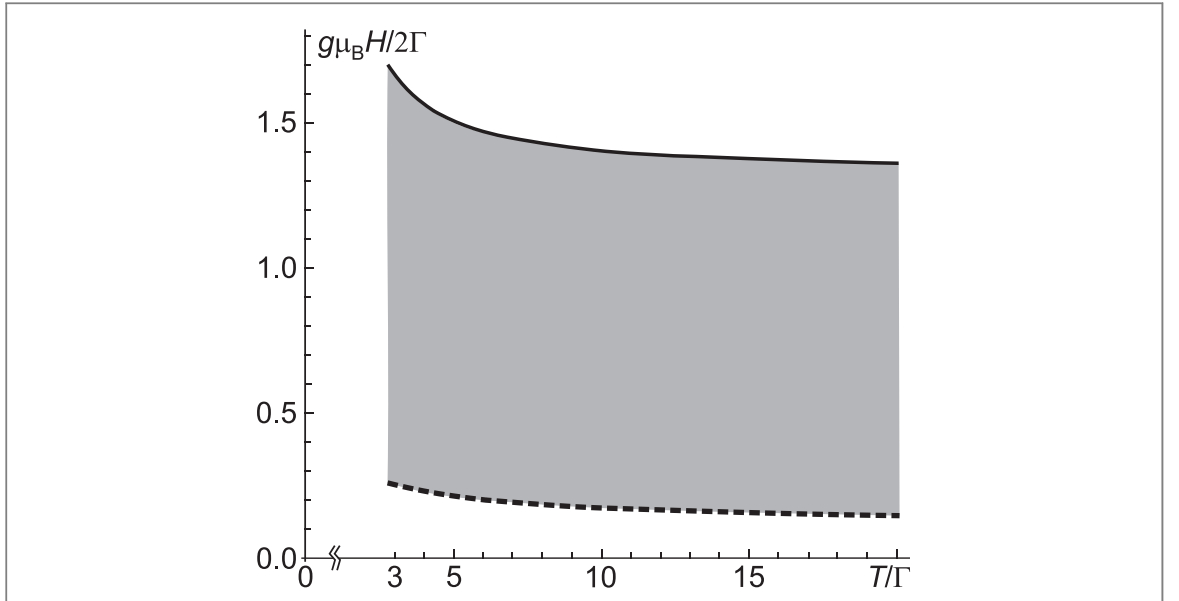
$$\Omega_{Hc1(c2)}^2 = \Gamma^2 \frac{C_2 \mp \sqrt{C_2^2 - 4C_1C_3}}{2C_1}. \quad (42)$$

The lower critical magnetic field  $\Omega_{Hc1}$  lies outside the range of applicability of our calculations. (We neglected the amplitude of shuttle oscillations compared to  $\Omega_H/\alpha$ .) Physically the existence of the lower critical magnetic field can be easily explained. Even in the absence of an external magnetic field (and in the absence of phenomenological friction) at finite temperature there is dissipation in the mechanical subsystem induced by magnetic forces and back-tunneling of electrons to the hot lead. The corresponding friction coefficient  $\gamma_f(T)$  (in what follows we will call it magnetic friction) can be estimated from simple physical considerations. Magnetic friction appears due to a finite work performed by magnetic driving force along the closed trajectory of oscillating QD and therefore it is proportional to the coordinate derivative of Fermi distribution function  $f[\varepsilon_1(x) - \mu]$ . Since magnetic force is nonzero only when the electron level is occupied, magnetic friction depends on the dot-lead coupling energy  $\Gamma$ . By taking into account retardation effects<sup>7</sup> this contribution to magnetic friction is represented by a factor  $\Gamma/(\Gamma^2 + (\hbar\omega)^2)$ . As the result friction coefficient takes the form

$$r_f(T) \sim -\frac{\hbar\alpha^2}{m} \frac{\Gamma}{\Gamma^2 + (\hbar\omega)^2} \frac{1}{T} \cosh^{-2}\left(\frac{\delta\varepsilon}{2T}\right), \quad (43)$$

<sup>7</sup> Note that in our approximation the equation for the dot density matrix is local; retardation effects are related to the nonlocality of the effective force in the equation of motion for the oscillator coordinate (see equation (30)).





**Figure 2.** The lower ( $H_{c1}$ , dashed curve) and upper ( $H_{c2}$ , full curve) threshold magnetic fields plotted as functions of normalized temperature,  $T/\Gamma$ , for  $\delta\varepsilon/\Gamma = 2$  in the adiabatic regime,  $\omega \ll \Gamma/\hbar$ . These fields define the border between the shuttle regime ( $H_{c1} < H < H_{c2}$ , shaded region) and the vibronic regime (outside this interval). For  $T \rightarrow \infty$  the lower threshold field  $H_{c1}$  saturates to a constant value determined by the phenomenological friction coefficient  $\gamma_0$ .

where  $\delta\varepsilon = \varepsilon_0 - \mu$ . Note that friction coefficient is defined as  $\gamma_j(T) = -2r_j(T)$ . The calculation of the decrement of shuttle vibrations in the absence of external magnetic field ( $\Omega_H = 0$ ) by using equations (15), (18)–(25) leads to equation (43) with the numerical prefactor  $1/32$ . We see that in high- $T$  limit  $T \gg \delta\varepsilon$  magnetic friction is decreased with the growth of temperature. At temperatures  $\Gamma \ll T \ll \delta\varepsilon$  dissipation is exponentially small,  $r_j \propto \exp(-\delta\varepsilon/T)$ . Our calculations are not valid at temperatures  $T \ll \Gamma$  where resonant electron tunneling takes place. However it is evident from physical considerations that dissipation vanishes when  $T \rightarrow 0$ . Anomalous temperature behavior of  $r_j(T)$  is a specific feature of magnetic dissipation which takes maximum value at  $T \sim \Gamma \sim \delta\varepsilon$  and it vanishes in the limits of both small and high temperatures.

The shuttle instability appears when the increment of exponential growth of dot oscillations amplitude exceeds the decrement  $\gamma_j(T)/2$ . For small magnetic fields,  $\Omega_H \rightarrow 0$ , the increment reads

$$r(\Gamma, \Omega_H \rightarrow 0) \simeq \frac{14\hbar\alpha}{3m\lambda\Gamma^3} \Omega_H^2. \quad (44)$$

Therefore, by comparing equations (43) and (44) we can estimate the lower critical magnetic field in the high- $T$  limit as

$$\Omega_{Hc1} \simeq 0.1 \sqrt{\frac{\alpha\lambda}{T}} \Gamma. \quad (45)$$

The phenomenological friction coefficient  $\gamma_0 = \omega/Q$  can be neglected in comparison with the optimal intrinsic friction coefficient  $\gamma_j(T)$  if the quality factor  $Q$  of the mechanical subsystem is sufficiently large. We estimate the minimal quality factor required to be  $Q_{\min} \sim 10^2 \div 10^3$  for  $\Gamma \sim \hbar\omega \sim 1$  meV,  $J_L(0) \sim J_R(0) \sim 10$  meV, values taken from experimental work [6, 15] on  $C_{60}$ -based molecular transistors.

The shuttle instability domain (shaded region in figure 2) is plotted in  $T/\Gamma$ ,  $g\mu_B H/2\Gamma$  parameter space for  $\delta\varepsilon/\Gamma = 2$ . The shuttle domain is shown only for  $T \geq \Gamma$  because we solved the problem in the perturbation theory in small parameter  $\beta\Gamma \ll 1$ . Although our calculations are not valid at low temperatures, at  $T \rightarrow 0$  the increment  $r(\Gamma, \Omega_H)$  behaves as  $r \sim \exp[-2\beta(\delta\varepsilon - \Omega_H)]$ . Exponential smallness of  $r_T(\Omega_H)$  for  $T \rightarrow 0$  is physically reasonable result. In the high temperature limit,  $T \rightarrow \infty$ , we return to the result of equation (32) for  $H_{c2}$ . Leaving the next term in expansion in small parameter  $\beta\delta\varepsilon$ , we obtain such an asymptotic behaviour of the critical magnetic field at large temperatures,

$$\frac{g\mu_B H_{c2}}{2} \simeq \frac{\sqrt{7}}{2} \left[ 1 + \frac{2}{7} \frac{\delta\varepsilon}{T} \right] \Gamma. \quad (46)$$

In adiabatic limit ( $\omega \ll \Gamma$ ) we used the evolution operator of the dot,  $\hat{u}_d(t, t')$ , in the form of equation (16). However the criterion of validity of the expression for the evolution operator in this form for magnetic shuttle is not equivalent to condition  $\omega \ll \Gamma$ . In fact, the analysis shows that the criterion of the validity of equation (16) is ( $\Omega_H, \Gamma \neq 0$ )

$$\frac{\omega}{\Gamma} \frac{\alpha \lambda \Omega_H}{\Omega_H^2 + (\alpha \lambda)^2} \ll 1. \quad (47)$$

Therefore, in the limit  $\alpha \lambda / \Omega_H \ll 1$  the ratio  $\omega / \Gamma$  can take large values ( $\omega / \Gamma \geq 1$ ) without violation of adiabaticity of mechanical motion.

Besides in our consideration we assume that the parameter  $\tilde{\alpha} = \alpha / (m \lambda \omega^2)$  is small,  $\tilde{\alpha} \ll 1$ . When both inequalities are taken into account one gets upper bound for frequencies

$$\omega \ll \omega_m = \left[ \frac{\Omega_H \Gamma}{m \lambda^2} \right]^{1/3} \quad (48)$$

when the evolution operator can be considered in the form corresponding to adiabatic motion.

When the conditions of equations (47), (48) are fulfilled one can use the system of kinetic equations, equations (18)–(21), and to analyze the behavior of the system at high frequencies similar to the previous calculations. As a result the shuttle instability at frequencies higher than  $\Gamma$  is defined by the inequality

$$|\Omega_H| / \omega < C(\Omega_H, T), \quad (49)$$

where

$$C(\Omega_H, T) = \sqrt{\frac{(2 - f_+)(4 - f_+)(2f_+^2 - f_-^2) + f_-^2(2f_+ - f_-^2)}{4(f_+^2 - f_-^2)[2f_+(2 - f_+) + f_-^2]}}. \quad (50)$$

(In formulas (49)–(50) we assumed  $\omega \gg \Gamma$ .)

The shuttle instability domain plotted in  $T / \hbar \omega$ ,  $g \mu_B H / 2 \hbar \omega$  parameter space has the same form as the shuttle instability domain at small frequencies plotted in figure 2.

We would like to note here another interesting fact. In the limit  $T \rightarrow \infty$  the problem under consideration can be solved exactly for arbitrary relationship between the model parameters  $\Omega_H, \Gamma, \omega$ . Physically the considered infinite temperature limit is realized for temperatures  $T \gg \max(\hbar \omega, \Gamma)$ . In this limit the kernel of collision integral in equation (9) can be replaced by  $\delta$ -function and the integro-differential equation for density operator becomes local in time. Indeed at  $T \rightarrow \infty$

$$\lim_{T \rightarrow \infty} \frac{T}{\sinh \pi(T\tau + i0)} = -i\delta(\tau) \quad (51)$$

and the function  $K_L(t, t')$  that defines the kernel of collision integral, equation (9), is reduced to  $K_L(t, t') = \pi \nu_L \delta(t - t')$ . As a consequence the evolution operator of the dot is trivial (unit operator) and the system of kinetic equations for the components of the density operator has a Markovian form. It is obvious that in the limit  $\Gamma < \omega \ll \omega_m$  this system coincides with equations (18)–(21) for adiabatic case in the limit  $T \rightarrow \infty$ . Therefore the dot dynamics is described by equation (30) and the criterion of shuttle instability (the range of magnetic field) for high frequencies is

$$\left| \frac{g \mu_B H}{2} \right| < \frac{g \mu_B H_c 2}{2} = \frac{\sqrt{7}}{2} \hbar \omega. \quad (52)$$

This result is in agreement with equations (49), (50).

The increment  $r(\Gamma, \Omega_H, \omega)$  of the exponential growth of shuttle center-of mass coordinate in the limit of high temperatures (note that in our model  $\delta T = T$ ) takes the form (we restore the dimensions)

$$r(\Gamma, \Omega_H, \omega) = \frac{\tilde{\alpha} \Gamma^3 \Omega_H^2}{8 \hbar \Delta D} \left[ \frac{7}{4} (\hbar \omega)^2 - \Omega_H^2 \right], \quad (53)$$

where  $\Delta$  is defined by equation (27) and

$$D = [(\hbar \omega)^2 - 4\Omega_H^2]^2 + \left( \frac{\Gamma}{\hbar \omega} \right)^2 \left[ \frac{11}{4} (\hbar \omega)^2 - 5\Omega_H^2 \right]^2. \quad (54)$$

The maximal value of the increment is reached at  $\Omega_H = \hbar \omega / 2$  when  $r_{\max}(\Gamma, \Omega_H = \hbar \omega / 2, \omega) = \tilde{\alpha} \Gamma / 60 \hbar$ .

## 4. Conclusions

We have shown that in a magnetic shuttle structure [4] a temperature gradient between the leads can trigger a shuttle instability, which leads to an exponential growth of the amplitude of shuttle oscillations, even in the absence of a voltage bias. This leads to a ‘mechanically supported thermal breakdown’ in the form of an exponential growth of the heat current (as well as of the electrical current) through the device. In our model [5] of fully (and oppositely) spin-polarized electrons in the leads a spin blockade prevents a current to flow in the absence of an external magnetic field. Lifting the spin blockade by applying such a field results in a shuttle

instability if the field strength exceeds a certain threshold value,  $H_{c1}$ , determined by the amount of dissipation in the mechanical subsystem. When the leads are kept at finite temperatures, there is an intrinsic dissipation mechanism [11] ('magnetic friction'; independent of magnetic field for low field strengths) caused by the magnetic force and the exchange of electrons between the QD and the leads. In addition there is phenomenological friction, which can be neglected if the quality factor of the mechanical subsystem is large enough. The amount of magnetic friction in our model is determined by the temperature of the 'hot' lead, the level energy  $\delta\varepsilon = \varepsilon_0 - \mu$ , the dot-lead coupling energy  $\Gamma$ , and the dot vibration frequency. In the general case of an asymmetric junction,  $\Gamma_L \neq \Gamma_R$ , and nonzero temperatures in both leads,  $T_L \neq T_R \neq 0$ , the magnetic friction is the sum of contributions produced by each lead. We predict that a specific feature of the magnetic friction is its anomalous temperature dependence. It vanishes in the limits of small and high temperatures and attains a maximum value at temperatures  $T \sim \Gamma \sim \delta\varepsilon$ . No shuttle instability occurs in such high magnetic fields,  $H > H_{c2}$ , that the spin-flip time exceeds the characteristic time scale determined by the maximum of the mechanical ( $\sim \omega^{-1}$ ) or electronic ( $\sim \hbar/\Gamma$ ) time scales. For sequential electron tunneling  $H_{c2}$  saturates at  $T \gg \Gamma$  and slightly increases with the decrease of temperature (see figure 2).

It is useful to qualitatively discuss the dependence of  $H_{c1}$  on the temperature difference between the two heat reservoirs when they are held at almost equal temperatures,  $\delta T \ll T$ . In this case the rate of increase,  $r$ , of the amplitude of the shuttle oscillations after an instability has occurred has a linear dependence on  $\delta T$  (for an electric shuttle the dependence of the corresponding rate on bias voltage  $V$  and model parameters,  $r \propto V\Gamma$ , was calculated in [16]). If  $T_L \simeq T_R \gg \Gamma$  our approach (using the density operator method) is valid and from physical considerations one can deduce that the rate of energy pumping is proportional to  $H_{c1}^2 \delta T$ . The temperature dependence of the magnetic friction is still determined by an equation similar to equation (43) and therefore the friction coefficient  $\gamma_f(T) \propto 1/T$ , where  $T$  is the average temperature. We see that now  $H_{c1} \propto 1/\sqrt{T\delta T}$  and that it is much larger than the corresponding field calculated for  $\delta T \simeq T$ . Therefore, it may be an unrealistic proposition to use such high values of the static external magnetic field in experiments.

The exponential increase of the amplitude of the center-of-mass oscillations of the dot saturates when the energy pumped into the dot vibrations equals the energy dissipated by the magnetic friction. From a general point of view our device works as a spintronic quantum heat engine [17]. A spin-polarized (spin-'up') electron tunnels from the hot lead to the vibrating QD and for a certain time it is localized in the dot. In the absence of an external magnetic field the only further dynamics of the spin-up electron allows it to tunnel back to the 'source' electrode. In this case the work done by the exchange forces results in the dot motion being damped.

An external magnetic field induces coherent electron spin dynamics in the dot (spin-up/down oscillations) and therefore a new channel of electron tunneling (from the dot to the 'drain' lead) is opened. This process results in positive work being done by the exchange forces, which amounts to pumping energy from the hot lead to the mechanical motion of the QD (the device becomes a spintronic single-electron heat engine). Note that the transformation of heat into mechanical energy in our device is carried out by strongly nonequilibrium and nonlinear processes. The shuttle instability is an intrinsically threshold phenomenon (there is a minimum temperature difference  $\delta T \sim \hbar\omega$  for which a mechanical instability can occur). Therefore it can not be described by thermoelectric coefficients obtained using linear response theory.

We speculate that the predicted phenomenon of a mechanically induced thermal breakdown could find useful applications in spintronic devices, when it is essential to avoid high temperature gradients on a chip.

## Acknowledgments

The authors thank LY Gorelik for useful discussions. OAI, SIK, and IVK acknowledge financial support from NAS Ukraine (Grant № 4/18-N and Scientific Programme 1.4.10.26.4). This publication is partly (IVK) based on the research provided by the grant support of the State Fund for Fundamental Research (Ukraine, project № Ф76/33683). This work was supported by the Institute for Basic Science in Korea (IBS-R024-D1). RIS and MJ acknowledge support from the Swedish Research Council (VR). IVK and RIS acknowledge hospitality of PCS IBS, Daejeon (Korea).

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