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Local heating in mesoscopic systems

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The thermal excitation of an impurity atom by an electron current in a mesoscopic system is investigated. Starting from the density matrix of the combined system of the electrons and the impurity, we obtain a solution to the master equation for the impurity atom in the presence of inelastic electron-impurity scattering. Explicit expressions are found for the effective temperature of the nonequilibrium electrons and for the relaxation rate of the impurity towards the thermally excited steady state. The effect of a phonon bath is included in our analysis. In the case of high bias and high lattice temperature, the impurity follows a Boltzmann distribution with a time-dependent temperature.

I. INTRODUCTION

Inelastic electron scattering in a mesoscopic system can have significant effects on electronic transport properties.[1–7] If the inelastic scattering is caused by impurity atoms, the momentum and energy transfer from the electrons will also affect the impurity's energy and spatial distribution, and this will be important in the electromigration phenomenon.[8,9] Although thermal transport by electrons in a mesoscopic system has been extensively studied, inelastic scattering and the associated dissipation is usually assumed to occur only in the reservoirs.[10–13]

Recently Ralls, Ralph, and Buhrman[14] have observed two-level fluctuations (TLF) in the resistance of a microscopic point contact. According to them, the TLF are caused by the motion of individual defects inside the nanometer-sized constriction, with inelastic scattering and electromigration playing important roles.[14] By relating the average time a defect spends in each of its two configurations to a defect local temperature in the context of electromigration theory, they were able to show that there is a local-heating process at the defect caused by the mesoscopic current. The notion of local heating also arises in the field of scanning tunneling microscopy (STM), where heating-assisted electromigration has been claimed to be the mechanism underlying the "atom switch," whereby an atom can be made to jump between a STM tip and a substrate upon application of a voltage.[15] The raising of electron temperature under nonequilibrium conditions at high current density has also been studied by Bergmann *et al.* for metallic microstructures.[16]

In this paper, we present a calculation of the thermal excitation of an impurity atom in a quasi-one-dimensional mesoscopic system due to electron current. The impurity is taken to be a harmonic oscillator that is only weakly coupled to the electrons and to the phonons. The electrons and the phonons act as thermal baths to the impurity and are treated separately. First we consider the density matrix of the combined system of the electrons and the impurity. Following the Landauer-Büttiker scattering theory formulation for mesoscopic systems,[17,18] we assume that the incident electron distribution, having temperature and chemical potential determined by the reservoirs, is not affected by the weak electron-impurity interaction. This allows us to trace out the electron degrees of freedom and arrive at a master equation for the impurity. The solution to the master equation shows that the current-carrying electrons act as a thermal bath for the impurity with an effective temperature determined by the voltage. Thermal heating is given in terms of impurity relaxation toward this elevated temperature. Phonons enter into the impurity master equation as an additional term, which attempts to bring the impurity back into thermal equilibrium with the lattice.

An overview of our paper is as follows. In Sec. II, starting from the density matrix of the combined system of the electrons and the impurity, we derive the master equation for the impurity in the presence of a weak electron-impurity interaction. The master equation is reduced to a differential equation in Sec. III, and its solution is characterized by a temperature that increases with time. In Sec. IV, we include the effect of a phonon bath in the master equation, and this gives rise to an additional relaxation term in the equation for the time-dependent temperature. Our calculation is generalized to a three-dimensional (3D) case in Sec. V. The connection of our results with some previous work is discussed in Sec. VI.

II. FORMULATION

We consider the density matrix of the combined system of the electrons and the impurity. Before being scattered by the impurity, the electrons are emitted by the reservoirs attached to the mesoscopic device, and their state is specified by a set of occupation numbers $\{n_k\}$, where k is the single-electron momentum. The impurity is taken to be a 1D particle bound by a harmonic potential, with energy eigenvalues labeled by ϵ. In the basis represented by $\{n_k\}$ and ϵ, we write the diagonal elements of the density matrix as $P(\epsilon,\{n_k\},t)$, which changes with time t due to electron-impurity scattering. In general, $P(\epsilon,\{n_k\},t)$ provides the desired information about the thermal excitation of the impurity.

The electron-impurity interaction is assumed to be

"switched on" at time $t=0$, and therefore at $t=0$ the density matrix is decoupled with respect to the electrons and the impurity, and it has only diagonal elements given by

$$P(\epsilon,\{n_k\},0)=P(\epsilon,0)P(\{n_k\}) , \tag{1}$$

where $P(\epsilon,0)$ is the initial distribution of the impurity just before the electron-impurity interaction is switched on. $P(\{n_k\})$ is the distribution of the incident electron stream established by the reservoirs. We have

$$\langle c_k^\dagger c_k\rangle=\begin{cases} f(E_k-\frac{1}{2}eV), & k>0 \\ f(E_k+\frac{1}{2}eV), & k<0 , \end{cases} \tag{2}$$

where $c_k^\dagger$ and c_k are the creation and annihilation operators for an electron at momentum k and energy E_k. The bracket $\langle\ \rangle$ stands for

$$\Sigma_{\{n_k\}}P(\{n_k\})\langle\{n_k\}|\cdots|\{n_k\}\rangle ,$$

which yields a Fermi distribution, and eV is the chemical potential difference between the reservoirs maintained by the bias voltage V. The Fermi distribution function f is given by $f(E)=1/(e^{\beta(E-E_F)}+1)$, where β is the inverse temperature of the reservoirs, and E_F is the Fermi energy.

Starting from the initial value given by Eq. (1), $P(\epsilon,\{n_k\},t)$ will change due to the electron-impurity interaction, which we write as

$$H_1=\frac{1}{2\pi}\int dk\int dk' V(k-k')e^{i(k-k')X}c_{k'}^\dagger c_k , \tag{3}$$

where $V(k-k')$ is the Fourier transform of the electron-impurity potential, and X is the impurity's coordinate relative to its equilibrium position. For weak H_1, and with the assumption that the density matrix is diagonal at $t=0$, one has[19,20]

$$\frac{\partial}{\partial t}P(\epsilon,\{n_k\},t)=-\sum_{\epsilon'}\sum_{\{n_k'\}}W(\epsilon',\{n_k'\};\epsilon,\{n_k\})[P(\epsilon,\{n_k\},t)-P(\epsilon',\{n_k'\},t)] , \tag{4}$$

where $W(\epsilon',\{n_k'\};\epsilon,\{n_k\})=W(\epsilon,\{n_k\};\epsilon',\{n_k'\})$ is the transition rate between state $|\epsilon,\{n_k\}\rangle$ and $|\epsilon',\{n_k'\}\rangle$ as given by the first-order Born approximation.

Equation (4) is known as the master equation[19,20] for a Markovian process, and can be derived from the quantum-mechanical equation of motion. Although the master equation gives the time variation of the diagonal elements of the density matrix, no assumption is made concerning the diagonality of the density matrix itself except for its initial form. In other words, the repeated application of the random-phase approximation is not necessary for the absence of interference effects as is suggested by Eq. (4). For a detailed analysis of this aspect, one is referred to Van Hove's classic 1955 paper.[19]

As an additional constraint to Eq. (4) based on the electron reservoir picture, it is reasonable to assume that the distribution of electrons as initially given by the reservoirs is not modified by the weak electron-impurity interaction to any significant extent; consequently, we replace $P(\epsilon,\{n_k\},t)$ appearing in the right-hand side of Eq. (4) by a simpler form:[21]

$$P(\epsilon,\{n_k\},t)=P(\epsilon,t)P(\{n_k\}) , \tag{5}$$

where $P(\{n_k\})$ is the same electron distribution as in Eq. (1).

Starting from Eq. (4), with the assumption concerning the right-hand side of the equation given above, one may wish to calculate the electron current through the mesoscopic system. The current equals the net incident current from the reservoirs minus $d/dt\int_{k>0}dk\langle c_k^\dagger c_k\rangle$, which is the rate at which the electrons that are incident from the reservoir to the left are backscattered. The result obtained in this way is consistent with our conductance calculation in Ref. 6. In the present work, we are concerned with the behavior of the impurity rather than the conductance.

Tracing out the electron degrees of freedom on both sides of Eq. (4) with the use of Eqs. (5) and (2), we obtain

$$\frac{\partial}{\partial t}P(\epsilon,t)=-\sum_{\epsilon'}\{W(\epsilon',\epsilon)P(\epsilon,t)-W(\epsilon,\epsilon')P(\epsilon',t)\} , \tag{6}$$

where $W(\epsilon',\epsilon)$ is the transition rate from state $|\epsilon\rangle$ to state $|\epsilon'\rangle$, and $W(\epsilon,\epsilon')$ refers to the reverse process. Explicitly, we have

$$W(\epsilon',\epsilon)=\sum_{\{n_k\}}\sum_{\{n_k'\}}W(\epsilon',\{n_k'\};\epsilon,\{n_k\})P(\{n_k\}) , \tag{7}$$

where in general $W(\epsilon',\epsilon)\neq W(\epsilon,\epsilon')$. Elastic electron scattering by the impurity with $\epsilon'=\epsilon$ drops out from the right-hand side of Eq. (6) and therefore has no effect on $P(\epsilon,t)$.

Applying Eqs. (2) and (3) to Eq. (7) with the first-order approximation for the transition-rate calculation, we get

$$W(\epsilon',\epsilon)=\frac{1}{2\pi\hbar}|r|^2\int_0^\infty dE\int_0^\infty dE'|\langle\epsilon'|e^{2ik_fX}|\epsilon\rangle|^2\delta(E-E'+\epsilon-\epsilon')$$
$$\times\{f(E-\tfrac{1}{2}eV)[1-f(E'+\tfrac{1}{2}eV)]+f(E+\tfrac{1}{2}eV)[1-f(E'-\tfrac{1}{2}eV)]\} , \tag{8}$$

where $|r|^2=(m/\hbar^2k_F)^2|V(2k_F)|^2$ is the elastic reflectivity at the Fermi level. The dynamical distribution of the inelastic process is governed by the matrix element $\langle\epsilon'|e^{2ik_FX}|\epsilon\rangle$. Since the Fermi distribution factor $f(1-f)$ in Eq. (8) takes a significant value only around the Fermi energy, we have replaced the electron density of states and the electron momentum change by the corresponding Fermi-level value. The reverse transition rate $W(\epsilon,\epsilon')$ is obtained from Eq. (8) by interchanging ϵ and ϵ'.

In deriving Eq. (8), we have taken into account only the backscattering of the electrons by the impurity. This approximation is valid because the momentum transfer $\Delta k\sim(m/\hbar^2k_F)(\epsilon'-\epsilon)$, with m being the electron mass, is small for inelastic forward scattering. Such scattering processes only account for a small fraction of the transition rate given roughly by $|\langle\epsilon'|e^{i\Delta kX}|\epsilon\rangle|^2/|\langle\epsilon'|e^{2ik_FX}|\epsilon\rangle|^2$ multiplied by the ratio $|V(\Delta k)|^2/|V(2k_F)|^2$. Expanding the exponentials in this expression to the linear term in X, we have $|\langle\epsilon'|e^{i\Delta kX}|\epsilon\rangle|^2/|\langle\epsilon'|e^{2ik_FX}|\epsilon\rangle|^2\simeq(\Delta k/2k_F)^2=\frac{1}{16}[(\epsilon'-\epsilon)/E_F]^2$. In the present problem, we expect this ratio to be exceedingly small.[22] Therefore as long as the ratio $|V(\Delta k)|^2/|V(2k_F)|^2$ is not anomalously large (which is true for a screened potential in a metallic system), the inelastic forward scattering contributions to the transition rate can always be neglected.

After the integration over E and E', Eq. (8) gives

$$W(\epsilon',\epsilon)=\frac{1}{2\pi\hbar}|r|^2|\langle\epsilon'|e^{2ik_FX}|\epsilon\rangle|^2[\beta_e^{-1}(eV+\epsilon-\epsilon')+\beta_e^{-1}(eV-\epsilon+\epsilon')+(\epsilon-\epsilon')] \tag{9}$$

whose derivation can be found in the Appendix and is valid for $\beta^{-1}\ll E_F$. The function β_e appearing in Eq. (9) is defined by

$$\beta_e(x)=\beta\frac{\tanh(\beta x/2)}{(\beta x/2)} . \tag{10}$$

In the next section, we will show the physical significance of this function. Equation (6) together with the transition rate given by Eqs. (9) and (10) is the basic result of this section.

III. LOCAL HEATING DUE TO ELECTRON CURRENT

Before going into detailed calculations based on Eq. (6), we mention here that the blocking effect due to the Pauli exclusion principle as treated in our previous work on mesoscopic conductance[6] is also present for the present problem, and the effect becomes apparent when the reservoir temperature and the applied bias are low. Then, as we discuss in Ref. 6, the frozen Fermi distribution given by the reservoirs sets a restriction on the electron final states, and excitations of the impurity will take place only when the offset in chemical potential between the reservoirs is larger than the electron energy loss. To see this effect on the transition rate of the impurity, we look at Eq. (9), which as $\beta^{-1}\to0$ becomes

$$W(\epsilon',\epsilon)=\frac{1}{2\pi\hbar}|r|^2|\langle\epsilon'|e^{2ik_FX}|\epsilon\rangle|^2\times\{\tfrac{1}{2}|eV+\epsilon-\epsilon'|+\tfrac{1}{2}|eV-\epsilon+\epsilon'|+(\epsilon-\epsilon')\} , \tag{11}$$

where we have used the property $\beta_e^{-1}(x)=|x|/2$ as $\beta^{-1}\to0$. For impurity excitation, $\epsilon'-\epsilon>0$, and we have

$$W(\epsilon',\epsilon)=\frac{1}{2\pi\hbar}|r|^2|\langle\epsilon'|e^{2ik_FX}|\epsilon\rangle|^2(|eV|-\epsilon'+\epsilon)\times\theta(|eV|-\epsilon'+\epsilon) , \tag{12}$$

where θ is the step function given by $\theta(x)=1$ when $x>0$, and $\theta(x)=0$ otherwise. Clearly, as $\beta^{-1}\to0$, it is necessary that $|eV|>\epsilon'-\epsilon$ for the impurity to obtain energy from the electrons, while impurity excitation is blocked when $|eV|<\epsilon'-\epsilon$. For finite temperatures, the edge of the step function in Eq. (12) is softened, and it has a finite width given by β^{-1}.

In our subsequent calculations, we consider the situation when the effect of Pauli blocking is unimportant and thus the excitation of the impurity by the electrons is fully realized. This happens in the high-bias limit in which $|eV|\gg\delta\epsilon$, where $\delta\epsilon$ is the probable step size of energy transfer.[22] Since local heating is expected to occur when the current density at the impurity is high, using the high-bias limit to obtain a steady-state solution to the master equation (6) is relevant. In the high-bias, high-temperature regime which we will discuss later, we can treat ϵ as a continuous variable and expand the right-hand side of Eq. (6) [with the transition rate given by Eq. (9)] as a series in terms of the moments of energy transfer $\sum_{\epsilon'}|\langle\epsilon'|e^{2ik_FX}|\epsilon\rangle|^2(\epsilon'-\epsilon)^n$ up to $n=2$. After shifting the energy variable $\epsilon\to\epsilon-R/2$, we obtain

$$\frac{\partial P}{\partial t}=\frac{1}{\tau_e}\left[\frac{1}{\beta_e}\frac{\partial P}{\partial\epsilon}+P\right]+\frac{1}{\tau_e}\epsilon\left[\frac{1}{\beta_e}\frac{\partial^2P}{\partial\epsilon^2}+\frac{\partial P}{\partial\epsilon}\right] , \tag{13}$$

where $1/\tau_e=(R/\pi\hbar)|r|^2$, $\beta_e=\beta_e(eV)$, and $R=(2\hbar k_F)^2/2M$, with M being the mass of the impurity. The quantity R is the recoil energy of the impurity for electron backscattering at the Fermi level. In deriving Eq. (13), we have used the following identities which concern the probable range of energy transfer:

$$\sum_{\epsilon'}|\langle\epsilon'|e^{2ik_FX}|\epsilon\rangle|^2(\epsilon'-\epsilon)=R \tag{14}$$

and

$$\sum_{\epsilon'}|\langle\epsilon'|e^{2ik_FX}|\epsilon\rangle|^2(\epsilon'-\epsilon)^2=R^2+2\epsilon R . \tag{15}$$

Equation (13) is a Fokker-Planck equation.[20] The normalized steady-state solution to this equation is given by $P=\beta_e e^{-\beta_e\epsilon}$, which makes both terms on the right-hand side of the equation vanish. The error in the steady-state solution comes from neglecting higher-order terms in $\beta_e(eV)(\epsilon'-\epsilon)$ and $(\epsilon'-\epsilon)/eV$ in the expansions of $P(\epsilon',t)$ and $[\beta_e(eV+\epsilon-\epsilon')+\beta_e(eV-\epsilon+\epsilon')]$ appearing in Eq. (9).

The quantity $\beta_e^{-1}=\beta_e^{-1}(eV)$ is free from dynamical de-

tails of the electron-impurity scattering, and it has the statistical property of a thermodynamical temperature. The steady-state solution $P=\beta_e e^{-\beta_e \epsilon}$ represents local heating of the impurity to an effective electron temperature β_e^{-1}. We notice that the appearance of $\beta_e^{-1}(eV)$ in our formulation comes from the difference in electron chemical potential between the initial and final states in electron inelastic backscattering. In Fig. 1, β_e^{-1} is plotted as a function of eV (solid curve), with the reservoir temperature at 100 K. As $V\rightarrow 0$, the system is at equilibrium and $\beta_e^{-1}=\beta^{-1}$. For very large voltages, $\beta_e^{-1}=|eV|/2$. The curve is symmetrical about $V=0$, and it is quadratic in V when V is small, linear for larger V. The shape of the β_e^{-1} curve is qualitatively similar to that obtained numerically by Ralls, Ralph, and Buhrman.[14]

We now assume that at $t=0$, just before the electron current is turned on, the impurity atom is in thermal equilibrium, such that

$$P(\epsilon,0)=\beta e^{-\beta\epsilon} , \tag{16}$$

where β in front of the exponential acts as a normalization factor. For the subsequent result to be valid, we restrict our calculation to the high-temperature limit where $\beta^{-1}\gg\delta\epsilon$. With Eq. (16) as the initial condition, we find by direct substitution that the exact solution to Eq. (13) is

$$P(\epsilon,t)=\beta_t e^{-\beta_t\epsilon} , \tag{17}$$

with

$$\beta_t^{-1}=\beta_e^{-1}-(\beta_e^{-1}-\beta^{-1})e^{-t/\tau_e} , \tag{18}$$

where the subscript t in β_t denotes the time variable. Equation (17) together with Eq. (18) gives the solution to the master equation with initial condition Eq. (16) in the high-temperature limit. From Eq. (18) we obtain the relaxation equation for the impurity temperature:

$$\dot{\beta}_t^{-1}=-\frac{\beta_t^{-1}-\beta_e^{-1}}{\tau_e} \tag{19}$$

Clearly, $\tau_e^{-1}=(R/\pi\hbar)|r|^2$ is a relaxation rate characterizing the electron-impurity scattering.

We now generalize our calculation to the case where there is an elastic potential barrier in the mesoscopic system, and the impurity atom is seen as an additional weak scatterer outside the barrier. The elastic scattering of electrons by the static barrier is treated exactly, and the interaction of the electrons with the impurity atom is taken to be a perturbation. Then, Eq. (2) in Sec. II is taken to be the average occupation of the electron-scattering states due to the static barrier, with k as the asymptotic momentum of the incident plane wave. The perturbation H_1 given by Eq. (3) is replaced by the interaction between the impurity atom and the electrons in the elastic scattering states due to the barrier. In the high-bias, high-temperature limit, we again arrive at Eq. (17) with a new relaxation equation for the impurity temperature:

$$\dot{\beta}_t^{-1}=-\frac{\beta_t^{-1}-\beta_e^{-1}}{\tau_e}-\frac{\beta_t^{-1}-\beta^{-1}}{\tau_e'} , \tag{20}$$

where $1/\tau_e=(R/\pi\hbar)|r|^2|t_0|^2$ and $1/\tau_e'=(R/\pi\hbar)|r|^2(1-|t_0|^2)[1-\cos(4k_F X_0+\alpha)]$. In these expressions $|t_0|^2$ is the transmission coefficient of the static barrier, X_0 is the equilibrium position of the impurity atom relative to the barrier, and the phase angle α is given by the structure of the barrier potential. The definitions of other quantities in τ_e and τ_e' remain the same. To obtain Eq. (20), we neglect the inelastic forward scattering of the asymptotic plane waves by the impurity in calculating $W(\epsilon',\epsilon)$, and we also assume that the amplitude of the impurity oscillation X is small compared to k_F^{-1}, so that $\sin 2k_F X\simeq 2k_F X$. When $|t_0|^2=1$, Eq. (20) reduces to Eq. (19). In the extreme case where $|t_0|^2=0$, the two reservoirs are isolated from each other, and the impurity relaxes toward the equilibrium temperature β^{-1}. The cosine function in the relaxation rate $1/\tau_e'$ reflects the interference of the scattered waves by the potential barrier and the impurity. In general, the steady-state temperature, given by $(\tau_e\beta^{-1}+\tau_e'\beta_e^{-1})/(\tau_e+\tau_e')$, also depends on the position of the impurity through τ_e'. Note that the presence of a static potential barrier lowers the steady-state temperature of the impurity due to reduced transmission of electrons in the mesoscopic system.

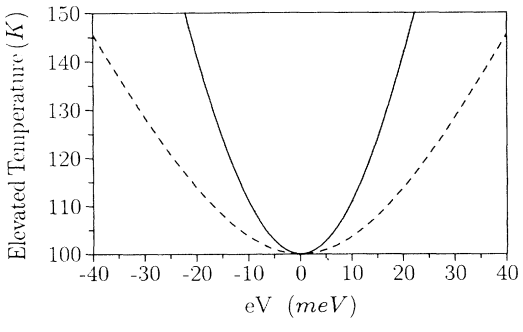

FIG. 1. Effective temperatures due to local heating. The solid curve is the effective temperature of nonequilibrium electrons (β_e^{-1}). The dashed curve is the defect temperature (β_d^{-1}) in the presence of a phonon bath. The lattice is at 100 K.

IV. EFFECT OF PHONON BATH

We now turn our attention to the effect of a phonon bath. In general, both nonequilibrium electrons and phonons are coupled to the impurity, and local heating by electrons occurs when the phonon coupling is relatively weak. As an example, we consider an interaction between the impurity and the phonons in the simple form

$$\sum_k g_k(a_k b^\dagger+b a_k^\dagger),$$

where g_k is the coupling constant between the impurity and the lattice, $b^\dagger=[\sqrt{(M\Omega/2\hbar)}X-(1/\sqrt{2M\hbar\Omega})(d/dX)]$ and $b=[\sqrt{(M\Omega/2\hbar)}X+(1/\sqrt{2M\hbar\Omega})(d/dX)]$ are the creation and annihilation operators for impurity oscillation with frequency Ω, and $a_k^\dagger, a_k$ are the creation and annihilation operators for a lattice phonon with wave vector k. The phonon distribution is given by

$$n(\omega_k)=\langle a_k^\dagger a_k\rangle=\frac{1}{e^{\beta\hbar\omega_k}-1}\ , \tag{21}$$

where $\langle\ \rangle$ denotes the ensemble average, ω_k is the frequency for lattice mode k, and β is the inverse lattice temperature which is taken to be the same as the inverse temperature of the electron reservoirs. In the first-order Born approximation, the transition rate of the impurity due to phonon scattering is given by

$$W(\epsilon',\epsilon)=\frac{2\pi}{\hbar}|\langle\epsilon'|b^\dagger|\epsilon\rangle|^2\,|g(\Omega)|^2\Gamma(\Omega)n(\Omega)+\frac{2\pi}{\hbar}|\langle\epsilon'|b|\epsilon\rangle|^2\,|g(\Omega)|^2\Gamma(\Omega)[n(\Omega)+1]\ , \tag{22}$$

where $\Gamma(\Omega)$ is the phonon density of states at $\omega_k=\Omega$, and $|g(\Omega)|^2$ is $|g_k|^2$ averaged over all orientations in k space at $\omega_k=\Omega$.

For a weakly bound impurity, Ω lies within the spectrum of ω_k, and the impurity forms a resonant mode[23] with a decay rate given by Eq. (22). When Ω lies outside the range of ω_k, $W(\epsilon',\epsilon)=0$, and the impurity gives rise to a localized mode whose lifetime can be calculated provided that there is anharmonic coupling between the impurity and the lattice.[24] In the present work, we consider the case where the impurity is weakly bound and forms a resonant mode. For simplicity we also assume that $\hbar\Omega$ is small in comparison with the experimental temperature β^{-1}.

We consider a single impurity coupled to electrons and phonons in the absence of any additional static potential barrier. To obtain a differential equation for P, we substitute the transition rates due to electron and phonon scattering, Eqs. (9) and (22), into Eq. (6), and expand the probability distribution $P(\epsilon',t)$ to second order in $(\epsilon'-\epsilon)$ for the phonon terms.[25] Repeating the previous operations for electron scattering, after shifting the origin for ϵ we obtain

$$\frac{\partial P}{\partial t}=\frac{1}{\tau_e}\left[\frac{1}{\beta_e}\frac{\partial P}{\partial\epsilon}+P\right]+\frac{1}{\tau_e}\epsilon\left[\frac{1}{\beta_e}\frac{\partial^2 P}{\partial\epsilon^2}+\frac{\partial P}{\partial\epsilon}\right]+\frac{1}{\tau_p}\left[\frac{1}{\beta}\frac{\partial P}{\partial\epsilon}+P\right]+\frac{1}{\tau_p}\epsilon\left[\frac{1}{\beta}\frac{\partial^2 P}{\partial\epsilon^2}+\frac{\partial P}{\partial\epsilon}\right]\ , \tag{23}$$

where $1/\tau_p=(2\pi/\hbar)|g(\Omega)|^2\Gamma(\Omega)$. For the initial condition given by Eq. (16), the solution to Eq. (23) is

$$P(\epsilon,t)=\beta_t e^{-\beta_t\epsilon}\ , \tag{24}$$

with

$$\beta_t^{-1}=\beta_d^{-1}-(\beta_d^{-1}-\beta^{-1})e^{-t/\tau}\ , \tag{25}$$

where $\beta_d^{-1}=(\tau_e\beta^{-1}+\tau_p\beta_e^{-1})/(\tau_e+\tau_p)$, $\tau^{-1}=\tau_e^{-1}+\tau_p^{-1}$. From Eq. (25),

$$\dot\beta_t^{-1}=-\frac{\beta_t^{-1}-\beta_d^{-1}}{\tau}=-\frac{\beta_t^{-1}-\beta_e^{-1}}{\tau_e}-\frac{\beta_t^{-1}-\beta^{-1}}{\tau_p}\ . \tag{26}$$

Equation (26) shows that the impurity-phonon coupling provides an additional relaxation term for the impurity's thermal energy. Local heating takes place as the impurity relaxes toward a weighted defect temperature β_d^{-1} at a rate given by τ^{-1}. The dotted curve in Fig. 1 shows β_d^{-1} as a function of eV, with $\tau_p/\tau_e=0.5$. We see that the defect temperature is lower than the effective electron temperature, due to coupling to a phonon bath.

We remark that the effect of a static potential barrier can be readily included in our analysis by following the procedure leading to Eq. (20). The result is an additional term $-(\beta_t^{-1}-\beta^{-1})/\tau_e'$ to the relaxation equation (26) for β_t^{-1}, with a modified value of τ_e as in Eq. (20).

In this analysis of the effect of a phonon bath, we have considered the interaction of phonons only with the impurity. There is, of course, interaction between phonons and electrons, and this will cause the incoming and outgoing electrons to have a finite lifetime. For mesoscopic systems, however, this lifetime is considerably larger than the time taken by the electrons to traverse the system. Hence, the electron-phonon interaction does not play a major role in the local heating of an impurity by the electron gas.

V. THREE-DIMENSIONAL CASE

To generalize our calculation to a 3D mesoscopic system, we consider a point-contact structure with transverse dimensions very large in comparison with the Fermi wavelength of the electrons. The impurity is taken to be an isotropic harmonic oscillator with mass M and angular frequency Ω located at the center of the microstructure, and interacting with the electrons through a contact potential (given by a δ function). In this case, an incident electron state can be specified by the momentum, with the z component taken along the direction of the mesoscopic channel. According to the reservoir picture, the distribution of the incident electrons is given by

$$\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}}\rangle=\begin{cases}f(E_{\mathbf{k}}-\frac{1}{2}eV), & k_z>0\\ f(E_{\mathbf{k}}+\frac{1}{2}eV), & k_z<0\ ,\end{cases} \tag{27}$$

where $\langle\ \rangle$ denotes an ensemble average over the internal states of the reservoirs, and $c_{\mathbf{k}}^\dagger, c_{\mathbf{k}}$ are the creation and annihilation operators for an electron with momentum $\mathbf{k}$.

Along the lines presented in Sec. II for the 1D case, we obtain a master equation for the impurity distribution $P(\epsilon_i)$, with ϵ_i being the energy of the impurity at state $|i\rangle$:

$$\frac{\partial P(\epsilon_i)}{\partial t}=-\sum_f[W(f,i)P(\epsilon_i)-W(i,f)P(\epsilon_f)]\ . \tag{28}$$

As an approximation, we take the impurity distribution as a function of the impurity energy only. Thus we exclude from our calculation the possible dependence of the distribution function on other quantum numbers of the impurity, and this enables us to concentrate on the local-heating aspect of the electron-impurity collisions.

The transition rate $W(f,i)$ is obtained from the first-order golden-rule calculation. Since $W(f,i)$ contains Fermi distribution factors similar to those appearing in Eq. (8) which are appreciable only around the Fermi energy, we replace the electron density of states per unit volume by its Fermi-level value $g(E_F)$, and replace the magnitude of the electron momentum appearing in the exponential [see Eqs. (29) and (30)] by the Fermi momentum k_F. We have $W(f,i)=W_0(f,i)+\delta W(f,i)$, where

$$W_0(f,i)=\frac{1}{(4\pi)^2}g(E_F)\sigma v_F \times \int d\Omega \int d\Omega' |\langle f|e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{X}}|i\rangle|^2 \times \left[\beta_e^{-1}(\epsilon_i-\epsilon_f)+\frac{(\epsilon_i-\epsilon_f)}{2}\right] \quad (29)$$

and

$$\delta W(f,i)=\frac{1}{(4\pi)^2}g(E_F)\sigma v_F \int d\Omega \int d\Omega' |\langle f|e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{X}}|i\rangle|^2 \times [\beta_e^{-1}(\epsilon_i-\epsilon_f+eV)+\beta_e^{-1}(\epsilon_i-\epsilon_f-eV)-2\beta_e^{-1}(\epsilon_i-\epsilon_f)] . \quad (30)$$

Due to approximations for performing integrations over the electron energy [see Eqs. (A4) and (A5) in the Appendix], Eqs. (29) and (30) are valid when $\beta^{-1}\ll E_F$. In Eqs. (29) and (30), β_e is the function given by Eq. (10) of Sec. II, v_F is the Fermi velocity, σ is the total cross section for the electron-impurity elastic scattering, and $\mathbf{X}$ is the impurity's coordinate relative to the equilibrium position. The integrations are carried out over solid angles Ω,Ω' in momentum space; in Eq. (29), Ω and Ω' are defined for the full 4π solid angle, and in Eq. (30) they take values for solid angles with $k_z>0$ and $k_z<0$, respectively.

In the high-bias, high-temperature regime as discussed in the 1D case, we can write the master equation (28) as a differential equation through series expansion in terms of the change of impurity energy up to second order. Since the distribution function is a function of impurity energy only, we can take an average of the result of the expansion over all impurity states $|i\rangle$ with $\epsilon_i=\epsilon$. After performing the integration over solid angles, we obtain

$$\frac{\partial P}{\partial t}=\frac{3}{\tau_e}\left[\frac{1}{\beta_e'}\frac{\partial P}{\partial \epsilon}+P\right]+\frac{1}{\tau_e}(\epsilon+R)\left[\frac{1}{\beta_e'}\frac{\partial^2 P}{\partial \epsilon^2}+\frac{\partial P}{\partial \epsilon}\right] +\frac{R}{16\tau_e}(\beta_e^{-1}-\beta^{-1})\frac{\partial^2 P}{\partial \epsilon^2} , \quad (31)$$

where $\beta_e'^{-1}=(5\beta_e^{-1}+3\beta^{-1})/8$, with $\beta_e=\beta_e(eV)$, and $\tau_e^{-1}=\frac{1}{6}g(E_F)\sigma v_F R$, with $R=(2\hbar k_F)^2/2M$. Since in most cases we are interested in the excited states of the impurity with $\epsilon\gg R$, the last term on the right-hand side of Eq. (31) is neglected. Making the transformation $\epsilon\rightarrow\epsilon-R$, we obtain

$$\frac{\partial P}{\partial t}=\frac{3}{\tau_e}\left[\frac{1}{\beta_e'}\frac{\partial P}{\partial \epsilon}+P\right]+\frac{\epsilon}{\tau_e}\left[\frac{1}{\beta_e'}\frac{\partial^2 P}{\partial \epsilon^2}+\frac{\partial P}{\partial \epsilon}\right] . \quad (32)$$

For the impurity which is treated as a three-dimensional harmonic oscillator, the density of states is proportional to $\epsilon^2/2$. For convenience, we can choose the density of states to be $\epsilon^2/2$. The normalized distribution function at time $t=0$, when the impurity is in equilibrium with the lattice, is then

$$P(\epsilon,0)=\beta^3 e^{-\beta\epsilon} . \quad (33)$$

With Eq. (33) as the initial condition, the solution to the differential equation (32) is

$$P(\epsilon,t)=\beta_t^3 e^{-\beta_t\epsilon} , \quad (34)$$

where

$$\beta_t^{-1}=\beta_e'^{-1}-(\beta_e'^{-1}-\beta^{-1})e^{-t/\tau_e} , \quad (35)$$

from which we have

$$\dot{\beta}_t^{-1}=-\frac{\beta_t^{-1}-\beta_e'^{-1}}{\tau_e} . \quad (36)$$

A significant difference between 3D and 1D systems with a single inelastic scatterer is that in the 3D case electrons not only act as the agent for local heating but also act as a dissipative thermal bath. This is because, in the 3D as opposed to the 1D case, the inelastic scattering of electrons is not confined to backscattering; forward-angle scattering is responsible for impurity relaxation toward the common reservoir temperature β^{-1} through the usual electron-hole-pair creation mechanism. The effective electron temperature $\beta_e'^{-1}=(5\beta_e^{-1}+3\beta^{-1})/8$ in Eq. (36) includes the effect of nonequilibrium local heating (the β_e^{-1} term) as well as electron-hole-pair-mediated relaxation toward the equilibrium temperature β^{-1}.

We now consider an impurity-phonon interaction of the form $\sum_{\alpha=x,y,z}\sum_{\mathbf{k}} g_{\alpha\mathbf{k}}(a_{\mathbf{k}}^\dagger b_\alpha+b_\alpha^\dagger a_{\mathbf{k}})$, where $a_{\mathbf{k}}^\dagger$ and $a_{\mathbf{k}}$ are the creation and annihilation operators for the lattice phonons, $b_\alpha^\dagger$ and b_α are the creation and annihilation operators for the α component of the impurity oscillation. In the high-temperature limit for which $\beta^{-1}\gg\hbar\Omega$, we can follow the procedure in Sec. III for the 1D case. We then find that the phonon bath contributes an additional term to Eq. (36), which becomes

$$\dot{\beta}_t^{-1}=-\frac{\beta_t^{-1}-\beta_e'^{-1}}{\tau_e}-\frac{\beta_t^{-1}-\beta^{-1}}{\tau_p} , \quad (37)$$

with $\tau_p^{-1}=(2\pi/\hbar)\Gamma(\Omega)|g(\Omega)|^2$, where $|g(\Omega)|^2$ is $|g_{\alpha\mathbf{k}}|^2$ averaged over the 4π solid angle in $\mathbf{k}$ space and is independent of α, and $\Gamma(\Omega)$ is the phonon density of states at the impurity frequency Ω.

The impurity thus follows a Boltzmann distribution,

with the time-dependent temperature given by Eq. (37). This generalizes our calculation in Secs. III and IV to a 3D case.

VI. DISCUSSION

We now discuss our results in the light of previous work. For the electron-impurity interaction part, the present work agrees with the steady-state numerical calculation of Ref. 14 in that the nonequilibrium electrons from the shifted Fermi distribution of Eqs. (2) and (27) provide a thermal interface to the impurity with an effective temperature higher than the reservoir temperature β^{-1}. Notable in our derivation are the explicit expressions for the effective electron temperature and for the relevant relaxation times associated with local heating. In the presence of a phonon bath, we are able to incorporate the effect of impurity-phonon coupling into the same framework as for the electrons, and thereby arrive at relations (26) and (37) as suggested by the experimental result of Ref. 14.

When a current driven by the chemical potential difference eV flows across a mesoscopic system, the effective temperature of the electrons is a fraction of eV on the energy scale. For applied voltages from 10 to 1000 mV, the temperature ranges from 10 to 10^3 K. For a quasiclassical metallic point-contact structure, $\tau_e^{-1} \simeq 10^{10}$ s^{-1} for an electron-impurity cross section $\sigma = 1$ Å^2. Therefore, local heating is effectively an instantaneous process, and is capable of ripping an isolated impurity atom out of its potential well in a very short time. A limitation to such a dramatic effect is due to the impurity-phonon coupling, characterized by the relaxation rate τ_p^{-1}. For strong impurity-phonon coupling, $\tau_p^{-1} \gg \tau_e^{-1}$, and local heating will be insignificant. On the other hand, when τ_p^{-1} is smaller than or comparable to τ_e^{-1}, local heating is significant, and one expects to see local-heating-assisted electromigration at high sample biases. In Ref. 14, τ_p^{-1} is found experimentally to be comparable to or slightly smaller than τ_e^{-1}, and indeed electromigration resulting in permanent sample resistance change has been deduced from experiment.[14]

The present paper can be considered as a complement to our previous work concerning inelasticity in mesoscopic systems.[6] There, starting from the same model, we investigated the effect of inelastic electron-impurity scattering on the transport properties of electrons. Although the nonlinearity found in our previous work is essentially due to energy transfer from the electrons to the impurity, we assumed that the impurity was in constant thermal contact with the lattice and that the impurity was at the equilibrium lattice temperature. In the present work, we deal with the problem of inelasticity with an emphasis on the behavior of the scatterer itself. However, our previous results concerning electron transport can be generalized by replacing the impurity temperature by the elevated temperature due to local heating.

To summarize, we have obtained a solution to the master equation for a single impurity subject to electron and phonon scattering in mesoscopic systems. In the case of high bias and high lattice temperature, we are able to show that the impurity follows a Boltzmann distribution with a time-dependent temperature relaxing toward the steady-state local temperature. Hence, in this case local heating and time-dependent temperature are concepts having thermodynamic justification.

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APPENDIX

We derive Eq. (9) from Eq. (8). From Eq. (8), we have

$$W(\epsilon',\epsilon)=\frac{2\pi}{\hbar}|r|^2\int_0^\infty dE\int_0^\infty dE'|\langle\epsilon'|e^{2ik_FX}|\epsilon\rangle|^2\,\delta(E-E'+\epsilon-\epsilon')$$
$$\times\{f(E-\tfrac{1}{2}eV)[1-f(E'+\tfrac{1}{2}eV)]+f(E+\tfrac{1}{2}eV)[1-f(E'-\tfrac{1}{2}eV)]\}\ . \tag{A1}$$

Performing integration over E', we obtain

$$W(\epsilon',\epsilon)=\frac{1}{2\pi\hbar}|r|^2\,|\langle\epsilon'|e^{2ik_FX}|\epsilon\rangle|^2\int_0^\infty dE\{f(E-\tfrac{1}{2}eV)[1-f(E+\epsilon-\epsilon'+\tfrac{1}{2}eV)]+f(E+\tfrac{1}{2}eV)[1-f(E+\epsilon-\epsilon'-\tfrac{1}{2}eV)]\} \tag{A2}$$

for $\epsilon'-\epsilon<0$, and

$$W(\epsilon',\epsilon)=\frac{1}{2\pi\hbar}|r|^2|\langle\epsilon'|e^{2ik_FX}|\epsilon\rangle|^2\int_0^\infty dE\{f(E+\epsilon'-\epsilon-\tfrac{1}{2}eV)[1-f(E+\tfrac{1}{2}eV)]$$
$$+f(E+\epsilon'-\epsilon+\tfrac{1}{2}eV)[1-f(E-\tfrac{1}{2}eV)]\} \tag{A3}$$

for $\epsilon'-\epsilon>0$. To go further, we consider the integral

$$I=\int_0^\infty dx f(x+x_1)[1-f(x+x_2)] \tag{A4}$$

and define a new variable $y=e^{\beta x}$ and two constants $A=e^{\beta(x_1-E_F)}$, $B=e^{\beta(x_2-E_F)}$. The integral of Eq. (A4) becomes

$$I=\beta^{-1}\frac{B}{A-B}\int_1^\infty dy\left[\frac{1}{y+\frac{1}{A}}-\frac{1}{y+\frac{1}{B}}\right]$$

$$=\beta^{-1}\frac{B}{A-B}\left[\ln\left[\frac{A}{B}\right]+\ln\left[\frac{1+B}{1+A}\right]\right]$$

$$=\frac{x_1-x_2}{e^{\beta(x_1-x_2)}-1}-\beta^{-1}\frac{B}{A-B}\sum_{n=1}^{\infty}(-1)^{n+1}\frac{1}{n}(A^n-B^n)\ . \tag{A5}$$

We restrict ourselves to the case $\beta^{-1},|\epsilon'-\epsilon|\ll E_F$. Then, when Eq. (A5) is applied to Eqs. (A2) and (A3), the second term in the last equation of Eq. (A5) can be neglected. We obtain

$$W(\epsilon',\epsilon)=\frac{1}{2\pi\hbar}|r|^2|\langle\epsilon'|e^{i2k_FX}|\epsilon\rangle|^2\left[\frac{\epsilon'-\epsilon-eV}{e^{\beta(\epsilon'-\epsilon-eV)}-1}+\frac{\epsilon'-\epsilon+eV}{e^{\beta(\epsilon'-\epsilon+eV)}-1}\right]\ . \tag{A6}$$

Application of the identity $x/(e^x-1)=[(x/2)/\tanh(x/2)]-x/2$ to Eq. (A6) gives Eq. (9).

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