Scattering Approach to Backaction in Coherent Nanoelectromechanical Systems

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We present theoretical results for the backaction force noise and damping of a mechanical oscillator whose position is measured by a mesoscopic conductor. Our scattering approach is applicable to a wide class of systems; in particular, it may be used to describe point contact position detectors far from the weak tunneling limit. We find that the backaction depends not only on the mechanical modulation of transmission probabilities, but also on the modulation of scattering phases, even in the absence of a magnetic field. We illustrate our general approach with several simple examples, and use it to calculate the backaction for a movable, Au atomic point contact modeled by *ab initio* density functional theory.

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Quantum mechanics requires that any detector used to measure an object's position unavoidably exerts a backaction force, imposing a fundamental limit on continuous position detection [1,2]. Recent experiments with nanoelectromechanical systems (NEMS) have come remarkably close to realizing this limit by using quantum electronic conductors as position detectors of nanomechanical oscillators [3–5]. In these systems, position detection is achieved using the influence of the mechanics on the current through the conductor; thus, it is natural to associate backaction with the position sensitivity of the electron transmission probability. This is indeed the picture that emerges from theoretical studies in the limit of weak tunneling [6–8]; however, several recent experiments are far from this limit [5,9–11], and it is not clear that the weak tunneling results apply.

In this Letter, we study the backaction of a mesoscopic position detector using a general noninteracting scattering approach that is not limited to the weak tunneling limit. Scattering theory has been used extensively to study various aspects of mesoscopic conductors, and we adapt it here to study the backaction heating and damping of a mechanical oscillator coupled to a conductor. Surprisingly, we find that backaction arises not only from transmission probabilities, but also from the position sensitivity of scattering phases, and we present several simple but illustrative examples where the phases play a pronounced role. We emphasize that these phases may be important despite intact time reversal symmetry, which we assume throughout, unlike Aharanov-Bohm phases due to a magnetic field [8]. Finally, we apply our general results to calculate the backaction from an atomic point contact (APC) between Au electrodes, using a scattering matrix obtained from density functional theory (DFT).

Our approach significantly extends the seminal work of Yurke and Kochanski, who first considered force noise in a tunnel junction using a scattering approach [12]. Unlike their work, which is limited to particular scattering potentials, we rely only on general properties of the scattering matrix. As a result, we can describe a wide class of systems, including arbitrary scattering potentials, various forms of electromechanical coupling, and multichannel scatterers. Moreover, we calculate not only the backaction force noise, but also the backaction damping, which is important in experiments (e.g. it is the basis of backaction cooling [4]) and up to now has not been dealt with in the scattering approach.

Scattering approach.—We consider a two-terminal device consisting of a coherent scattering region coupled to left and right leads, each of which supports N transverse modes. Electrons are scattered by a potential $U(\vec{r}_e, x)$, where $\vec{r}_e = (x_e, y_e, z_e)$ is the electron position, and the potential depends on the position x of a mechanical oscillator. Incoming and outgoing waves are related by the scattering matrix $s(x)$, which depends on x through $U(\vec{r}_e, x)$. We will show that a knowledge of s and $\partial s/\partial x$ is sufficient to calculate the backaction.

For the usual experimental regime of weak electromechanical coupling, the change in the electronic potential due to small changes in x is generally linear and may be written $\mathcal{H}_{\rm int} = -x\hat{F}$, where the force on the oscillator is $\hat{F} = -\int d\vec{r}_e \hat{\rho}(\vec{r}_e)\partial U(\vec{r}_e, x)/\partial x$, and $\hat{\rho}(\vec{r}_e)$ is the electron density operator. By relating small and slow changes in the potential, $U(\vec{r}_e, x)$, to the parametric derivative of the scattering matrix [13–15], we can express $\hat{F}$ in the scattering state basis as

$$\hat{F} = \sum_{\alpha\beta} \int d\epsilon \int d\epsilon' \hat{a}^\dagger_\alpha(\epsilon) W_{\alpha\beta}(\epsilon, \epsilon')\hat{a}_\beta(\epsilon'), \tag{1}$$

where $\hat{a}_\alpha(\epsilon)$ destroys a scattering state of energy ϵ incident in the lead and transverse mode indexed by α, and

$$W(\epsilon, \epsilon) = \frac{1}{2\pi i}\left[s^\dagger(\epsilon, x)\frac{\partial s(\epsilon, x)}{\partial x}\right]_{x=0}. \tag{2}$$

We require only the diagonal-in-energy part of W since we focus on the zero frequency noise properties of $\hat{F}$; this is sufficient for the experimentally relevant case when the oscillator period is much longer than time scales in the conductor. Derivatives of the scattering matrix similar to Eq. (2) are familiar from studies of charge noise [16] and parametric pumping [17]. Here we use the parametric derivative with respect to x to calculate the backaction on the oscillator directly in terms of the scattering matrix, without the need for detailed knowledge of $U(\vec{r}_e, x)$ and $\hat{\rho}(\vec{r}_e)$ in the scattering region. In the following we work to lowest order in $\mathcal{H}_{\rm int}$, valid for weak coupling.

Fluctuations of the backaction force cause momentum diffusion and heating of the oscillator. Heating is determined by the classical, frequency-symmetric part of the backaction force noise, $\bar{S}_F[\omega] = (S_F[\omega] + S_F[-\omega])/2$, where the quantum noise spectral density is $S_F[\omega] = \int dt e^{i\omega t}\langle \hat{F}(t)\hat{F}(0)\rangle$ and averages are taken with respect to the uncoupled conductor [18]. These averages are easily taken using Eq. (1), and the backaction heating is directly determined by W. The zero frequency force noise is ($k_B = 1$, $\bar{S}_F \equiv \bar{S}_F[0]$)

$$\bar{S}_F = 2\pi\hbar \sum_{\alpha\beta} \int d\epsilon\, \mathrm{tr}\{W_{\alpha\beta}W_{\beta\alpha}\} f_\alpha (1 - f_\beta), \qquad (3)$$

where the trace is over transverse modes, assumed to be the same in both leads, and the matrixes $W_{\alpha\beta}$ are the $N \times N$ blocks of W in Eq. (2), which may be ϵ dependent. The Fermi functions are $f_\alpha = (1 + e^{(\epsilon-\mu_\alpha)/T_{\rm el}})^{-1}$, where μ_α is the chemical potential in lead α and $T_{\rm el}$ is the electronic temperature.

In addition to heating, the oscillator also experiences backaction damping as a result of energy exchange with the conductor. The damping rate is given by the quantum, asymmetric-in-frequency part of the force noise, $\gamma[\omega] = (S_F[\omega] - S_F[-\omega])/2M\hbar\omega$, where M is the oscillator mass. Taking the $\omega \to 0$ limit, we find

$$\gamma = \frac{2\pi\hbar}{M} \sum_{\alpha\beta} \int d\epsilon\, \mathrm{tr}\{W_{\alpha\beta}W_{\beta\alpha}\} f_\alpha \left(-\frac{\partial f_\beta}{\partial \epsilon}\right). \qquad (4)$$

By considering the ratio of $\bar{S}_F[\omega]$ to $\gamma[\omega]$, one can associate a frequency-dependent effective temperature $T_{\rm eff}[\omega]$ with the backaction; this amounts to using the standard fluctuation-dissipation relation to *define* the effective temperature at each frequency from the system's force noise and damping [2,6,18]. $T_{\rm eff}[\omega]$ characterizes the conductor as an effective thermal environment. In the $\omega \to 0$ limit, the relation is simply $T_{\rm eff} \equiv \bar{S}_F/2M\gamma$. If backaction dominates over intrinsic sources of dissipation, $T_{\rm eff}$ corresponds to the physical temperature of the oscillator.

Single channel.—We first consider the case of single-channel leads. For simplicity, we also focus on the limit of small applied bias, ignoring the possible energy dependence of s. We assume time reversal symmetry (i.e. no magnetic field), but allow for broken left-right inversion symmetry. In this case the scattering matrix may be parametrized as

$$s(\epsilon, x) = e^{i\phi}\begin{pmatrix} \sqrt{\mathcal{R}}e^{i\theta} & i\sqrt{\mathcal{T}} \\ i\sqrt{\mathcal{T}} & \sqrt{\mathcal{R}}e^{-i\theta} \end{pmatrix}, \qquad (5)$$

where $\mathcal{T}$ ($\mathcal{R} = 1 - \mathcal{T}$) is the transmission (reflection) probability, ϕ is the overall scattering phase, and θ parametrizes broken inversion symmetry; i.e. $\theta = 0$ for an inversion-symmetric conductor. In general, all of the scattering parameters depend on x through the potential, $U(\vec{r}_e, x)$.

Inserting Eq. (5) into Eq. (3) we obtain the symmetrized force noise for a single channel,

$$\bar{S}_F = \frac{\hbar}{2\pi}\frac{(\partial\mathcal{T}/\partial x)^2}{4\mathcal{R}\mathcal{T}} eV\left[(1 + \mathcal{R}\mathcal{T}\Delta_\theta)\coth\left(\frac{eV}{2T_{\rm el}}\right) + (\Delta_\phi + \mathcal{R}^2\Delta_\theta)\frac{2T_{\rm el}}{eV}\right], \qquad (6)$$

where V is the bias, and the phase terms enter as

$$\Delta_\zeta = 4\mathcal{R}\mathcal{T}\left(\frac{\partial\zeta/\partial x}{\partial\mathcal{T}/\partial x}\right)^2, \qquad (7)$$

for $\zeta = \phi, \theta$. In the limit $eV \gg T_{\rm el}$, the first term (independent of Δ_ϕ and Δ_θ) in Eq. (6) represents the expected, quantum-limited backaction of our position detector; it is simply the sensitivity of a position measurement made by monitoring the current, and reflects the fact that a stronger measurement leads to increased backaction. This term scales as the square of the measurement gain, $\chi_{IF} \propto \partial\mathcal{T}/\partial x$, and inversely with the shot noise in the current, $\bar{S}_I = e^2 V\mathcal{R}\mathcal{T}/2\pi\hbar$; in the limit $\mathcal{T} \ll 1$ it reproduces the well-known result obtained from a tunnel Hamiltonian calculation [6,7]. The second term in Eq. (6) is independent of $\partial\mathcal{T}/\partial x$ and is thus not directly related to a measurement of the current. Instead, it results from the oscillator's modulation of the phase θ. This phase contribution to $\bar{S}_F$ is proportional to $\mathcal{R}\mathcal{T}$ and thus vanishes when $\mathcal{T} \ll 1$. The remaining two terms ($\propto T_{\rm el}/eV$) are also independent of $\partial\mathcal{T}/\partial x$ and represent additional thermal noise at finite $T_{\rm el}/eV$.

The damping for a single channel is

$$\gamma = \frac{\hbar}{2\pi M}\frac{(\partial\mathcal{T}/\partial x)^2}{4\mathcal{R}\mathcal{T}}(1 + \Delta_\phi + \mathcal{R}\Delta_\theta). \qquad (8)$$

In the small bias limit, γ is strictly positive and independent of $T_{\rm el}$. Similar to $\bar{S}_F$, the first term in Eq. (8) is the backaction associated with a measurement of the current and reduces to the tunnel Hamiltonian result in the limit $\mathcal{T} \ll 1$. More interestingly, the second and third terms correspond to corrections due to scattering phases; unlike $\bar{S}_F$, these phase contributions to γ are present even for a symmetric detector and, as we will see, do not necessarily vanish in the weak tunneling limit. The overall phase ϕ is directly connected to the density of states in the scattering region via the Friedel sum rule [19]. An x-dependent ϕ implies that the mechanical oscillator can change the scattering-induced electronic density of states; this means that the total electronic free energy becomes x dependent, resulting in a force whose quantum noise contributes to damping.

Equations (6) and (8) show that the backaction properties of a general conductor cannot simply be extrapolated from the weak tunneling limit; scattering phases play a role in both the heating and damping of the oscillator. Further, the phases can have a dramatic influence on the effective backaction temperature $T_{\rm eff}$ of the detector. For a single channel, using Eqs. (6) and (8), in the limit $T_{\rm el} \ll eV$ we find

$$T_{\rm eff} = \frac{eV}{2}\left(\frac{1 + \mathcal{R}\mathcal{T}\Delta_\theta}{1 + \Delta_\phi + \mathcal{R}\Delta_\theta}\right). \tag{9}$$

If the mechanical motion does not modify the scattering phases, then we simply obtain the tunnel Hamiltonian result [6,7], $T_{\rm eff} = eV/2$, independent of $\mathcal{T}$. However, in the more general case including the backaction from scattering phases, $T_{\rm eff}$ is not solely determined by the voltage. The phase corrections always decrease the effective temperature; they arise from the diagonal elements of W, which correspond to transitions between scattering states in the same lead. At $T_{\rm el} = 0$ such transitions can only occur if an electron absorbs energy, because the scattering states in each lead are filled up to the Fermi level. Thus, phase corrections lead to increased absorption of energy from the oscillator, lowering $T_{\rm eff}$. Including a nonzero lead temperature $T_{\rm el}$, one finds that $T_{\rm eff}$ can be lowered to a minimum value of $T_{\rm el}$; as $T_{\rm el} \ll eV$, this could still be quite useful.

Square potential barrier.—To demonstrate that backaction from scattering phases plays a role even in the simplest scattering model, we calculate the backaction for a one-dimensional symmetric square barrier potential whose width depends on the oscillator position. The force noise for this model was first considered in Ref. [12]; our general method further provides γ and $T_{\rm eff}$ and allows us to identify the role of scattering phases. Incoming electrons of wave vector k and energy ϵ are scattered in one dimension by a square potential barrier of height U_0 and width $w = L + x$. The inverse decay length of the wave function under the barrier is $\kappa = \sqrt{2m_e(U_0 - E)}/\hbar$. It is straightforward to find $\mathcal{T}$ and ϕ as functions of U_0 and w, and $\theta = 0$ due to inversion symmetry. We obtain

$$\Delta_\phi = \left(1 + \frac{4k^2\kappa^2}{(k^2 - \kappa^2)^2\mathcal{T}}\right)^{-1}, \tag{10}$$

and the phase terms become important when $\mathcal{T} \sim 1$. For a high but narrow barrier ($U_0 \gg \epsilon$, $\kappa L \ll 1$), we find [via Eq. (9)] that $T_{\rm eff}$ may be reduced by up to a factor of 2 compared to the tunnel Hamiltonian result of $eV/2$. For a low barrier ($U_0 \ll \epsilon$), we find $T_{\rm eff} \to T_{\rm el}$.

Resonant level model.—We now apply our general results to a prototypical resonant level model (RLM), where a single electronic level of energy ϵ_d is connected to the left (right) lead via the tunneling rate Γ_L (Γ_R). If ϵ_d depends on the position of a mechanical oscillator [see Fig. 1(a)], one has the electromechanical analog of a dispersively coupled optomechanical system [20], and a simple model of quantum-dot–based NEMS studied in recent experiments [21,22]. Beginning from the scattering matrix for the RLM, $s_{\alpha\beta} = \delta_{\alpha\beta} - i\hbar\sqrt{\Gamma_\alpha\Gamma_\beta}/(\epsilon - \epsilon_d + i\hbar\Gamma/2)$, where $\Gamma = \Gamma_L + \Gamma_R$, and assuming linear coupling, we obtain $\gamma \propto (\Gamma/\Gamma_L\Gamma_R)^2\mathcal{T}^2$ [23]. We also find $\Delta_\phi = 1 + \mathcal{R}\Delta_\theta$, independent of the tunneling rates and the detuning of the incident electron energy ϵ from ϵ_d. Comparing with Eq. (8), this implies that the phases play a crucial role: the x dependence of the overall scattering phase ϕ always accounts for half of the damping, as seen in Fig. 1(b). Further, in the limit of asymmetric tunneling rates we find $\mathcal{R}\Delta_\theta \gg 1$, and the damping is almost entirely due to the combined ϕ and θ. Also striking is the cotunneling limit, where the detuning is large compared to the level broadening, i.e. $|\epsilon - \epsilon_d| \gg \hbar\Gamma$. In this limit tunneling is suppressed, $\mathcal{T} \ll 1$, and the level charge only fluctuates virtually; as a result, one might expect that the system is equivalent to a single junction in the weak tunneling limit, and that γ should be given by the tunnel Hamiltonian result, i.e., the first term in Eq. (8). However, this is not the case: due to phase corrections, the damping is *twice* the tunnel Hamiltonian result [see the inset of Fig. 1(b)]. This shows that the phases can play a role even when $\mathcal{T}$ is small. Note that backaction in this model was recently studied theoretically using a path integral approach [24,25], although backaction due to phases was not discussed.

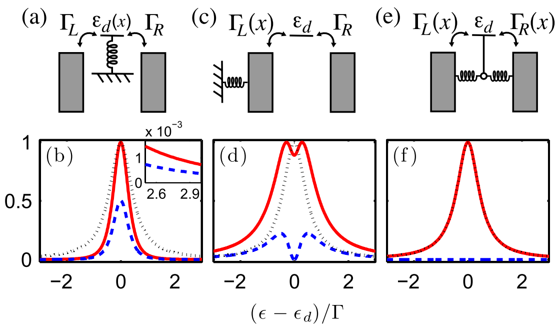

FIG. 1 (color online). Schematic setups and backaction damping for RLM with dispersive (a,b), dissipative (c,d), and shuttle (e,f) mechanical coupling. In all plots, the full backaction damping (red solid line) and the damping without phase corrections (blue dashed line) are shown, with $\mathcal{T}$ (black dotted line) also shown for reference. We took $\Gamma_L(0) = \Gamma_R(0)$.

Our general theory also allows us to consider variations of the above RLM, where the mechanical position modulates the tunneling rates Γ_L and Γ_R. This is the electromechanical analog of a dissipatively coupled optomechanical system [26], and could be achieved experimentally using a quantum dot coupled to two leads via tunnel junctions, with the tunneling rates modified by an on-board [5] or off-board [10] mechanical oscillator. First, we consider a setup where only the left tunneling rate is x dependent [see Figs. 1(c) and 1(d)]. In this case, interference between

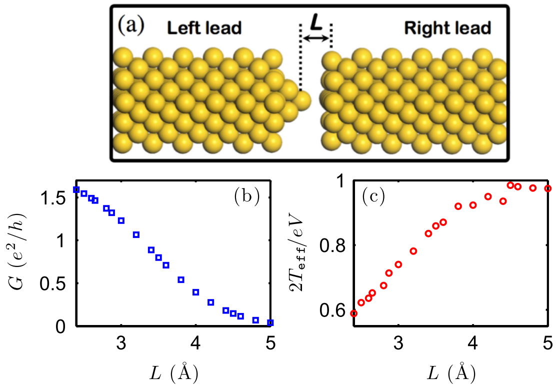

FIG. 2 (color online). (a) APC in a 5×5 atom Au (100) quantum wire. (b) Conductance through the APC versus gap size (for small L, several channels contribute to transport and G exceeds e^2/h [23]). (c) Effective backaction temperature versus gap size. For small L, $T_{\mathrm{eff}} < eV/2$ due to phase corrections. The Au-Au interatomic distance in bulk gold is 2.87 Å.

resonant charge fluctuations (on the level) and nonresonant charge fluctuations (in the leads) results in a Fano line shape and suppression of γ at zero detuning [23], similar to the optomechanical case [26]. Second, we consider mechanical coupling to both tunneling rates with opposite sign, corresponding to a quantum shuttle [see Figs. 1(e) and 1(f)]. Here we find $\gamma \propto (\Gamma/\Gamma_L\Gamma_R)^2\mathcal{T}$; moreover, all of the damping is due to the scattering phases, since (for $\Gamma_L = \Gamma_R$) the transmission has no linear dependence on x [23].

Atomistic model.—While the above examples show that phases contribute to backaction in simple model potentials, our approach allows us to investigate phase contributions in fully atomistic calculations of mesoscopic conductors. We demonstrate this by applying our theory to an APC using the scattering matrix obtained from DFT [27]. We model the APC as a single-atom constriction in a 5×5 atom Au quantum wire (see Fig. 2), and take x to modify the gap size of the APC to $L + x$. This geometry is motivated by recent experimental setups using an APC [5] or a scanning tunneling microscope [9] with one mechanically compliant electrode. We approximate the surface electrode of experiments by the flat 5×5 edge of the wire on the right; this is justified since the transport properties of the APC are expected to be dominated by the few atoms closest to the tip. We find 11 scattering channels contributing to transport, consistent with recent *ab initio* studies of similar Au wires [28]. After obtaining s and $\partial s/\partial x$ [23], we calculate the backaction using Eqs. (3) and (4), assuming $T_{\mathrm{el}} \ll eV$. We find that phase corrections are important when the APC transmission deviates from the weak tunneling limit; it leads to a significant reduction in T_{eff} from the tunnel Hamiltonian result of $eV/2$, as seen in Fig. 2. While transmission properties are often studied using DFT, an important feature of our calculation is our explicit use of the scattering phases obtained from an atomistic calculation of a quantum electronic device.

Conclusions.—We have presented a scattering approach to backaction in NEMS and demonstrated the importance of backaction from scattering phases. This work is particularly relevant to NEMS based on quantum or atomic point contacts which are often far from the weak tunneling limit. Our results may also be easily extended to describe strong electromechanical coupling in the low oscillator frequency limit, by making an adiabatic approximation such that the noise spectra of $\hat{F}$ effectively become x dependent [18].

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