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Phonon Effects on Electric and Thermal Properties in a Single Electron Transistor

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We investigate the effects on the transport characteristics of a single electron transistor caused by dynamic deformations of the device configuration due to phonons. We formulate the electron-phonon interaction that originates from changes in capacitances and tunnel resistances caused by the breathing and oblong vibrations of the island that forms part of the transistor. We derive transport properties by means of the master equation. For a single electron transistor with a gold nanoparticle island with a radius of 1 nm, we demonstrate the contribution to the transport properties that originates from tunneling channels associated with THz phonon emission and absorption.

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I. INTRODUCTION

In molecular devices, coupling between molecular vibrations and electron tunneling causes phonon-mediated electron transport channels, giving rise to characteristic I-V curves that reflect multi-phonon emission and absorption [1–3], where the coupling occurs in two possible ways [3]: electron tunneling induces internal vibrations owing to rearrangement of that atomic configuration, and the charged molecules are driven in the bias electric field. In contrast, electron transport characteristics that reflect multi-phonon emission and absorption are not expected in a metal-based single electron transistor (SET) because the elements of the device are stiff and atomic configuration changes are not expected.

We anticipate another electron-phonon interaction mechanism in SETs that will influence the I-V characteristics. Central to the operation of an SET is a metal island positioned between two electrodes. The gaps between the island and electrodes set the key electronic parameters for the device: the capacitances and tunnel resistances. Surface displacement of the island due to phonons will modify the gaps, which is expected to affect the current through the SET.

In this work, we explore the effects of gap modulation on the electron transport in the SET. In order to understand the character and magnitude of possible phonon effects, we model an SET containing a metal nanoparticle island between the source and the drain (Fig. 1). Considering an ideal case, we assume that the particle has an almost stress-free surface and will have relatively large amplitude surface vibrations due to phonons. Since only the breathing modes of spherical symmetry change the intrinsic capacitance of the

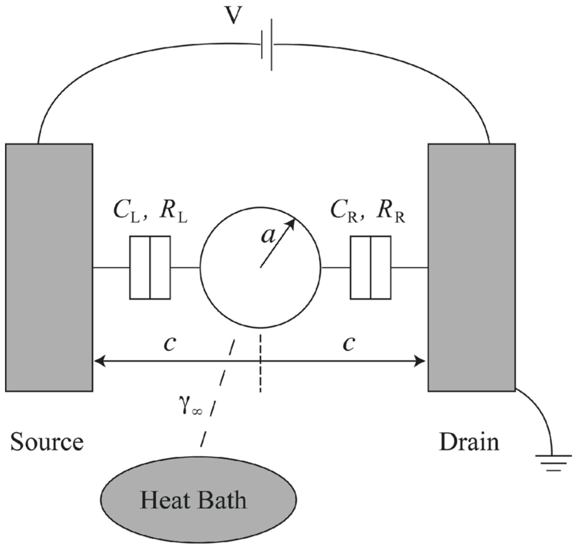

FIG. 1: Model of a SET. The metal nanoparticle is linked electrically to the source and drain, which are conducting planes. $C_{L(R)}$ and $R_{L(R)}$ are the capacitance and tunnel resistance between the particle and the left (right) electrode, respectively. a and c are the radius of the metal particle and the distance between the particle and the leads. The oval below the particle represents a heat bath.

island and the oblong modes modify tunnel resistances significantly more than other modes [4], we investigate the contributions of breathing and oblong mode phonons to the transport, respectively, as the representative cases.

The paper is planned as follows; In Sec. II, we describe the system to be studied in this work, and introduce the Hamiltonian of the system. The phonon-mediated tunneling is formulated in this section. In Sec. III, the density matrix and associated master equations are introduced. In Sec. IV, we give numerical results for the thermal and transport properties. Finally, Sec. V provides a discussion and summary of the work.

II. MODEL

We consider the island to be a spherical nanoparticle a in radius, firmly suspended centrally between the source and drain, which are assumed to be conducting planes (Fig.1). The electron transport is due to single electron tunneling between the island and the electrodes in the Coulomb blockade regime. The island is connected to a heat bath with a coupling strength γ_∞.

We first evaluate the change in the tunnel resistances and capacitances between the island and electrodes due to phonons. Supposing the island as an isotropically elastic sphere, the phonon modes in the island are derived by means of a scalar and two vector potentials. The normal phonons modes in the elastic sphere are spheroidal and toroidal modes [4], the former of which gives rise to surface vibrations of the sphere, but the latter does not.

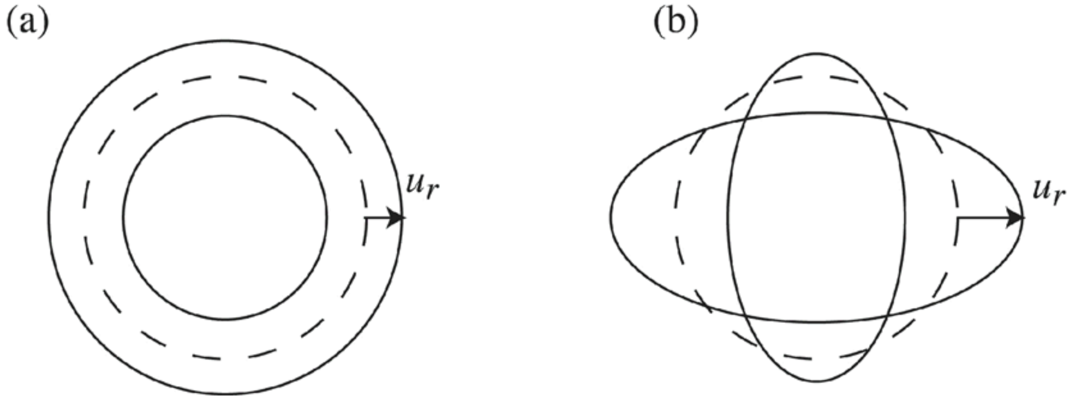

FIG. 2: The displacement of (a) the breathing mode and (b) the oblong mode. $u_r$indicates the surface displacement of the particle.

The spheroidal modes are classified into the breathing mode having the spherical symmetry for the displacement, the oblong mode showing ellipsoidal deformation, and others on the basis of the angular momentum of phonons. Although all the spheroidal modes can cause surface vibrations, in this work, we focus only on the breathing and oblong modes (Fig.2) since only the breathing modes of spherical symmetry change the intrinsic capacitance of the island and the oblong modes modify tunnel resistances significantly more than other modes [5], as mentioned in the previous section.

Expressing the surface displacement u_r for the breathing modes, the radius of the sphere modulated by phonons becomes $r = a + u_r$. We express the tunnel resistances that change exponentially with respect to the radius as

$$R_{L,R}(r) = R_{L,R}(a)e^{\frac{2(r-a)}{\lambda}}, \tag{1}$$

where λ is a characteristic length of tunneling.

The capacitance between a sphere and a conducting plane is evaluated by using a method of image charge [6] as

$$C_{\text{sphere}}(r) = 4\pi\varepsilon^*\varepsilon_0 r \left(1 + \alpha + \frac{\alpha^2}{1-\alpha^2} + \dots\right), \tag{2}$$

where $\alpha = r/2c$. Here, c is the distance between the center of the particle and the conducting plane, and then $\alpha < 1/2$. The total capacitance $C(r)$ of the SET comprises C_L and C_R, each of which is given by Eq.(2). Since the particle is positioned at the midpoint between the source and drain, $C_L = C_R$ and then the total capacitance becomes twice of Eq.(2) [7], i.e., $C(r) = 2C_{\text{sphere}}(r)$. For small displacement in comparison with radius, i.e., $|u_r| \ll a$, $C(r)$ is approximated as

$$\frac{1}{C(r)} \approx \left(1 - \beta\frac{u_r}{a}\right)\frac{1}{C_0}, \tag{3}$$

where $C_0 = C(a)$ and the factor β for the breathing mode is defined by $\beta_{\rm B} = 1 + a/2c$.

It is known that the intrinsic capacitance of a substance with finite volume is a minimum for a sphere [8]. Then the change in the intrinsic capacitance for the oblong modes depends on u_r^2, and the change in the capacitance is mainly due to the change in the gaps between the island and electrodes. Considering only the change in α in Eq.(2), for the oblong mode, we obtain $\beta_{\rm O} = a/2c$, where we suppose that the sphere is stretched toward the electrodes, and regard u_r as the surface displacement in the direction. The change in the tunnel resistance for the oblong mode is same as Eq.(1) because of the assumption. $\beta_{\rm O}$ is not only for the oblong modes but also common to all the spheroidal modes except for the breathing mode.

The surface displacement u_r toward the electrodes is expressed in a quantized form by

$$u_r = \kappa_K a(b_K + b_K^\dagger), \tag{4}$$

where $b_K$and $b_K^\dagger$ are the annihilation and creation operators, respectively, of breathing (K = B) and oblong mode phonons (K = O). In Eq.(4), κ_K is the ratio of the surface displacement to a, which is evaluated as $\kappa_{\rm B} = 2.33 \times 10^{-22} a^{-2}$ for the breathing mode at the fundamental frequency $\omega_{\rm B}$, and $\kappa_{\rm O} = 29.87 \times 10^{-22} a^{-2}$ for the oblong mode at the fundamental frequency $\omega_{\rm O}$ [5].

Here, we introduce the Hamiltonian of electrons and phonons in the island;

$$H_S = \sum_k (\varepsilon_{D,k} + \Delta\mu_D) c_{D,k}^\dagger c_{D,k} + E_C \left(\sum_k c_{D,k}^\dagger c_{D,k} \right)^2 - \eta_K^2 \frac{E_C^2}{\hbar\omega_K} \left(\sum_k c_{D,k}^\dagger c_{D,k} \right)^4$$
$$+ H_{phonon}, \tag{5}$$

where $E_C = e^2/2C_0$ and $\eta_K = \beta_K \kappa_K$. $c_{D,k}^\dagger$ and $c_{D,k}$ are the creation and annihilation operators of electrons in the island, and $\Delta\mu_D$ is the change in the chemical potential in the island due to the bias. H_{phonon} represents phonon energy in the island, including the breathing and oblong modes. The tunnel Hamiltonian $H_T$between the island and electrodes becomes

$$H_T = \sum_{k,k'} \left[t_L^0 c_{L,k}^\dagger c_{D,k'} B_K + t_L^{0*} B_K^\dagger c_{D,k'}^\dagger c_{L,k} + t_R^0 c_{R,k}^\dagger c_{D,k'} B_K + t_R^{0*} B_K^\dagger c_{D,k'}^\dagger c_{R,k} \right], \tag{6}$$

where $B_K = e^{z_1 b_K^\dagger - z_2 b_K}$,$z_1 = \eta_K \frac{E_C}{\hbar\omega_K} + \kappa_K \frac{a}{\lambda}$ and $z_2 = \eta_K \frac{E_C}{\hbar\omega_K} - \kappa_K \frac{a}{\lambda}$. $t_{L,R}^0$ is the tunnel coefficient.

III. MASTER EQUATION

In order to formulate transport properties such as current and conductance, we introduce a reduced density matrix defined by $\rho_{nn}^{mm}(t) = {\rm Tr}[\rho(t)]_{n,m}$, where $m(= m_K)$ is the number of breathing/oblong mode phonons in the island. Considering the case that only the two states with $n = 0$ and 1 are involved in transport, we derive equations of motion of ρ_{nn}^{mm} for each n. Using a von Neumann equation, the master equation yields

$$\dot{\rho}_{00}^{mm} = \sum_{m'} \Gamma_{00}^{mm'} \rho_{00}^{m'm'} + \sum_{m'} \Gamma_{01}^{mm'} \rho_{11}^{m'm'} \tag{7}$$

$$\dot{\rho}_{11}^{mm} = \sum_{m'} \Gamma_{10}^{mm'} \rho_{00}^{m'm'} + \sum_{m'} \Gamma_{11}^{mm'} \rho_{11}^{m'm'}. \tag{8}$$

The matrix elements are

$$\Gamma_{01}^{mm'} = \frac{1}{R_T e^2} \sum_{\alpha=L,R} \left|\left\langle m \left| B_K \right| m' \right\rangle\right|^2 F(-\Delta\mu_\alpha + E_C + \Delta\mu_D + (m'-m)\hbar\omega_K) \tag{9}$$

$$\Gamma_{10}^{mm'} = \frac{1}{R_T e^2} \sum_{\alpha=L,R} \left|\left\langle m' \left| B_K \right| m \right\rangle\right|^2 F(\Delta\mu_\alpha - E_C - \Delta\mu_D - (m-m')\hbar\omega_K) \tag{10}$$

$$\Gamma_{00}^{mm'} = -\delta_{m,m'} \sum_{m''} \Gamma_{10}^{m''m} - 2\gamma_\infty N(\omega_K)[(m+1)\delta_{m,m'} - m\delta_{m-1,m'}]$$

$$-2\gamma_\infty[N(\omega_K)+1][m\delta_{m,m'} - (m+1)\delta_{m+1,m'}] \tag{11}$$

$$\Gamma_{11}^{mm'} = -\delta_{m,m'} \sum_{m''} \Gamma_{01}^{m''m} - 2\gamma_\infty N(\omega_K)[(m+1)\delta_{m,m'} - m\delta_{m-1,m'}]$$

$$-2\gamma_\infty[N(\omega_K)+1][m\delta_{m,m'} - (m+1)\delta_{m+1,m'}], \tag{12}$$

where we put $R_T = R_L(a) = R_R(a)$ and $F(x) = x/(1 - e^{-x/k_B T})$. The changes in the chemical potentials are related to the bias voltage as follows; $\Delta\mu_L = eV, \Delta\mu_R = 0, \Delta\mu_D = eV/2$.

The Franck-Condon factor can be computed as

$$\left|\left\langle m \left| B \right| m' \right\rangle\right|^2 = e^{-z_1 z_2} z^{2|m-m'|} \frac{p!}{q!} \left[L_p^{|m-m'|}(z_1 z_2)\right]^2, \tag{13}$$

where$z = z_1\Theta(m-m') - z_2\Theta(m'-m)$, $p = \min(m, m')$ and $q = \max(m, m')$, and $L_p^{|m-m'|}$ is the associated Laguerre polynomial. The diagonal elements of Eq.(13) decay from unity as the product $z_1 z_2$increases from 0. On the other hand, the off-diagonal elements related to tunneling associated with multi-phonon emission or absorption increase.

Equations (7) and (8) comprise the terms of electron tunneling with or without phonon mediation, and the phonon exchange terms with the heat bath in the Lindblad form [9] as seen in Eqs.(11) and (12), where $N(\omega_K)$is the Bose-Einstein distribution function of phonons in the heat bath at the same frequency as the breathing or oblong mode phonons.

The current in the steady state that may be described as

$$I = e \sum_{m \geq 0} \Gamma_{10}^{mm} \rho_{00}^{mm} + I_{ph}, \tag{14}$$

which is derived from the master equations (7) and (8), provided that $\langle \dot{n} \rangle = 0$. The relevant phonon-mediated component I_{ph} is

$$I_{ph} = e \sum_{m \geq 0} \sum_{m' \geq -m} \Gamma_{10}^{m+m',m} \rho_{00}^{mm}. \tag{15}$$

IV. RESULTS

We investigate the thermal and transport properties of a SET of gold nanoparticle $a = 1$nm in radius, by numerically solving Eqs. (7) and (8) self-consistently by means of the Runge-Kutta method of the fourth order. We substitute the temperature T in $F(x)$ by the temperature T' in the island calculated from the averaged number of phonons discussed below in order to incorporate thermal equilibration among phonons and electrons. Used parameters are $\omega_B/2\pi = 1.516$THz, $\kappa_B = 2.426 \times 10^{-4}$, $\beta_B = 1.5$, $z_1 = 1.62 \times 10^{-2}$, $z_2 = 6.517 \times 10^{-3}$ for the breathing mode, and $\omega_O/2\pi = 0.515$THz, $\kappa_O = 29.876 \times 10^{-4}$, $\beta_O = 0.5$, $z_1 = 1.97 \times 10^{-1}$, $z_2 = 7.750 \times 10^{-2}$ for the oblong mode. We assume the characteristic tunneling rates $\gamma(\equiv 1/R_T C_0)$ to be $\gamma \ll \omega_K$.

Phonon emission and absorption induced by electron tunneling are expected to heat or to cool the island, and then, we first examine the temperature on the particle. In steady state, i.e., $\dot{\rho}_{nn}^{mm} = 0$, thermal properties depend on the ratio γ_∞/γ.

In steady state, the total phonon occupation probability ρ^{mm} $(= \rho_{00}^{mm} + \rho_{11}^{mm})$ is expected to obey the canonical distribution. On the other hand, it is known that ρ^{mm} deviates from the canonical distribution when electron tunneling associated with multi-phonon emission and absorption takes place in the molecular devices. The present system also shows such deviation of ρ^{mm} from the canonical distribution, which is, however, limited to the voltage region of the onset of Coulomb blockade, and the deviation is subtle. As a consequence, we may evaluate the temperature in the island from the averaged number of phonons $\langle m_K \rangle [= \mathrm{Tr}(m\rho_{nn}^{mm})]_K$, using the Bose-Einstein distribution function;

$$T' = \frac{\hbar\omega_K}{k_B} \left[\ln \left(\frac{1}{\langle m_K \rangle} + 1 \right) \right]^{-1}. \tag{16}$$

In Fig.3, we plot T' versus V at $T = 4$K and 40K for each case of the breathing and oblong mode phonons, with $\gamma_\infty = 0.01\gamma$, 0.1γ and 0.5γ. Here, the bias voltage V is

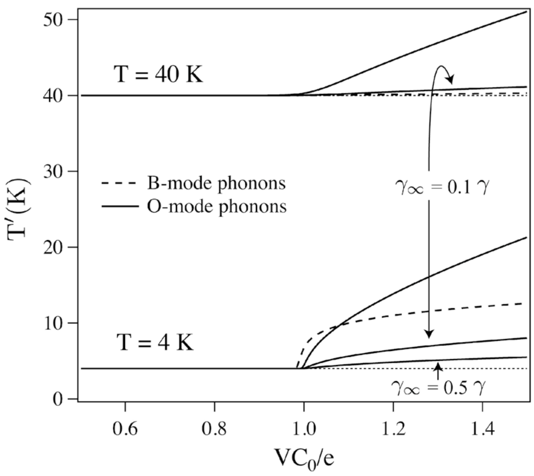

FIG. 3: The temperature T' in the island versus V at $T = 4$K for $\gamma_\infty = 0.01\gamma$, 0.1γ and 0.5γ. The data lines of $\gamma_\infty = 0.1\gamma$ and 0.5γ are denoted by arrows. $T$is the temperature of the heat bath.

expressed in unit of e/C_0, and $VC_0/e = 1$ that is equivalent to $eV/2 = E_C$is the threshold bias voltage for tunneling without phonon mediation. The rate at which T' increases with bias depends on how fast the phonon energy dissipates to the heat bath and becomes small for large γ_∞/γ.

The onset of the temperature increase depends on the phonon modes. The temperature rise begins at a lower bias voltage for the breathing mode than that for the oblong mode because the threshold voltage associated with phonon absorption is lower for the breathing mode; $\omega_{\mathrm{B}} > \omega_{\mathrm{O}}$. Even below the threshold bias for tunneling associated with phonon emission, the island gains phonon energy by phonon emission as mentioned above. As a consequence, the temperature for the breathing mode rises more steeply at lower bias voltage. Conversely, the increasing rate is larger for the oblong mode than that for the breathing mode, which is seen clearly at the heat bath temperature of $T = 40$K.

We plot the total current I and the current I_{ph} only due to phonon-mediated electron tunneling versus V at $T = 4$K in Fig.4. Figure 4(a) shows the results for the breathing mode. The total current I begins to flow at $VC_0/e = 1$ and increases almost linearly with increasing V. On the other hand, I_{ph} arises at $VC_0/e = 1 + \hbar\omega_B/E_C \approx 1.03$ that is the threshold bias voltage for tunneling associated with single phonon emission. Because I_{ph} amounts, at most, to 0.004% of the total current, the signature of phonon effects on I is obscured. Figure 4(b) plots I and I_{ph} due to the oblong mode. I_{ph} begins to arise at $VC_0/e = 1 + \hbar\omega_O/E_C \approx 1.01$, and increases nonlinearly with respect to V. Although I_{ph} is three orders of magnitude larger than that for the breathing mode, it is still too small to cause apparent modifications to the total current I.

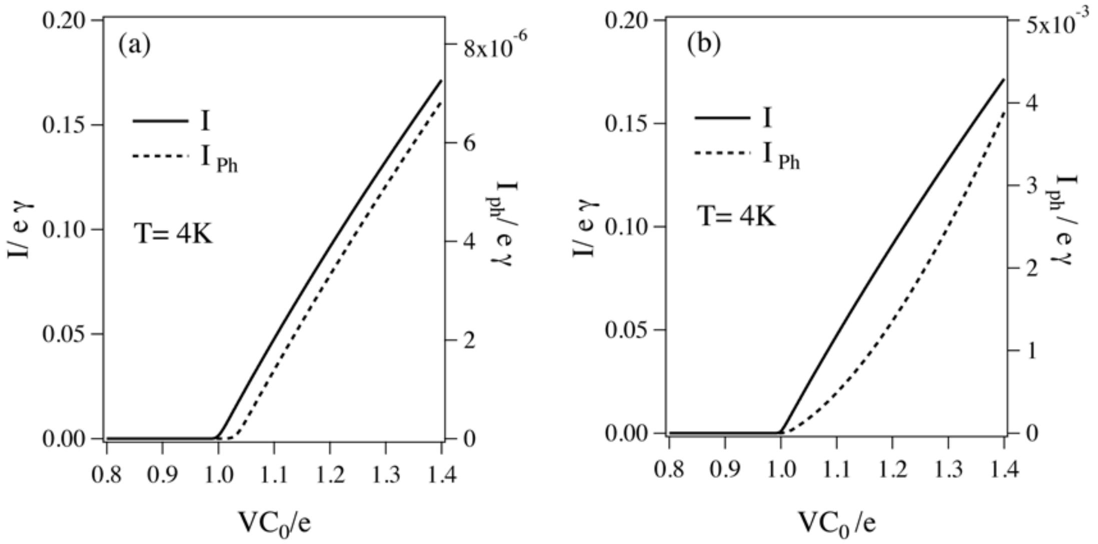

FIG. 4: The total current I and phonon-mediated current I_{ph} for (a) the breathing and (b) oblong modes versus V at 4K.

In order to resolve the subtle phonon effects on the current, we investigate the second derivative of current with respect to V. Figure 5(a) shows $d^2I/dV^2$and d^2I_{ph}/dV^2 versus V for the breathing mode at various heat bath temperatures from 4K to 40K. d^2I/dV^2has a main peak at $VC_0/e = 1$, which lowers and broadens with increasing temperature. On the other hand, at $T = $ 4K, d^2I_{ph}/dV^2shows sidebands at $VC_0/e = 1 \pm 0.03$ due to single phonon absorption (-) and emission (+). These two peaks are too small to be resolved in d^2I/dV^2. As the temperature increases, the peak due to the phonon absorption becomes larger and broadens, while the peak due to phonon emission flattens. The peaks eventually merge at $T \geq$ 20K, and the effects of phonon absorption and emission become indistinguishable above 20K.

Figure 5(b) plots d^2I/dV^2 and d^2I_{ph}/dV^2 versus V for the oblong mode, and there are sidebands in d^2I_{ph}/dV^2, indicating single phonon absorption and emission at $VC_0/e = 1 \pm 0.01$. Because the two sidebands are close in energy, the peak corresponding to phonon absorption is only just resolved at low temperature. The two peaks merge with increasing temperature and become indistinguishable at $T =$ 20K. Although we expected other sidebands associated with multi-phonon absorption/emission at, for example, $VC_0/e = 1.00 \pm 0.02$, no evidence of extra peaks was found in d^2I_{ph}/dV^2, indicating that the nonlinear increase in I_{ph} for the oblong mode is not primarily the result of multi-phonon-mediated tunneling.

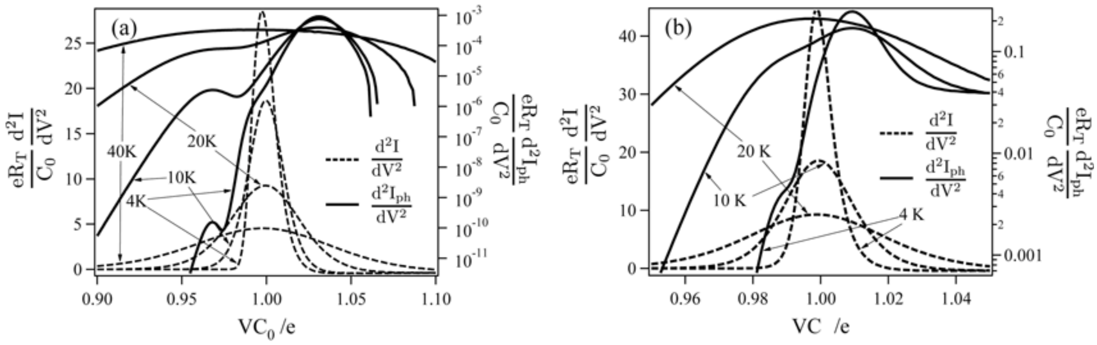

FIG. 5: The second differential conductance of the total current d^2I/dV^2 and that of the phonon-mediated current $d^2I_{\rm ph}/dV^2$ versus V at 4K for (a) the breathing mode and (b) oblong mode.

V. SUMMARY AND CONCLUSION

We have discussed how phonons associated with the island of an SET influence the electron transport of the device. We have formulated the tunnel Hamiltonian to incorporate the changes in the capacitances and tunnel resistances caused by phonons. On the basis of this result, we set up the master equations for the density matrix and formulate the current and differential conductance.

Applying the model to an ideal SET containing a spherical gold particle with a radius of 1nm, we calculated the effects of the breathing and oblong mode phonons on the thermal properties of the island and on the electron transport. Phonon emission associated with tunneling raises the temperature in the island, and multi-phonon emission makes the phonon occupation number in the island deviate from the canonical distribution even at steady state in the bias region close to the tunneling threshold. The current through the SET is dominated by tunneling without phonon mediation. The second derivative of the phonon-mediated current exhibits peaks associated with single phonon absorption and emission similar to phonon signatures found by inelastic electron energy spectroscopy [2] in other systems. In the system studied, peaks associated with multi-phonon emission are smeared. We conclude that the dominant effect of the dynamic deformation of the particle island induced by phonons is on the thermal properties of the island rather than the electronic properties of the SET. It appears that molecular vibrations such as vibrons have the most dominant signatures of island dynamics on the transport [1–3, 10–14].

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References

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[1] M. Galperin, M. A. Ratner and A. Nitzan, J. Phys. :Condens. Matter **19**, 103201(2007).

[2] M. Galperin, A. Nitzan and M. A. Ratner, Phys. Rev. B **78**, 15320 (2008).

[3] A. Mitra, I. Aleiner and A. J. Millis, Phys. Rev. B**69**, 245302 (2004).

[4] A. E. H. Love, *A Treatise on the Mathematical Theory of Elasticity* (New York, Dover, 1944), Chap. 12.

[5] N. Nishiguchi and M.N.Wybourne, Journal of Phys.:Condens. Matter **22**, 065301(2010).

[6] D. K. Cheng, *Field and Wave Electromagnetics*, (Addison-Wesley Publishing, Reading, Massachusetts, 1989), 2nd edition, pp. 172-174.

[7] G.-L.Ingold and Yu. V. Nazarov, in *Single Charge Tunneling: Coulomb Blockade Phenomena in Nanostructures* (NATO Science Series B: Physics)(Springer, 1992) edited by H. Grabert and M. H. Devoret, pp. 67.

[8] G. Pòlya and G. Szego, *Isoperimetric Inequalities in Mathematical Physics: Annals of Mathematical Studies* (Princeton University Press, Princeton, 1951).

[9] G. Lindblad, Commun. Math. Phys. **48**, 119 (1976).

[10] D. Boese and H. Schoeller, Europhys. Lett. **54**, 668 (2001).

[11] S. Braig and K. Flensberg, Phys. Rev. B**68**, 205324 (2003).

[12] M. R. Wegewijs and K. C. Nowack, New Journal of Physics **7**, 239 (2005).

[13] J. Koch, von Oppen F, Phys. Rev. Lett. **94**, 206804 (2005).

[14] J. Koch, Semmelhack M, von Oppen F, Nitzan A, Phys. Rev. B **73**, 155306 (2006).