

Quantum Theory of Triboelectricity



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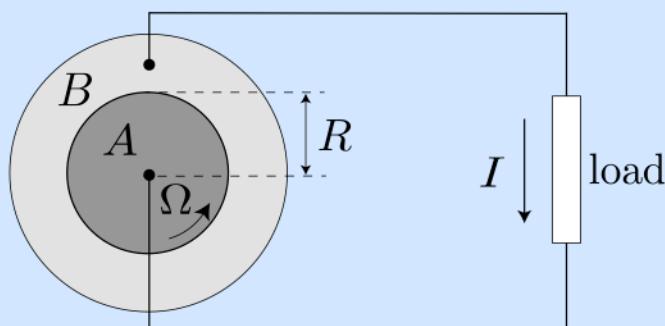
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Graphical abstract:

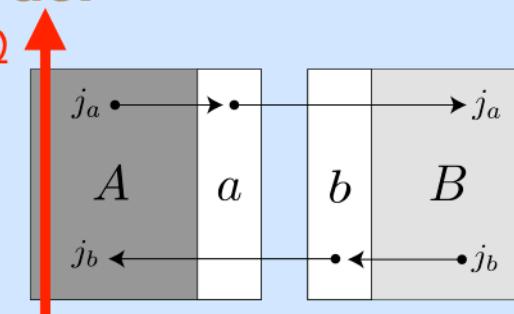
Bulk material A with surface a, rubbing against bulk B with surface b

Minimal tribogenerator:



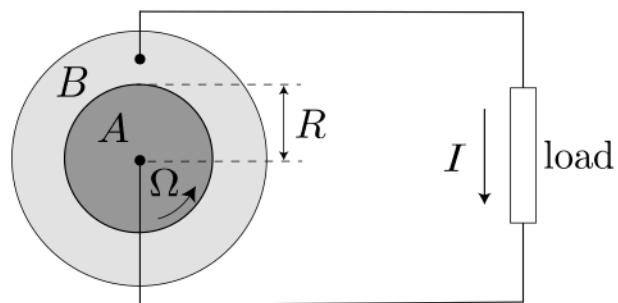
Tribocurrents for each electronic surface mode:

$$V_s = R \Omega$$



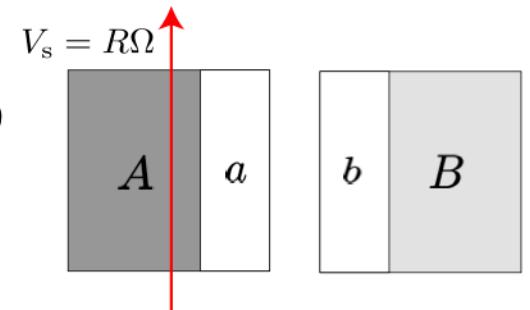
Tribovoltage: $e\phi_{oc} = |\mu_A - \mu_B|_{\text{at zero current}} \lesssim \hbar k_F V_s$

Open quantum system



system: surfaces $a + b$

2 baths: bulks A & B



At rest:

$$H_0^x = \sum_{\sigma, m} \omega_x(\sigma, m) c_x^\dagger(\sigma, m) c_x(\sigma, m) \quad \text{for } x = a, b$$

$$H_0^X = \sum_{\kappa, m} \omega_X(\kappa, m) c_X^\dagger(\kappa, m) c_X(\kappa, m) \quad \text{for } X = A, B$$

In motion:

(Doppler shift)

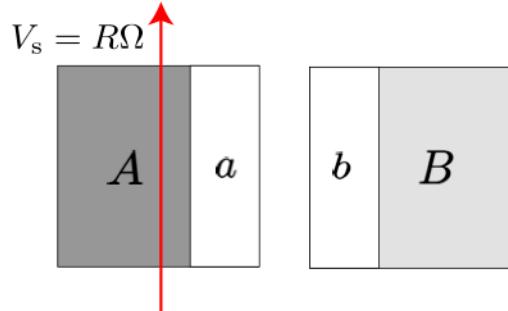
$$H_\Omega^a = \sum_{\sigma, m} [\omega_a(\sigma, m) - m\Omega] c_a^\dagger(\sigma, m) c_a(\sigma, m)$$

$$H_\Omega^A = \sum_{\kappa, m} [\omega_A(\kappa, m) - m\Omega] c_A^\dagger(\kappa, m) c_A(\kappa, m)$$

See also: R. Alicki & AJ, *Ann. Phys. (NY)* **395**, 69 (2018) [[arXiv:1702.06231](https://arxiv.org/abs/1702.06231)]

Surface-bulk tunneling: $H_X^x = \sum_{\kappa, \sigma, m} g_X^x(\kappa, \sigma, m) c_X^\dagger(\kappa, m) c_x(\sigma, m) + \text{h.c.}$

Kinetic eqs.



Total Hamiltonian:

$$H_{\text{tot}} = H_{\Omega}^a + H_0^b + H_{\Omega}^A + H_0^B + H_A^a + H_B^a + H_A^b + H_B^b$$

Kinetic eq. for each surface electronic mode.:

$$\dot{n}_x = \gamma_{\uparrow}^{xA} + \gamma_{\uparrow}^{xB} - (\gamma_{\downarrow}^{xA} + \gamma_{\downarrow}^{xB} + \gamma_{\uparrow}^{xA} + \gamma_{\uparrow}^{xB}) n_x$$

KMS conditions: $\gamma_{\uparrow}^{aA}(\sigma, m) = e^{-\beta(\omega_a(\sigma, m) - \mu_A)} \gamma_{\downarrow}^{aA}(\sigma, m)$

$$\gamma_{\uparrow}^{aB}(\sigma, m) = e^{-\beta(\omega_a(\sigma, m) - m\Omega - \mu_B)} \gamma_{\downarrow}^{aB}(\sigma, m)$$

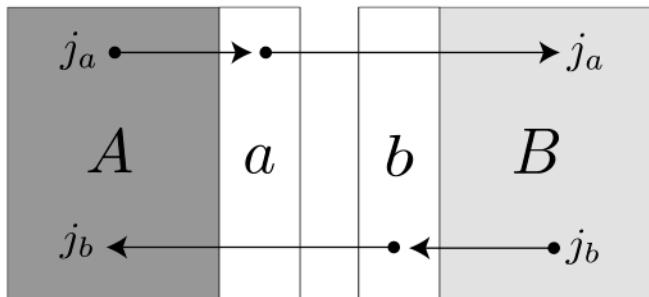
(Doppler shift)

Steady state: $n_a = \bar{n}_a \equiv (\gamma_{\uparrow}^{aA} + \gamma_{\uparrow}^{aB}) / \Gamma^a = \text{const.}$

$$n_b = \bar{n}_b \equiv (\gamma_{\uparrow}^{bA} + \gamma_{\uparrow}^{bB}) / \Gamma^b = \text{const.}$$

$$\Gamma^a \equiv \gamma_{\uparrow}^{aA} + \gamma_{\downarrow}^{aA} + \gamma_{\uparrow}^{aB} + \gamma_{\downarrow}^{aB}; \quad \Gamma^b \equiv \gamma_{\uparrow}^{bA} + \gamma_{\downarrow}^{bA} + \gamma_{\uparrow}^{bB} + \gamma_{\downarrow}^{bB}$$

Tribocurrents



$$j_a = \gamma_{\uparrow}^{aA} - (\gamma_{\downarrow}^{aA} + \gamma_{\uparrow}^{aA}) \bar{n}_a = \frac{\gamma_{\uparrow}^{aA} \gamma_{\downarrow}^{aB} [1 - e^{\beta(m\Omega + \mu_B - \mu_A)}]}{\Gamma^a}$$

$$j_b = \gamma_{\uparrow}^{bB} - (\gamma_{\downarrow}^{bB} + \gamma_{\uparrow}^{bB}) \bar{n}_b = \frac{\gamma_{\downarrow}^{bA} \gamma_{\uparrow}^{bB} [1 - e^{-\beta(m\Omega + \mu_B - \mu_A)}]}{\Gamma^b}$$

Net current:
$$J = -e \left(\sum_{\sigma, m} j_a(\sigma, m) + \sum_{\sigma', m} j_b(\sigma', m) \right)$$

Sign of J depends on relative magnitudes of $\gamma_{\uparrow}^{aA} \gamma_{\downarrow}^{aB} / \Gamma^a$ and $\gamma_{\downarrow}^{bA} \gamma_{\uparrow}^{bB} / \Gamma^b$

Only surface modes satisfying $m\Omega < \mu_A - \mu_B$ contribute to $j_a \Rightarrow j_a > 0$

Only surface modes satisfying $m\Omega > \mu_A - \mu_B$ contribute to $j_b \Rightarrow j_b > 0$

As charging increases $|\mu_A - \mu_B|$, fewer modes contribute to corresponding j_x , and more modes to the **opposing** j_x

Tribovoltage & emf

- In cylindrical coords. $\mathbf{k} = (k_m, k_z)$

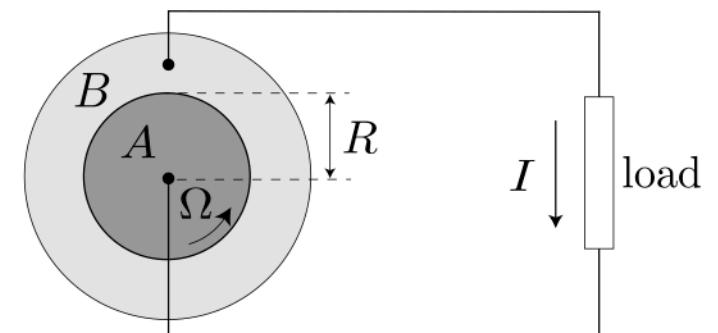
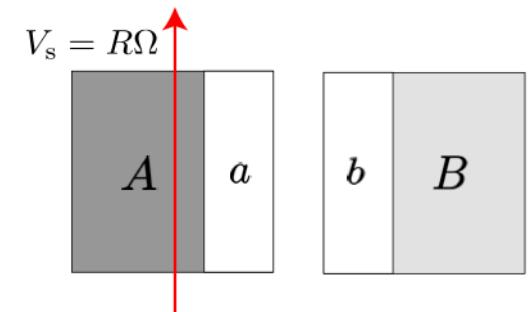
- Fermi wave vector $k_F \geq \sqrt{k_m^2 + k_z^2}$

$$|m\Omega| = |k_m V_s| \leq k_F V_s$$

- Bound on open-circuit tribovoltage ($j_a \gg j_b$, or vice-versa):

$$e\phi_{oc} = |\mu_A - \mu_B|_{\text{at zero current}} \lesssim \hbar k_F V_s$$

- This is an actual **electromotive force (emf)**, corresponding to active pumping of charges
- Can drive current along a closed circuit



Phenomenology & outlook

- For $k_F \approx 10^{10} \text{ m}^{-1}$ (**inter-atomic**) and $V_s \approx 1 \text{ m/s}$, we get $\phi_{oc} \lesssim 10^{-5} \text{ V}$; voltage enhanced by **mechanical separation** of electrified surfaces
- Increase from inter-atomic to meter scale gives $\phi_{oc} \lesssim 10^5 \text{ V}$, as in **Van de Graaf generator**
- Consistent with other qualitative features of triboelectrification, including some reported very recently (see paper)
- Precise control over V_s needed for further experimental testing
- We've extended **quantum-thermodynamic** analysis of work extraction by an open system coupled to external disequilibrium to fermion fields

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