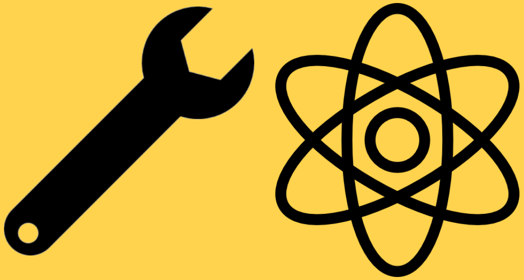
PUTTING QUANTUM INTO MECHANICS



Julian Iacoponi
MSci Project Viva

OVERVIEW

MOTIVATION & CONTEXT

→ Why do this?

→ Where did we start?

→ What's new?

INITIAL RESULTS & GRAPHS

→ Current

→ Thermal Power

DEVELOPING THE MODEL

→ Theory

→ More results and graphs

→ Entanglement?

WHY THIS PROJECT?

STUDY THE THEORY OF *NEMS*

→ Model *single electron current* across a junction of 2 leads

→ Add a quantum harmonic oscillator (QHO) to the model

BENEFITS

→ Philosophy

- *entanglement of macro-objects?*
- *measurement of the ground state?*

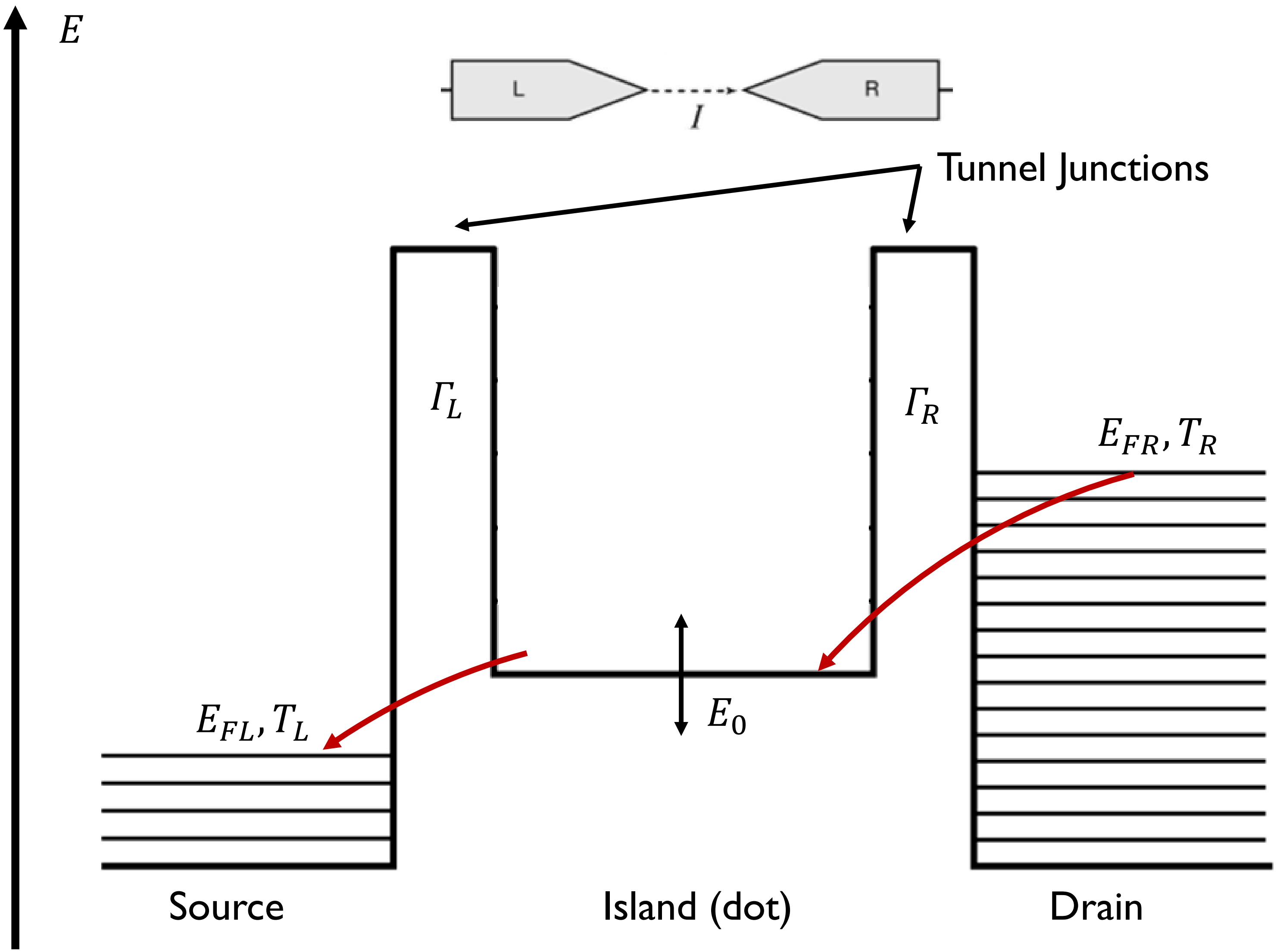
→ Applications

-MEMS have revolutionised our technology

-qubits; atom resolution microscopy[1]

[1] Roukes, Michael. "Nanoelectromechanical systems face the future." *Physics World*, February 2001: p25-31.

MODEL SCHEMATIC



WHAT DID WE START FROM?

TAHIR'S PHD[2]

→ Self-energies (advanced, retarded, lesser)

- *contribution to dot energy due to leads* ($\alpha = L, R$)

$$\Sigma_\alpha^< = f_\alpha(\Sigma_\alpha^a - \Sigma_\alpha^r) \qquad \Sigma_\alpha^a = (\Sigma_\alpha^r)^* = \frac{i\Gamma_\alpha}{2}$$

→ Green's functions (advanced, retarded, lesser)

- $G^<$ *propagates electrons*

$$G^< = G^r \Sigma^< G^a \qquad G^{r(a)} = (E - E_0 - \Sigma^{r(a)})^{-1}$$

[2] Tahir, Muhammad. Quantum Behaviour in Nano-Mechanical Systems. PhD Thesis: Imperial College, Condensed Matter Theory Group, 2010.

ORIGINS OF THE MODEL

$$\rho = \frac{1}{2\pi i}\int_{-\infty}^{\infty} G^{<} dE \qquad \hat{I}_{\alpha}/\tfrac{e}{\hbar} = i\sum_{j}(V_{0\alpha}c_0^{\dagger}c_{\alpha j} - c_{\alpha j}^{\dagger}c_0 V_{\alpha 0})$$

$$\begin{aligned} I_{\alpha} &= \mathrm{Tr}(\rho \hat{I}_{\alpha}) \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \Sigma_{\alpha}^{<}(G^{r} - G^{a}) + G^{<}(\Sigma_{\alpha}^{a} - \Sigma_{\alpha}^{r}) dE \end{aligned}$$

$\longrightarrow$ Current in units of $\frac{e}{\hbar}$

$\longrightarrow$ Electron creation/annihilation operators:

- *propagates from dot to leads (and vice versa) via* $G^{<}$

$\longrightarrow$ Hopping potentials related to tunneling fraction

- *self-energy is included*

CURRENT EQUATION

$$I = I_L - I_R$$
$$= \frac{1}{2\pi}\int_{-\infty}^{\infty}(\Sigma_L^< - \Sigma_R^<)(G^r - G^a)dE - (\Gamma_L - \Gamma_R)\rho$$

DENSITY

$\longrightarrow$ Affects current only when $\Gamma_L \neq \Gamma_R$

$\longrightarrow$ 'Leaks' more in one direction if tunnelling barriers are not equal

WHAT'S NEW?

→ Normal form of Fermi function hard to integrate

→Tahir assumed T→0; Fermi function going to a step function

$$f_\alpha = \left(e^{\frac{E-E_{F\alpha}}{k_B T_\alpha}} + 1\right)^{-1}$$

→Prof. MacKinnon set us up with <u>*Matsubara*</u> technique

→*Mathematica* can do the integral, and then the sum

$$f_\alpha = \frac{1}{2} - \sum_{q=-\infty}^{\infty} \left(\frac{E-E_{F\alpha}}{k_B T_\alpha} - i(2q+1)\pi\right)^{-1}$$

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Can now explore the theory at finite temperatures!

DERIVED RESULTS

MOST GENERAL CASE

→ Algebraically simplifies very nicely

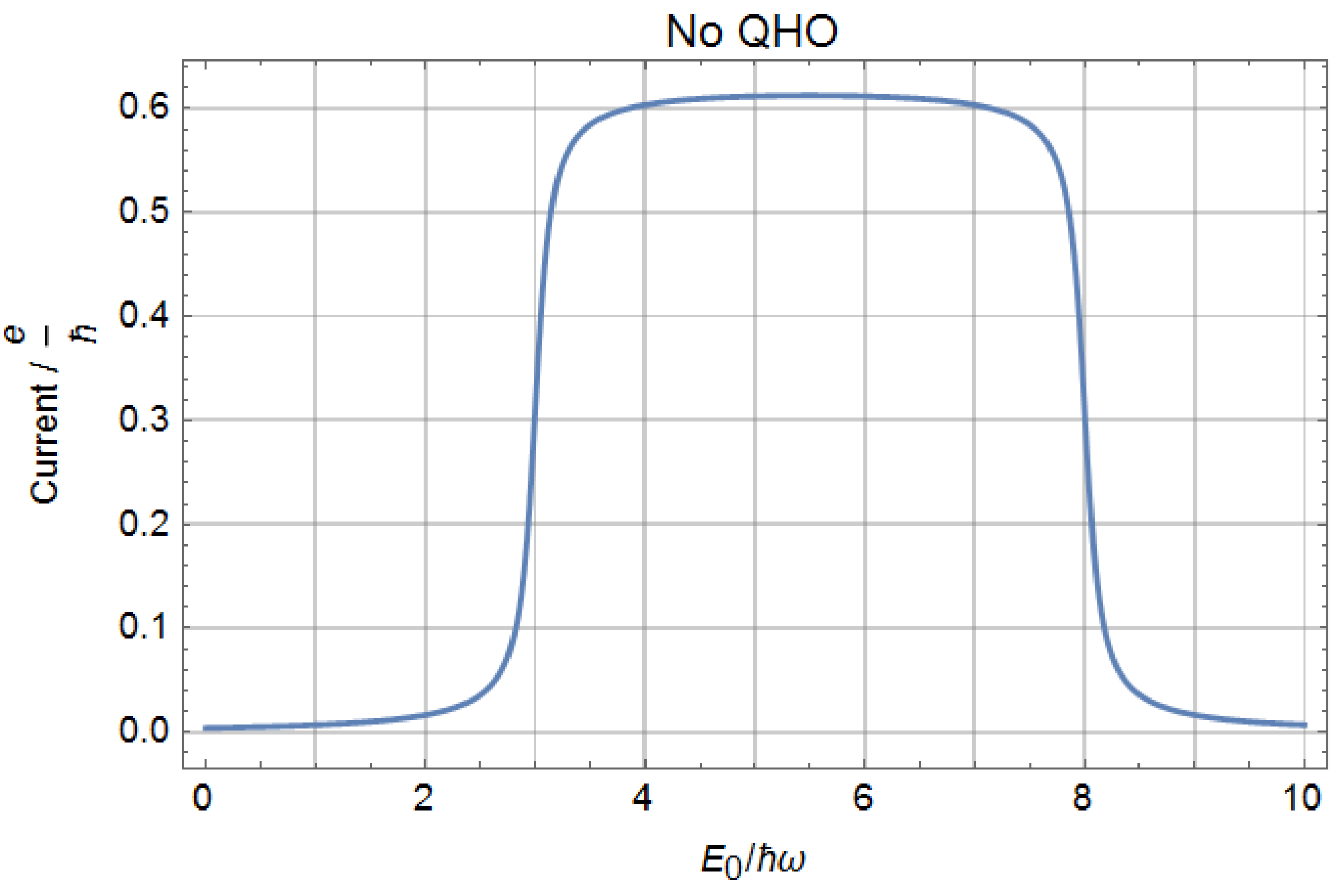
$$I = \frac{1}{2\pi} . \frac{\Gamma_L \Gamma_R}{\bar{\Gamma}} . i(\Delta\psi(z_L) - \Delta\psi(z_R))$$

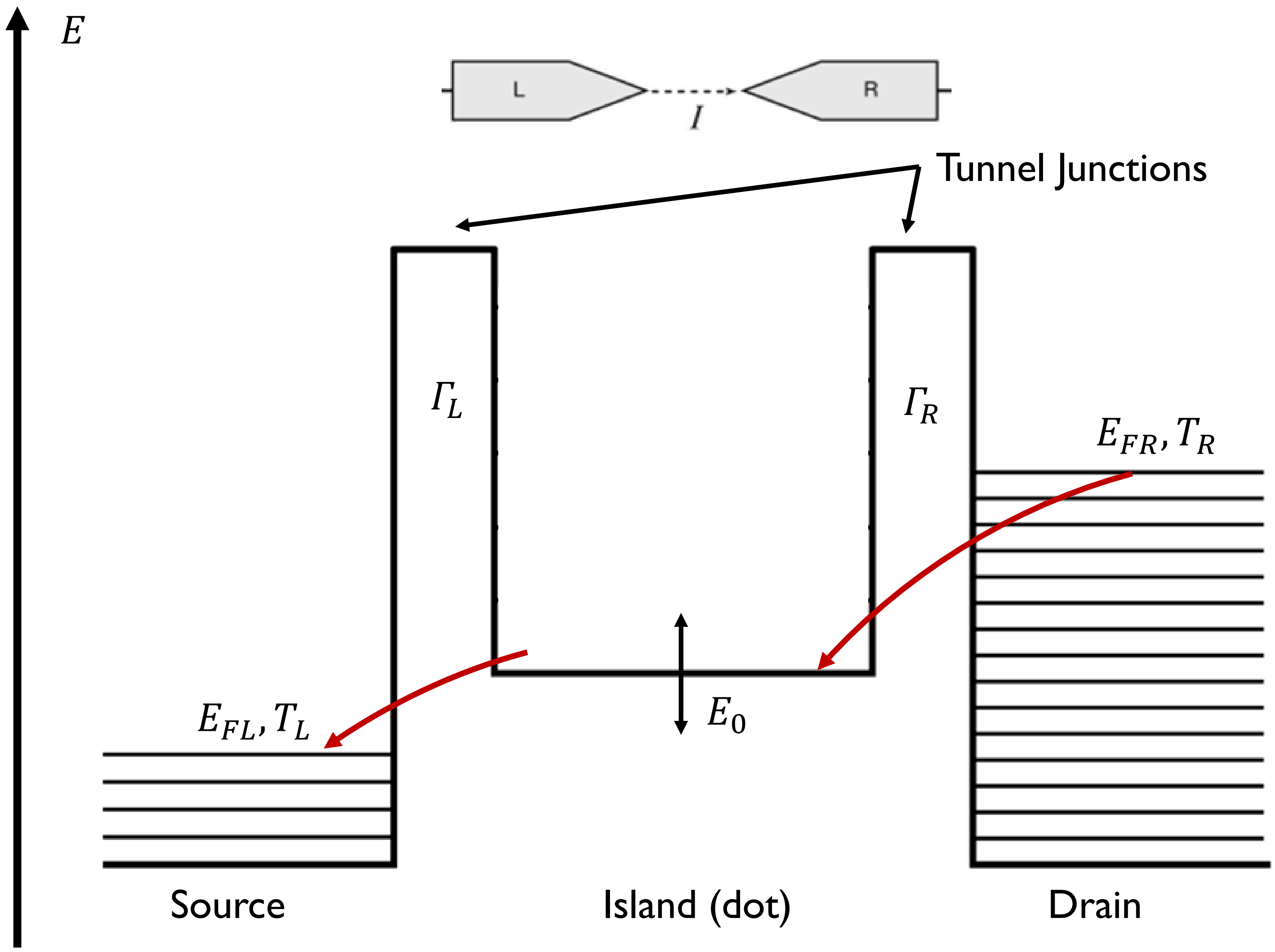
$$\Delta\psi(z) = \psi(z) - \psi(z^*) \qquad z_\alpha = \frac{1}{2} + \frac{\bar{\Gamma} + i(E_{F\alpha} - E_0)}{2\pi k_B T_\alpha}$$

→ Gives: Digamma functions depending on the difference in dot and Fermi energies

→Symmetric to exchanging left and right, as required

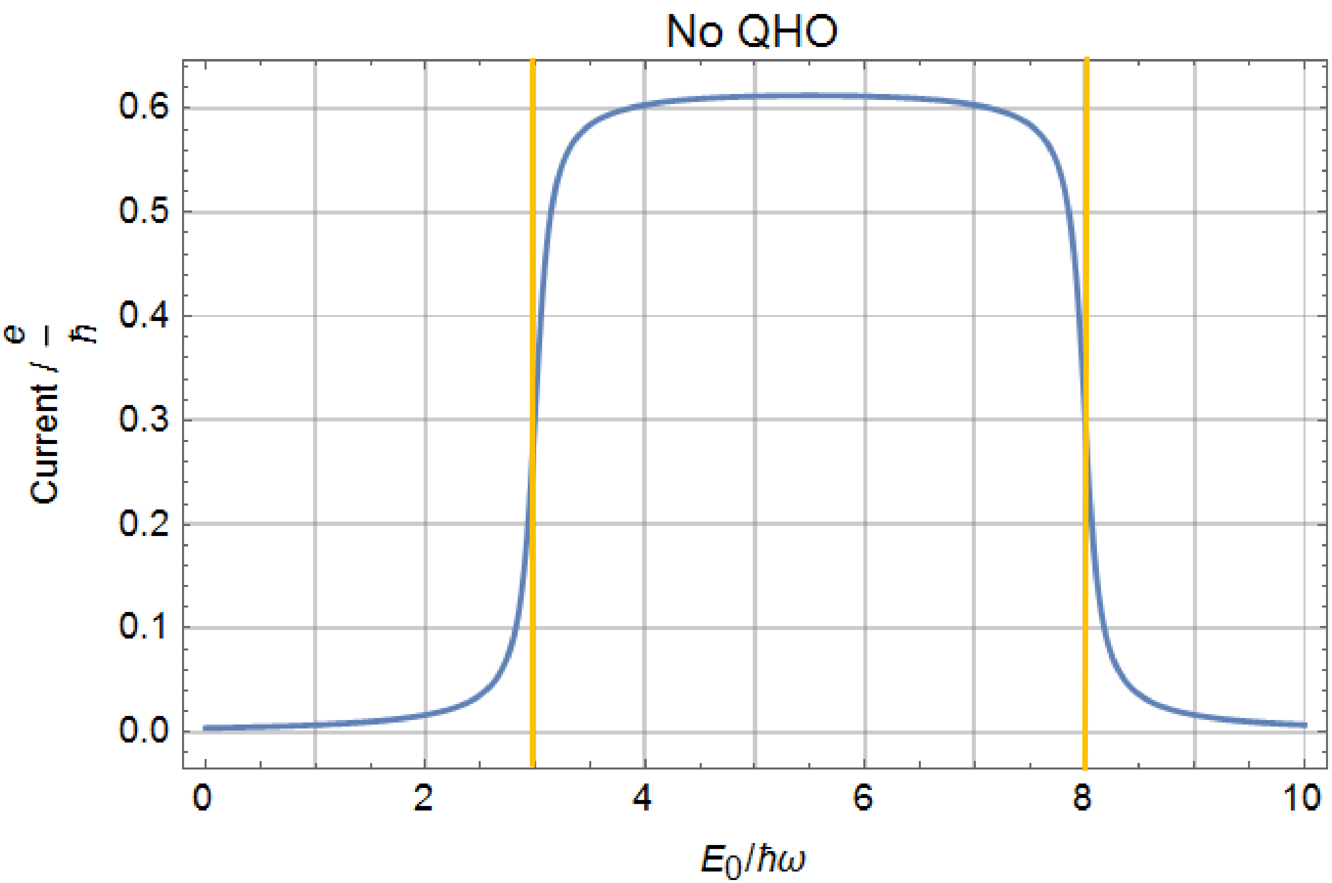
CURRENT GRAPH





E
L
R
I
Tunnel Junctions
Γ_L
Γ_R
E_{FR}, T_R
E_{FL}, T_L
E_0
Source
Island (dot)
Drain

CURRENT GRAPH



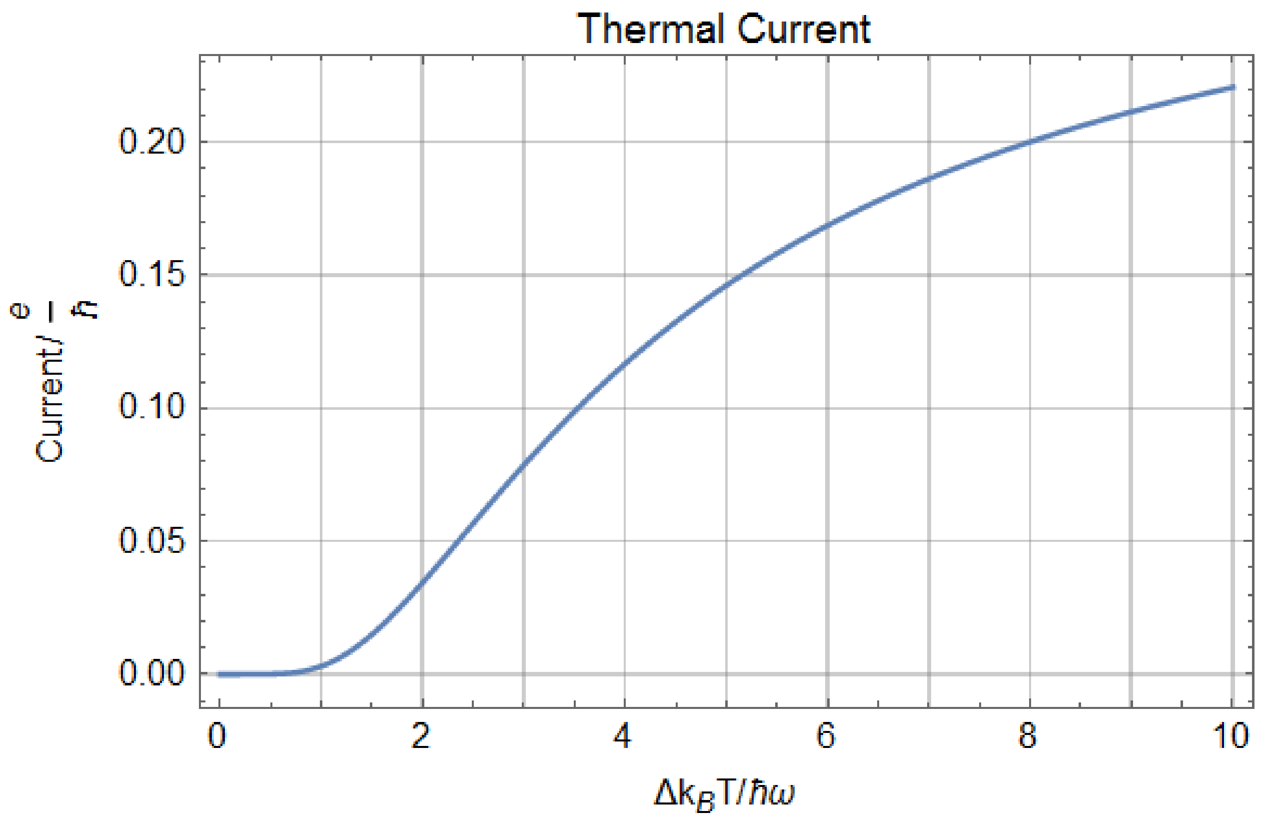
→ Double step shape because of 2 transitions

→ Smoothing at Fermi level transition due to temperature

THERMAL POWER

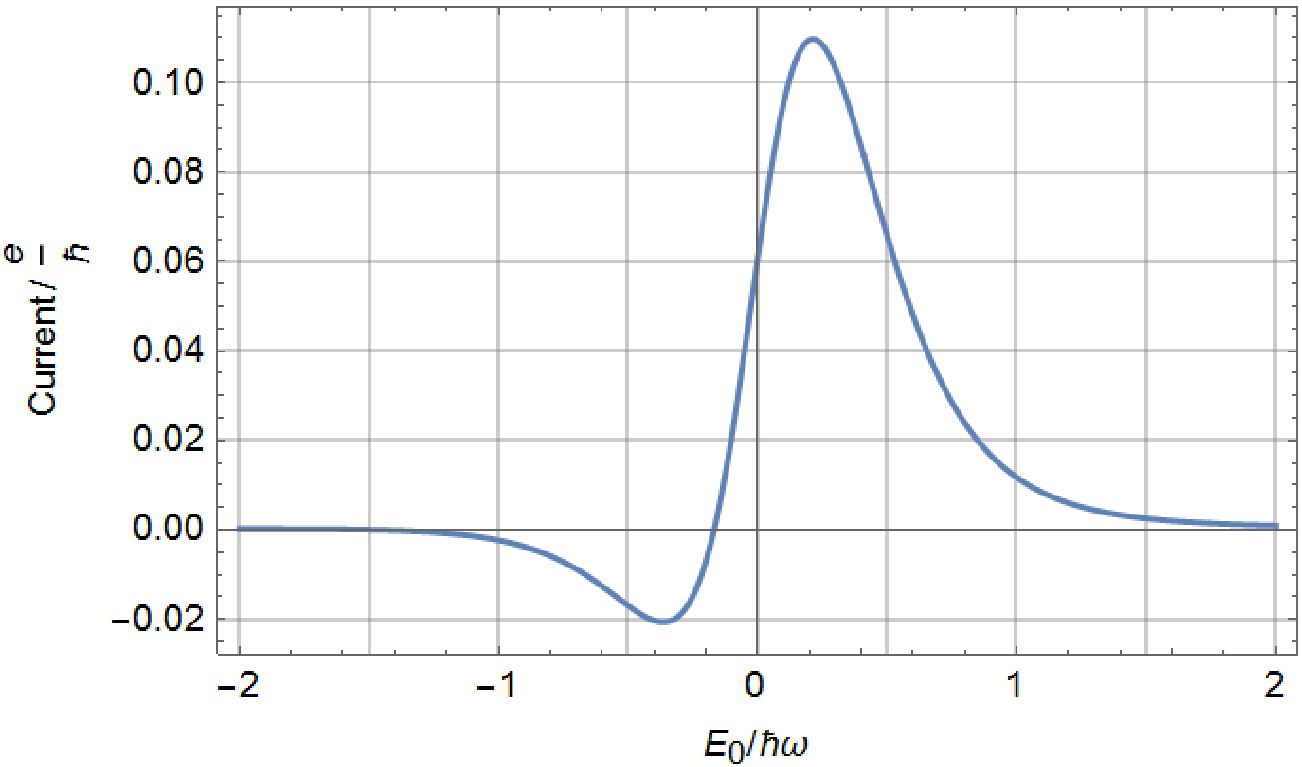
→ Set $E_{FL} = E_{FR} \neq E_0$

→ Difference in lead temperatures produces a current!



THERMAL POWER

→ Set $\Delta k_B T \approx \Delta E_F$



→ Thermal power reverses normal current at transition!

SATURATION CURRENT

$$E_{FL} \to \infty \Rightarrow f_L \to 0$$

$$E_{FR} \to -\infty \Rightarrow f_R \to 1$$

$$\Rightarrow \quad I = \frac{1}{2\pi} \cdot \frac{\Gamma_L \Gamma_R}{\bar{\Gamma}}$$

$\longrightarrow$ Depends on tunnelling fractions only
$\longrightarrow$ More tunnelling = more current flow
$\longrightarrow$ Symmetric to right/left, as required

ADDING AN OSCILLATOR

QHO THEORY

$\longrightarrow$ Add QHO energies!

$$E_{F\alpha} \longrightarrow E_{F\alpha} + (n + \tfrac{1}{2})\hbar\omega$$

$$E_0 \longrightarrow E_0 + (n + \tfrac{1}{2})\hbar\omega$$

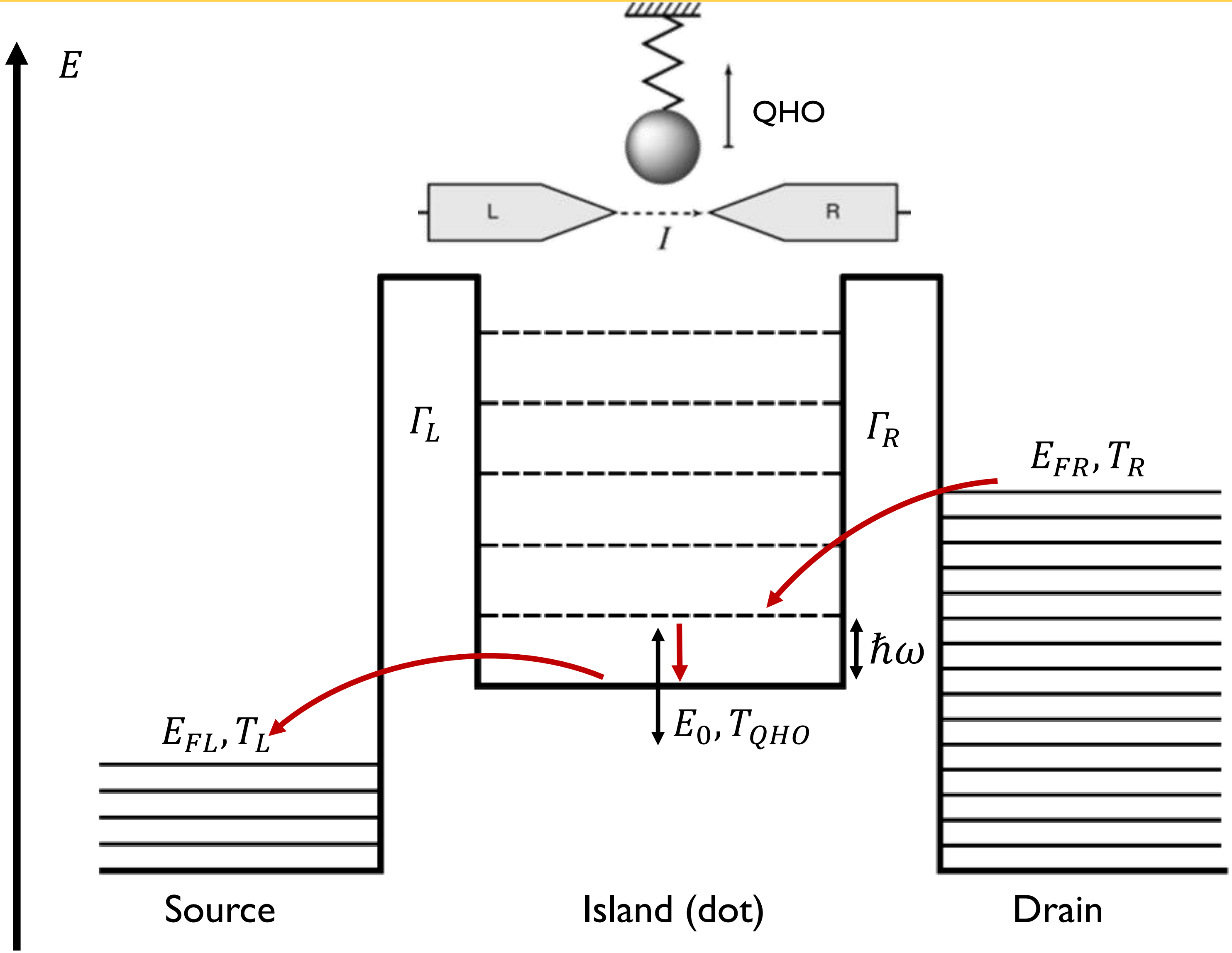
$\longrightarrow$ S-matrices (Φ_{nm}) relate initial and final QHO states

$\longrightarrow$ Add indices to indicate these states

$\longrightarrow$ Self-energy has Boltzmann factor

$$\Sigma^{<}_{\alpha n} = i\Gamma_\alpha f_{\alpha n} B_n$$

SCHEMATIC (WITH QHO)



RESULTS WITH QHO

CURRENT

$\longrightarrow$ Take $\Gamma_L = \Gamma_R = \Gamma$ case to simplify current equation

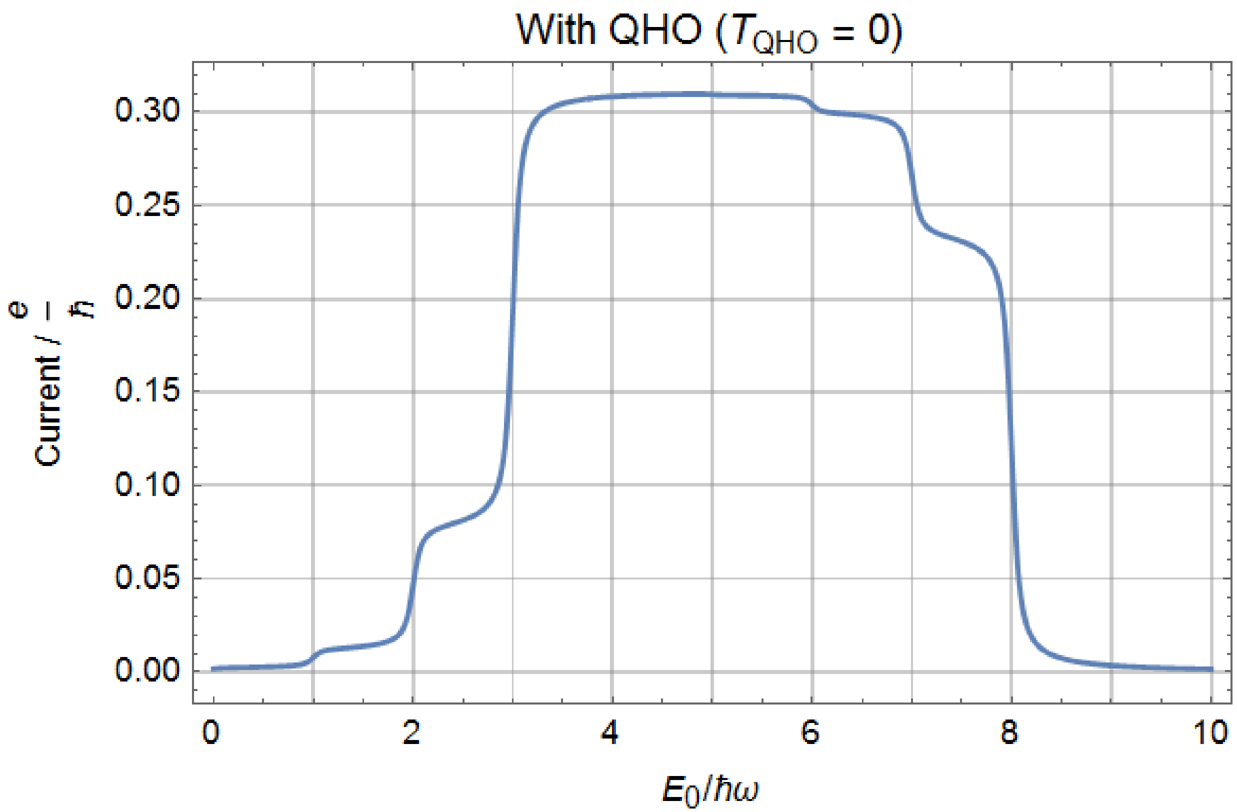
$$I = \sum_{nm} B_n |\Phi_{nm}|^2 . i\Gamma(\Delta\psi(z_{Lnm}) - \Delta\psi(z_{Rnm}))$$

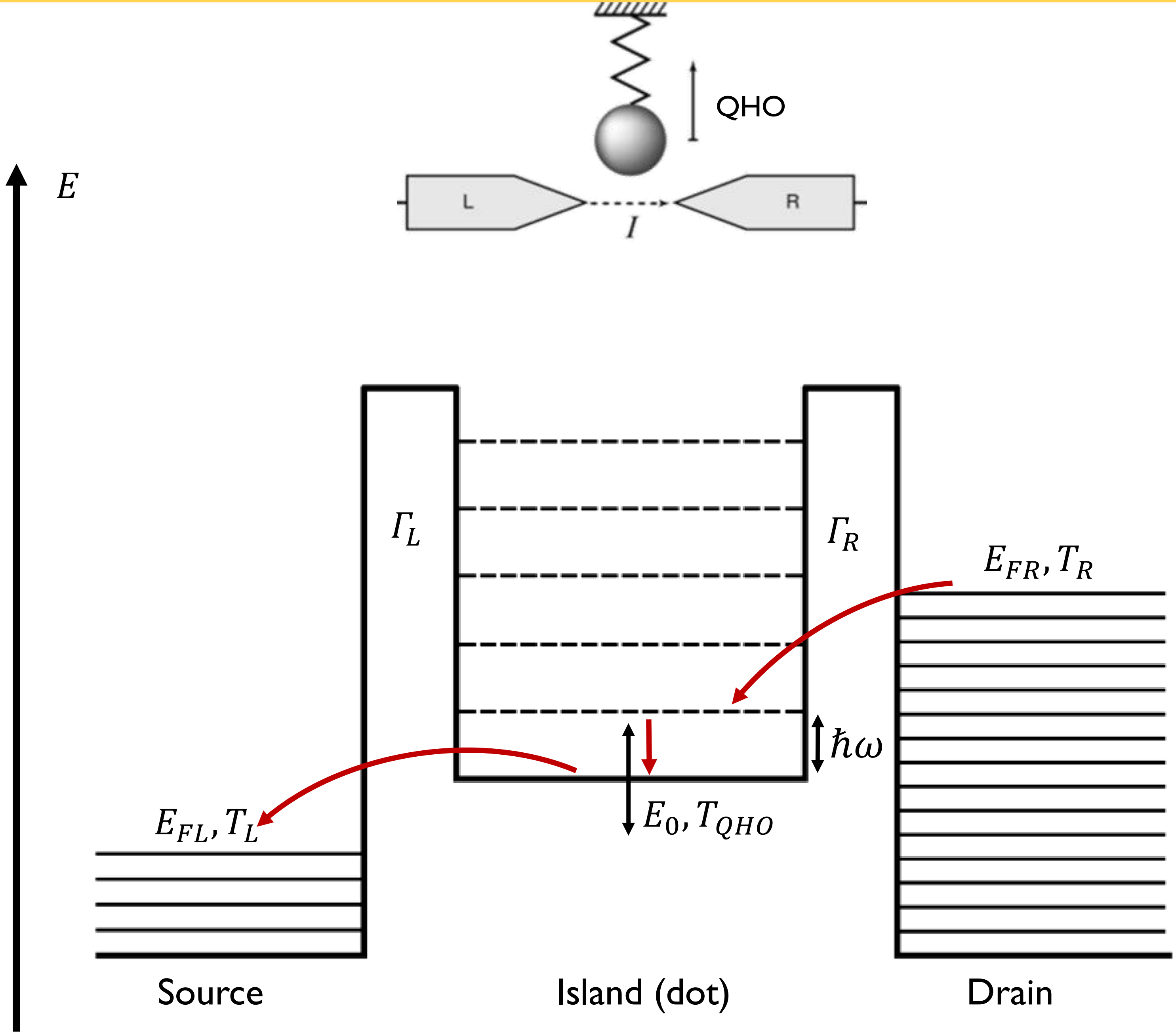
$$z_{\alpha nm} = \frac{1}{2} + \frac{\Gamma + i((E_{F\alpha} + (n + \frac{1}{2})\hbar\omega) - (E_0 + (m + \frac{1}{2})\hbar\omega)}{2\pi k_B T_\alpha}$$

$\longrightarrow$ Again, Digammas depending on difference in dot and lead energies

$\longrightarrow$ Ground state cancels!

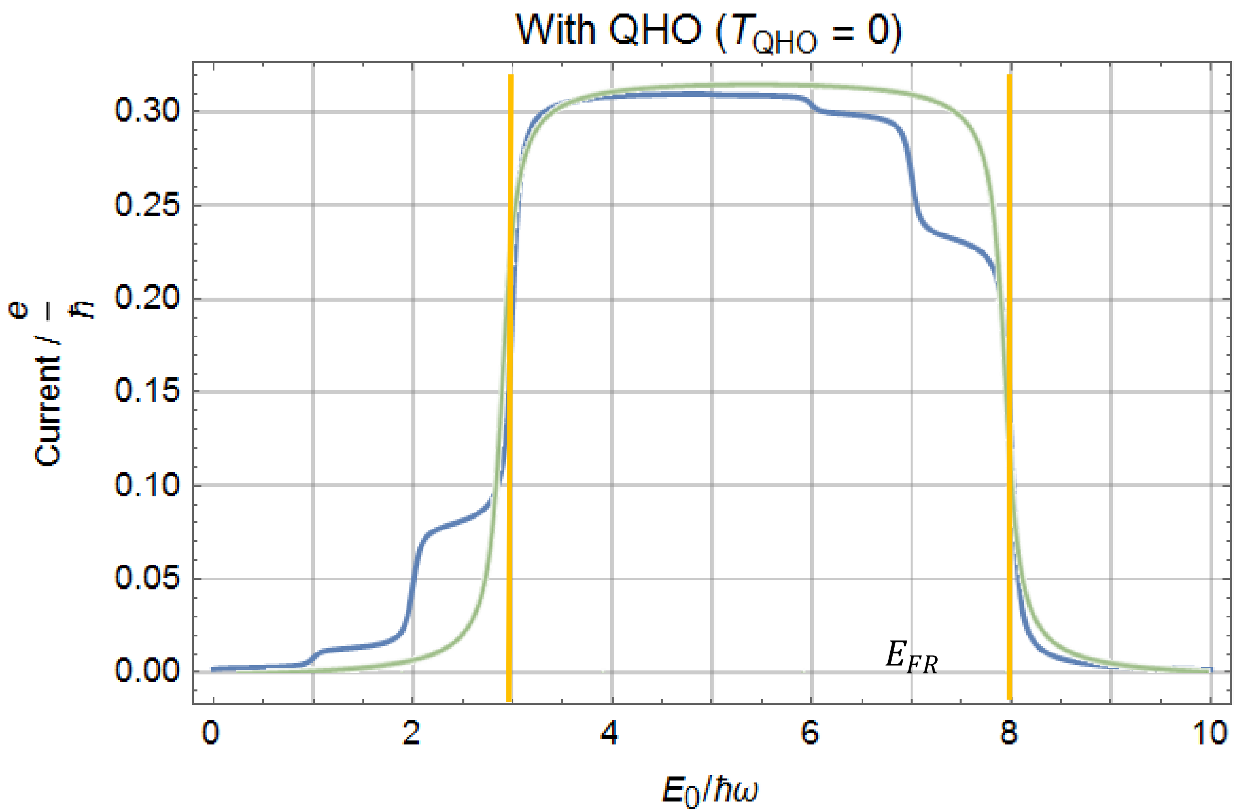
T_{QHO}=0 CURRENT





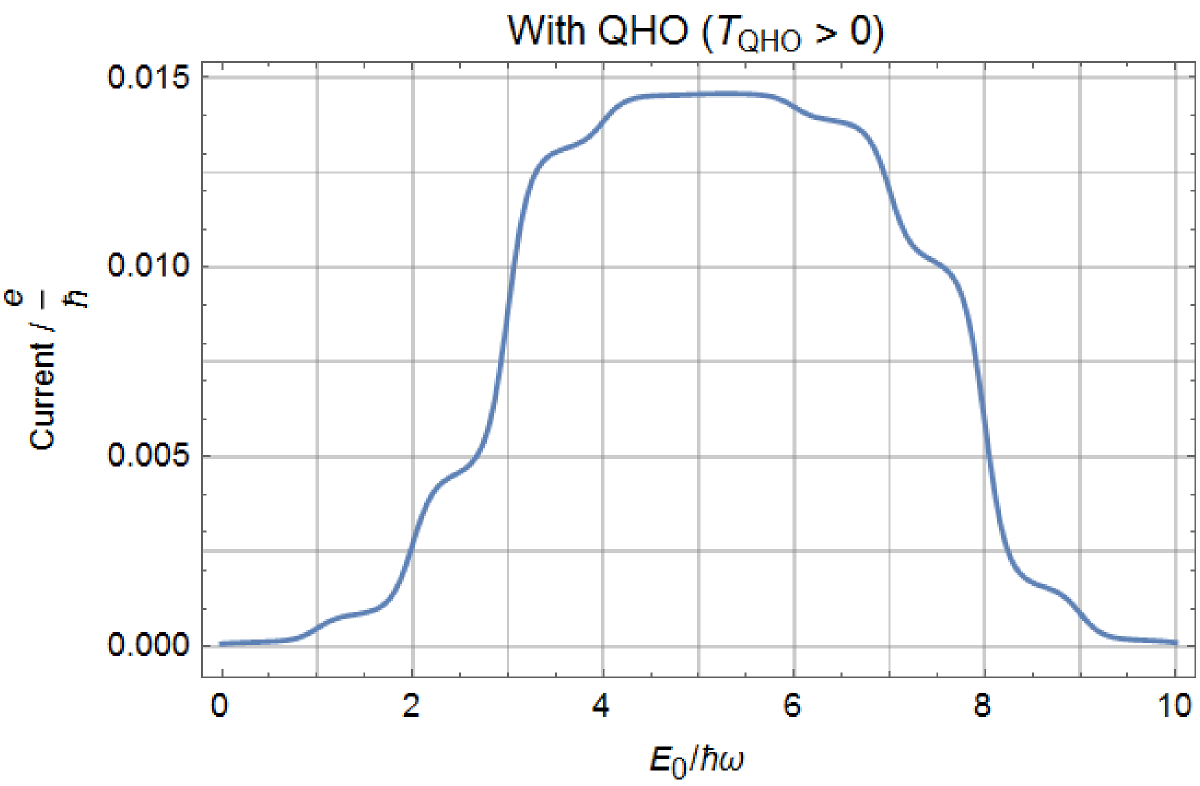
QHO
L
R
I
E
Γ_L
Γ_R
E_{FR}, T_R
$\hbar\omega$
E_0, T_{QHO}
E_{FL}, T_L
Source
Island (dot)
Drain

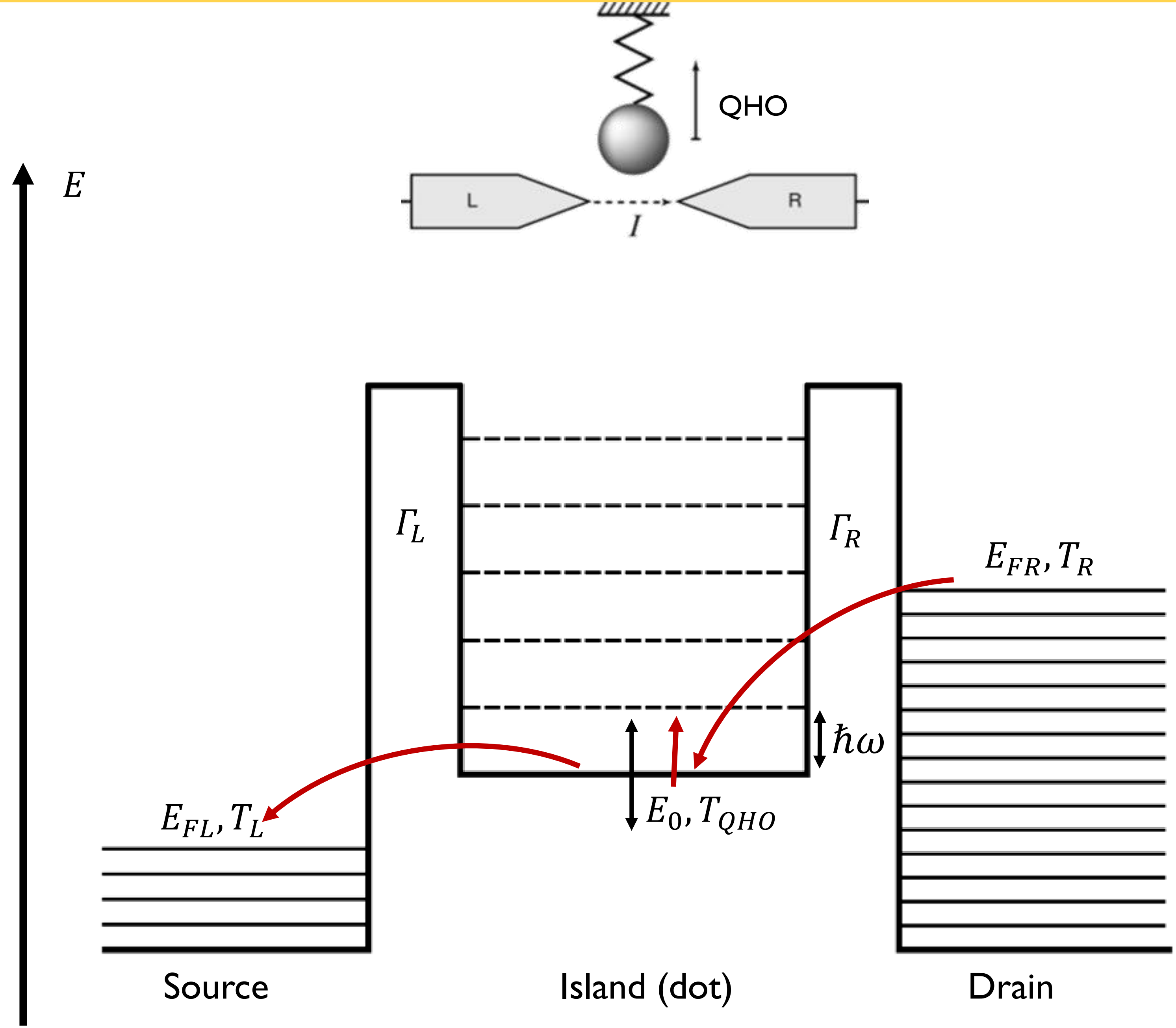
T_{QHO}=0 CURRENT



→ Phonon creation routes **raise** *(lower)* current **<u>before</u> entry** *(exit)* of Fermi energy gap

T_{QHO}>0 CURRENT




QHO
L
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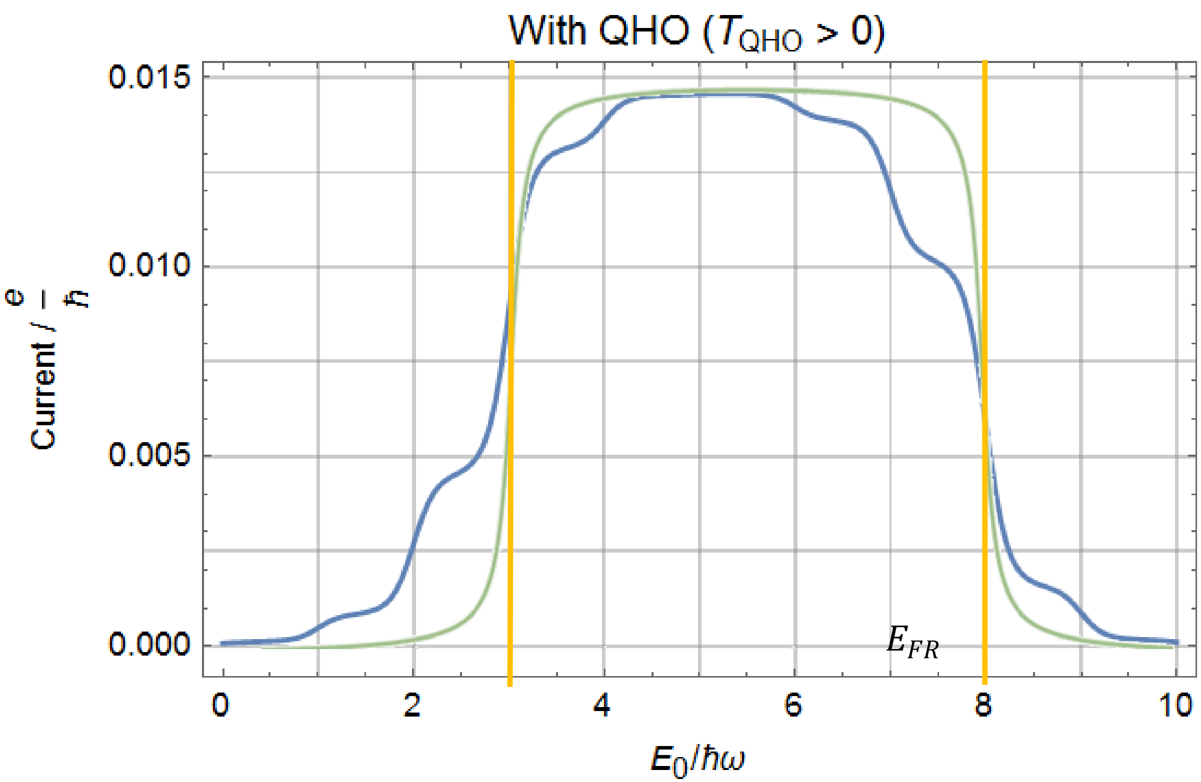
$T_{QHO}>0$ CURRENT



→ Phonon annihilations **lower** *(raise)* current **<u>after</u> entry** *(exit)* of Fermi energy gap

ENTANGLEMENT?

DENSITY MATRIX

$$\rho_{nn'} = \frac{1}{2\pi i}\int_{-\infty}^{\infty} G^{<}_{nn'}\, dE$$

$$G^{<}_{nn'} = \sum_{m} G^{r}_{nm}\Sigma^{<}_{m}G^{a}_{mn'}$$

→Non-zero diagonal elements suggest mixed states
→Eigenvectors correspond to phonons
→Eigenvalues correspond to electrons

QUANTUM ENTROPY?

VON NEUMANN DEFINITION

$$S(\rho) = -\mathrm{Tr}(\rho \ln \rho)$$

→ Quantifiable measure for extent of entanglement
× Our density matrix is 'missing' density, so approach not currently working

SUMMARY

MOTIVATION & CONTEXT

→ Important for philosophy and technology

→ Based off Tahir's PhD

→ New Matsubara technique for Fermi function!

INITIAL RESULTS & GRAPHS

→ Digammas gives step-like current

→ Thermal power

→ Saturation current

DEVELOPING THE MODEL

→ Coupled QHO

→ Bumps in current due to phonons

→ Evidence of entanglement

THANK YOU FOR LISTENING ☺