Energy, momentum, and angular momentum transfers mediated by photons

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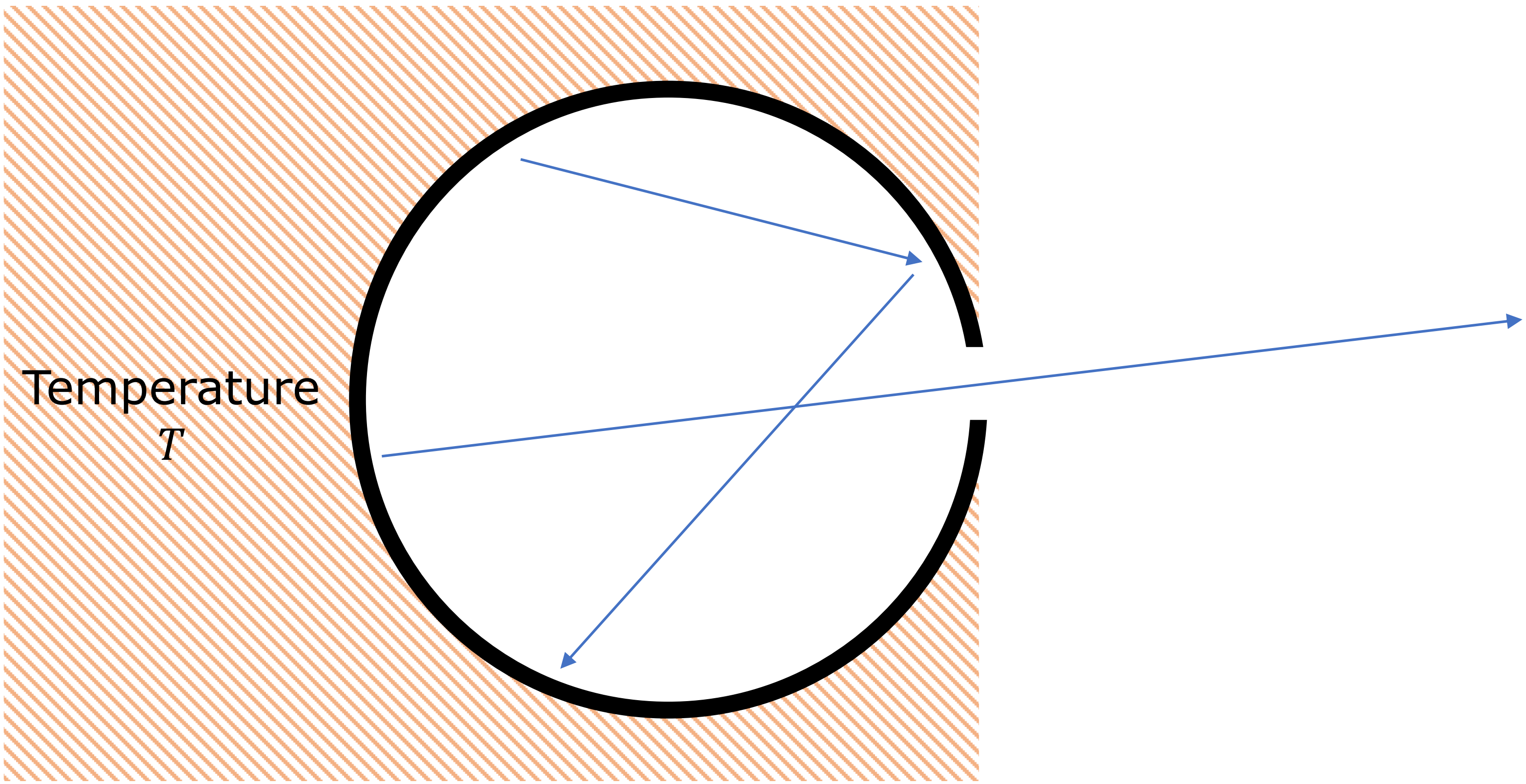
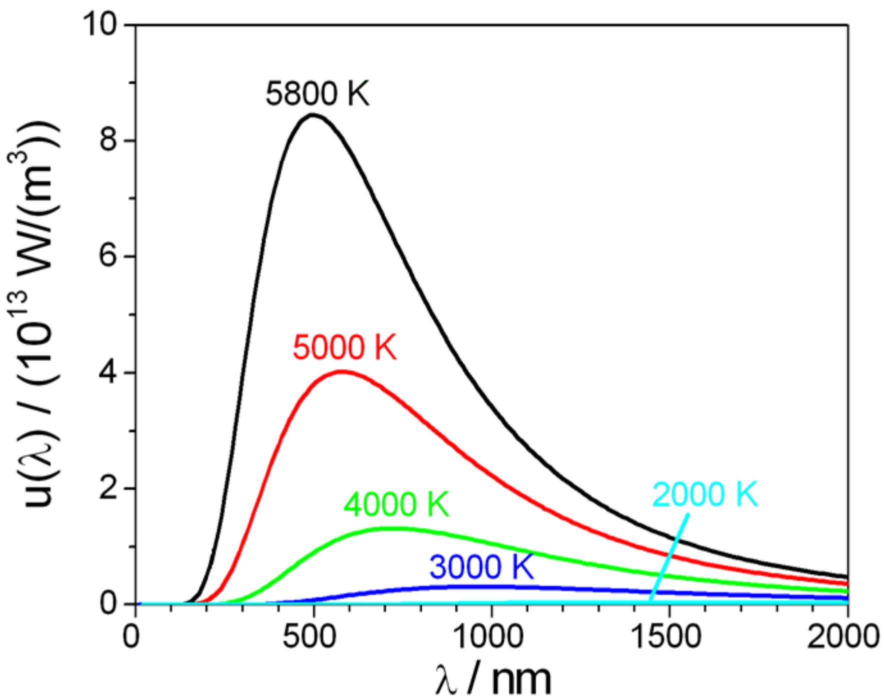
Outline

- Radiative (heat & momentum) transfer, experimental background
- NEGF theory of energy, momentum, and angular momentum transfer
  - N + 1 objects, bath at infinity
  - Meir-Wingreen/Landauer formula
  - Zero-point motion, when it contributes?
- Applications
  - Near-field heat transfer between graphene objects
  - Angular momentum emission from current-driven benzene molecule
  - Nonreciprocity, graphene edge effect

Blackbody radiation



Experimental background, blackbody radiation



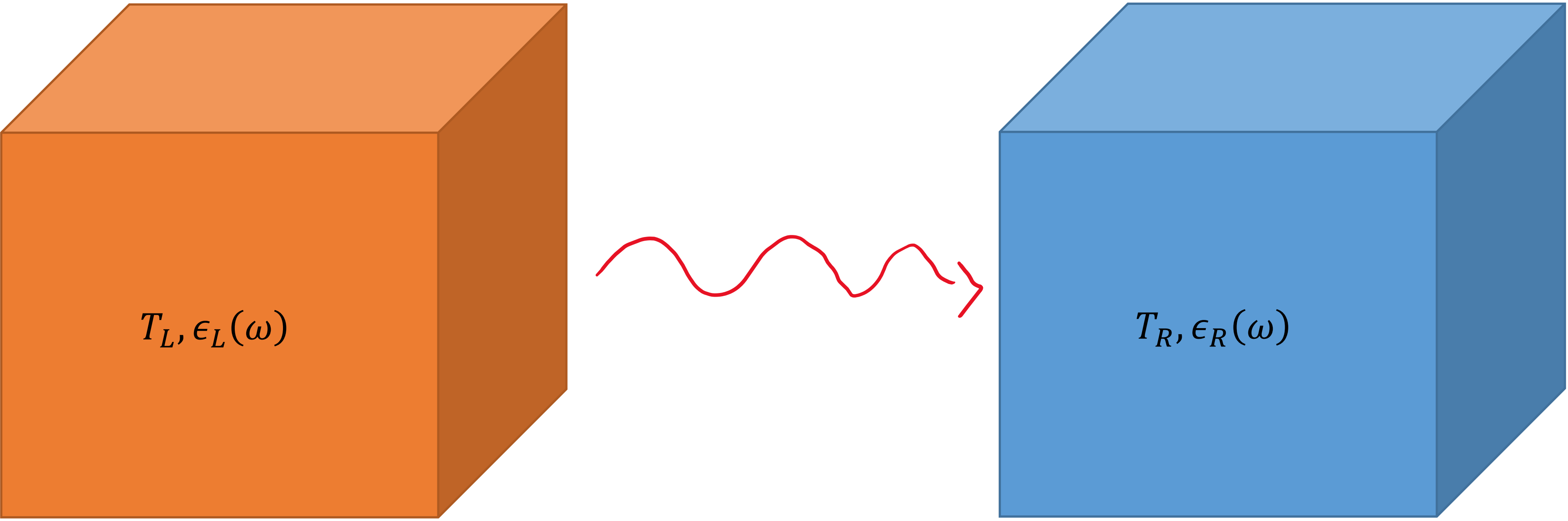
Stefan-Boltzmann law:

$$\langle S \rangle = \sigma T^4$$

Poynting vector

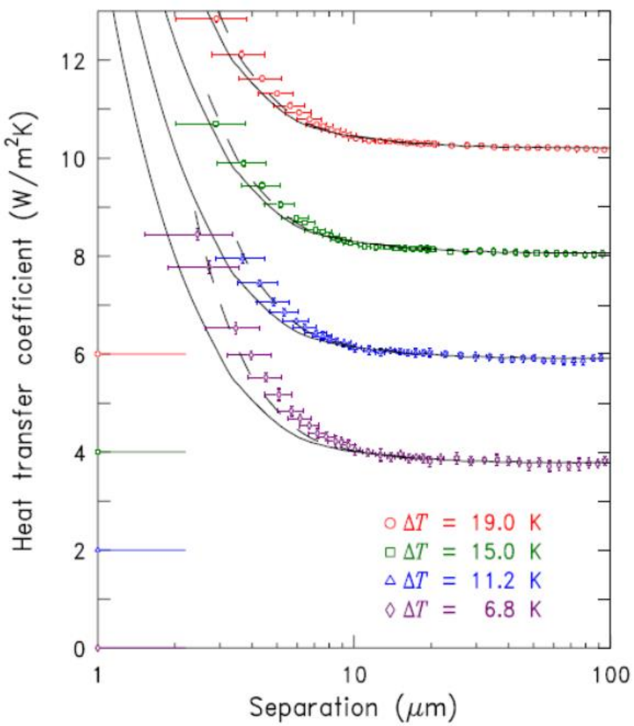
$$\mathbf{S} = \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B}$$

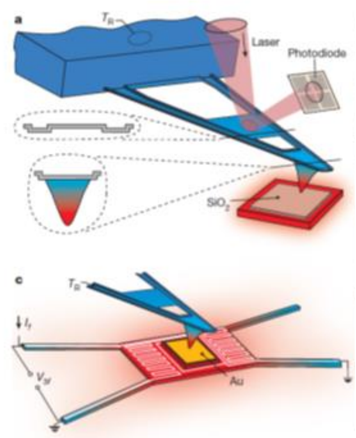
Heat transfer between (grey) bodies

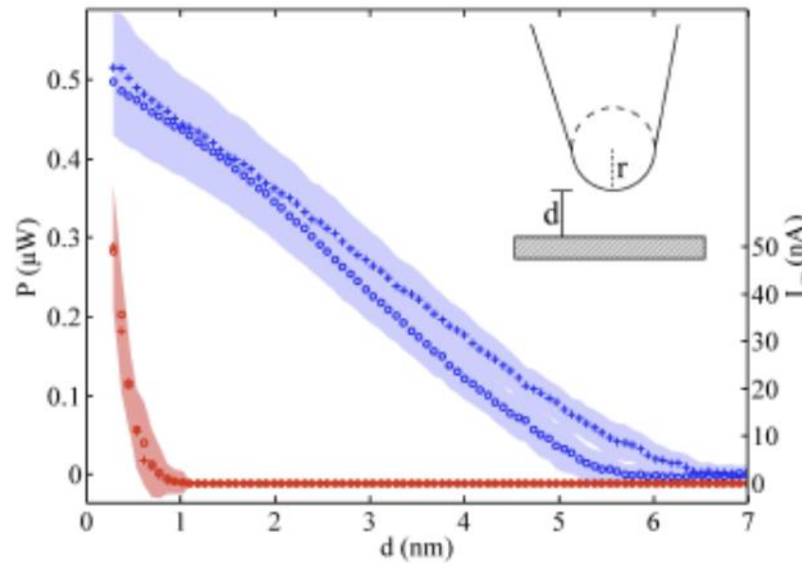


Polder & van Hove problem (1971)

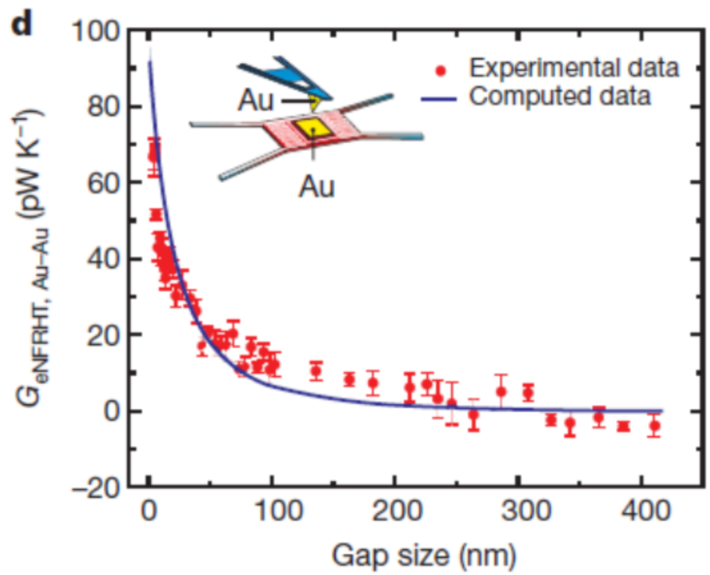
Near-field heat transfer







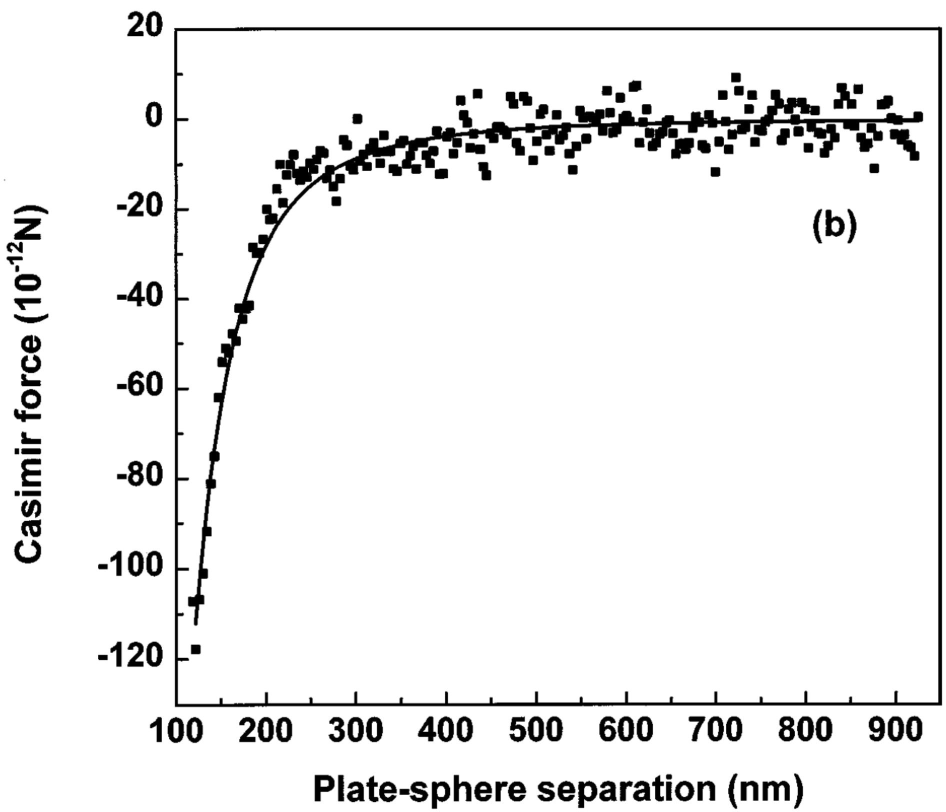
↑ Kloppstech, et al, Nature Comm (2017).

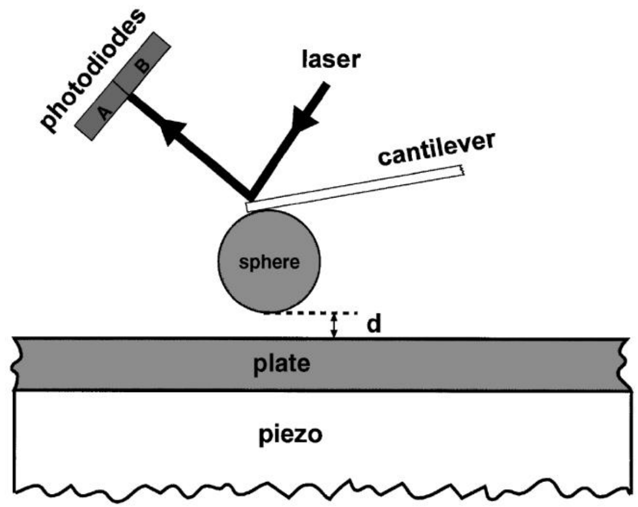


↑ Ottens, et al PRL (2011).

→ Kim et al, Nature (2015).

(Casimir) force

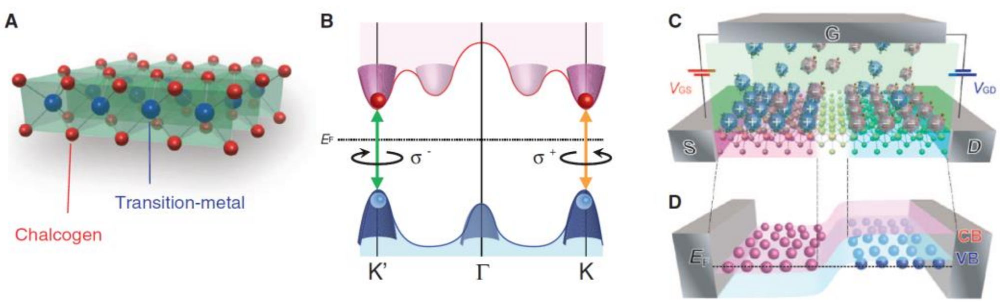




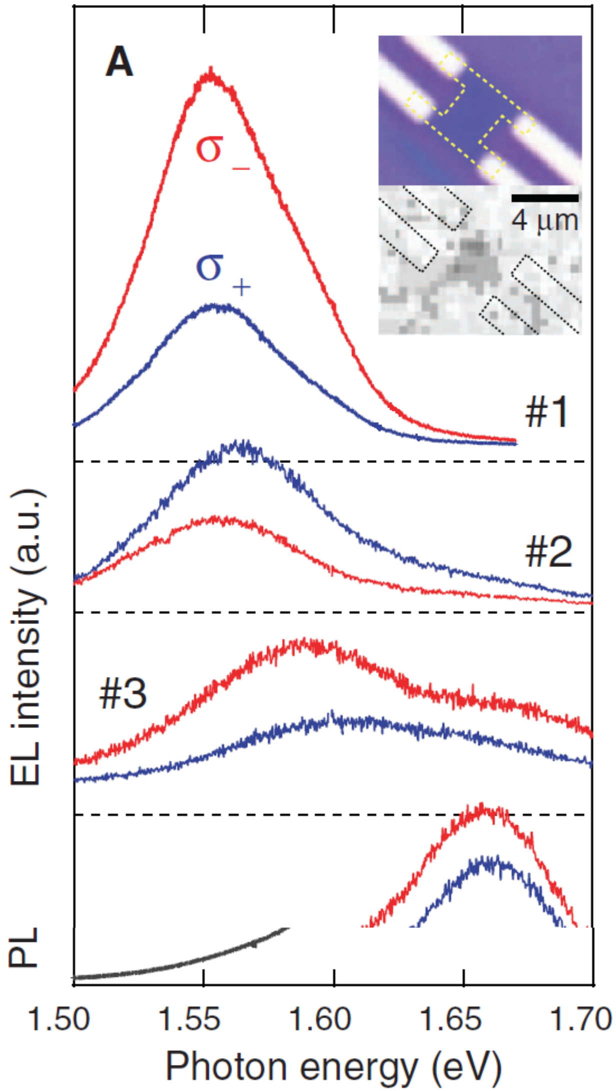
Casimir force in plate-sphere geometry, from Mohideen and Roy, PRL (1998).

$$F \approx -\frac{\pi^3 R\hbar c}{360\, d^3}$$

Angular momentum emission



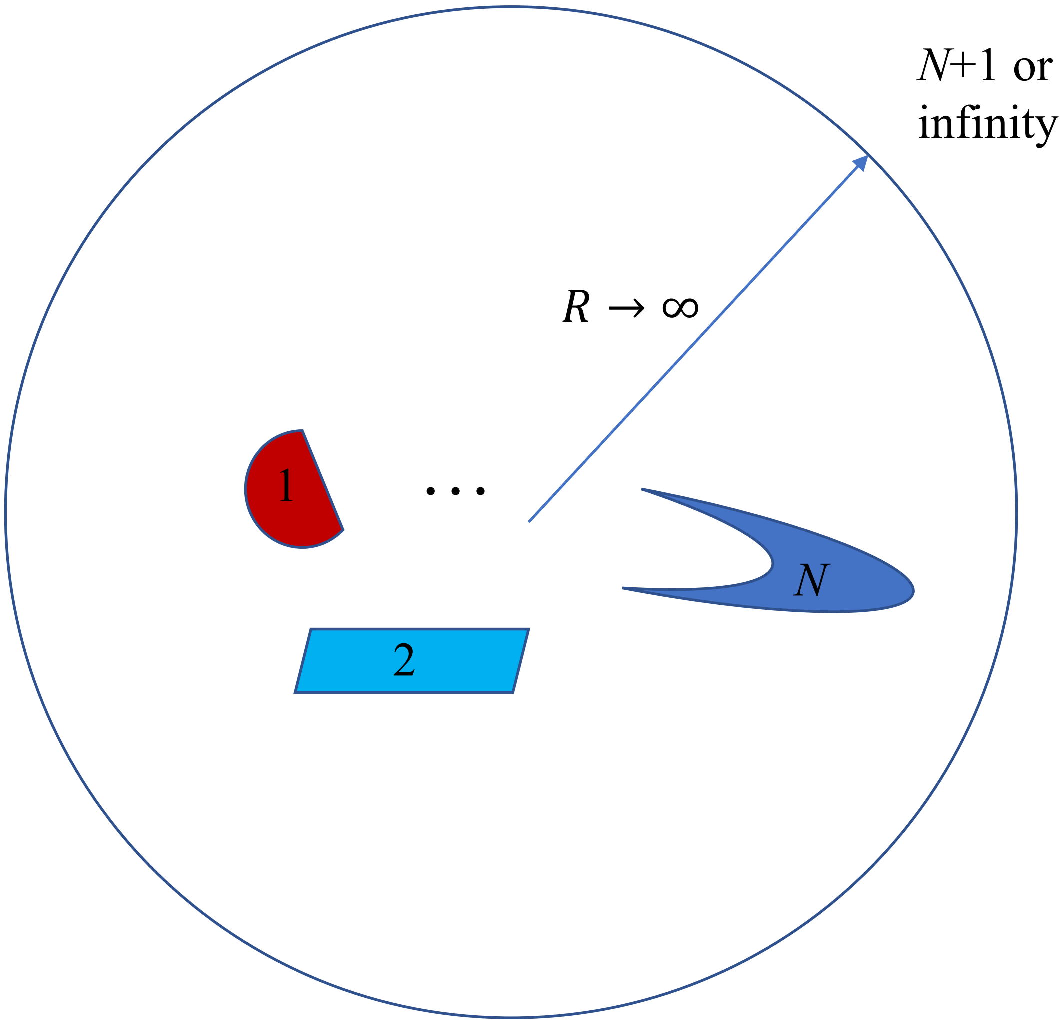
2D semiconductor junction made of WSe_2 that can emit polarized light. From Y. J. Zhang, et al., Science 344, 725 (2014).



Nonequilibrium Green's function (NEGF) theory

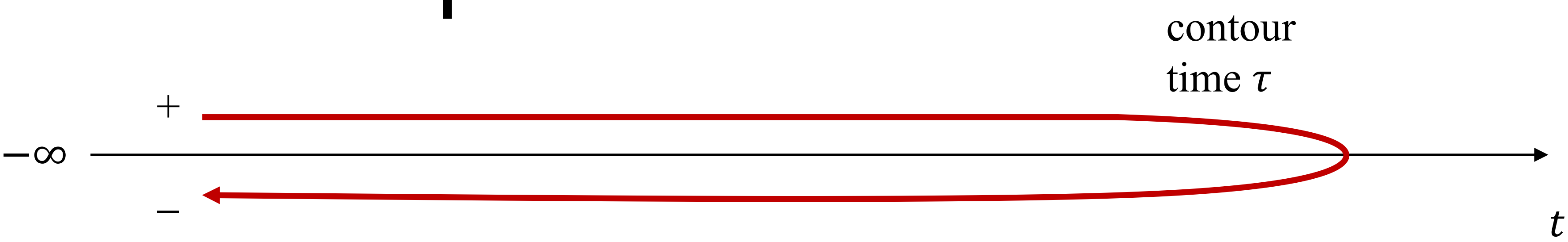
https://phyweb.physics.nus.edu.sg/~phywjs/NEGF/review-2022.pdf

System setup



Question: what are the energy emitted, force and torque applied to, for each of the object 1 to *N*+1.

NEGF preliminaries



$$D_{\mu\nu}(\mathbf{r},\tau;\mathbf{r}',\tau') = \frac{1}{i\hbar}\left\langle T_\tau\, A_\mu(\mathbf{r},\tau) A_\nu(\mathbf{r}',\tau')\right\rangle \;\rightarrow\; \begin{bmatrix} D^t & D^< \\ D^> & D^{\bar{t}} \end{bmatrix} \qquad \mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla\times\mathbf{A}$$

$$\tau = (t, \pm) \qquad\qquad \mathbf{A} \rightarrow A_\mu, \quad \mu = x, y, z$$

$$D^r = D^t - D^<$$

$$D^t + D^{\bar{t}} = D^> + D^< = D^K, \qquad D^> - D^< = D^r - D^a, \qquad D^t - D^{\bar{t}} = G^r + G^a$$

$$D = v + v\Pi D \;\rightarrow\; \begin{cases} D^< = D^r(\Pi^< + \Pi^<_\infty)D^a \\ D^r = v^r + v^r\Pi^r D^r \end{cases} \qquad v^{-1} = -\varepsilon_0\left(\frac{\partial^2}{\partial\tau^2}U + c^2\nabla\times\nabla\times\right)$$

In equilibrium: $D^< = N(\omega)\left(D^r - D^a\right), \qquad N(\omega) = \dfrac{1}{e^{\beta\hbar\omega} - 1}$

NEGF definitions

$$D^{>}_{\mu\nu}(\mathbf{r},t;\mathbf{r}'t') = \frac{1}{i\hbar}\left\langle A_\mu(\mathbf{r},t)A_\nu(\mathbf{r}',t')\right\rangle$$

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A}$$

$$\mathbf{A} \to A_\mu, \quad \mu = x, y, z$$

$$D^{<}_{\mu\nu}(\mathbf{r},t;\mathbf{r}'t') = \frac{1}{i\hbar}\left\langle A_\nu(\mathbf{r}',t')A_\mu(\mathbf{r},t)\right\rangle$$

$$\langle \ldots \rangle = \mathrm{Tr}\left(\rho \cdots\right)$$

$$D^r = \theta(t-t')\left(D^> - D^<\right)$$

$$D^> + D^< = D^K, \qquad D^> - D^< = D^r - D^a = -iA$$

Fluctuation-dissipation theorem in thermal equilibrium

$$D^{<} = N\left(D^{r} - D^{a}\right), \qquad D^{>} = (N+1)\left(D^{r} - D^{a}\right)$$

$$D^{a} = \left(D^{r}\right)^{\dagger}$$

$$N = \frac{1}{e^{\beta\hbar\omega} - 1}$$

$$D^{<} \quad \rightarrow \quad D^{<}_{\mu\nu}(\omega; \mathbf{r}, \mathbf{r}')$$

$$\left(D^{<}\right)^{\dagger} = -D^{<}$$

Dyson equations

$$D = v + v\Pi D \quad \rightarrow \quad \begin{cases} D^< = D^r \left(\Pi^< + \Pi^<_\infty \right) D^a \\ D^r = v^r + v^r \Pi^r D^r \end{cases}$$

$$v^{-1} = -\varepsilon_0 \left(\frac{\partial^2}{\partial \tau^2} U + c^2 \nabla \times \nabla \times \right)$$

$$-\varepsilon_0 \left(\frac{\partial^2}{\partial t^2} U + c^2 \nabla \times \nabla \times \right) D^r(\mathbf{r}, \mathbf{r}'; t - t') = U \delta(t - t') \delta(\mathbf{r} - \mathbf{r}') +$$

$$\int d^3\mathbf{r}'' \int dt'' \, \Pi^r(\mathbf{r}, \mathbf{r}'', t - t'') D^r(\mathbf{r}'', \mathbf{r}', t'' - t')$$

$$U = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\mathbf{j} = -\Pi^r \mathbf{A}$$

Keldysh equation

$$D = v + v\Pi D \quad \rightarrow \quad \begin{cases} D^{<} = D^{r}\left(\Pi^{<} + \Pi_{\infty}^{<}\right)D^{a} \\ D^{r} = v^{r} + v^{r}\Pi^{r}D^{r} \end{cases}$$

$$v^{-1} = -\varepsilon_0\left(\frac{\partial^2}{\partial t^2}U + c^2\nabla\times\nabla\times\right)$$

$$\begin{aligned} D^{<} &= v^{<} + v^{r}\Pi^{r}D^{<} + v^{r}\Pi^{<}D^{a} + v^{<}\Pi^{a}D^{a} \\ &= D^{r}\Pi^{<}D^{a} + (I + D^{r}\Pi^{r})v^{<}(I + \Pi^{a}D^{a}) \\ &= D^{r}\left(\Pi^{<} + N_{\infty}\left((-v^{r})^{-1} + (v^{a})^{-1}\right)\right)D^{a} \end{aligned}$$

environment: $v^{<} = N_{\infty}(v^{r} - v^{a})$

$$\Pi_{\infty}^{r} = (-v^{r})^{-1}$$

φ = 0 gauge, fundamental equation for vector potential **A**

$$v^{-1}\mathbf{A} = -\varepsilon_0\left(\frac{\partial^2}{\partial t^2} + c^2\nabla\times\nabla\times\right)\mathbf{A} = -\mathbf{j}$$

$$\mathbf{A} = -v\,\mathbf{j}, \qquad \mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} \qquad \text{dyadic Green's function } \overleftrightarrow{\mathbf{G}} = -v/\mu_0$$

Quantization:

$$\left[A_\mu(\mathbf{r}), E_\nu(\mathbf{r}')\right] = -\frac{i\hbar}{\varepsilon_0}\delta_{\mu\nu}\delta\left(\mathbf{r}-\mathbf{r}'\right)$$

Complication in $\varphi = 0$ gauge

- Gauss's law not reflected in the equation of motion

- States need to be selected such that

$$\left(\nabla \cdot \mathbf{E} - \frac{\rho}{\varepsilon_0} \right) \left| \Psi \right\rangle = 0$$

Poynting theorem, steady state average

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{S} = -\mathbf{E} \cdot \mathbf{j} \qquad u = \frac{1}{2}\left(\varepsilon_0 \mathbf{E}^2 + \frac{1}{\mu_0} \mathbf{B}^2 \right)$$

$$\left\langle \frac{\partial u}{\partial t} \right\rangle = \frac{\partial}{\partial t} \langle u \rangle = 0 \qquad \mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t}$$

so $\langle \nabla \cdot \mathbf{S} \rangle = -\langle \mathbf{E} \cdot \mathbf{j} \rangle$ or $\oint d\mathbf{\Sigma} \cdot \langle \mathbf{S} \rangle = -\int dV \langle \mathbf{E} \cdot \mathbf{j} \rangle$

Momentum and angular momentum conservation

$$-\frac{1}{c^2}\frac{\partial \mathbf{S}}{\partial t} + \nabla \cdot \overleftrightarrow{\mathbf{T}} = \rho \mathbf{E} + \mathbf{j} \times \mathbf{B} = \mathbf{f}$$

$$\overleftrightarrow{\mathbf{T}} = \varepsilon_0 \mathbf{E}\mathbf{E} + \frac{1}{\mu_0}\mathbf{B}\mathbf{B} - u\mathbf{U}$$

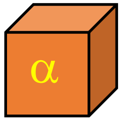
angular momentum density

$$\mathbf{l} = \mathbf{r} \times \mathbf{S} / c^2 = \varepsilon_0 \mathbf{r} \times \left(\mathbf{E} \times \mathbf{B} \right)$$

$$-\frac{\partial \mathbf{l}}{\partial t} - \nabla \cdot \left(\overleftrightarrow{\mathbf{T}} \times \mathbf{r} \right) = \mathbf{r} \times \mathbf{f}$$

From surface integral to volume integral

$$I_\alpha = \int d\mathbf{\Sigma}\cdot(\mathbf{E}\times\mathbf{B})\frac{1}{\mu_0} = -\int dV\,\mathbf{E}\cdot\mathbf{j} = \int dV\,\frac{\partial\mathbf{A}}{\partial t}\cdot\mathbf{j}$$



$$\mathbf{F}_\alpha = \int d\mathbf{\Sigma}\cdot\mathbf{T} = \int dV\,\mathbf{f} = \int dV\sum_\nu(\nabla A_\nu)j_\nu$$

$$\mathbf{N}_\alpha = \int \mathbf{r}\times\mathbf{T}\cdot d\mathbf{\Sigma} = \int dV\,\mathbf{r}\times\mathbf{f} = \int dV\left(\sum_\nu(\mathbf{r}\times\nabla A_\nu)\,j_\nu + \mathbf{j}\times\mathbf{A}\right)$$

$$\mathbf{f} = \rho\mathbf{E} + \mathbf{j}\times\mathbf{B}$$

$$\mathbf{T} = \varepsilon_0\mathbf{E}\mathbf{E} + \frac{1}{\mu_0}\mathbf{B}\mathbf{B} - u\mathbf{U}, \qquad u = \frac{1}{2}\left(\varepsilon_0\mathbf{E}^2 + \frac{1}{\mu_0}\mathbf{B}^2\right)$$

A-j correlation function

$$F^{\alpha}_{\mu\nu}(\mathbf{r}\tau;\mathbf{r}'\tau') = \frac{1}{i\hbar}\left\langle T_\tau A_\mu(\mathbf{r},\tau)\, j^{\alpha}_{\nu}(\mathbf{r}',\tau')\right\rangle$$

$$\sum_\alpha F^{\alpha} = -D\Pi \quad \to \quad \sum_\lambda \int d^3\mathbf{r}'' \int d\tau''\, D_{\mu\lambda}(\mathbf{r}\tau;\mathbf{r}''\tau'')\Pi_{\lambda\nu}(\mathbf{r}''\tau'';\mathbf{r}'\tau')$$

Assuming additivity: $\Pi \approx \sum_{\alpha=1}^{N} \Pi^{\alpha}$, then $F^{\alpha} = -D\Pi^{\alpha}$

In frequency domain, using Langreth rule, we have:

$$F^K = F^> + F^< = -(D\Pi)^K = -D^r\Pi^K - D^K\Pi^a$$

Hamiltonian, electron-photon system, temporal gauge

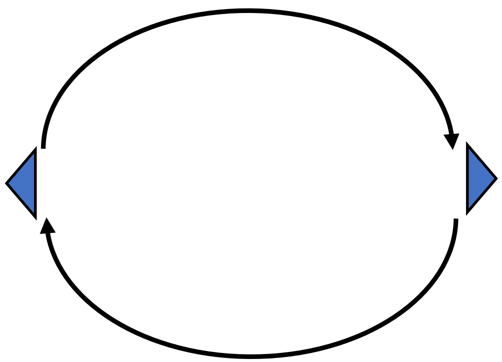
$$\hat{H} = \frac{\varepsilon_0}{2}\int dV\left[\left(\frac{\partial \mathbf{A}}{\partial t}\right)^2 + c^2\left(\nabla\times\mathbf{A}\right)^2\right]$$

$$+\sum_{j,l} c_j^\dagger H_{jl} c_l \exp\left(-i\frac{e}{\hbar}\int_l^j \mathbf{A}\cdot d\mathbf{r}\right)$$

electron charge is $-e$

Self energy Π

RPA



Aslamazov-Larkin diagram
(superconductivity, Coulomb drag)

$$H = H_0 + H_{\text{int}}$$

$$\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c} \approx \frac{1}{137}$$

$$H_{\text{int}} = -\int dV \mathbf{A} \cdot \mathbf{j} = \sum_{jkl\mu} c_j^\dagger M_{jk}^{l\mu} c_k A_\mu(\mathbf{r}_l)$$

$$D = v + v\Pi D$$

$$\Pi^r = \omega^2 \varepsilon_0 \left(1 - \varepsilon\right)$$
$$= -i\omega\sigma$$

$$\Pi_{l\mu,l'\nu}(\tau,\tau') = -i\hbar \,\mathrm{Tr}_e \left(M^{l\mu} G(\tau,\tau') M^{l'\nu} G(\tau',\tau) \right)$$

Operator order: normal or symmetric order?

$A^\dagger = A,\ B^\dagger = B,$ but $\langle AB \rangle$ is not a real number

Two choices: $\frac{1}{2}\langle AB + BA \rangle$ or normal order $\langle : AB : \rangle$

$$\frac{1}{2}\langle AB + BA \rangle = \mathrm{Re}\ i\hbar \int_0^\infty \frac{d\omega}{2\pi} G_{AB}^K(\omega)$$

$$G_{AB}(\tau, \tau') = \frac{1}{i\hbar}\langle A(\tau) B(\tau') \rangle \qquad G^K = G^> + G^<$$

Meir-Wingreen formula

$$\begin{pmatrix} I_\alpha \\ \mathbf{F}_\alpha \\ \mathbf{N}_\alpha \end{pmatrix} = -\int_0^\infty \frac{d\omega}{2\pi} \operatorname{Re}\operatorname{Tr}\left[\begin{pmatrix} -\hbar\omega \\ \hat{\mathbf{p}} \\ \hat{\mathbf{J}} \end{pmatrix} F_\alpha^K(\omega) \right], \qquad \alpha = 1, 2, \cdots, N, N+1$$

$$-F_\alpha^K = D^r \Pi_\alpha^K + D^K \Pi_\alpha^a \qquad F_{\mu\nu}(\mathbf{r}, \mathbf{r}', \omega)$$

$$\hat{\mathbf{p}} = \frac{\hbar}{i}\nabla, \quad \hat{\mathbf{J}} = \mathbf{r} \times \hat{\mathbf{p}} + \hat{\mathbf{S}}, \quad S_{\nu\lambda}^\mu = (-i\hbar)\varepsilon_{\mu\nu\lambda}$$

Bath at infinity

Eckhardt, PRA 29, 1991 (1984)

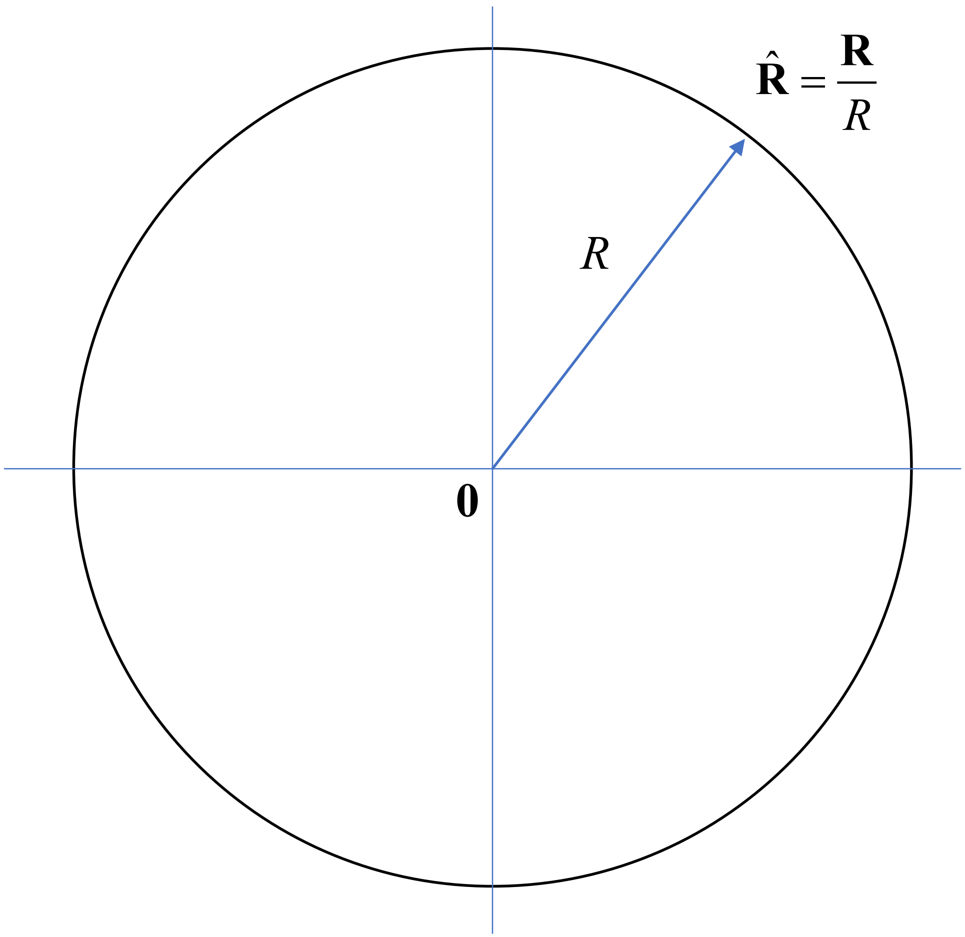
Krüger, et al, PRB 86, 115423 (2012)

$$\Pi_{\infty}^{r} = -(v^{r})^{-1}$$

$$\Pi_{\infty}^{r} = -i\varepsilon_{0} c\omega \left(\mathbf{U} - \hat{\mathbf{R}}\hat{\mathbf{R}} \right)$$

$$\hat{\mathbf{R}} = \frac{\mathbf{R}}{R}$$

Recover blackbody Planck result



$$\Pi_{\infty}^{r} = -i\varepsilon_0 c\omega\left(\mathbf{U} - \hat{\mathbf{R}}\hat{\mathbf{R}}\right)$$

$$\hat{\mathbf{R}} = \frac{\mathbf{R}}{R}$$

$$u = \frac{1}{2}\left(\varepsilon_0 \mathbf{E}^2 + \frac{\mathbf{B}^2}{\mu_0}\right)$$

$$\left\langle u(\mathbf{r}=\mathbf{0})\right\rangle = \int_0^\infty \frac{d\omega}{2\pi} i\hbar \,\mathrm{Tr}_\mu \left[\varepsilon_0 \omega^2 D^< - \frac{1}{\mu_0}\nabla_{\mathbf{r}} \times D^< \times \nabla_{\mathbf{r}'}\right]_{\mathbf{r}=\mathbf{r}'=\mathbf{0}}$$

$$= \int_0^\infty d\omega \frac{\omega^2}{\pi^2 c^3} \hbar\omega N(\omega)$$

$$D^< = D^r \Pi_\infty^< D^a, \quad \Pi_\infty^< = N(\omega)\left(\Pi_\infty^r - \Pi_\infty^a\right)$$

$$D^r \approx -\frac{e^{i\frac{\omega}{c}R}}{4\pi\varepsilon_0 c^2 R}\left(\mathbf{U} - \hat{\mathbf{R}}\hat{\mathbf{R}}\right)$$

From Meir-Wingreen to Landauer: local equilibrium approximation

$$-F_\alpha^K = D^r \Pi_\alpha^K + D^K \Pi_\alpha^a$$

$$\Pi_\alpha^K = -i\left(2N_\alpha + 1\right)\Gamma_\alpha$$

$$\Gamma_\alpha = i\left(\Pi_\alpha^r - \Pi_\alpha^a\right)$$

$$D^K = D^r \sum_{\beta=1}^{N+1} \Pi_\beta^K \, D^a$$

No Landauer form for force and torque!

$$I_\alpha = \int_0^\infty \frac{d\omega}{2\pi} \hbar\omega \sum_{\beta=1}^{N+1} \left(N_\alpha - N_\beta\right) \mathrm{Tr}\left(D^r \Gamma_\beta D^a \Gamma_\alpha\right)$$

When zero-point-motion contribution is cancelled?

temperature $T \to 0$

$N \to 0$ when $\omega > 0$

$$\int_0^\infty \frac{d\omega}{2\pi} \mathrm{Tr}\left[\hat{O} \left(D^r (\Pi_\alpha^r - \Pi_\alpha^a) + D^r \sum_{\beta=1}^{N+1} \left(\Pi_\beta^r - \Pi_\beta^a \right) D^a \Pi_\alpha^a \right) \right] = 0\,?$$

$\hat{O} = -\hbar\omega$ or $\hat{\mathbf{p}}$ or $\hat{\mathbf{J}}$

Emission to infinity

$$\begin{pmatrix} I_\infty \\ \mathbf{F}_\infty \\ \mathbf{N}_\infty \end{pmatrix} = \int_0^\infty \frac{d\omega}{2\pi} \operatorname{Re}\operatorname{Tr}\left[\begin{pmatrix} -\hbar\omega \\ \hat{\mathbf{p}} \\ \hat{\mathbf{J}} \end{pmatrix} D^r \Pi^< D^a \Pi_\infty^a \right]$$

$$\Pi_\infty^a = i\omega\varepsilon_0 c\left(\mathbf{U} - \hat{\mathbf{R}}\hat{\mathbf{R}}\right)$$

$$\hat{\mathbf{p}} = \frac{\hbar}{i}\nabla, \quad \hat{\mathbf{J}} = \mathbf{r}\times\hat{\mathbf{p}} + \hat{\mathbf{S}}, \quad S_{\nu\lambda}^{\mu} = (-i\hbar)\varepsilon_{\mu\nu\lambda}$$

Far field approximations

- Ignore screening or multiple reflection: $D^r \approx v^r$
- Multiple expansion: $D^r(\mathbf{R},\mathbf{r}) = D^r(\mathbf{R},0) - \mathbf{r}\cdot\nabla_{\mathbf{R}} D^r(\mathbf{R},0) + \cdots$
- Integrating over solid angle analytically, eigenmode representation for Π^r

$$-I_\infty = \frac{4\alpha}{3\hbar c^2}\sum_{\mu,n,n'}\left(\varepsilon_n - \varepsilon_{n'}\right)^2 \theta(\varepsilon_n - \varepsilon_{n'})\left|\langle n | V^\mu | n'\rangle\right|^2 f_n(1-f_{n'})$$

Fermi golden rule

$$\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \approx \frac{1}{137}$$

Torque and force on object

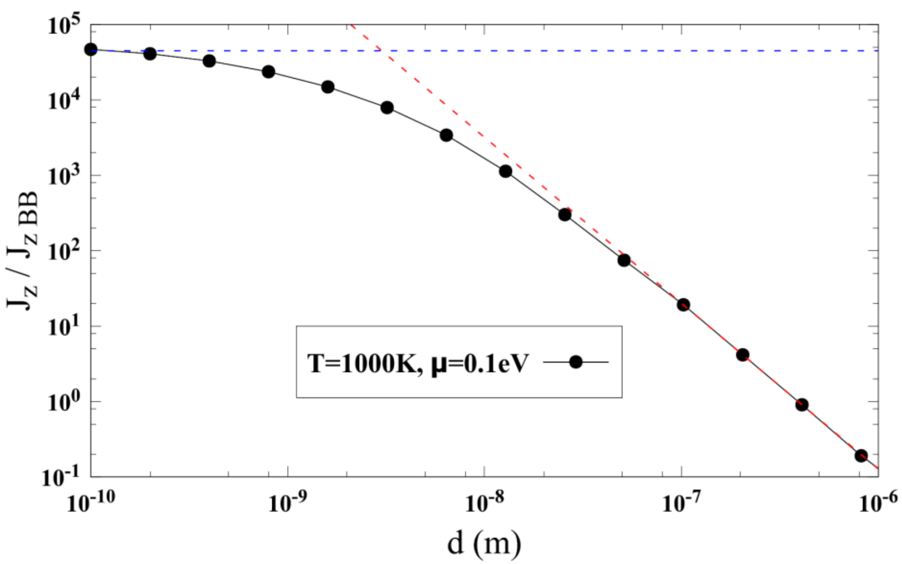
$$N_{\infty}^{\mu} = \int_{0}^{\infty} d\omega \frac{\hbar\omega}{6\pi^2\varepsilon_0 c^3} \sum_{\alpha,\beta} \varepsilon_{\mu\alpha\beta} \Pi_{\beta\alpha}^{<}, \qquad \mu = x, y, z$$

$$F_{\infty}^{\mu} = \int_{0}^{\infty} d\omega \frac{\hbar\omega^3}{60\pi^2\varepsilon_0 c^5} \sum_{l,l',\alpha} \left[4\Pi_{l\alpha,l'\alpha}^{<} \left(r_{\mu}^{l} - r_{\mu}^{l'} \right) - \left(r_{\alpha}^{l} - r_{\alpha}^{l'} \right) \Pi_{l\alpha,l'\mu}^{<} - \Pi_{l\mu,l'\alpha}^{<} \left(r_{\alpha}^{l} - r_{\alpha}^{l'} \right) \right]$$

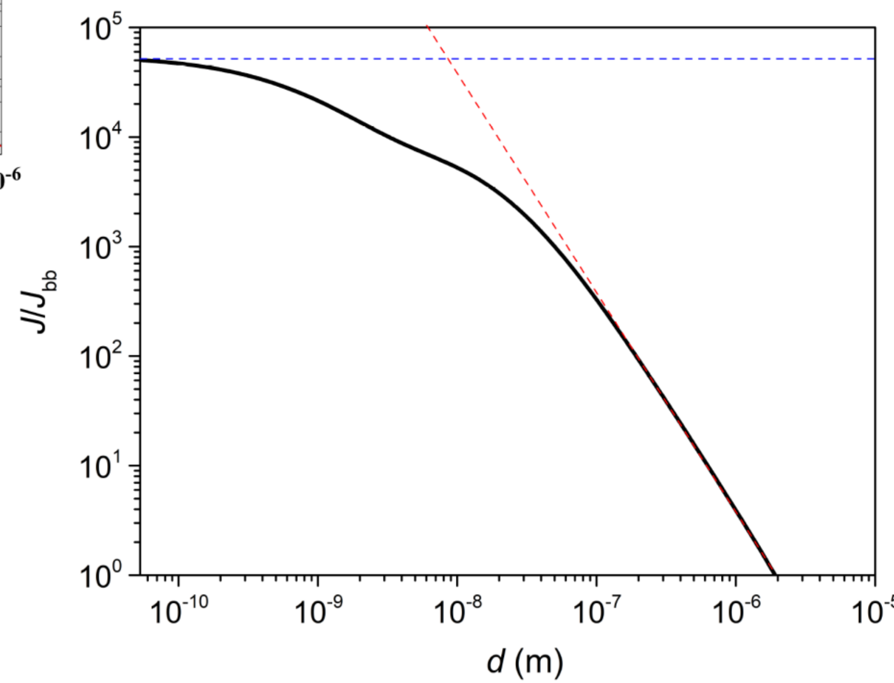
Force is zero if system is reciprocal, i.e., if $(\Pi^{<})^{T} = \Pi^{<}$

Applications

Heat transfer between two graphene sheets

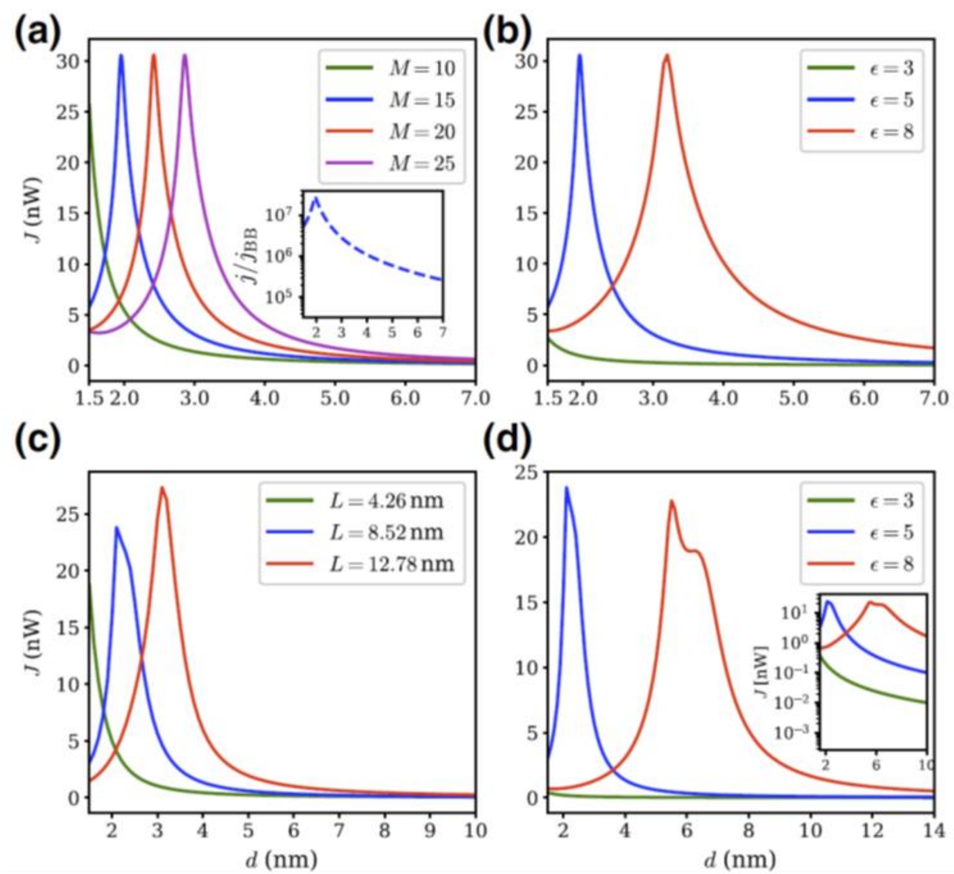


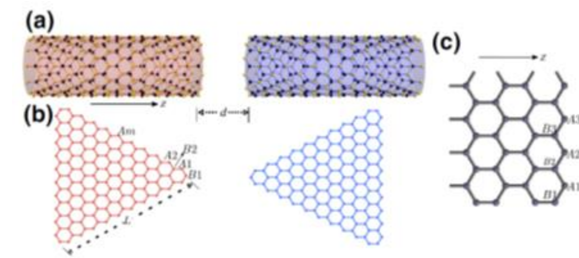
↓ First principles QE/BerkeleyGW calculation for the ratio of energy transfer to blackbody value between two graphene sheets at temperatures 300 K and 1000 K, η = 0.05 eV, electron chemical potential at Dirac point. Zhu & Wang, PRB 104, L121409 (2021).



↑ Heat transfer ratio based on electron tight-binding model with nearest neighbor hopping t = 2.8 eV, between 300 K and 1000 K sheets at chemical potential μ = 0.1 eV. Slope ≈ 2.2. Jiang & Wang, PRB 96, 155437 (2017).

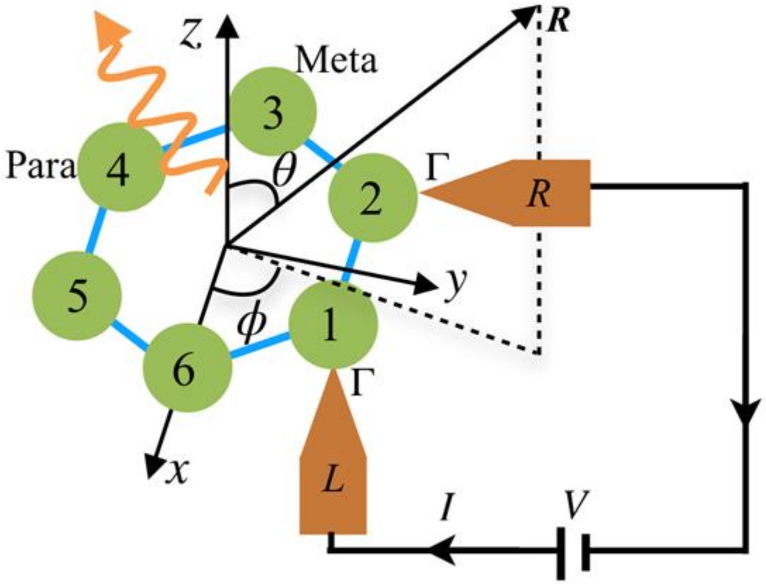
Heat transfer between zigzag nanotubes or triangles





Heat transfer from 400K to 300K objects. (a), (b) zigzag carbon nanotubes. (c), (d) nano-triangles. *d*: gap distance, *M*: nanotube circumference, *L*: triangle length. ε: dielectric constant. From Tang, Yap, Ren, and Wang, Phys. Rev. Appl. 11, 031004 (2019).

Angular momentum emission from a benzene molecule



$$P = -\int_0^\infty d\omega \frac{\hbar\omega^2}{6\pi^2\varepsilon_0 c^3} \,\mathrm{Im} \sum_{l,l',\mu} \Pi^<_{l\mu,l'\mu}(\omega)$$

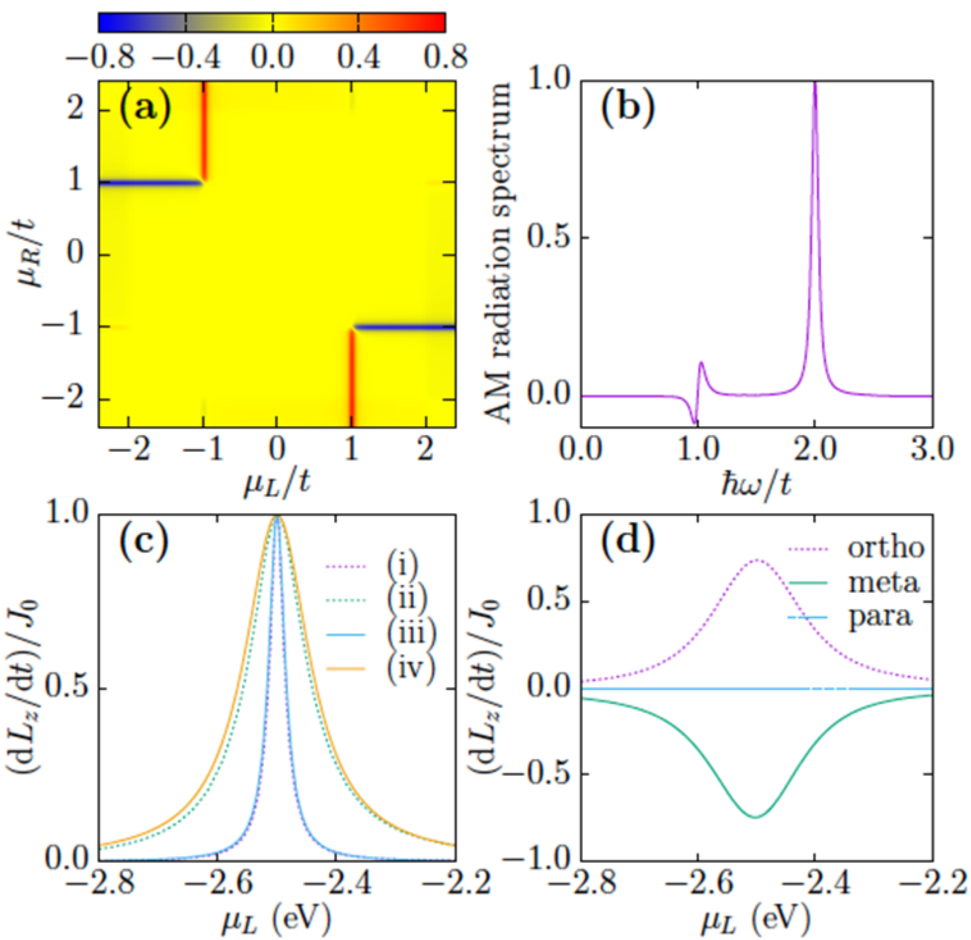
$$-N^z = \frac{dL^z}{dt} = \int_0^\infty d\omega \frac{\hbar\omega}{6\pi^2\varepsilon_0 c^3} \sum_{l,l'} \left(\Pi^<_{lx,l'y}(\omega) - \Pi^<_{ly,l'x}(\omega) \right)$$

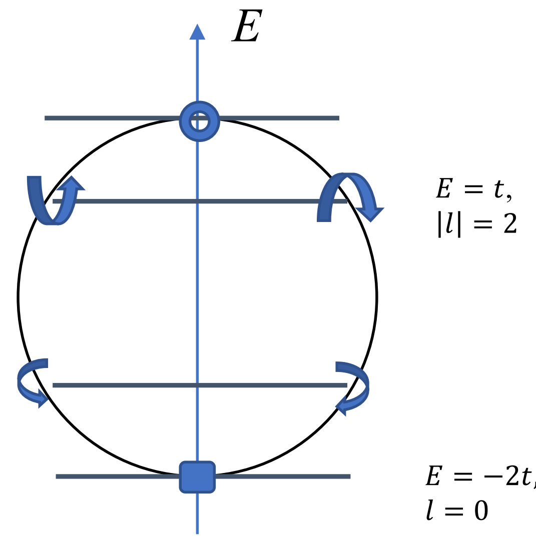
$$\Pi^<_{l\mu,l'\nu}(\omega) = -i \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \mathrm{Tr}\left[M^{l\mu} G^<(E) M^{l'\nu} G^>(E - \hbar\omega) \right]$$

$$H_{\mathrm{int}} = \sum_{l,\mu,j,k} c_j^\dagger M_{jk}^{l\mu} c_k A_\mu(\mathbf{r}_l)$$

Far field monopole approximation (all atoms are at the origin), ignore screening/multiple scatterings.

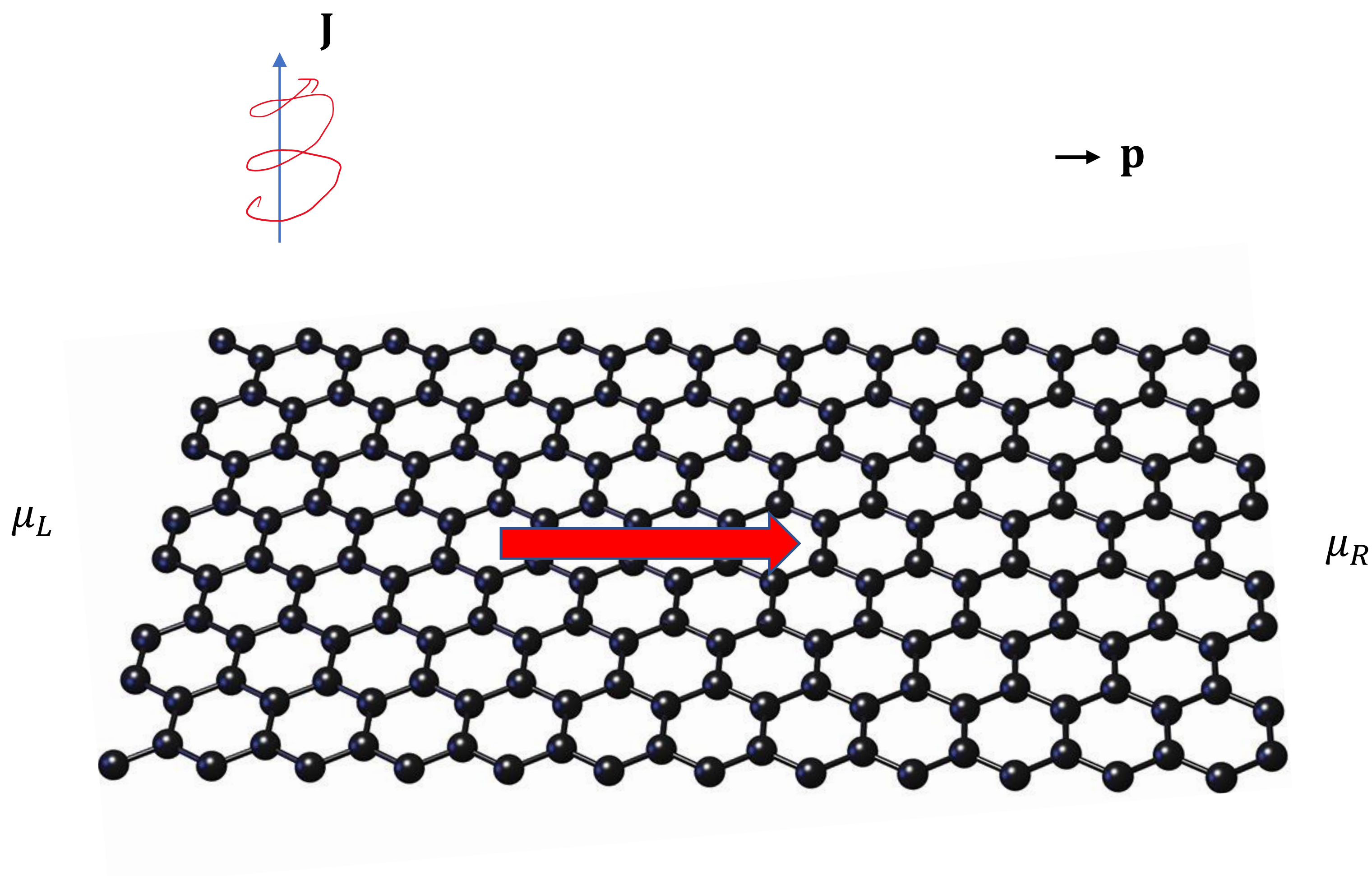
Angular momentum emission resonance effect



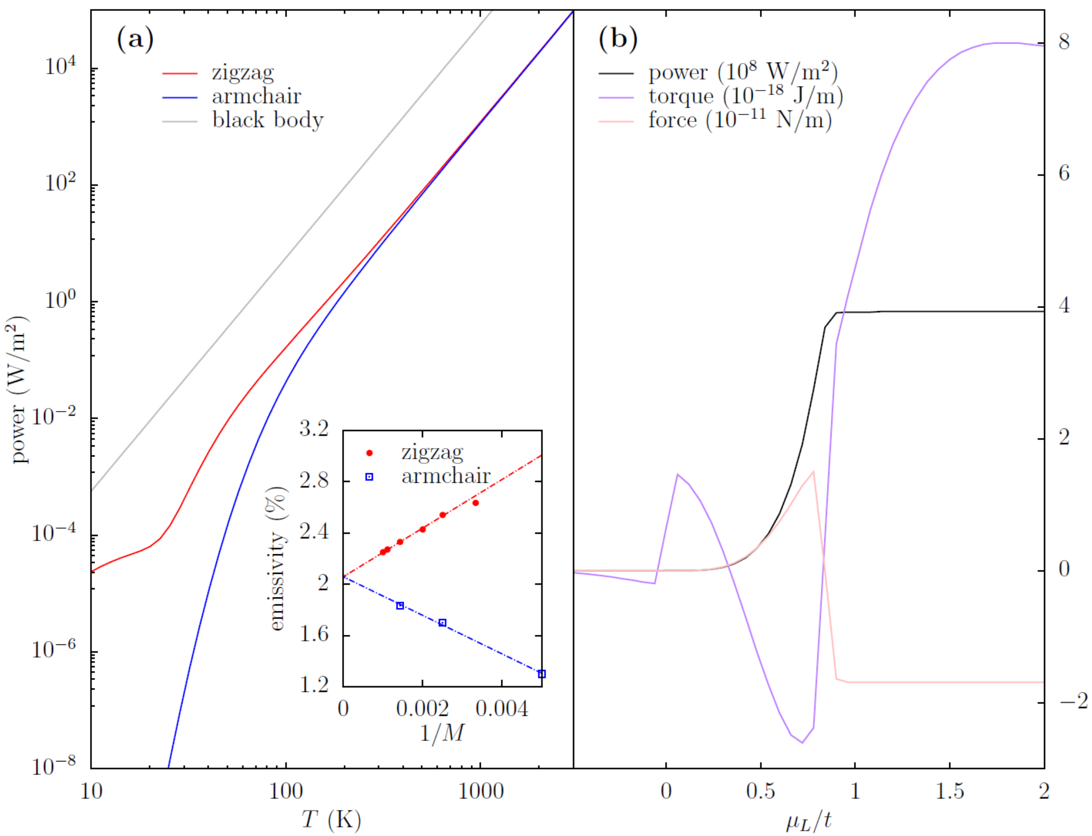


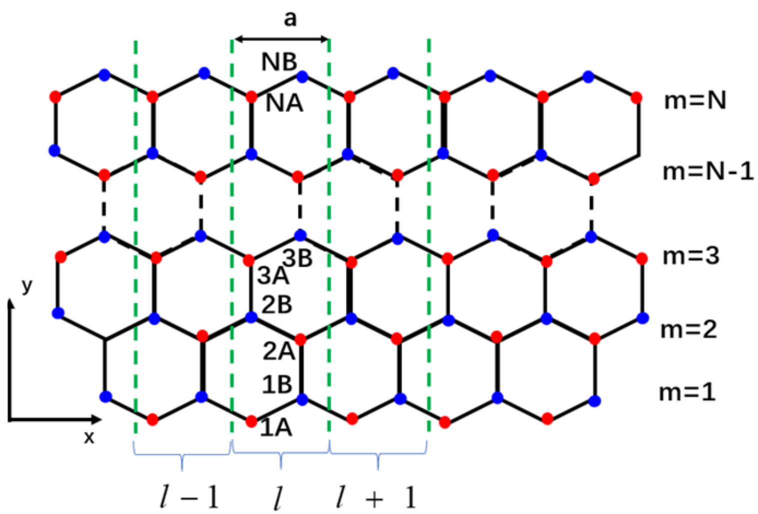
Largest angular momentum emission when one of the chemical potential meets the $E = +t$ energy level. From Zhang, Lü, and Wang, PRB 101, 161406(R) (2020).

Force and torque from the nonequilibrium edge

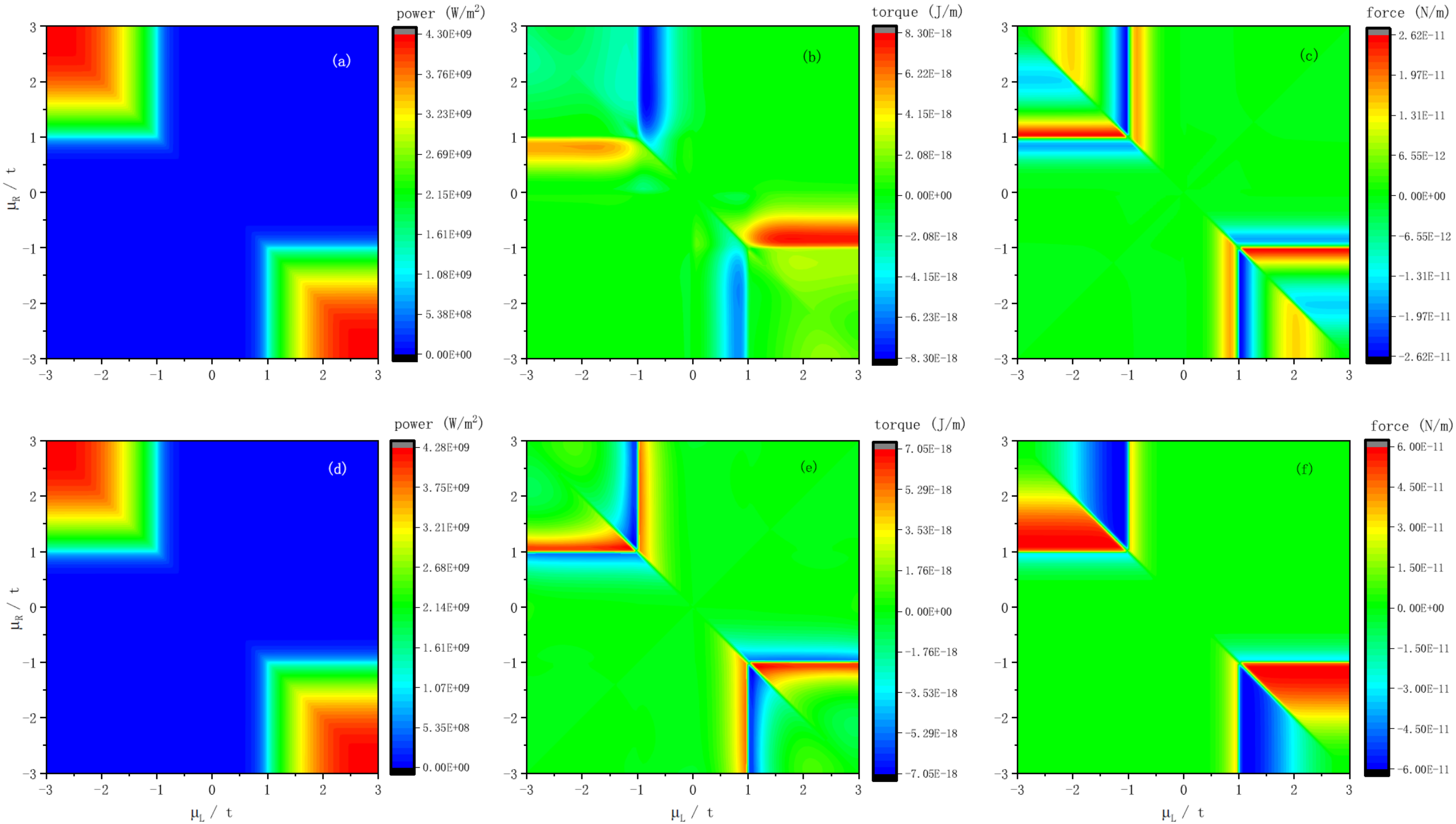


Emission from graphene edge





(a) Emission power as a function of temperature, (b) P, N, F as a function of μ_L fixing $\frac{\mu_R}{t} = -0.8$. Y.-M. Zhang, etc.



I, N, F scan μ_R vs μ_L. System size width 700 unit cells, k-point 401. From Zhang, et al, PRB 105, 205421 (2022).

Summary of NEGF approach

- Determine Π_α the photon-self energy for each object serving as bath
- Solve the Dyson equation $D^r = v + v\Pi^r D^r$
- Field distribution/correlation by the Keldysh equation $D^< = D^r \Pi^< D^a$
- Apply Meir-Wingreen or Landauer (when we have local equilibrium) formula to compute transport quantities: energy, momentum, and angular momentum

NEGF advantage

- Fully quantum-mechanical
- Local equilibrium or not, reciprocal or not, the theory is the same
- Strong coupling regime? E.g., cavity QED (different free Green's function v), or need self-consistent $\Pi_L(G_L, G_R)$?
- First-principle based materials properties, i.e., Π.

- Challenges: Large system sizes? Moving objects?

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left to right: Dr. Zhang Yong-Mei, Dr. Zhu Tao, Dr. Gao Zhibin, Prof. Wang Jian-Sheng, Mr. Sun Kangtai, and Dr. Zhang Zuquan.