Energy, momentum, and angular momentum transfers mediated by photons

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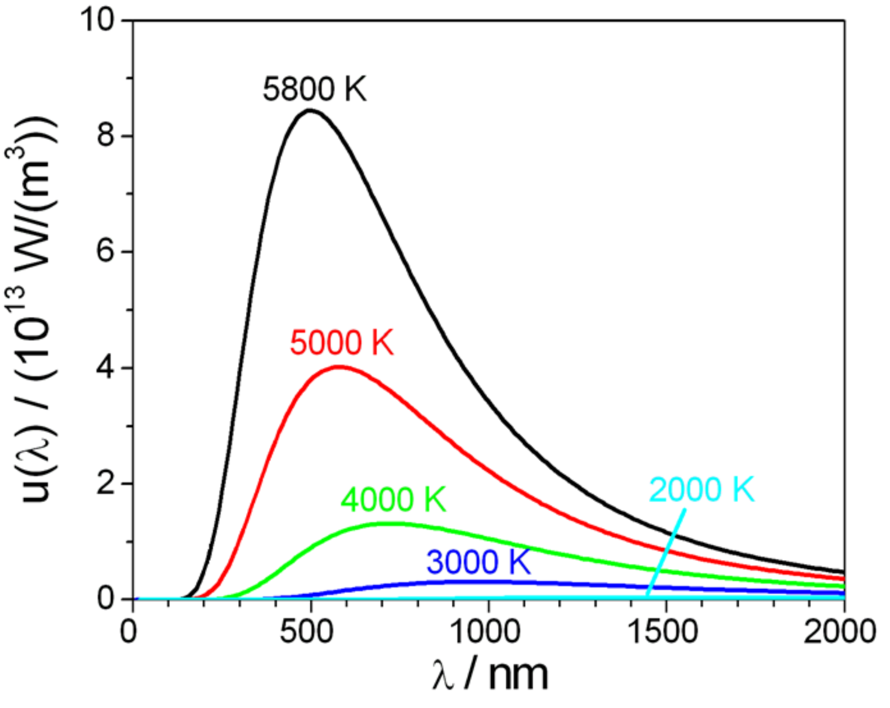
Outline

- Radiative (heat) 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
  - Graphene edge effect

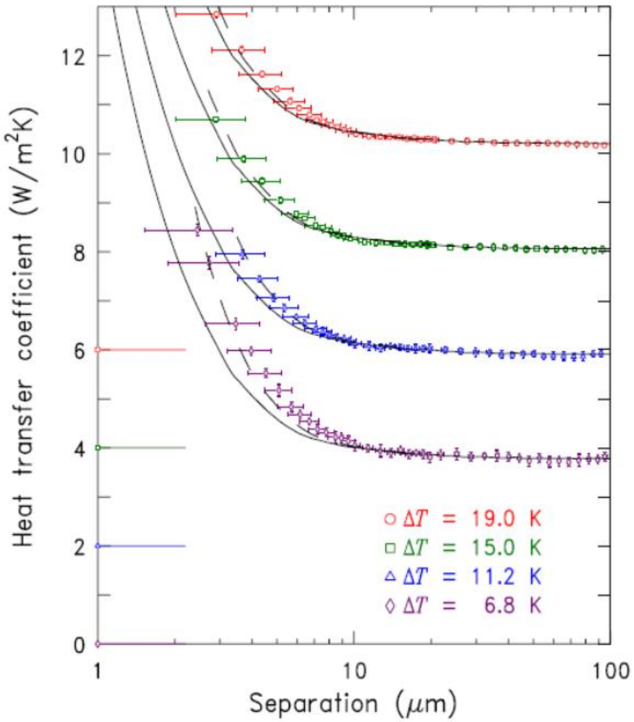
Experimental background, blackbody radiation

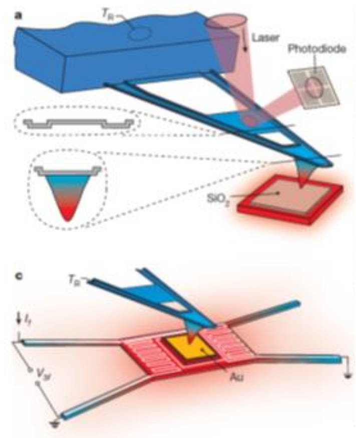


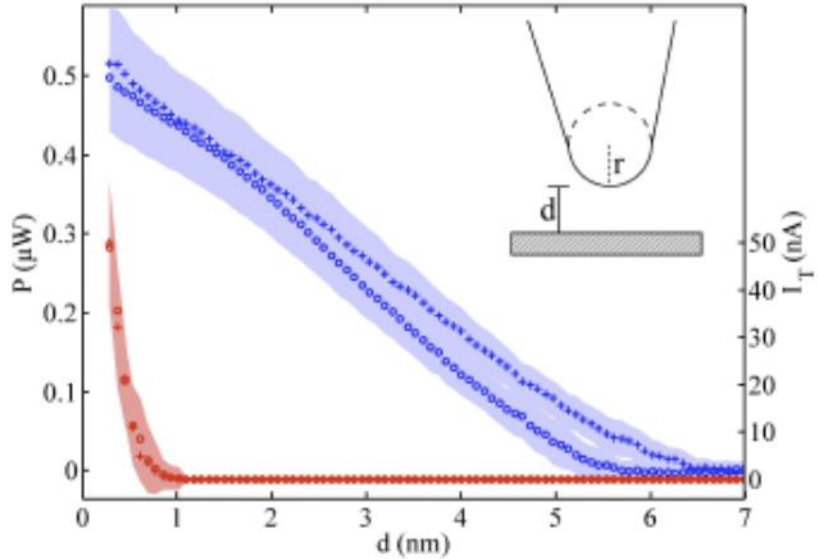
Stefan-Boltzmann law:

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

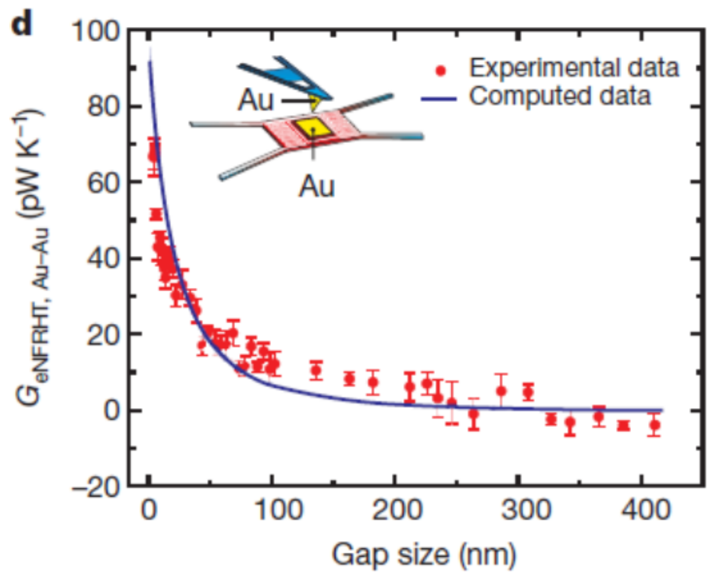
Near-field heat transfer







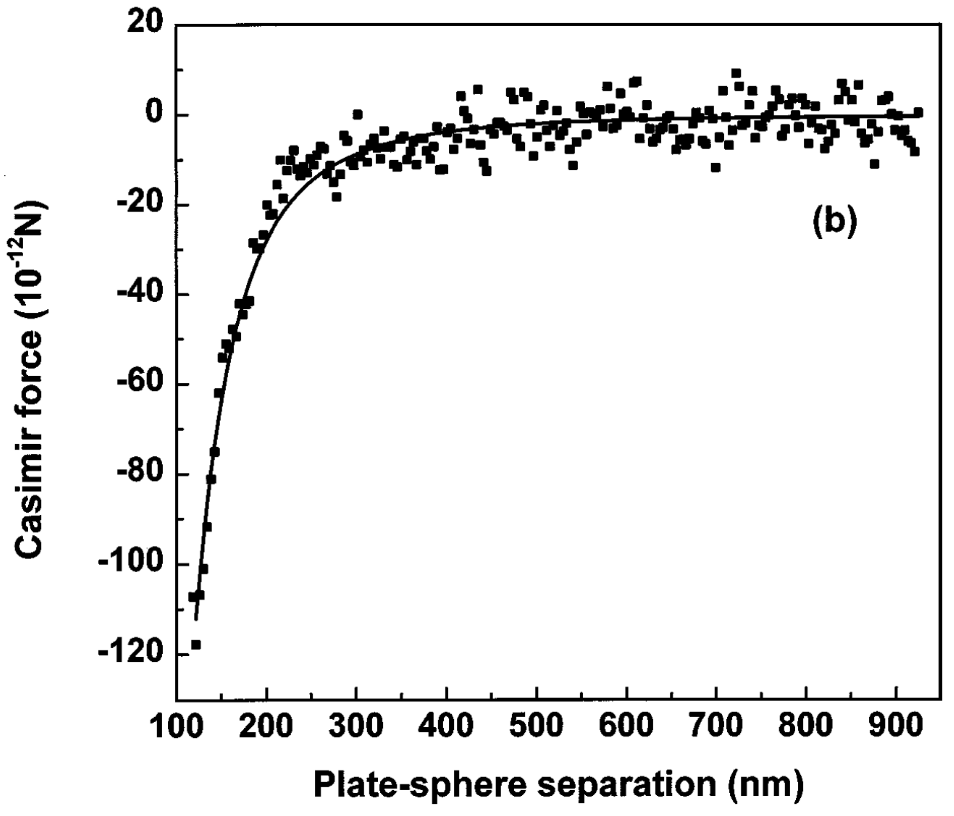
↑ Ottens, et al PRL (2011).

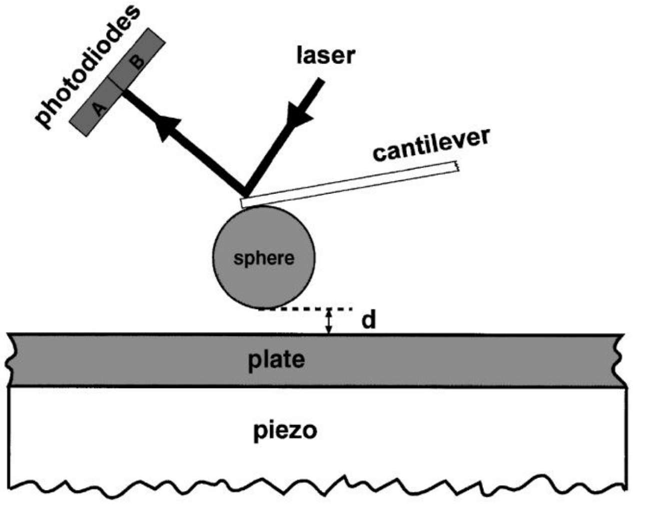


→ Kim et al, Nature (2015).

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

(Casimir) force

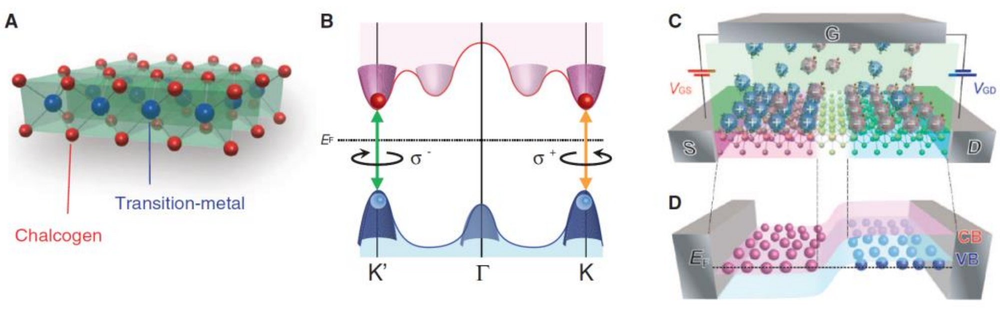


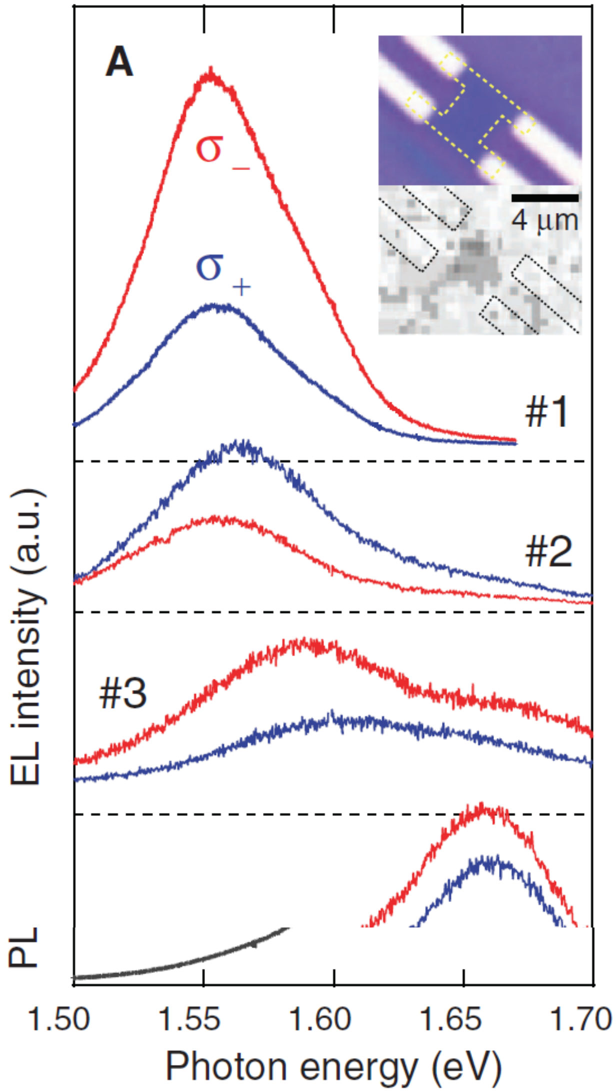


Casimir force in plate-sphere geometry, from Mohideen and Roy, PRL (1998).

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

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).

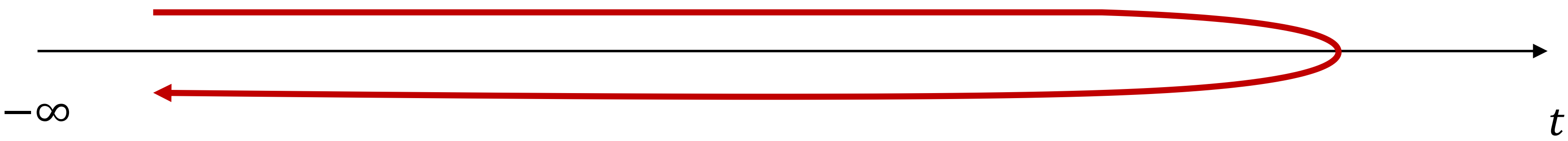
Nonequilibrium Green's function (NEGF) theory

A brief history of NEGF

- Schwinger 1961
- Kadanoff and Baym 1962
- Keldysh 1965
- Caroli, Combescot, Nozieres, and Saint-James 1971
- Meir and Wingreen 1992
- …

- J.-S. Wang, J. Wang, and J. T. Lü, “Quantum thermal transport in nanostructures,” Eur. Phys. J. B 62, 381 (2008); J.-S. Wang, B. K. Agarwalla, H. Li, and J. Thingna, “Nonequilibrium Green’s function method for quantum thermal transport,” Front. Phys. 9, 673 (2014).

Evolution on Keldysh contour

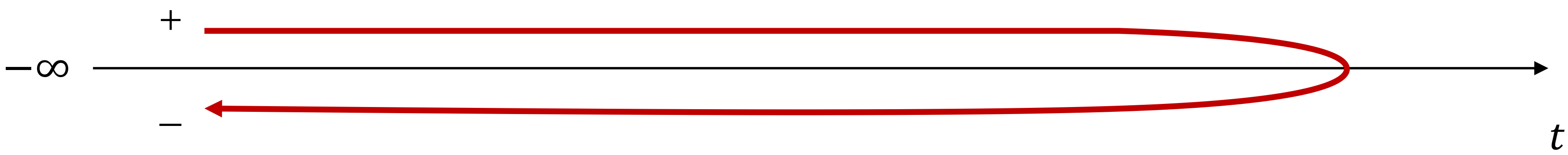


$$U(\tau_2,\tau_1) = T_\tau \exp\left(-\frac{i}{\hbar}\int_{\tau_1}^{\tau_2} H_\tau d\tau\right), \qquad \tau_2 \succ \tau_1$$

$$O(\tau) = U(t_0^+,\tau) O U(\tau, t_0^+)$$

$$i\hbar \frac{dO(\tau)}{d\tau} = [O(\tau), H]$$

NEGF preliminaries



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

$$\tau = (t, \pm)$$

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

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

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

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

$$D = v + v\Pi D \quad \rightarrow \quad \begin{cases} D^< = D^r \Pi^< D^a \\ D^r = v^r + v^r \Pi^r D^r \end{cases}$$

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

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

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

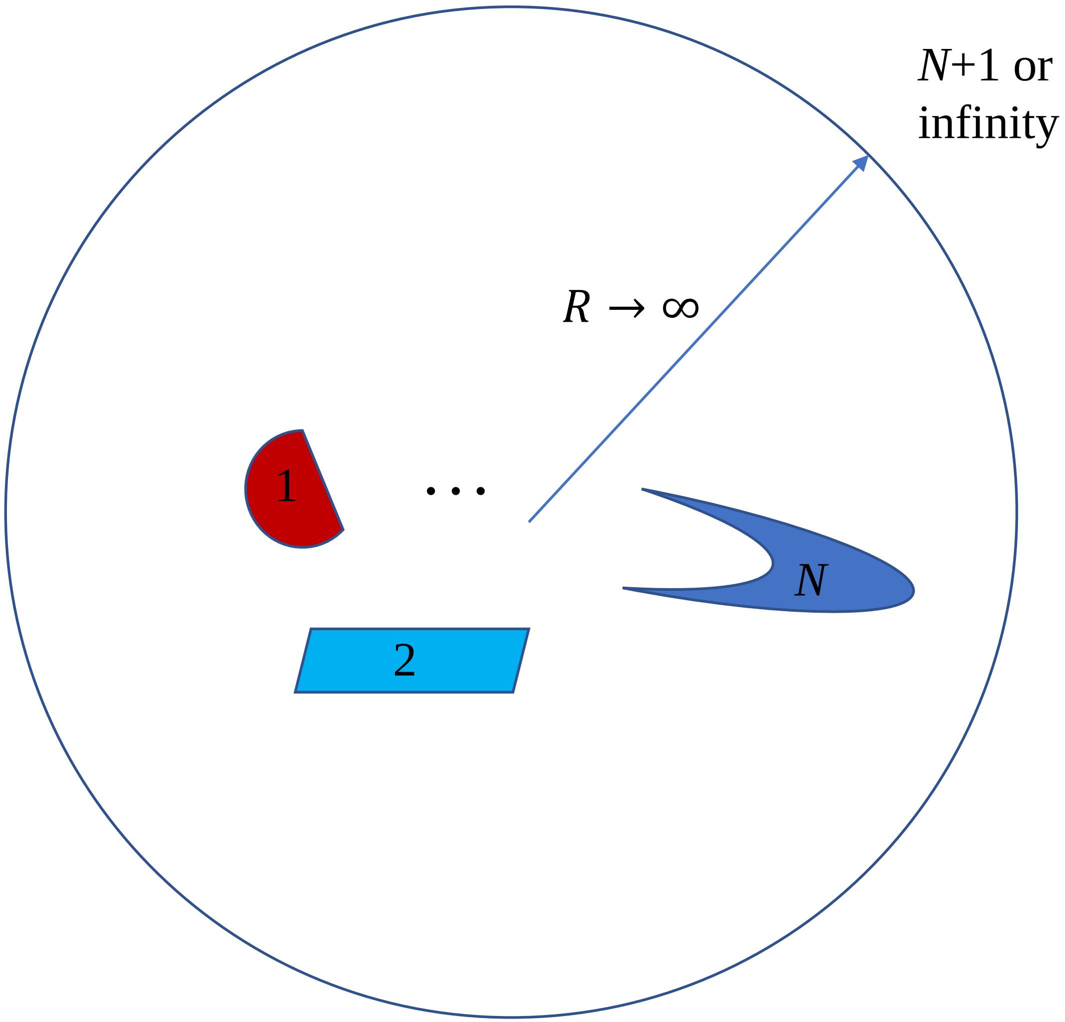
$$v^{-1}\mathbf{A} = -\varepsilon_0\left(\frac{\partial^2}{\partial t^2} + c^2\nabla\times\nabla\times\right)\mathbf{A} = -\mathbf{j}$$

$$\mathbf{A} = -v\,\mathbf{j}, \qquad \mathbf{E} = -\frac{\partial\mathbf{A}}{\partial t}$$

Quantization:

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

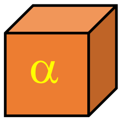
System setup



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

From surface integral to volume integral

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



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

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

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

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

A-j correlation function

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

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

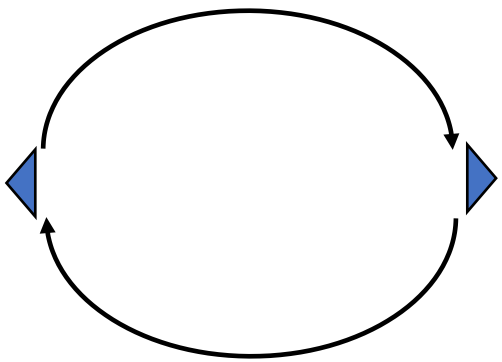
Assuming additivity: $\Pi \approx \sum_{\alpha=1}^{N+1} \Pi^{\alpha}$, then $F^{\alpha} = -D\Pi^{\alpha}$

In frequency domain, using Langreth rule, we have:

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

Self energy Π

RPA



Aslamazov-Larkin diagram

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

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

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

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

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

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

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 $\langle :AB: \rangle$

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

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

Meir-Wingreen formula

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

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

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

Bath at infinity

Eckhardt, PRA 29, 1991 (1984)

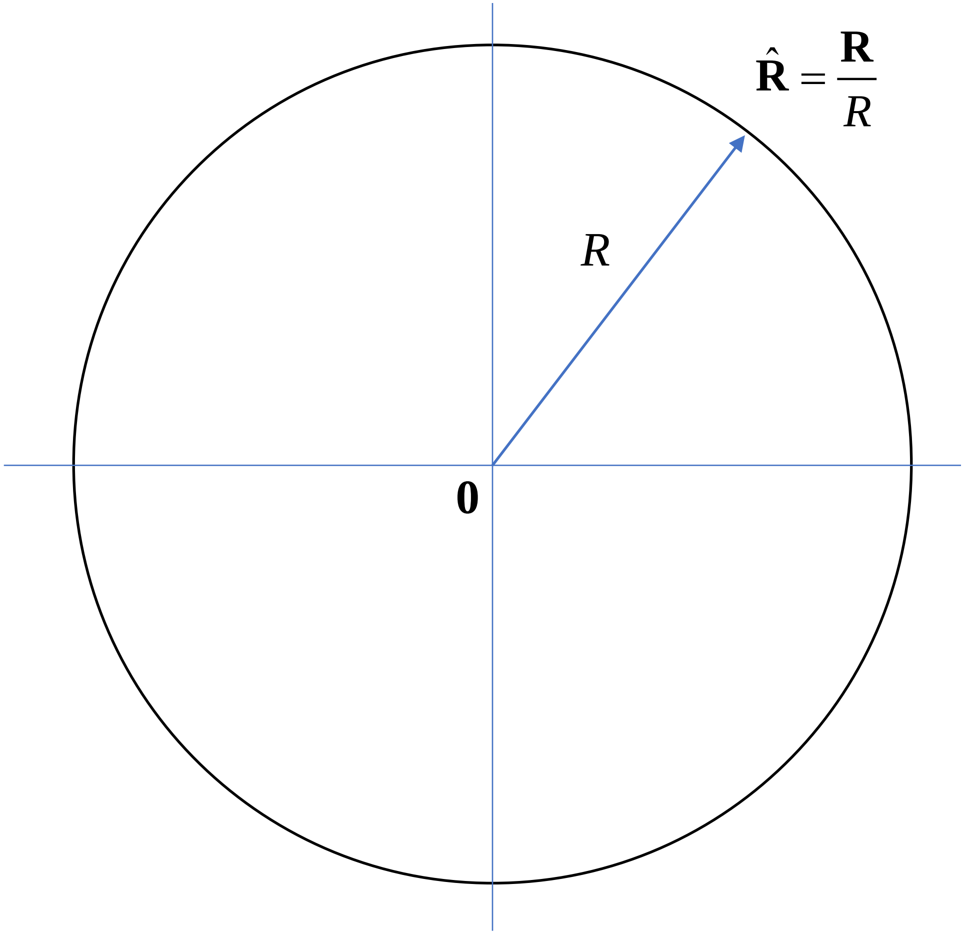
Krüger, et al, PRB 86, 115423 (2012)

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

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

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

Recover blackbody Planck result



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

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

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

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

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

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

$$D_0^r \approx -\frac{e^{i\frac{\omega}{c}R}}{4\pi\varepsilon_0 c^2 R}\left(\mathbf{U} - \hat{\mathbf{R}}\hat{\mathbf{R}}\right)$$

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?

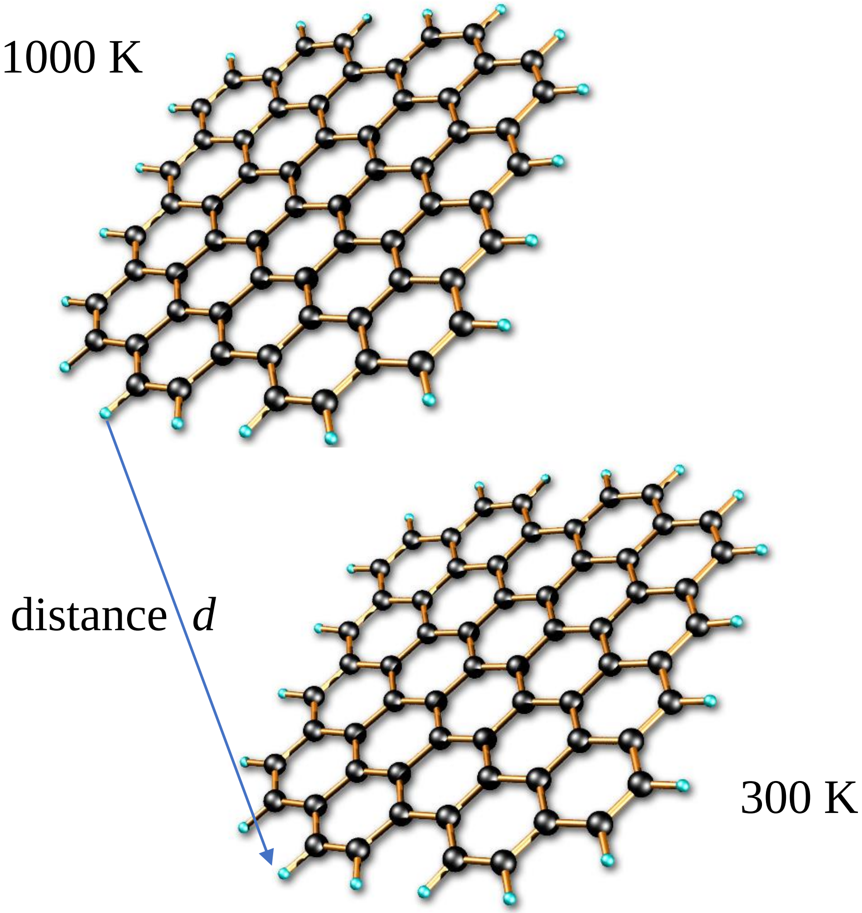
temperature $T \to 0$

$N \to 0 \quad \text{when} \quad \omega > 0$

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

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

“scalar field” theory, non-retardation limit



$$H = c^{\dagger} H c + H_{\phi} + H_{\text{int}}$$

$$H_{\phi} = -\frac{\varepsilon_0}{2}\int d^3\mathbf{r}\left[\left(\frac{\dot{\phi}}{\tilde{c}}\right)^2 + \left(\nabla\phi\right)^2\right], \qquad \tilde{c} \to \infty$$

$$H_{\text{int}} = -e\sum_{j\in\text{system}} c_j^{\dagger} c_j \phi(\mathbf{r}_j)$$

$$D(\mathbf{r},\tau;\mathbf{r}',\tau') = -\frac{i}{\hbar}\left\langle T_{\tau}\phi(\mathbf{r},\tau)\phi(\mathbf{r}',\tau')\right\rangle$$

$$G_{jk}(\tau;\tau') = -\frac{i}{\hbar}\left\langle T_{\tau} c_j(\tau) c_k^{\dagger}(\tau')\right\rangle$$

$$J_1 = \int_0^{\infty}\frac{d\omega}{2\pi}\hbar\omega\, T(\omega)\left(N_1 - N_2\right),$$

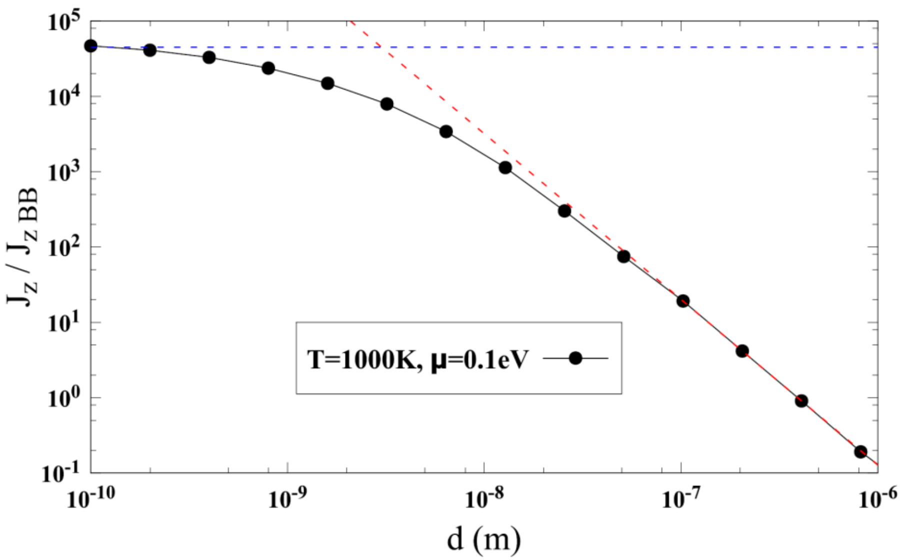
$$T(\omega) = \mathrm{Tr}\left(D^r\Gamma_1 D^a\Gamma_2\right)$$

$$\Gamma_{\alpha} = i\left(\Pi_{\alpha}^r - \Pi_{\alpha}^a\right), \qquad \alpha = 1,2$$

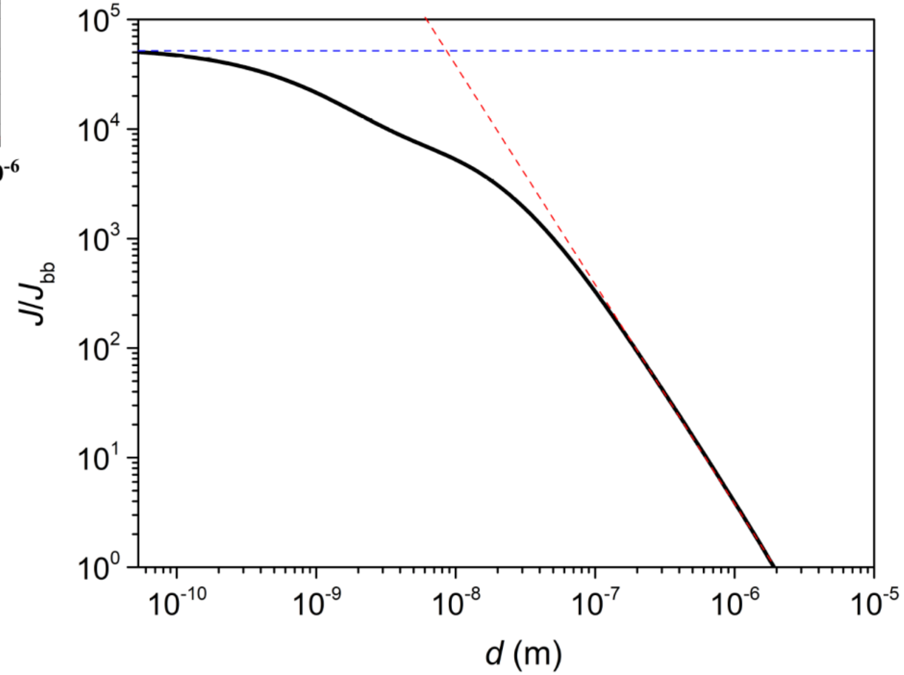
$$\Pi_{jk}(\tau,\tau') = -i\hbar e^2 G_{jk}(\tau,\tau') G_{kj}(\tau',\tau)$$

Applications

Heat transfer between two graphene sheets

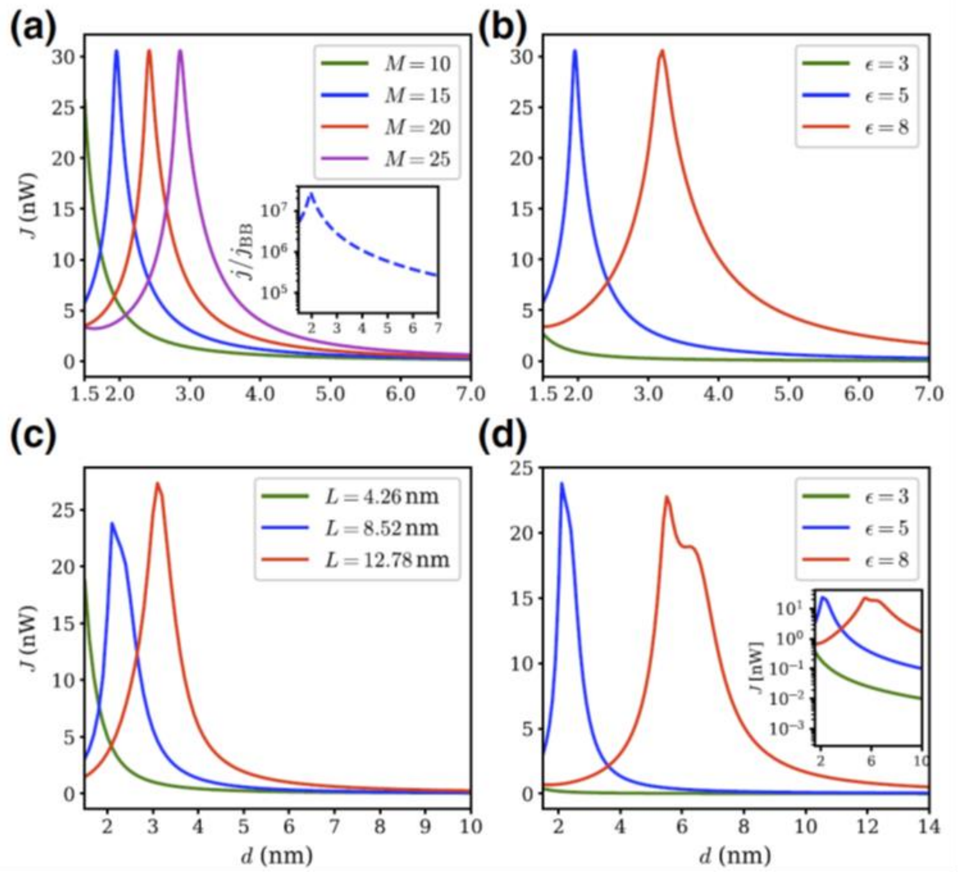


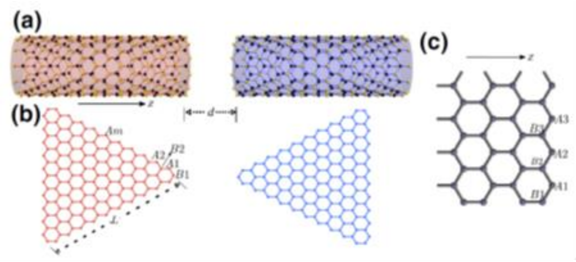
↓ First principles QE/BerkeleyGW calculation for the ratio of energy transfer to blackbody value between two graphene sheets at temperatures 300 K and 1000 K, η = 0.05 eV, electron chemical potential at Dirac point. Zhu & Wang, arXiv:2105.02422.



↑ 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).

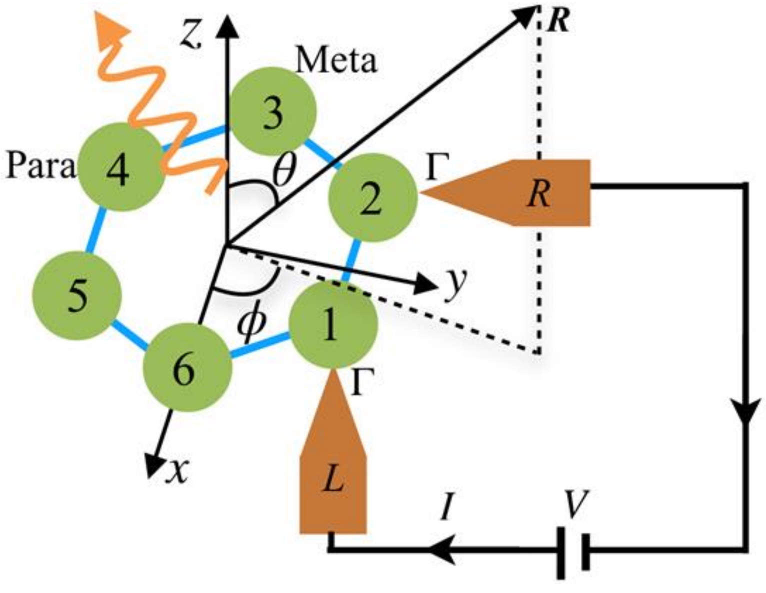
Heat transfer between zigzag nanotubes





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



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

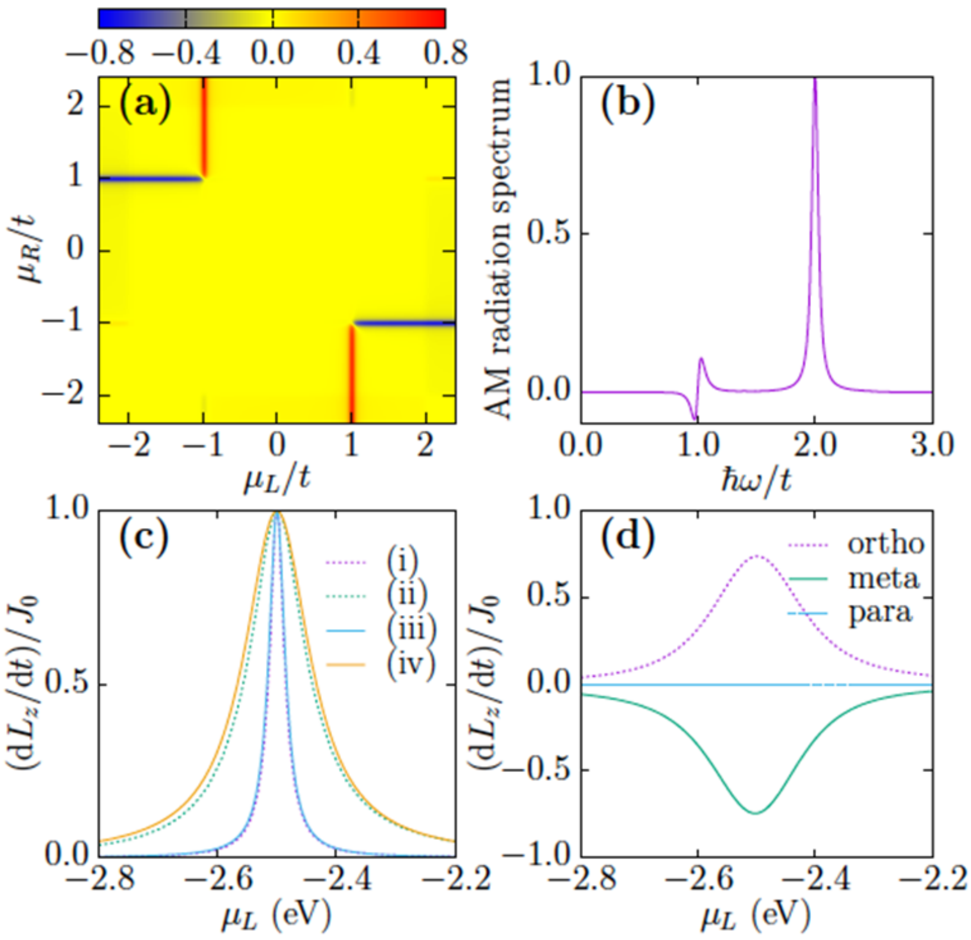
$$-N^z = \frac{dL^z}{dt} = \int_0^\infty d\omega \frac{\hbar\omega}{6\pi^2\varepsilon_0 c^3} \sum_{l,l'} \left(\Pi^<_{lx,l'y}(\omega) - \Pi^<_{ly,l'x}(\omega) \right)$$

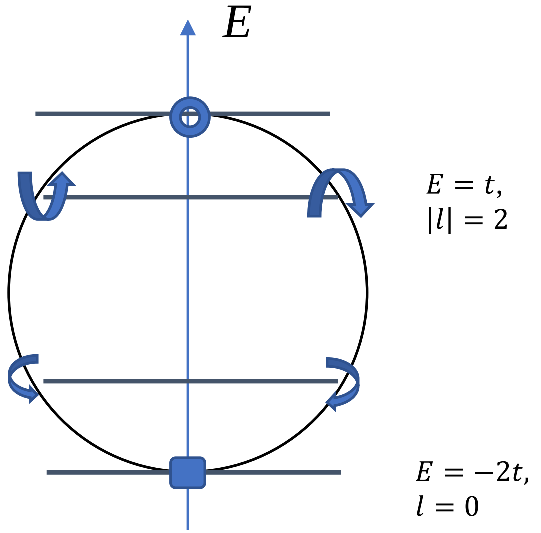
$$\Pi^<_{l\mu,l'\nu}(\omega) = -i \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \operatorname{Tr}\left[M^{l\mu} G^<(E) M^{l'\nu} G^>(E - \hbar\omega) \right]$$

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

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

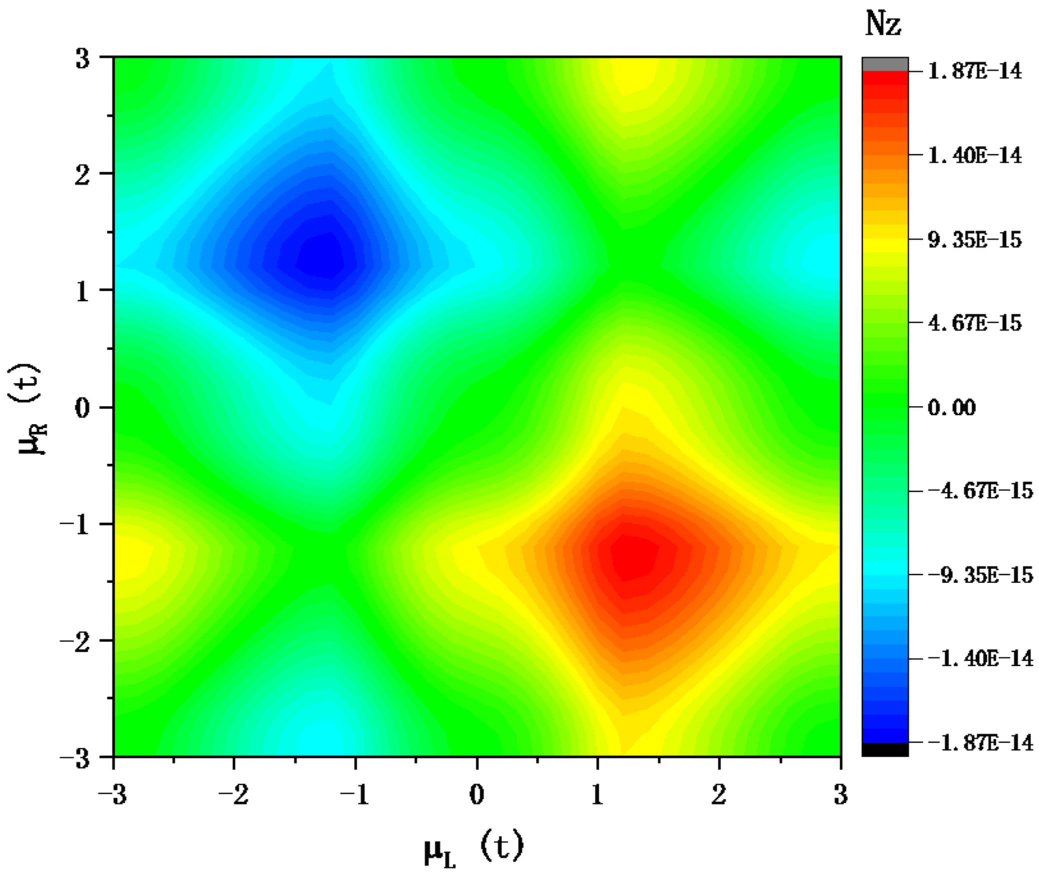
Angular momentum emission resonance effect

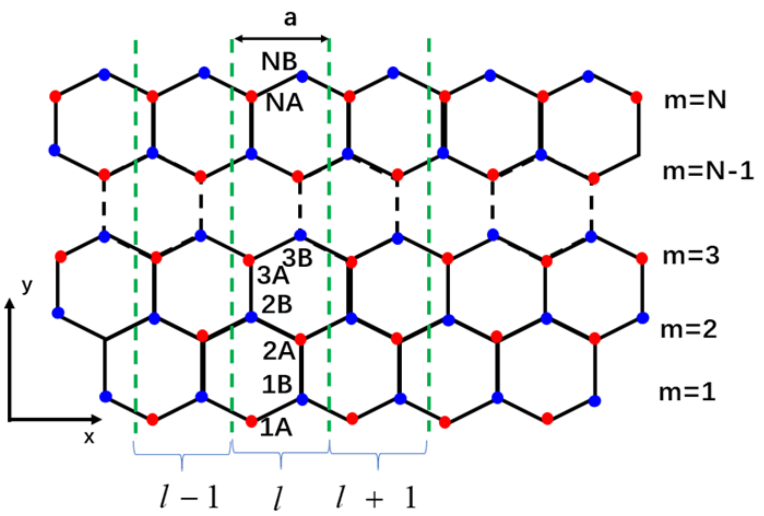




Largest angular momentum emission when one of the chemical potential meets the $E = +t$ energy level. From Zhang, Lü, and Wang, PRB 101, 161406(R) (2020).

Angular momentum emission from graphene edge





Angular momentum emission intensity (atomic units), as chemical potential bias, at temperature of 300 K. Unpublished, Y.-M. Zhang, etc.

Acknowledgements

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