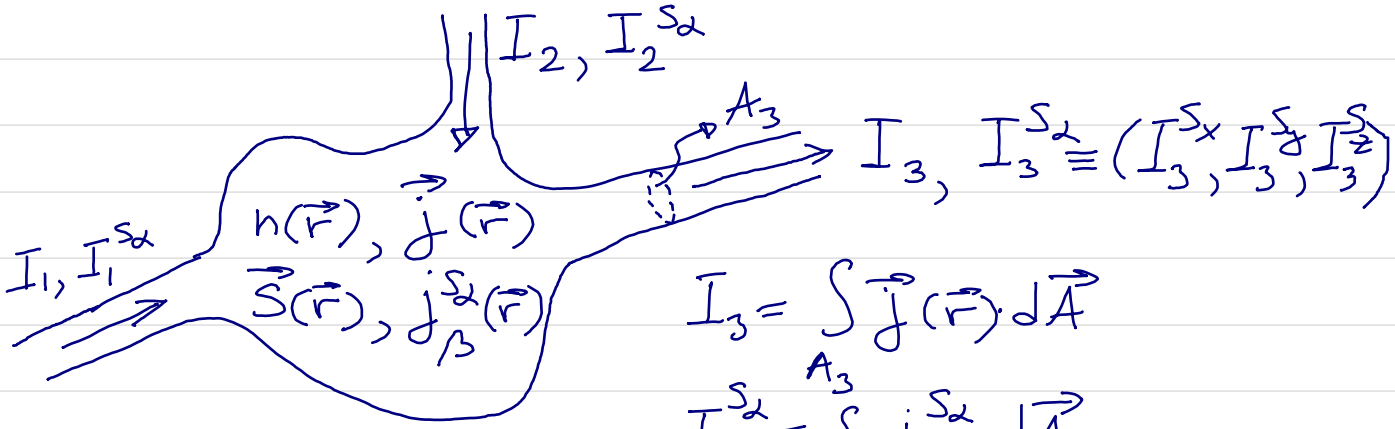
LECTURE 2: Survey of quantum statistical tools

1° Basic quantities that are most frequently measured or calculated in a multiterminal nanostructure



$$I_3 = \int_{A_3} \vec{j}(\vec{r}) \cdot d\vec{A}$$

$$I_3^{S_\alpha} = \int_{A_3} j_\beta^{S_\alpha} \cdot d\vec{A}$$

$\hookrightarrow$ 3×3 tensor

$$S_z(\vec{r}) = \frac{\hbar}{2}\left[n_\uparrow(\vec{r}) - n_\downarrow(\vec{r})\right] \rightarrow z\text{-component of spin density}$$

$\hookrightarrow$ spin-resolved particle density

$$M_z(\vec{r}) = g\mu_B\left[n_\uparrow(\vec{r}) - n_\downarrow(\vec{r})\right] \rightarrow z\text{-component of magnetization density}$$

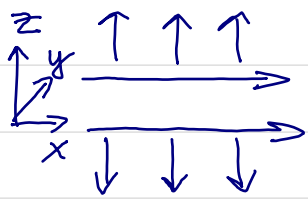
$n(\vec{r})$ is the key quantity in DFT
$n_\uparrow(\vec{r})$, $n_\downarrow(\vec{r})$ are the key quantities in collinear DFT
$n(\vec{r})$, $\vec{M}(\vec{r})$ are the key quantities in noncollinear DFT

$$I_p = I_p^\uparrow + I_p^\downarrow \quad ; \quad I_p^{S_z} = \frac{\hbar}{2e}\left(I_p^\uparrow - I_p^\downarrow\right)$$

$\hookrightarrow$ spin-resolved charge current

EXAMPLE: Charge and spin currents

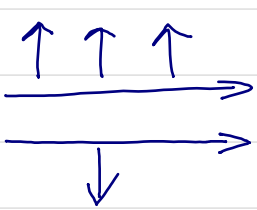
i) conventional unpolarized charge current:



$I = 6\ e/s$

$I^{S_z} = 0$

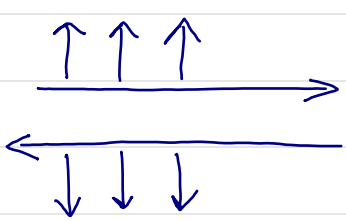
ii) spin-polarized charge current:



$I = 4\ e/s$

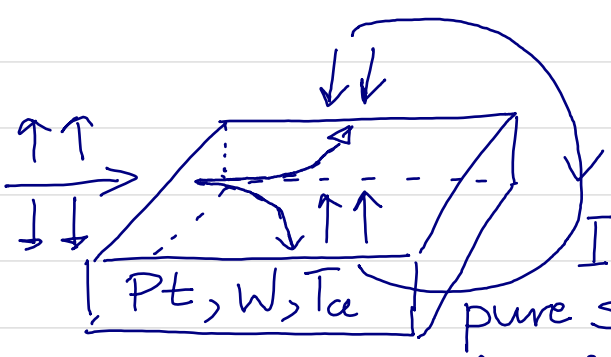
$I^{S_z} \equiv 2\ \frac{\hbar}{2}\ s^{-1}$

iii) pure spin current:



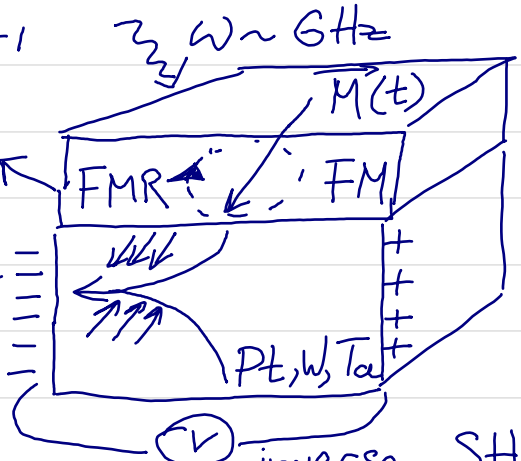
$I = 0\ e/s$ → no charge current, so spin currents is "pure"

$I^{S_z} = 6 \cdot \frac{\hbar}{2} \cdot s^{-1}$



pumps pure spin current into heavy metal

pure spin Hall current

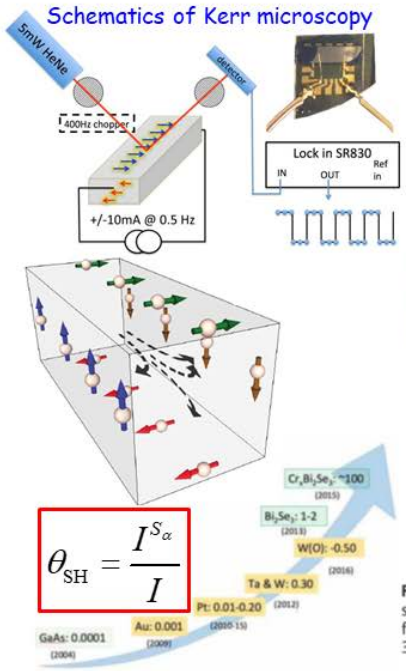


EXAMPLE: Experimental imaging of $S(\vec{r})$ or $S(\vec{r},t)$

1910 10 DECEMBER 2004 VOL 306 SCIENCE

Observation of the Spin Hall Effect in Semiconductors

Y. K. Kato, R. C. Myers, A. C. Gossard, D. D. Awschalom*



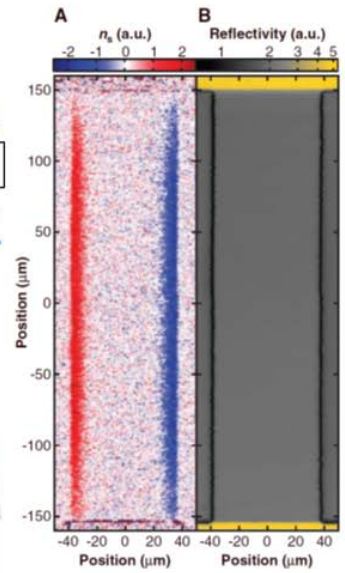


Fig. 2. (A and B) Two-dimensional images of spin density n_s and reflectivity R, respectively, for the unstrained GaAs sample measured at T = 30 K and E = 10 mV μm^{-1}.

ARTICLES
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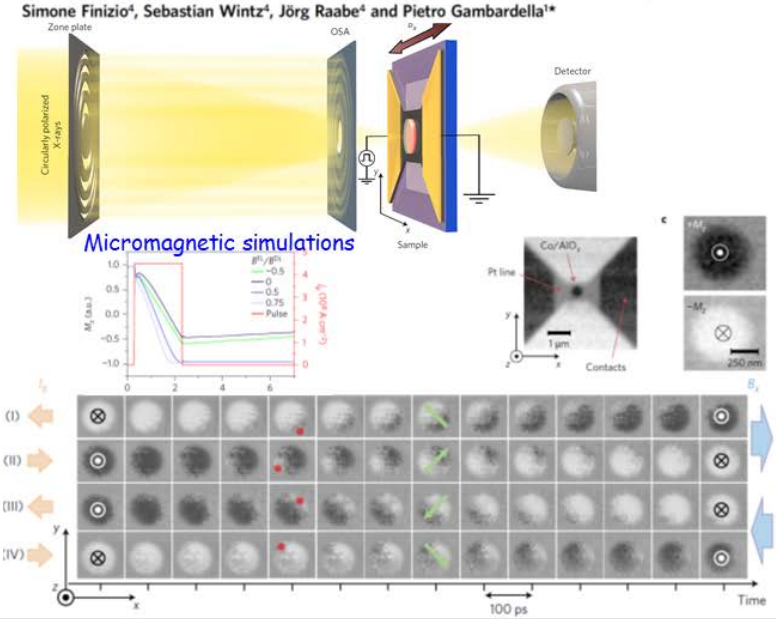
nature nanotechnology

Spatially and time-resolved magnetization dynamics driven by spin–orbit torques

Manuel Baumgartner[1]*, Kevin Garello[1,2]*, Johannes Mendil[1], Can Onur Avci[1], Eva Grimaldi[1], Christoph Murer[1], Junxiao Feng[1], Mihai Gabureac[1], Christian Stamm[1], Yves Acremann[3], Simone Finizio[4], Sebastian Wintz[4], Jörg Raabe[4] and Pietro Gambardella[1]*



EXAMPLE: Experimental imaging of $\vec{j}(\vec{r})$

Article

Imaging viscous flow of the Dirac fluid in graphene

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https://doi.org/10.1038/s41586-020-2507-2
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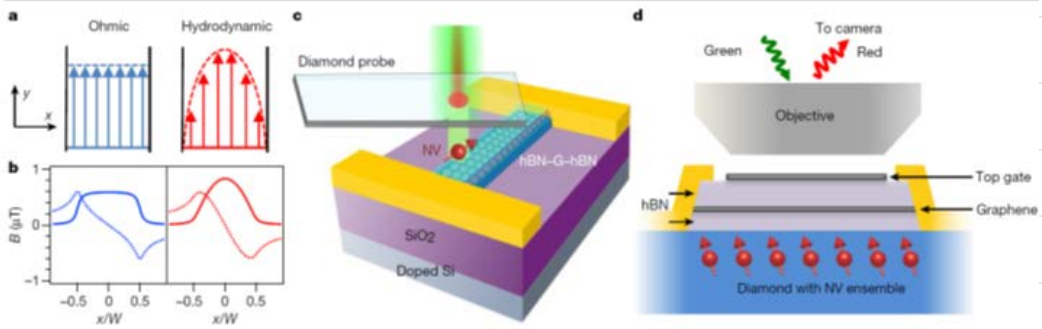
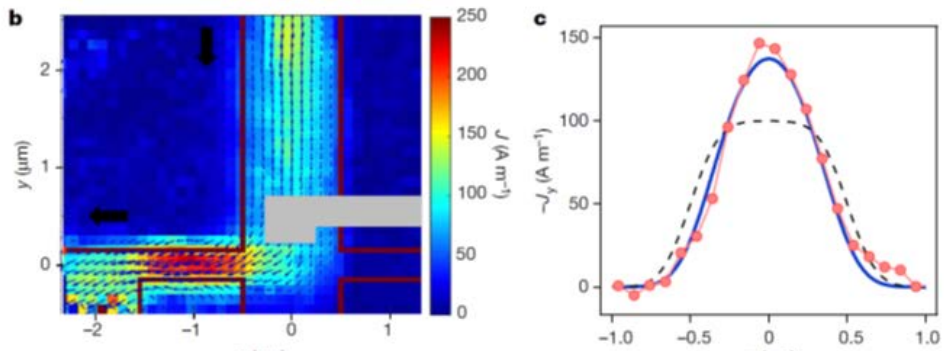
Mark J. H. Ku, Tony X. Zhou, Qing Li, Young J. Shin, Jing K. Shi, Claire Burch, Laurel E. Anderson, Andrew T. Pierce, Yonglong Xie, Assaf Hamo, Uri Vool, Huiliang Zhang, Francesco Casola, Takashi Taniguchi, Kenji Watanabe, Michael M. Fogler, Philip Kim, Amir Yacoby & Ronald L. Walsworth





2° Quantum Theories

$T=0$ → Quantum Mechanics

$T\neq 0$ → EQUILIBRIUM Quantum Statistical Mechanics

due to $\mu_1 \neq \mu_2$, $\mu_1 \neq \mu_2$, $T_1 \neq T_2$, $\omega \neq 0$ → NONEQUILIBRIUM Quantum Statistical Mechanics

describes fluxes of charge, spin and heat $A \bullet \xrightarrow{\vec{j}_s(\vec{r})} \bullet B$

i) Quantum Mechanics overview

$|\psi\rangle \in \mathcal{H}$, $\hat{A}: \mathcal{H} \mapsto \mathcal{H}$, $\hat{A}^+ = \hat{A}$

none of fundamental objects is directly measurable

$\alpha|\psi_1\rangle + \beta|\psi_2\rangle$ is behind "wave-particle duality" or "quantum interference & coherence"

Schrödinger equation

$$i\hbar \frac{\partial|\psi\rangle}{\partial t} = \hat{H}|\psi\rangle ; \quad \hat{A}|a_n\rangle = a_n|a_n\rangle$$

$\hookrightarrow \in \mathbb{R}$ and measurable

$$|\psi\rangle = \int d^3r \, |\vec{r}\rangle\langle\vec{r}|\psi\rangle = \int d^3r \, \psi(\vec{r})|\vec{r}\rangle$$

or $\hat{I}$

$$= \sum_n |a_n\rangle\langle a_n|\psi\rangle = \sum_n \psi_n |a_n\rangle$$

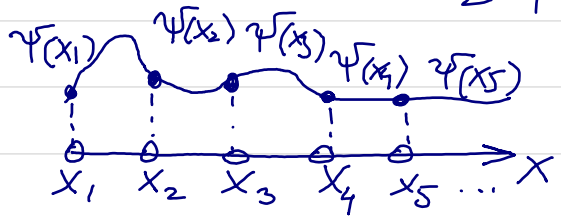
$\hat{I}$

$[\hat{x}, \hat{p}_x] = i\hbar$ means $\mathcal{H}$ and, therefore, these vectors are infinite but they have to be truncated in the computer

$|\psi\rangle \rightarrow \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_N \end{pmatrix}$

$\psi(\vec{r})$ has to be discretized → $\begin{pmatrix} \psi(\vec{r}_1) \\ \vdots \\ \psi(\vec{r}_N) \end{pmatrix}$

1D lattice example ←



spectral decomposition

$$\hat{A} = \sum_n a_n |a_n\rangle\langle a_n| \Rightarrow \underbrace{\langle \hat{A} \rangle \equiv A}_{\langle \psi|\hat{A}|\psi\rangle = \sum_n a_n \langle\psi|a_n\rangle\langle a_n|\psi\rangle}$$

$$\langle N \rangle = 1\cdot\frac{1}{6} + 2\cdot\frac{1}{6} + 3\cdot\frac{1}{6} + 4\cdot\frac{1}{6} + 5\cdot\frac{1}{6} + 6\cdot\frac{1}{6} = 3.5$$

$$= \sum_n a_n |\langle a_n|\psi\rangle|^2$$

prob a_n is

akin to any probabilistic theory

Function of an operator: ▷ in case continuous spectrum is also present

$$F(\hat{A}) = \sum_n F(a_n)|a_n\rangle\langle a_n| + \int da\, F(a)|a\rangle\langle a|$$

$$\hat{n} = |\vec{r}\rangle\langle\vec{r}| \Rightarrow n = \langle\psi|\vec{r}\rangle\langle\vec{r}|\psi\rangle = |\psi(\vec{r})|^2$$

$$\vec{S} = \langle\psi|\left(|\vec{r}\rangle\langle\vec{r}| \otimes \frac{\hbar}{2}\hat{\vec{\sigma}}\right)|\psi\rangle = \frac{\hbar}{2}|\phi(\vec{r})|^2 \cdot \langle\Sigma|\hat{\vec{\sigma}}|\Sigma\rangle$$

$|\psi\rangle = |\phi\rangle \otimes |\Sigma\rangle \in \mathcal{H}_0 \otimes \mathcal{H}_s$ ▷ tensor product in theory

numpy.kron in Numpy practice

or

$|\psi\rangle = \alpha|\phi_\uparrow\rangle \otimes |\uparrow\rangle + \beta|\phi_\downarrow\rangle \otimes |\downarrow\rangle$ if spin-orbit coupling $\neq 0$

classical currents	$\mapsto$	quantum operators
$\vec{j} = e n \vec{v}$	$\mapsto$	$\hat{\vec{j}} = \frac{e}{2}(\hat{n}\hat{\vec{v}} + \hat{\vec{v}}\hat{n})$
$j_\alpha^\beta = \frac{\hbar}{2}\sigma_\beta v_\alpha$	$\mapsto$	$\hat{j}_\alpha^\beta = \frac{\hbar}{4}(\hat{\sigma}_\beta \otimes \hat{v}_\alpha + \hat{v}_\alpha \otimes \hat{\sigma}_\beta)$

heuristic since there is no spin or $\hbar/2$ in classical physics

$$\vec{v} = \frac{d\vec{r}}{dt} \mapsto \hat{\vec{v}} = \frac{d\hat{\vec{r}}}{dt} = \frac{1}{i\hbar}[\hat{\vec{r}}, \hat{H}]$$

refresher from elementary quantum mechanics

→ more formal is to use continuity equations:

$$d\hat{n}/dt = \frac{1}{i\hbar}[\hat{n}, \hat{H}] \Rightarrow e\frac{d\hat{n}}{dt} + \nabla\cdot\hat{\vec{j}} = 0$$

↳ $\hat{\vec{j}} = \frac{e}{2}(\hat{n}\hat{\vec{v}} + \hat{\vec{v}}\cdot\hat{n})$

$$d\hat{\vec{S}}/dt = \frac{1}{i\hbar}[\vec{S}, \hat{H}] \Rightarrow \frac{d\hat{\vec{S}}}{dt} + \nabla\hat{j}_\alpha \neq 0$$ in the presence of spin-orbit coupling

↳ $\hat{j}_\alpha = \frac{\hbar}{4}(\hat{\sigma}_\beta\otimes\hat{v}_\alpha + \hat{v}_\alpha\otimes\hat{\sigma}_\beta)$

$$\vec{j}(\vec{r}) = \langle\psi|\hat{\vec{j}}|\psi\rangle = \frac{e}{2}\left(\langle\psi|\vec{r}\rangle\langle\vec{r}|\hat{\vec{v}}|\psi\rangle + \langle\psi|\hat{\vec{v}}|\vec{r}\rangle\langle\vec{r}|\psi\rangle\right)$$

$$= \frac{e}{2}\int d^3x d^3y \Big(\langle\psi|\vec{x}\rangle\underbrace{\langle\vec{x}|\vec{r}\rangle}_{\delta(\vec{x}-\vec{r})}\underbrace{\langle\vec{r}|\hat{\vec{v}}|\vec{y}\rangle}_{i\hbar\partial_y\delta(\vec{r}-\vec{y})/m}\langle\vec{y}|\psi\rangle +$$

$$+ \langle\psi|\vec{x}\rangle\underbrace{\langle\vec{x}|\hat{\vec{v}}|\vec{r}\rangle}_{-i\hbar\partial_x\delta(\vec{x}-\vec{r})}\underbrace{\langle\vec{r}|\vec{y}\rangle}_{\delta(\vec{r}-\vec{y})}\langle\vec{y}|\psi\rangle\Big)$$

$$\delta(x-y) = \delta(y-x), \quad \int \partial_x\,\delta(x-y)\,f(x)dx = -\partial_y f(y)$$

$$\langle x|\hat{p}|y\rangle = p_{xy} = i\hbar\,\partial_y\delta(x-y) = -i\hbar\,\partial_x\delta(x-y)$$

$$\vec{j}(\vec{r}) = \frac{e\hbar}{2im}\left[\psi^*(\vec{r})\frac{\partial\psi(\vec{r})}{\partial\vec{r}} - \psi(\vec{r})\cdot\frac{\partial\psi^*(\vec{r})}{\partial\vec{r}}\right]$$ ← textbook formula

→ on the computer:

$$\langle\psi|\hat{\vec{j}}|\psi\rangle = \sum_{m,n}\underbrace{\langle\psi|n\rangle}_{\downarrow}\underbrace{\langle n|\hat{\vec{j}}|m\rangle}_{\text{matrix representation of }\hat{\vec{j}}}\underbrace{\langle m|\psi\rangle}_{\downarrow}$$

$$= \begin{pmatrix}\psi_1^* & \dots & \psi_N^*\end{pmatrix}\begin{pmatrix}\text{matrix representation of } \hat{\vec{j}}\end{pmatrix}\begin{pmatrix}\psi_1\\ \vdots \\ \psi_N\end{pmatrix}$$

ii) Quantum Statistical Mechanics overview

$\hat{\rho}, \hat{A} : \mathcal{H} \mapsto \mathcal{H}$ $\quad \mathrm{Tr}\,\hat{\rho} = 1,\ \hat{\rho}^+ = \hat{\rho},\ \langle\psi|\hat{\rho}|\psi\rangle \geq 0$

$$\hat{\rho} = \sum_i w_i |\psi_i\rangle\langle\psi_i| \qquad \{|\psi\rangle \text{ from QM} \iff \hat{\rho} = |\psi\rangle\langle\psi|\}$$

von Neumann equation

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{H}, \rho]$$

$\alpha|\psi_1\rangle + \beta|\psi_2\rangle$ from QM $\Rightarrow \hat{\rho} = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix}$ quantum coherence & interference

$$A = \mathrm{Tr}\left(\hat{\rho}\cdot\hat{A}\right) = \sum_n \langle a_n| \sum_i w_i |\psi_i\rangle\langle\psi_i| \sum_m a_m |a_m\rangle\underbrace{\langle a_m|a_n\rangle}_{\delta_{nm}}$$

$$= \sum_i w_i \sum_n a_n \langle a_n|\psi_i\rangle\langle\psi_i|a_n\rangle$$

$$= \sum_i w_i \sum_n a_n \cdot \mathrm{prob}\, a_n = \sum_i w_i \langle\psi_i|\hat{A}|\psi_i\rangle$$

■ EXAMPLE: Volume average of current density

$$\vec{\bar{j}} = \frac{1}{\Omega}\int d^3r\, \vec{j}(\vec{r}) = \frac{1}{\Omega}\int d^3r\, \mathrm{Tr}\left[\hat{\rho}\cdot\hat{\vec{j}}\right] = \frac{1}{\Omega}\int d^3r \sum_{nm} \rho_{nm}\vec{j}_{mn}$$

$$\vec{j}_{mn}(\vec{r}) = \langle m|\hat{\vec{j}}|n\rangle = \frac{e}{2}\left(\langle m|\vec{r}\rangle\langle\vec{r}|\hat{\vec{v}}|n\rangle + \langle m|\hat{\vec{v}}|\vec{r}\rangle\langle\vec{r}|n\rangle\right)$$

$$\frac{1}{\Omega}\int d^3r\, \vec{j}_{mn}(\vec{r}) = \frac{1}{\Omega}\int d^3r \left(\langle m|\vec{r}\rangle\langle\vec{r}|\hat{\vec{v}}|n\rangle + \langle m|\hat{\vec{v}}|\vec{r}\rangle\langle\vec{r}|n\rangle\right)$$

$\int d^3|\vec{r}\rangle\langle\vec{r}| = \hat{I}$

$$= \frac{e}{2\Omega}\left(\langle m|\hat{\vec{v}}|n\rangle + \langle m|\hat{\vec{v}}|n\rangle\right)$$

$$= \frac{e}{\Omega}\langle m|\hat{\vec{v}}|n\rangle \Rightarrow \vec{\bar{j}} = \frac{1}{\Omega}\sum_{nm}\hat{\rho}_{nm}\frac{e}{\Omega}\hat{\vec{v}}_{mn} = \underbrace{\mathrm{Tr}\left(\hat{\rho}\cdot\frac{e}{\Omega}\hat{\vec{v}}\right)}_{\text{for one } e^-}$$

for N e^- $\longrightarrow$ $\mathrm{Tr}\left(\hat{\rho}\, ne\,\hat{\vec{v}}\right)$

EXAMPLE: Density matrix of spin-polarized current

$|\Sigma\rangle = |\downarrow\rangle$ or

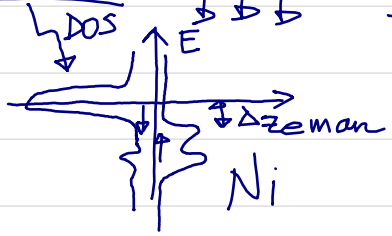
$\uparrow\uparrow I\neq 0$, $\downarrow\downarrow I^{S_z}=0$ → [half-metal FM] → $\downarrow\downarrow\downarrow$

$\hat{\rho}_{out} = |\downarrow\rangle\langle\downarrow| = \hat{\rho}_{out}^2 \Rightarrow \mathrm{Tr}\,\rho_{out}^2 = 1$

$\uparrow\uparrow I\neq 0$, $\downarrow\downarrow I^{S_z}=0$ → [conventional FM] → $\uparrow I\neq 0$, $\downarrow\downarrow\downarrow$ $I^{S_z}\neq 0$

$\hat{\rho}_{out} = \frac{1}{4}|\uparrow\rangle\langle\uparrow| + \frac{3}{4}|\downarrow\rangle\langle\downarrow|$ (w_1, w_2)

$\hat{\rho}_{in} = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow|$



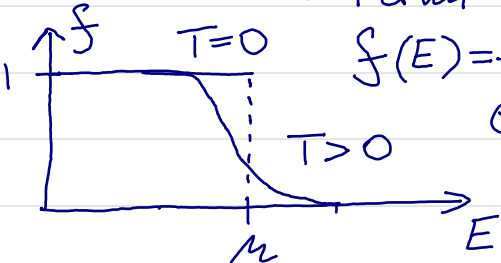
$\mathrm{Tr}\,\hat{\rho}_{out} = w_1 + w_2 = 1$

EXAMPLE: Equilibrium density matrix of electrons at $T\neq 0$

$[\hat{H}, \hat{\rho}_{eq}] = 0 \Rightarrow \hat{\rho}_{eq} = F(\hat{H}) \xrightarrow[\text{canonical}]{\text{grand}} \hat{\rho}_{eq} = \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{Z_G}$

$\hat{\rho}_{eq} = \sum_n f(\varepsilon_n - \mu)\,|\psi_n\rangle\langle\psi_n|$ → not normalized to $\mathrm{Tr}\,\hat{\rho}_{eq} = 1$

↳ Fermi-Dirac function



$f(E) = \frac{1}{e^{\frac{E-\mu}{k_B T}} + 1}$

$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$

$\hat{\rho}_{eq} = f(\hat{H} - \mu\cdot\hat{I})$

will be coded in Python

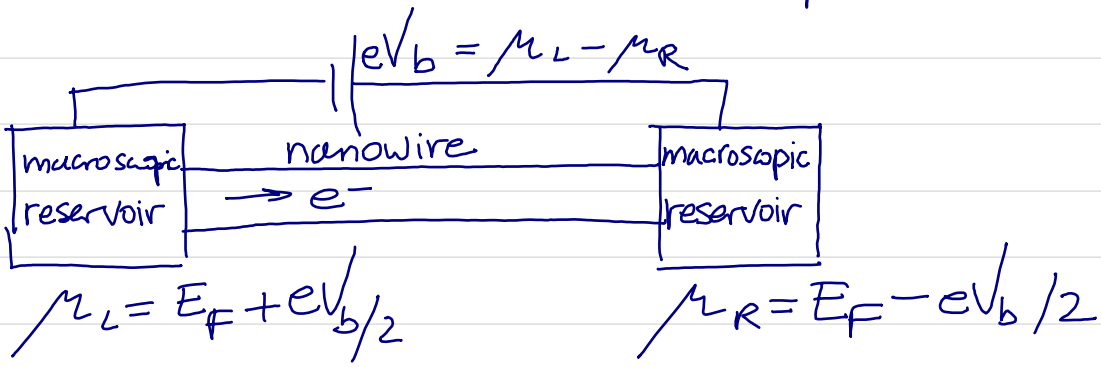
$$n(\vec{r}) = \mathrm{Tr}\left(\hat{\rho}_{eq}|\vec{r}\rangle\langle\vec{r}|\right) = \int d^3\vec{x}\,\langle\vec{x}|\hat{\rho}_{eq}|\vec{r}\rangle\langle\vec{r}|\vec{x}\rangle = \langle\vec{r}|\hat{\rho}_{eq}|\vec{r}\rangle \quad (\langle\vec{r}|\vec{x}\rangle = \delta(\vec{r}-\vec{x}))$$

$$= \sum_n f(E_n-\mu)\langle\vec{r}|\psi_n\rangle\langle\psi_n|\vec{r}\rangle = \sum_n f(E_n-\mu)\,|\psi_n(\vec{r})|^2$$

$$= \int dE \left[\sum_n |\psi_n(\vec{r})|^2 \delta(E-E_n)\right] f(E-\mu)$$

$d(\vec{r},E) \equiv$ local density of states probed by STM

■ EXAMPLE: Nonequilibrium density matrix of electrons in nanowire attached to two macroscopic reservoirs



→ naive: $n(\vec{r}) = \sum_n f(E_n - \mu) \cdot |\psi_n(\vec{r})|^2$ is INCORRECT using $\mu_R < \mu < \mu_L$ or $f \rightarrow f_{neq}$

→ CORRECT:

$$n(\vec{r}) = Tr\left(\hat{\rho}_{neq} |\vec{r}\rangle\langle\vec{r}|\right) = \sum_n \langle\psi_n|\hat{\rho}_{neq}|\vec{r}\rangle\langle\vec{r}|\psi_n\rangle$$

$$= \sum_{n,m} \langle\psi_n|\hat{\rho}_{neq}|\psi_m\rangle\langle\psi_m|\vec{r}\rangle\langle\vec{r}|\psi_n\rangle$$

$$= \sum_{n,m} \psi_n(\vec{r}) \cdot [\hat{\rho}_{neq}]_{nm} \psi_m^*(\vec{r})$$

→ general form of $\hat{\rho}_{neq}$ is not known; in steady-state transports it could be $\hat{\rho} = e^{-\beta(\hat{H} - \hat{Y})}/Z$ but $\hat{Y}$ operator which knows about bias voltage has been notoriously difficult to construct

→ for noninteracting electrons:

$$\hat{\rho}_{neq} = \frac{1}{2\pi i} \int \hat{G}^r(E) \left[i f(E - \mu_L) \hat{\Gamma}_L + i f(E - \mu_R) \hat{\Gamma}_R \right] \cdot \hat{G}^a(E)$$

→ need to learn about Green functions

■ EXAMPLE: Self-consistent charge loops in Poisson-Schrödinger and DFT schemes

$$\hat{H}_0 = \frac{\hat{\vec{p}}^2}{2m} + V_{ext}(\vec{r})$$

in DFT ▷ add $+ V_{xc}(\vec{r})$

$$n_{in}(\vec{r}) \longrightarrow \left[\hat{H}_0 + V_H(\vec{r})\right]\psi_n(\vec{r}) = E_n\psi_n(\vec{r})$$

$$n_{out}(\vec{r}) \longleftarrow \nabla\left[\varepsilon(\vec{r})\nabla V_H(\vec{r})\right] = -\frac{e^2}{\varepsilon}\left[n(\vec{r}) + n^d(\vec{r})\right]$$

stop when $\int d^3r\,|n_{out}(\vec{r}) - n_{in}(\vec{r})| < \delta_n$

OR $|E^{total}_{out} - E^{total}_{in}| < \delta_E$

in computational practice also mix $n^{(i+1)} = \beta n^{(i)} + (1-\beta)n^{(i-1)}$

$n^d(\vec{r})$ ▷ any charge density located elsewhere in the system, such as dopants or trapped charges

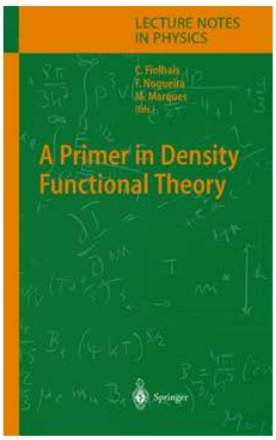
$V_{ext}(\vec{r}) = \sum_i V_i(\vec{r} - \vec{R}_i)$ is typically a sum of nuclear potentials centered at the atomic positions

$$V_{Hartree}(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int d^3r'\,\frac{n(\vec{r}')}{|\vec{r} - \vec{r}'|}$$

is Hartree potential from classical electrostatics

$$V_{xc}(\vec{r}) = \frac{\delta E_{xc}[n(\vec{r})]}{\delta n(\vec{r})}$$

is exchange-correlation potential in DFT



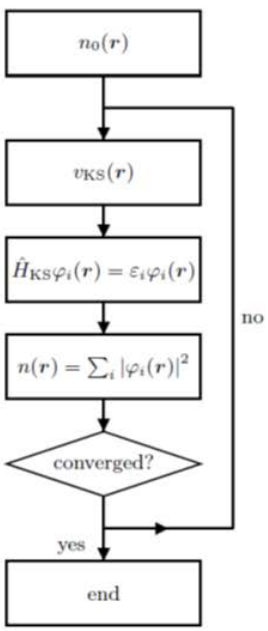


Fig. 6.1. Flow-chart depicting a generic Kohn-Sham calculation

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SciPost Phys. 7, 031 (2019)

The self-consistent quantum-electrostatic problem in strongly non-linear regime

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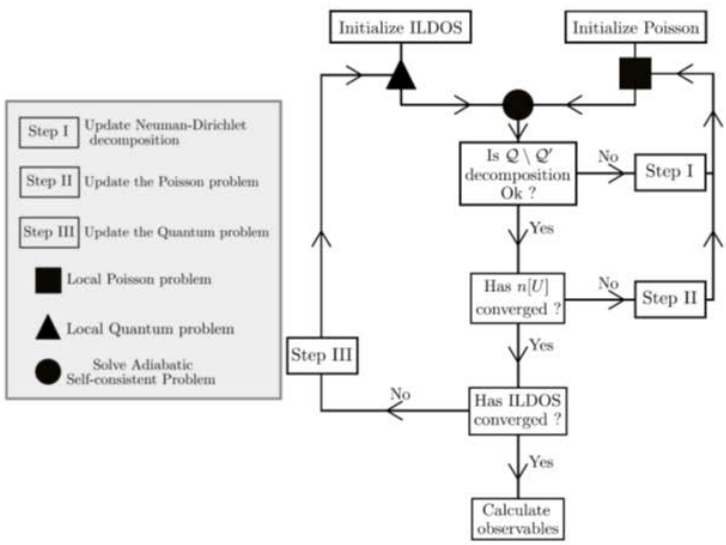

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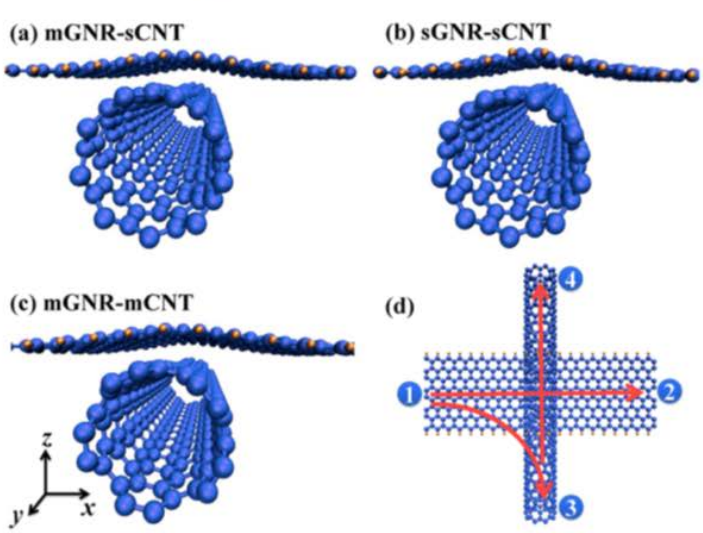
Negative differential resistance in graphene-nanoribbon–carbon-nanotube crossbars: a first-principles multiterminal quantum transport study

Kamal K. Saha · Branislav K. Nikolić



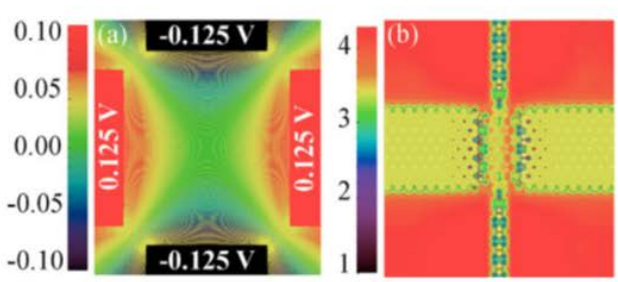


Fig. 2 (**a**) Solution of the Laplace equation within the xy-planes (of size 5.2 nm × 6.0 nm) of 3D real-space grid of points enclosing mGNR-sCNT crossbar in Fig. 1(a) whose central region is removed and where voltages applied to the four electrodes provide the boundary conditions. This solution is used as the initial guess for solving the Poisson equation on 3D real-space grid enclosing central region of mGNR-sCNT crossbar, where self-consistent solution within the plane positioned between mGNR and sCNT is shown in panel (**b**) (Color figure online)

3° Single particle or many-particle Quantum Theory?

$\Psi(\vec{r})$ or $\hat{\xi}(\vec{r},\vec{r}')$ ← $\Psi(\vec{r}_1,\dots,\vec{r}_N)$ or $\hat{\xi}(\vec{r}_1,\dots\vec{r}_N;\vec{r}_1',\dots\vec{r}_N')$

↳ due to e-e, e-phonon, e-magnon interactions

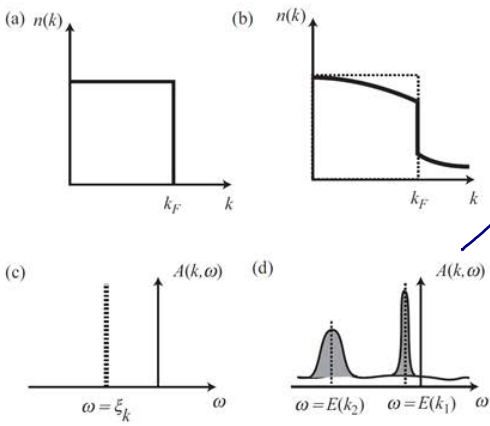
i) Why is quantum description of electrons in solids necessary?

MO⇔OM $a \simeq 3\text{Å}$ is typical lattice spacing between ions

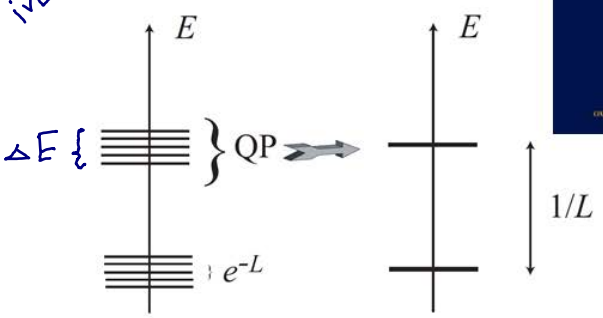
$\lambda_{ion} = h/\sqrt{2M k_B T} \simeq 10^{-11}\,m \ll a$; $\lambda_{e^-} = h/\sqrt{2m k_B T} \simeq 10^{-9}\,m \gg a$

↳ can use classical mechanics (like molecular dynamics) except at low T

ii) Crash course on Landau quasielectrons



same as LDOS but in k-space



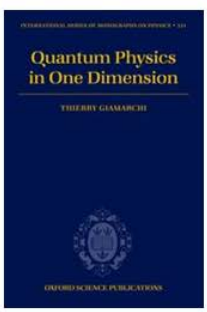


FIG. 1.1. (a) Free electrons: the occupation n_k has a discontinuity of amplitude 1 at the Fermi surface. The spectral function $A(k,\omega)$ (see text) is a delta function peak, showing excitations without damping and a well-defined frequency–momentum relation $\omega = \xi(k)$. The excitations are made of the individual particles of a given momentum. (b) Fermi liquid: it is *essentially* similar to a free electron gas, with some differences. The occupation n_k still has a discontinuity at the Fermi wavevector $k = k_F$, but with a reduced amplitude $Z < 1$. The excitations become sharper when they get closer to the Fermi surface. The total weight in these excitations (quasiparticles) is Z. The quasi-free excitations (quasiparticles) are electrons dressed by the particle–hole excitations of the electron gas.

FIG. 1.2. A quasiparticle 'state' is in fact made of a very large number of *exact* eigenstates of the interacting system. The separation in energy of these states is exponentially small in the system size L and thus irrelevant physically, for reasonable systems. The cluster of all these states form the quasiparticle with its average energy and lifetime (inverse of the broadening in energy).

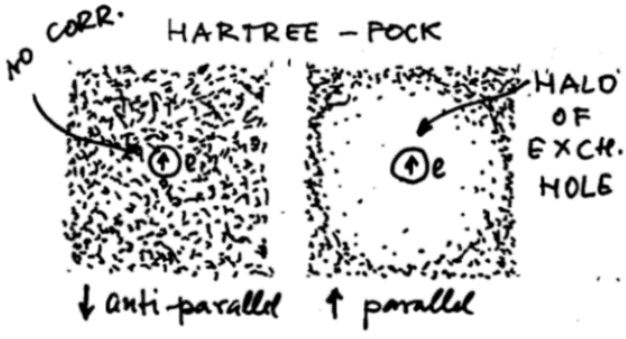
$$\varepsilon(\vec{k}) \mapsto \varepsilon(\vec{k}) + i\Delta E$$

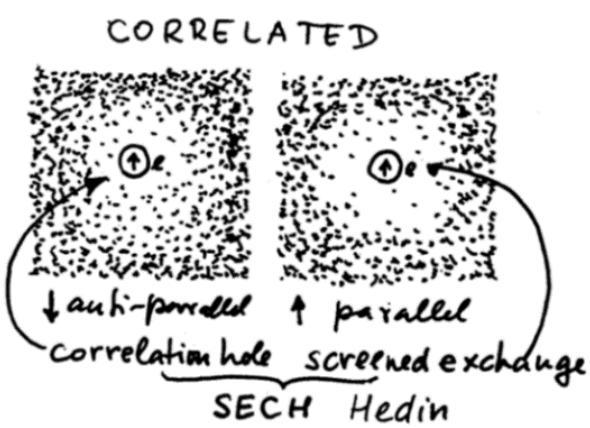
$$\Psi(\vec{r},t) \propto e^{-i\varepsilon(\vec{k})t/\hbar}\, e^{-t/\tau}$$

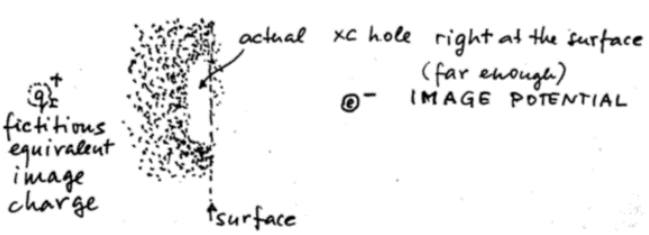
$\tau = \hbar/\Delta E$ is finite due scattering between quasielectrons

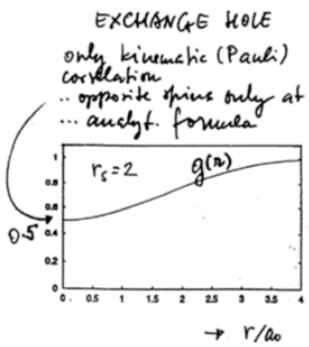
$\tau \to \infty$ close to the Fermi level since phase space to scatter is reduced

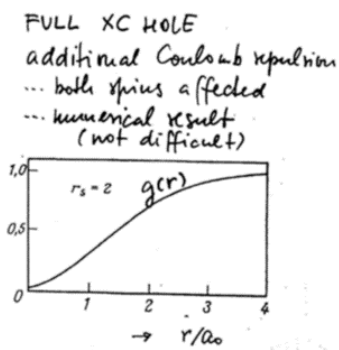
iii) exchange-correlation hole around electron in DFT











iv) Quantifying effects of long-range Coulomb interaction

$V/N = \frac{1}{n} = \frac{4}{3} r_s^3 \pi$, r_s is typical inter-electron distance given in units of Bohr radius $a_B = 5.29 \cdot 10^{-11} m$

$U = e^2/r_s$ ⇒ potential energy due to Coulomb interaction

$T = p^2/2m \sim \hbar^2/2m r_s^2$ since $p_F \sim \hbar/r_s$ by Heisenberg uncertainty

$U/T \sim r_s$ { < 1, perturbative
$2 < r_s < 6$, all metals with Landau quasielectrons
> 106, Wigner crystal in 3D
> 31, Wigner crystal in 2D

■ EXAMPLE: graphene $U = e^2 n^{1/2}/\varepsilon$, $T = \hbar v_F n^{1/2}$

$U/T = \alpha/\varepsilon$ is not function of r_s, $\alpha = \frac{e^2}{\hbar v_F} \approx 2.2$

EXAMPLE: Wigner crystal of electrons floating on liquid He

Selected for a Viewpoint in *Physics*

PHYSICAL REVIEW B **79**, 045406 (2009)

Addition spectra of Wigner islands of electrons on superfluid helium

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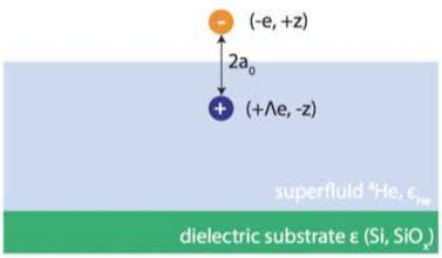

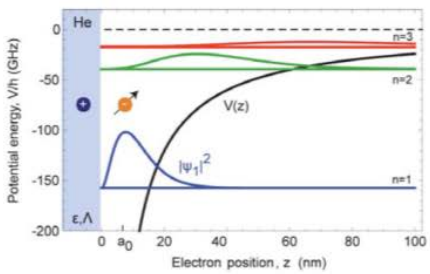

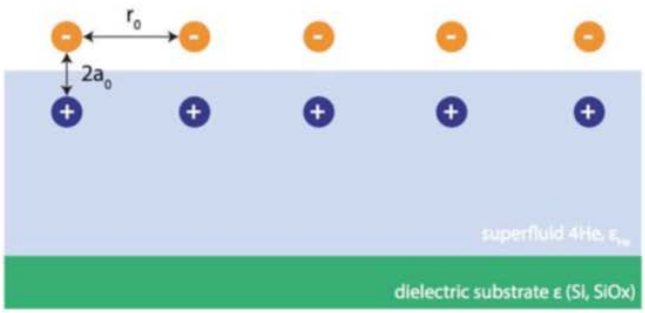

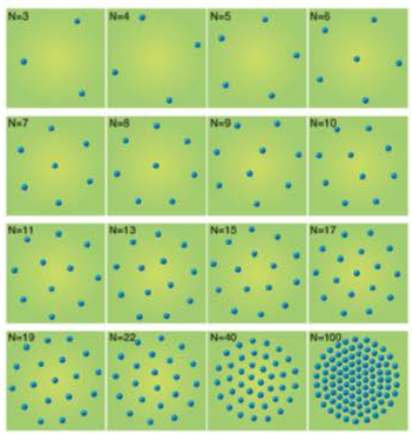

Ground state configurations for N=3 to 100

FIG. 1: A series of Wigner crystal structures showing the arrangement of electrons in a circular island from an occupation number of $N = 3$ to $N = 100$. The electrons form ring structures as more electrons are added. At $N = 15$ an inner ring of five electrons is formed, but at $N = 16$ the additional electron is forced to the center to start a new ring. For large N, a triangular Wigner lattice forms in the center, while the outer electrons remain in rings. (Illustration: Alan Stonebraker/`stonebrakerdesignworks.com`)

EXAMPLE: Wigner crystal of electrons within twisted TMD bilayer vdW heterostructure

Article

Mott and generalized Wigner crystal states in WSe_2/WS_2 moiré superlattices

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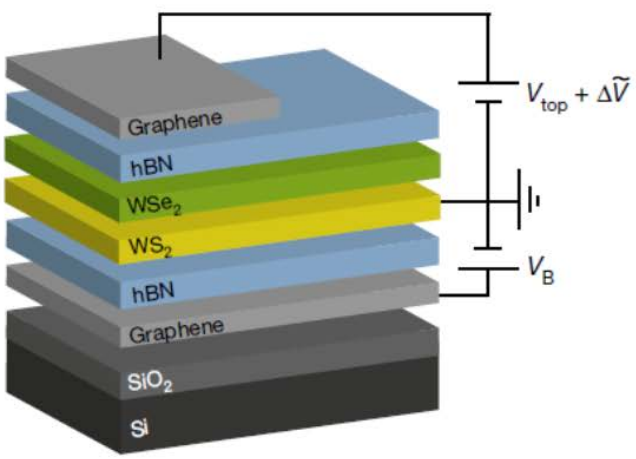


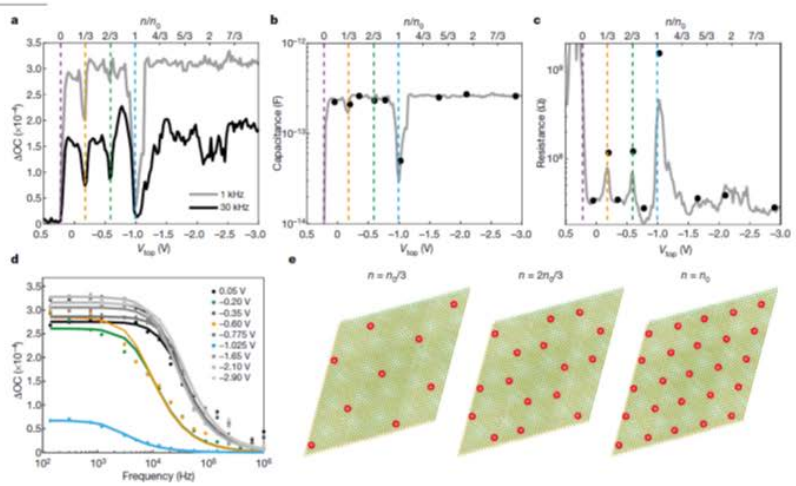


Fig. 2 | Doping-dependent resistance and capacitance probed by ODRC. **a**, ODRC signal at 1 kHz (grey) and 30 kHz (black) from charge-neutral to moderate hole doping. Strong gap-like features are observed at hole doping levels of $n = n_0/3$ (orange dashed line), $n = 2n_0/3$ (green dashed line) and $n = n_0$ (blue dashed line). The purple dashed line corresponds to $n = 0$. **b**–**d**, Capacitance C_{tot} (**b**) and resistance (**c**) of region 1. Grey curves are extracted from the data in **a**, and black dots are extracted from the frequency-dependent ODRC signal (**d**) at representative doping levels. In **d**, the dots are the frequency-dependent ODRC signal at the indicated values of V_{top} and the lines are the corresponding fits with the RC circuit model. The decreased capacitance and increased resistance indicate emerging insulating states at $n = n_0/3$, $n = 2n_0/3$ and $n = n_0$. All measurements are done at 3 K. **e**, Illustrations of generalized Wigner crystal ($n = n_0/3$, $n = 2n_0/3$) and Mott insulator states ($n = n_0$) in a WSe_2/WS_2 moiré superlattice.

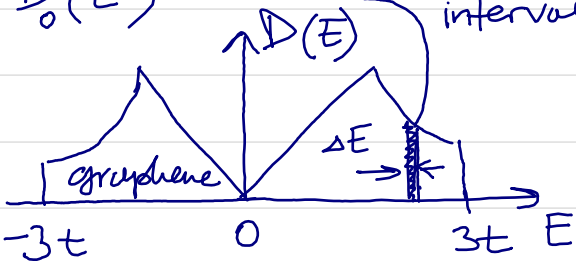
4° Total density of states (DOS)

$$N = \int n(\vec{r})\,d^3r = 2_s \int dE \underbrace{\left[\int d^3r \sum_n |\psi_n(\vec{r})|^2 \delta(E-E_n)\right]}_{d(\vec{r},E)\text{ is local DOS}} f(E-\mu)$$

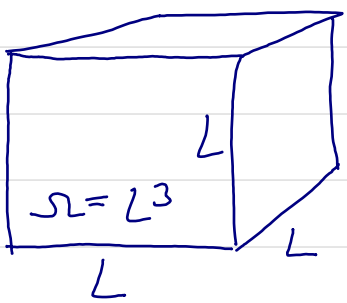
$$= 2_s \int dE \underbrace{\left[\sum_n \delta(E-E_n)\right]}_{\text{total DOS } D_0(E)} f(E-\mu)$$

physical meaning: $D(E)\Delta E$ is number of states within interval ΔE

$$D(E) = \underbrace{\frac{2_s}{\Omega}}_{\text{prefactor is a matter of convention}} \sum_n \delta(E-E_n)$$



EXAMPLE: Free electron gas in a box



$$\hat{H} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2\nabla^2}{2m}$$

$$\hat{H}\cdot\psi(\vec{r}) = E\psi(\vec{r}) \Rightarrow E_{\vec{k}} = \frac{\hbar^2 k^2}{2m},\quad \psi(\vec{r}) \propto e^{i\vec{k}\cdot\vec{r}}$$

has infinite $\int |\psi(\vec{r})|^2 d^3r$

→ enclose electrons in a box and use periodic BC:

$$\psi(x,y,z) = \psi(x+L,y,z) = \psi(x,y+L,z) = \psi(x,y,z+L)$$

$$e^{i\vec{k}\cdot\vec{L}} = 1 \Rightarrow \vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z) \quad n_{x,y,z} = 0, 1, 2, \ldots$$

$$\psi(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{r}},\quad E_{\vec{k}} = \frac{\hbar^2 k^2}{2m} \text{ are now discrete}$$

i) 2-dimensional electron gas

all states in this ring in k-space have the same energy

$$\frac{2k\pi\,dk}{(2\pi/L)^2} = \underbrace{D_0(E)dE}_{\text{number of states in } dE}$$

$\frac{2k\pi\,dk}{(2\pi/L)^2}$: number of states in the ring

$$D(E) = \frac{2s}{L^2}\cdot\frac{2k\pi}{4\pi^2}L^2\frac{dk}{dE}, \quad k = \frac{1}{\hbar}\sqrt{2mE} \Rightarrow \frac{dk}{dE} = \frac{1}{\hbar}\frac{m}{\sqrt{2mE}}$$

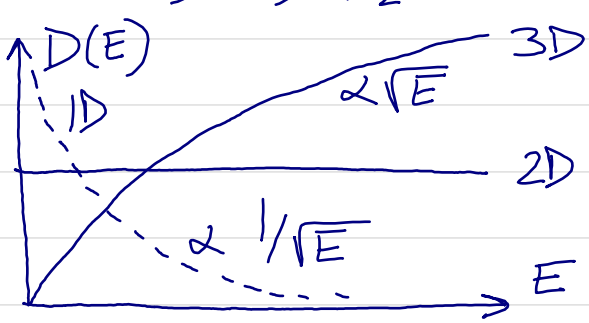
Introduce normalization factor

$$= \frac{1}{\pi}\frac{1}{\hbar}\sqrt{2mE}\cdot\frac{1}{\hbar}\frac{m}{\sqrt{2mE}} = \frac{m}{\pi\hbar^2}$$

ii) 3-dimensional electron gas

$$\frac{4k^2\pi\,dk}{\left(\frac{2\pi}{L}\right)^3} = D_0(E)dE$$

$$D(E) = \frac{2s}{L^3}\cdot\frac{L^3}{8\pi^3}\cdot 4\pi\frac{2mE}{\hbar^2}\cdot\frac{m}{\hbar\sqrt{2mE}} = \frac{m^{3/2}}{\hbar^3}\frac{\sqrt{2}}{\pi^2}\sqrt{E}$$



5° Rewrite $\hat{\rho}_{eq}$ by introducing Green functions

$$\hat{\rho}_{eq} = f(\hat{H} - \mu\hat{I}) \Leftrightarrow \hat{\rho}_{eq} = \int_{-\infty}^{+\infty} f(E-\mu)\,\delta(E\hat{I} - \hat{H})$$

→ one "realization" of δ-function is

$$2\pi\delta(x) = \lim_{\eta\to 0+} \frac{2\eta}{x^2+\eta^2} = \frac{i}{x+i\eta} - \frac{i}{x-i\eta}$$

$$\Rightarrow \delta(E\hat{I} - \hat{H}) = \frac{i}{2\pi}\left(\underbrace{[(E+i\eta)\hat{I} - \hat{H}]^{-1}}_{\text{retarded GF } \hat{G}^r} - \underbrace{[(E-i\eta)\hat{I} - \hat{H}]^{-1}}_{\text{advanced GF } \hat{G}^a = [\hat{G}^r]^+} \right)$$

$$\hat{\rho} = -\frac{1}{\pi}\int_{-\infty}^{\infty} \mathrm{Im}\,\hat{G}\, f(E-\mu)$$

$$\mathrm{Im}\,\hat{G} = \frac{\hat{G}^r - \hat{G}^a}{2i}$$

$$\langle \vec{r}|\hat{\rho}|\vec{r}\rangle = n(\vec{r}) = -\frac{1}{\pi}\int_{-\infty}^{\infty} \langle \vec{r}|\mathrm{Im}\,\hat{G}|\vec{r}\rangle\, f(E-\mu)$$

$$\Rightarrow -\frac{1}{\pi}\langle \vec{r}|\mathrm{Im}\,\hat{G}|\vec{r}\rangle = d(\vec{r}, E)$$

diagonal elements of matrix representation of $\mathrm{Im}\,\hat{G}$ give LDOS

EXAMPLE: DOS of 1-dim electron gas via $\mathrm{Im}\,\hat{G}$

$$\hat{G}^{r,a} = \frac{1}{(E\pm i\eta) - \hat{H}} \cdot \sum_k |k\rangle\langle k| \Rightarrow \langle x|\hat{G}^{r,a}|x'\rangle = \sum_k \frac{\langle x|k\rangle\langle k|x'\rangle}{E\pm i\eta - \frac{\hbar^2k^2}{2m}}$$

$$\sum_{\vec{k}}{}' F(\vec{k}) = \frac{1}{\Delta\vec{k}} \sum_{\vec{k}}{}' F(\vec{k})\Delta\vec{k} \xrightarrow{\Delta\vec{k}\to 0} \frac{L^d}{(2\pi)^d}\int d^dk\, F(\vec{k})$$

$$\langle x|\hat{G}^{r,a}|x\rangle = \frac{L}{2\pi}\int dk\, \frac{e^{ik(x-x')}}{(E\pm i\eta) - \frac{\hbar^2k^2}{2m}}$$

$$\langle x|\hat{G}^{r,a}|x'\rangle = \mp \frac{imL}{\hbar^2 k_0} e^{\pm i k_0 |x-x'|}$$

$$k_0 = \sqrt{\frac{2m|E|}{\hbar^2}} \geq 0, \quad E > 0$$

$$\langle x|\hat{G}^{r,a}|x'\rangle = -\frac{mL}{\hbar^2 k_0} e^{-k_0|x-x'|}, \quad E < 0$$

$$d_0(x,E) = -\frac{1}{\pi}\underbrace{\left[\langle x|\hat{G}^r|x\rangle - \langle x|\hat{G}^a|x\rangle\right]}_{-2\pi i\,\theta(E)\frac{m}{\pi\hbar^2 k_0}} = \theta(E) L \frac{\sqrt{m}}{\pi\hbar\sqrt{2}}\frac{1}{\sqrt{E}}$$

$$d(x,E) = \frac{2s}{L}\cdot \theta(E) L \frac{\sqrt{m}}{\pi\hbar\sqrt{2}}\frac{1}{\sqrt{E}} = \frac{\sqrt{2m}}{\pi\hbar}\frac{1}{\sqrt{E}}$$

6° Green functions as a tool to solve partial differential equations in classical physics

i) Solving Poisson equation with Green functions

$$\nabla^2 V(\vec{r}) = -\frac{1}{\varepsilon_0} n(\vec{r}) \xrightarrow{GF} \nabla^2 G(\vec{r}-\vec{r}') = \delta(\vec{r}-\vec{r}')$$

$$V(\vec{r}) = -\frac{1}{\varepsilon_0}\int d^3r'\, G(\vec{r}-\vec{r}')\, n(\vec{r}')$$

$$G(\vec{r}) = \int \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{r}} G(\vec{k}) \Rightarrow -|\vec{k}|^2 G(\vec{k}) = 1$$

Fourier

solution in k-space

$$G(\vec{k}) = -1/|\vec{k}|^2$$

$$G(\vec{r}) = -\int \frac{d^3k}{(2\pi)^3}\frac{e^{i\vec{k}\cdot\vec{r}}}{k^2} = -\frac{1}{4\pi r} \Rightarrow V(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int d^3r' \frac{n(\vec{r}')}{|\vec{r}-\vec{r}'|}$$

7° Green functions for time-dependent single-particle Schrödinger equation

$\hat{H}$ → assume, for simplicity, is time-independent

$$\left[i\hbar\frac{\partial}{\partial t} - \hat{H}\right]\cdot G(\vec{r},t;\vec{r}',t') = \delta(\vec{r}-\vec{r}')\,\delta(t-t')$$

satisfy:

$$G^r(\vec{r},t;\vec{r}',t') = -\frac{i}{\hbar}\theta(t-t')\langle\vec{r}|e^{-i\hat{H}(t-t')/\hbar}|\vec{r}'\rangle$$

$$G^a(\vec{r},t;\vec{r}',t') = \frac{i}{\hbar}\theta(t'-t)\langle\vec{r}|e^{-i\hat{H}(t-t')/\hbar}|\vec{r}'\rangle = [G^r]^\dagger$$

$$\frac{\partial}{\partial t}\theta(t-t') = \delta(t-t')$$

PHYSICAL MEANING:

$$\langle\vec{r}|\psi(t)\rangle = \langle\vec{r}|e^{-i\hat{H}(t-t')/\hbar}|\psi(0)\rangle \rightarrow \text{insert } \hat{I} = \int d^3r'|\vec{r}'\rangle\langle\vec{r}'|$$

$$= \int d^3r' \langle\vec{r}|e^{-i\hat{H}(t-t')/\hbar}|\vec{r}'\rangle\langle\vec{r}'|\psi(t)\rangle$$

$$\psi(\vec{r},t) = \int d^3r'\, G(\vec{r},t;\vec{r}',t')\,\psi(\vec{r}',t')$$

→ so $G(\vec{r},t;\vec{r}',t')$ determines conditional probability to find particle at $\vec{r},t$ if the particle was earlier at $\vec{r}',t'$

$$G^r(\vec{r},t;\vec{r}',t') = -\frac{i}{\hbar}\theta(t-t')\sum_n \langle\vec{r}|e^{-i\hat{H}(t-t')/\hbar}|E_n\rangle\langle E_n|\vec{r}'\rangle$$

$$= -\frac{i}{\hbar}\theta(t-t')\sum_n \psi_n^*(\vec{r}')\,\psi_n(\vec{r})\,e^{-iE_n(t-t')/\hbar}$$

$$\theta(t-t') = \frac{-1}{2\pi i}\int_{-\infty}^{\infty} dE\ \frac{e^{-iE(t-t')}}{E+i\eta},\quad \eta\to 0+$$

$$\Downarrow$$

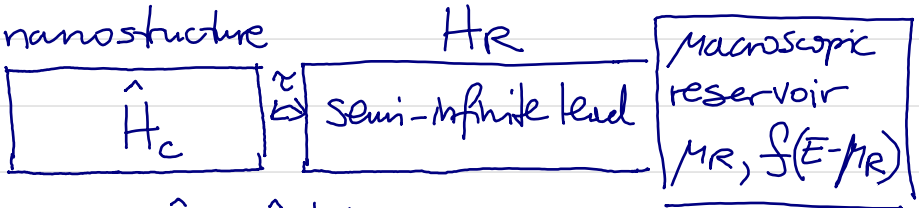
$$G^r(r,t;r',t') = \frac{1}{2\pi\hbar}\sum_n \psi_n(\vec{r}')\psi_n(\vec{r})\int_{-\infty}^{\infty} dE\ \frac{e^{-i(\overbrace{E}+E_n)(t-t')/\hbar}}{E+i\eta}$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dE\ \underbrace{\left[\sum_n \frac{\psi_n^*(\vec{r}')\psi_n(\vec{r})}{E-E_n+i\eta}\right]}_{G^r(E)} e^{-iE(t-t')/\hbar}$$

so two different retarded GFs we introduced or Fourier transforms of each other

$$G^r(E) = \int_{-\infty}^{\infty} dt\ \underbrace{G^r(\vec{r},\vec{r}';t-t')}_{\text{depends on } t-t' \text{ when } \hat{H} \text{ is time independent}} e^{iE(t-t')}$$

8° Equilibrium density matrix of open quantum system with continuous energy spectrum



$$\hat{H}_{total} = \begin{pmatrix} \hat{H}_c & \hat{\tau}^+ \\ \hat{\tau} & \hat{H}_R \end{pmatrix}$$

$$\hat{G}^r = \frac{1}{(E+i\eta)\hat{I} - \hat{H}_{total}} = \begin{pmatrix} \hat{G}^r_c & \hat{G}^r_{cR} \\ \hat{G}^r_{Rc} & \hat{G}^r_R \end{pmatrix}$$

$$\begin{pmatrix} \hat{G}^r_c & \hat{G}^r_{cR} \\ \hat{G}^r_{Rc} & \hat{G}^r_R \end{pmatrix} \cdot \begin{pmatrix} (E+i\eta)\hat{I}-\hat{H}_c & -\hat{\tau}^+ \\ -\hat{\tau} & (E+i\eta)\hat{I}-\hat{H}_R \end{pmatrix} = \begin{pmatrix} \hat{I} & 0 \\ 0 & \hat{I} \end{pmatrix}$$

$$[(E+i\eta)\hat{I}-\hat{H}_c]\cdot\hat{G}_c^r-\hat{\tau}\cdot\hat{G}_{cR}^r=\hat{I}$$

replace

$$-\hat{\tau}^+\hat{G}_c^r+[(E+i\eta)\hat{I}-\hat{H}_R]\cdot\hat{G}_{cR}^r=0$$

$$\Downarrow$$

$$\hat{G}_{cR}^r=\hat{g}_R^r\cdot\hat{\tau}^+\cdot\hat{G}_c^r \quad \text{where} \quad \hat{g}_R^r=[(E+i\eta)\hat{I}-\hat{H}_R]^{-1}$$

$$\hat{G}_c^r=[(E+i\eta)\hat{I}-\hat{H}_c-\tau\hat{g}_R^r\hat{\tau}^+]^{-1}$$

self-energy due to semi-infinite R lead

→ $\hat{\rho}_{eq}=-\frac{1}{\pi}\int dE\ \mathrm{Im}\hat{G}(E)f(E)$ is computationally much more expensive than $\hat{\rho}_{eq}=f(\hat{H}-\mu\hat{I})$ since in the former case one has to perform matrix inversion REPETEADLY over apparently infinite energy interval, while in the latter case one performs only ONE diagonalization; but the former approach works for OPEN quantum system such as nanodevices attached to external circuit, while the latter ONLY works for isolated quantum systems with discrete energy spectrum

→ computational algorithms for contour integration of $\mathrm{Im}\hat{G}f$

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Electron density and transport in top-gated graphene nanoribbon devices: First-principles Green function algorithms for systems containing a large number of atoms

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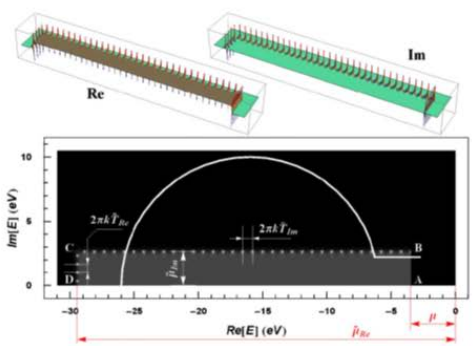

PHYSICAL REVIEW B **75**, 035123 (2007)

Continued fraction representation of the Fermi-Dirac function for large-scale electronic structure calculations

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