Nanodevices: Window into the realm of quantum physics

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Outline

1. Introduction – quantum microscopic laws & macroscopic world
   - Classical vs. quantum physics
   - Quantum macroscopic state
2. Mesoscopic systems – superconductivity & supercurrent
   - Measusrements & experimental realization
   - Quantum dot attached to superconductors
   - Model description & perturbation theory
3. Numerical and analytic results
   - Spin-symmetric state
   - Spin polarized state
4. Conclusions

Macroscopic vs. microscopic

Macroscopic phenomena do have microscopic origin

Experiment vs. theory

- Observers & observing devices are macroscopic
- Perception of the laws of Nature via complex composite objects
- Theory
  - Macroscopic – phenomenological (incomplete)
  - Fundamental (first principles) – microscopic
- Indirect interaction between experiment & theory
- Interpretation of microscopic dynamics via macroscopic objects

Devise microscopic laws complying with observed macroscopic behavior

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Classical physics – continuous world

- Space & time homogeneity – scale invariance (macroscopically observed)
- No fundamental universal space and time scale breaking macroscopic space-time homogeneity
- Downscaling to a mass point at instantaneous time
- Infinitesimal space and time changes (continuous space-time)
- Deterministic differential equations of motion – Newton's laws
- Macroscopic objects – superposition principle

Quantum physics – discrete world I

- Fundamental length scale: Bohr radius (hydrogen atom)

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} \doteq 5.29 \times 10^{-11} m$$

- Classical scale invariance broken at microscopic length scales
- Uncertainty principle for coordinate and momentum

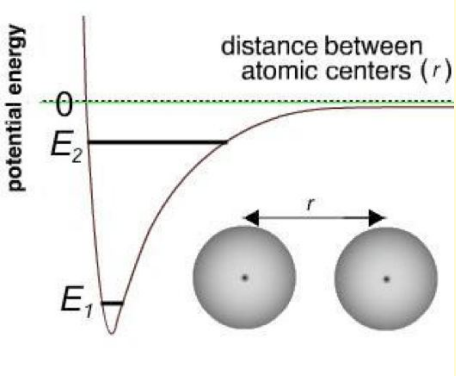
$$\Delta_x \Delta_p \geq \frac{\hbar}{2}$$

$$\hbar \doteq 1.054 \times 10^{-34} Js/rad$$

- Particle-wave duality
  - Local objects (particles) –no deterministic trajectory when measured (Feynman path integral)
  - Extended objects (waves) – deterministic Schrödinger equation when unobserved

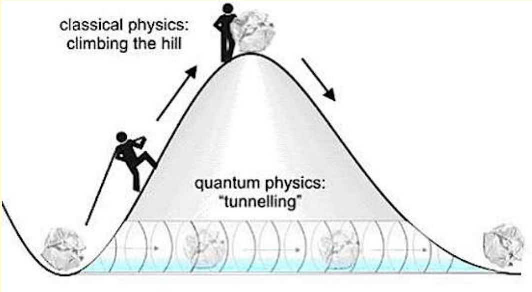
Quantum physics – discrete world II

- Bound states – world made discrete



Quantum physics – discrete world III

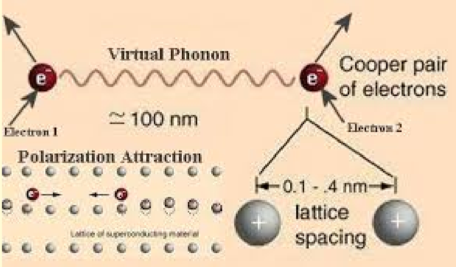
- Tunneling – particles can penetrate potential barriers



Microscopic world governed by quantum laws

Superconductivity – macroscopic quantum coherence I

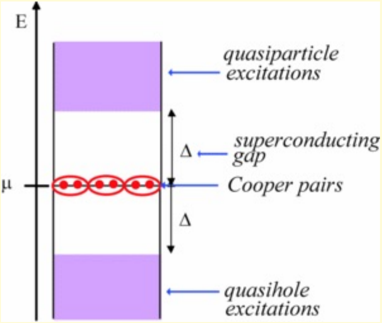
- Long-range quantum coherence – quantum phase
- Electron-phonon interaction – mediates electron attraction



- Cooper pairs – bound states of two electrons
- Bardeen-Cooper-Schrieffer (BCS) theory (weak coupling) – condensation of singlet Cooper pairs

Superconductivity – macroscopic quantum coherence II

- Order parameter – energy gap Δ for one-electron excitations



- Energy won by creating a Cooper pair Δ
- Cooper pairs form the ground state - are not excitations

Microscopic origin of macroscopic phenomena

Can we observe directly the quantum microscopic processes underlying the macroscopic long-range collective behavior?

Yes.
Thanks to high-resolution microscopy and improved technology of fabrication nanoscale structures with controlled properties.

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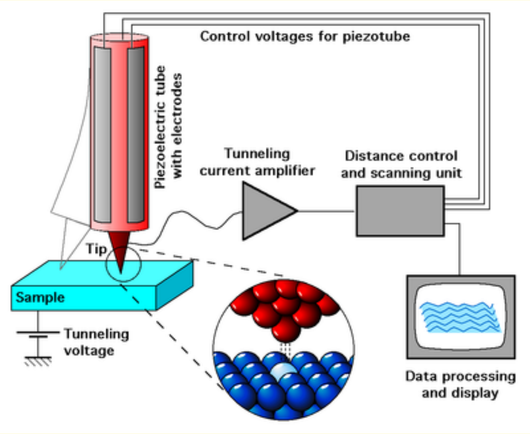
High-resolution probes

- Manipulation of individual atoms via scanning tunneling microscope



Superconductivity in nano-structures

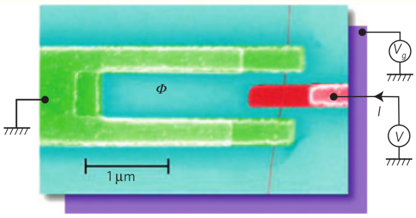
Experimental realization

- Carbon nanotubes with well separated energy levels and strong electron repulsion
- Nanotube attached to metallic leads – formation of local magnetic moment
- Nanotube attached to superconducting leads – tunneling of Cooper pairs

Theoretical description

- Singe-impurity Anderson model
- Metallic leads – no spontaneous magnetization (Kondo)
- BCS superconducting leads – induce superconducting gap on impurity

Experimental setup

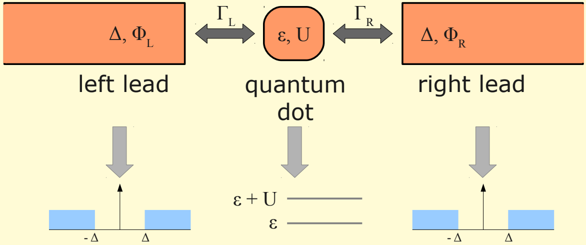


Quantum nanosystem

- doped silicon substrate + 1μm SiO_2 layer
- 700nm carbon nanotube ($\delta E \sim 0.7$meV)
- alluminium electrodes ($T_c = 1.2$K) (green)
- sc tunneling probe (red)
- magnetic flux ϕ through the loop generates phase difference $\Phi = (2e/\hbar)\phi$
- $T \sim 40$mK

J.-D. Pillet, C. Quay, P. Morfin, C. Bena, A. Levy Yeyati, P. Joyez, Nature Phys. 6, 965 (2010)

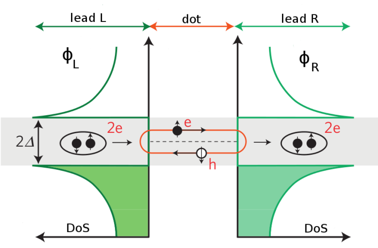
Model system

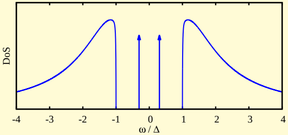


- U - on-site Coulomb interaction
- ε - on-site energy level
- Δ - superconducting gap
- Φ_α - phase of the superconducting wave function
- $\Phi = \Phi_R - \Phi_L$ - phase difference
- Γ_α - tunneling rate (dot-lead coupling)

Andreev reflections and gap states

- Electron at the right QD-S interface: Cooper pair created by reflecting hole to left
- Hole at the left QD-S interface: Cooper pair annihilated & electron reflected to right
- Multiple Andreev reflections form Andreev bound states at $\pm\omega_0$ ($\omega_0 < \Delta$ - gap states)





- Andreev bound states carry Josephson current (supercurrent)

$$J_{ABS} = \frac{2e}{\hbar}\frac{\partial \omega_0}{\partial \Phi}$$

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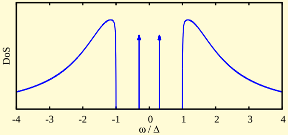

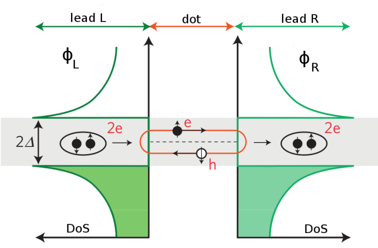

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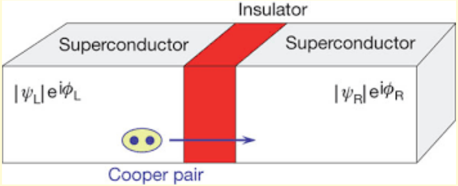
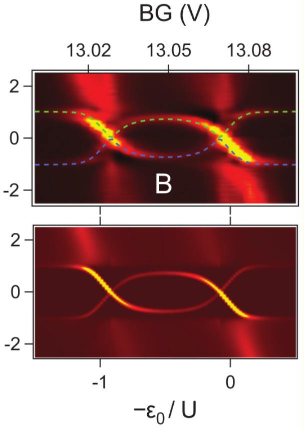
Supercurrent – Josephson effect

- Josephson junction: S-I-S



- Nonzero phase difference $\Phi = \Phi_R - \Phi_L$ induces tunneling of Cooper pairs trhough the insulating interface
- Josephson current (supercurrent) – dispersionless
- Supercurrent – equilibrium property (no excitation or external force needed)

Behavior of gap states with electron repulsion



ε_0 – impurity energy level (chemcal potential)

Crossing of gap states

- Experiment: continuous crossing of Andreev states at the Fermi level
- Numerical RG results in good agreement with experimental data
- Missing reliable analytic approach to explain the phenomenon

Single-impurity Anderson model with SC leads

- Generic operator Hamiltonian

$$\mathcal{H} = \mathcal{H}_{dot} + \sum_{\alpha=R,L} \left(\mathcal{H}^{\alpha}_{lead} + \mathcal{H}^{\alpha}_{c}\right)$$

- quantum dot (single - level):

$$\mathcal{H}_{dot} = \varepsilon \sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} + U d^{\dagger}_{\uparrow} d_{\uparrow} d^{\dagger}_{\downarrow} d_{\downarrow}$$

- BCS (s-wave) leads:

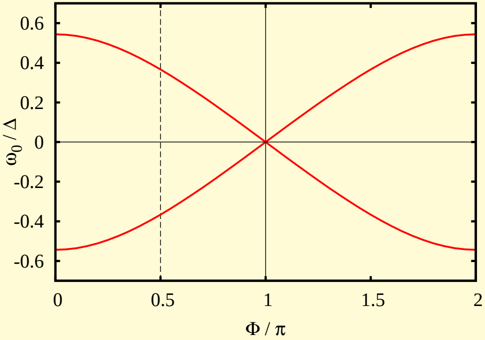
$$\mathcal{H}^{\alpha}_{lead} = \sum_{\mathbf{k}\sigma} \varepsilon(\mathbf{k}) c^{\dagger}_{\alpha,\mathbf{k}\sigma} c_{\alpha,\mathbf{k}\sigma} - \Delta \sum_{\mathbf{k}} \left(e^{i\Phi_{\alpha}} c^{\dagger}_{\alpha,\mathbf{k}\uparrow} c^{\dagger}_{\alpha,-\mathbf{k}\downarrow} + \text{H.c.}\right) \qquad \alpha = R, L$$

- coupling to the bath:

$$\mathcal{H}^{\alpha}_{c} = -t_{\alpha} \sum_{\mathbf{k}\sigma} \left(c^{\dagger}_{\alpha,\mathbf{k}\sigma} d_{\sigma} + \text{H.c.}\right) \qquad \Gamma_{\alpha} = 2\pi \rho_{\alpha} |t_{\alpha}|^{2}$$

Crossing of gap states – spin-symmetric solution I

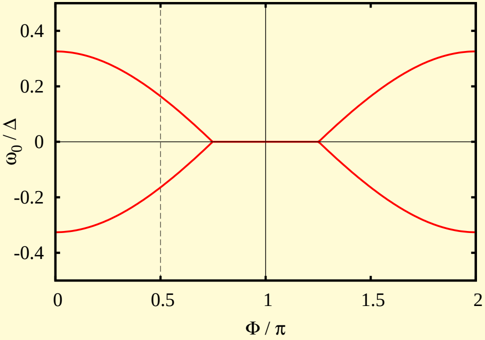
- No Coulomb repulsion ($U = 0$)
- Energy of gap (Andreev) states as a function of phase difference $\Phi = \Phi_L - \Phi_R$



- Energy yield of the creation of a Cooper pair: ω_0

Crossing of gap states – spin-symmetric solution II

- Effect of electron repulsion (Hartree-Fock solution)



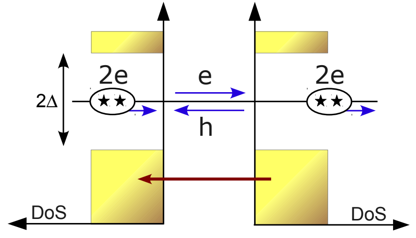
- 0 phase only for $\omega_0 > 0$ – Cooper pairs energetically favorable
- A new (π) phase – no Cooper pairs due to strong Coulomb repulsion

Crossing of gap states – spin-symmetric solution III

No crossing of gap states in the spin-symmetric state

Josephson current - gap & band states

$$J_{super} = -2\Delta\Gamma_0 \left[\frac{\mathrm{Res}[\mathcal{G}^*, -\omega_0]}{\sqrt{\Delta^2 - \omega_0^2}} + \int_{-\infty}^{-\Delta} \frac{d\omega}{\pi} \frac{\Re \mathcal{G}^*(\omega)}{\sqrt{\omega^2 - \Delta^2}} \right] \sin(\Phi/2)$$



$J_{ABS} \sim \sin(\Phi/2)$

$J_{band} \sim \sin(\Phi)$

- Contribution from Andreev bound states: direct current via the impurity level split to $\pm\omega_0$
- Contribution from band states: reverse tunneling current

0 and π phases – infinite superconducting gap

- Only discrete gap (Andreev) states – no band states
- 0 phase BCS singlet: $|\pm\rangle = \mp u_{\mp}|\uparrow\downarrow\rangle + u_{\pm}|0\rangle$

$$\omega_{\pm} = \pm\sqrt{\left(\varepsilon + \frac{U}{2}n\right)^2 + \cos^2(\Phi/2)\left(\Gamma_0 - U\nu\right)^2}$$

ν density of Cooper pairs

- Spin doublet – degenerate $|\uparrow\rangle, |\downarrow\rangle$ states at energy $E_d = 0$
- 0 phase being the ground state: $\omega_- < E_d = 0$
- $0 - \pi$ transition: $\omega_{\pm} = 0$
- Critical interaction: $0 - \pi$ transition

$$\frac{U_c}{2} = \sqrt{\left(\varepsilon + \frac{U_c}{2}\right)^2 + \cos^2(\Phi/2)\Gamma_0^2}$$

only for $\varepsilon < 0$

Analytic methods – diagrammatic expansion

Static mean field – spin polarized

- 0-π first order (no gap-state crossing)
- π phase bound with spurious magnetic state
- Numerically off wrt Numerical Renormalization Group (NRG)

Dynamical solutions – spin symmetric

- Dynamical corrections (DC) with only static self-consistence
- Fully dynamically self-consistent corrections (FDC)
- High numerical precision of 2^{nd} order (intermediate coupling)

Dynamical approximations by now applicable only in 0 phase and zero temperature

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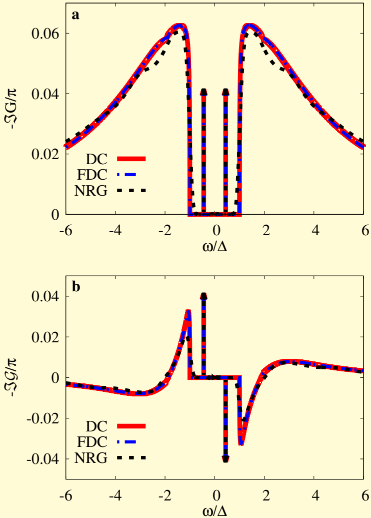
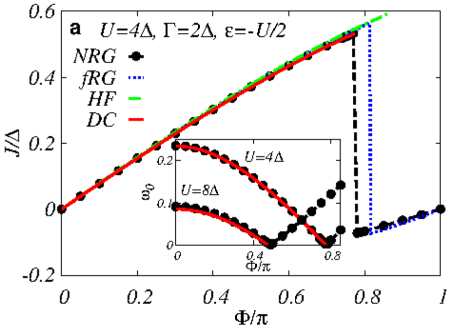
Normal & anomalous GF

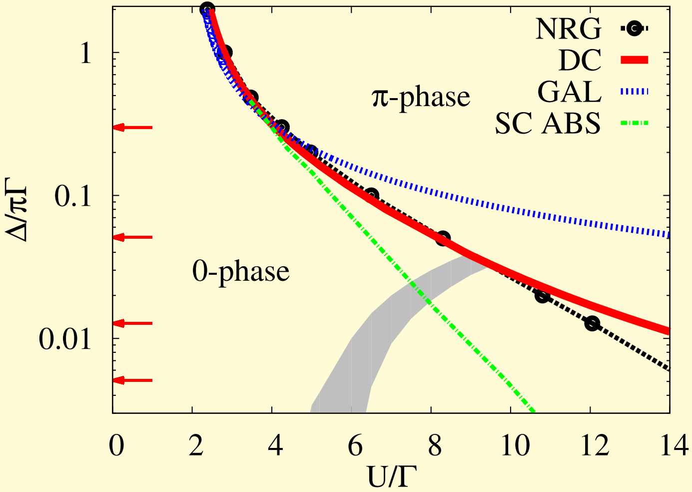


$0-\pi$ transition – change of sign of the supercurrent



- $0-\pi$ transition coincides with the crossing of gap states
- Supercurrent carried dominantly by Andreev states - zero phase (direct current)
- Supercurrent due to tunneling of band states - π phase (reverse current)

$U - \Delta$ Phase diagram



Beyond the crossing of gap states

What the crossing of gap states means?
How to describe π phase beyond MFT?

Suppressing spurious magnetic state due to band states in the spin polarized state.
Dynamical solution in magnetic field.

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Solution in an external magnetic field I

- Spin-dependent propagators $G_\sigma(\omega)$, $\mathcal{G}_\sigma(\omega)$ in magnetic field
- Denominator - spin dependent $(n = n_\uparrow + n_\downarrow,\ m = n_\uparrow - n_\downarrow)$

$$D_\sigma(\omega) = \left[\omega(1 + s(\omega)) + \sigma\left(h + \frac{U}{2}m\right)\right]^2 - \left(\epsilon + \frac{U}{2}n\right)^2 - \Delta_\Phi^2\left(s(\omega) - U\nu\right)^2$$

(Mean-field approximation)

- Reflection symmetry: $D_{-\sigma}(\omega) = D^*_\sigma(-\omega)$
- Four spin-dependent gap states

$$\omega_\sigma^\pm\left(1 + s_\sigma^\pm\right) = -\sigma\left(h + \frac{U}{2}m\right) \pm \sqrt{\left(\epsilon + \frac{U}{2}n\right)^2 + \Delta_\Phi^2\left(s_\sigma^\pm - U\nu\right)^2}$$

- Spin-reflection symmetry: $\omega_\sigma^\pm = -\omega_{-\sigma}^\mp$

Solution in an external magnetic field II

- Crossing of gap states ($h \searrow 0$): $\omega_\uparrow^+ = \omega_\downarrow^- = 0$
  - 0 phase: $\omega_\sigma = \omega$

$$n_c = -\frac{2\varepsilon}{U}\,, \qquad \Delta\nu_c = \frac{2\Gamma_0}{U}$$

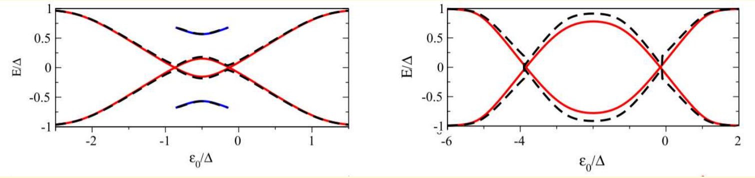
  - π phase: $\omega_\uparrow \neq \omega_\downarrow$

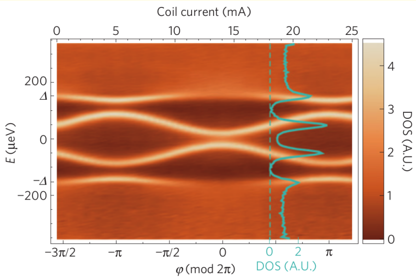
$$\frac{U^2}{4}m^2 = \left(\varepsilon + \frac{U}{2}n\right)^2 + \Gamma_0^2\cos^2(\Phi/2)$$

  - Atomic limit: $n_\downarrow = 0, m = n = 1, \nu = 0$, & exact critical U_c
- 0 phase: low-magnetic (singlet) state ($\omega_\uparrow^- < 0,\ \omega_\uparrow^+ > 0$)
- π phase: high-magnetic (doublet) state ($\omega_\uparrow^- < 0,\ \omega_\uparrow^+ < 0$)
- No Andreev bound states in π-phase

Spin polarized Andreev states

$U = \Delta$ $\qquad$ $U = 4\Delta$





- Four Gap states in the π phase
- Jump in particle density, magnetization & Josephson current
- Continuous crossing of gap states beyond Hartee-Fock solution (free of spurious magnetic transition due to band states)

SC interacting quantum dot – spectral representation

1. Induced SC gap on impurity - normal & anomalous GF
2. Gap states – remnants of the impurity level
3. Perturbation theory – convolutions of poles & cuts in GF

Andreev bound states & Josephson current

1. Two contributions to JC: Direct (ABS) & tunneling (inverse)
2. $0 - \pi$ transition – crossing of gap states to spin-dependent JC
3. Spin symmetric solution (beyond static HF):
   - Two Andreev states symmetric around FE
   - No crossing - saturation due to freezing at FE & vanishing of anomalous GF
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