# *General analytical solution to quantum states of open nanoelectronic systems*

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# I. Introduction and motivation

*quantum states*

*preparation* *manipulation* *detection*

*quantum information processing*

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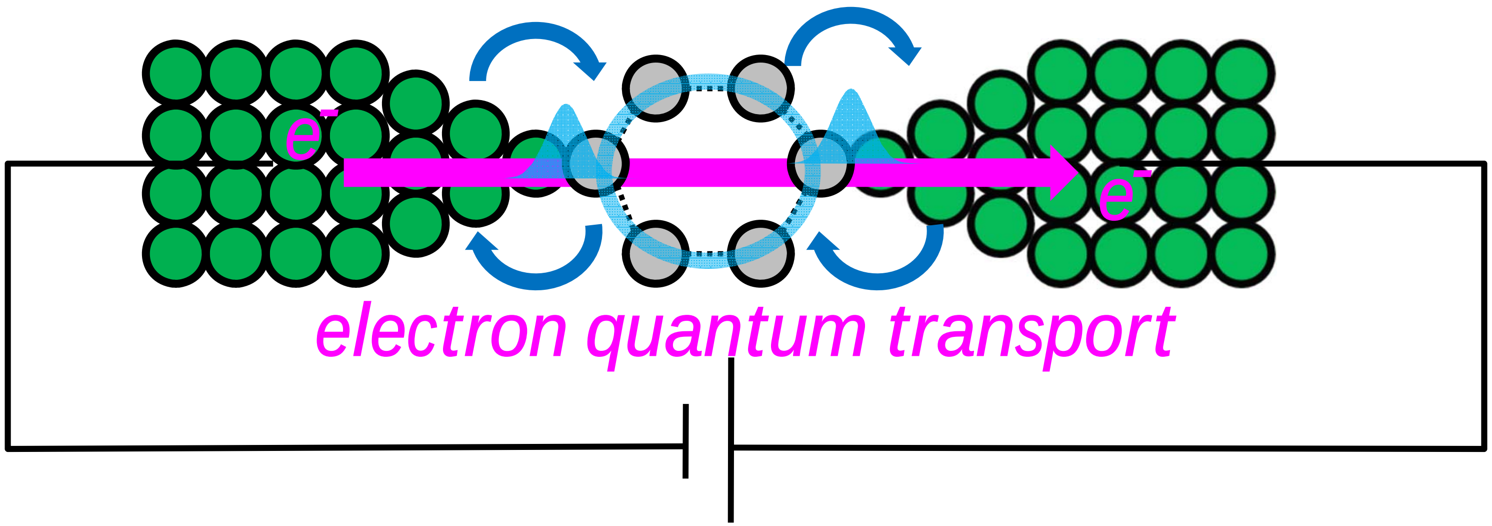
*nanoelectronic systems*

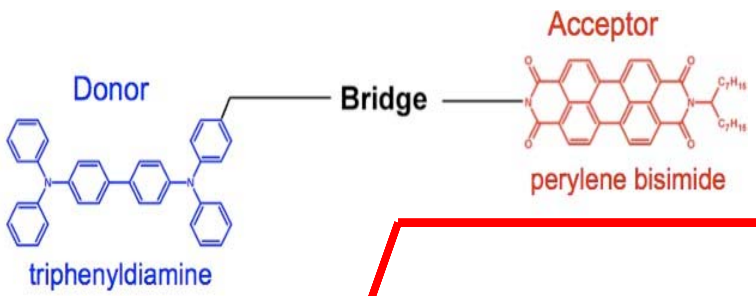



*electron quantum transport*

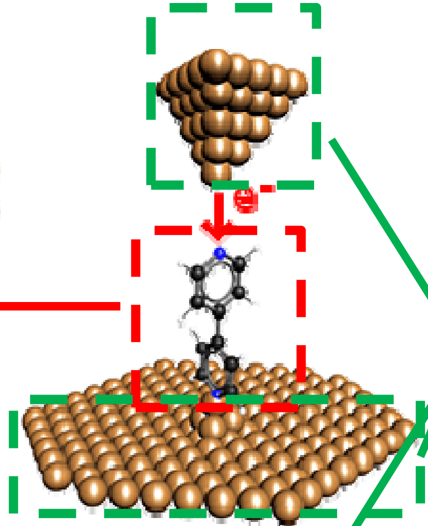
- **various tunable couplings**
- **adjustable energetic structures**
- **useful as quantum devices**

# I. Introduction and motivation

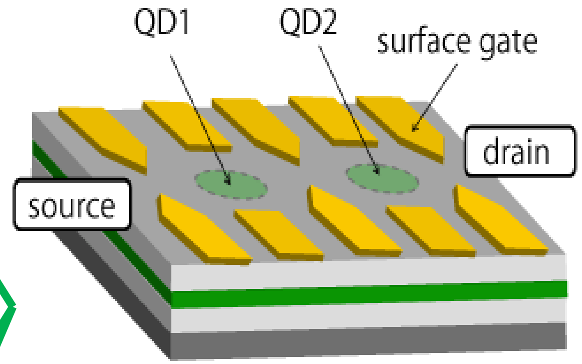
## *quantum transport and nanoelectronics*




charge transfer pair



STM probing surface absorbed molecule




semiconductor quantum dots

naturally occurred ＋ synthesized

**quantum transport systems are ubiquitous**

**central system** ＋ **environments**: electron reservoirs

electrodes continuous states in host materials

⬇

*open quantum systems*

# I. Introduction and motivation

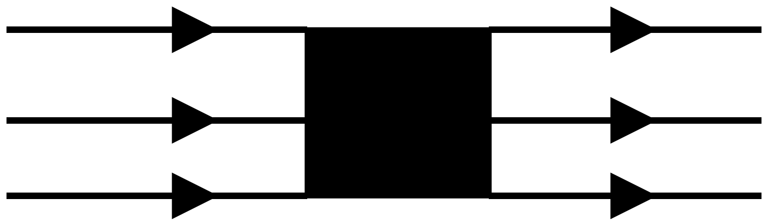
*theories for nanoelectronic transport setups*

- *Landauer-Bütikker formalism*

-- in terms of scattering amplitudes

--targeting at in-out relation

--the central system as a black box



- *Schwinger-Keldysh nonequilibrium Green function technique*

-- in terms of Green functions

--targeting at the transport currents

-- the state of the central system is averaged

✓ - *Feynman-Vernon's influence functional theory*

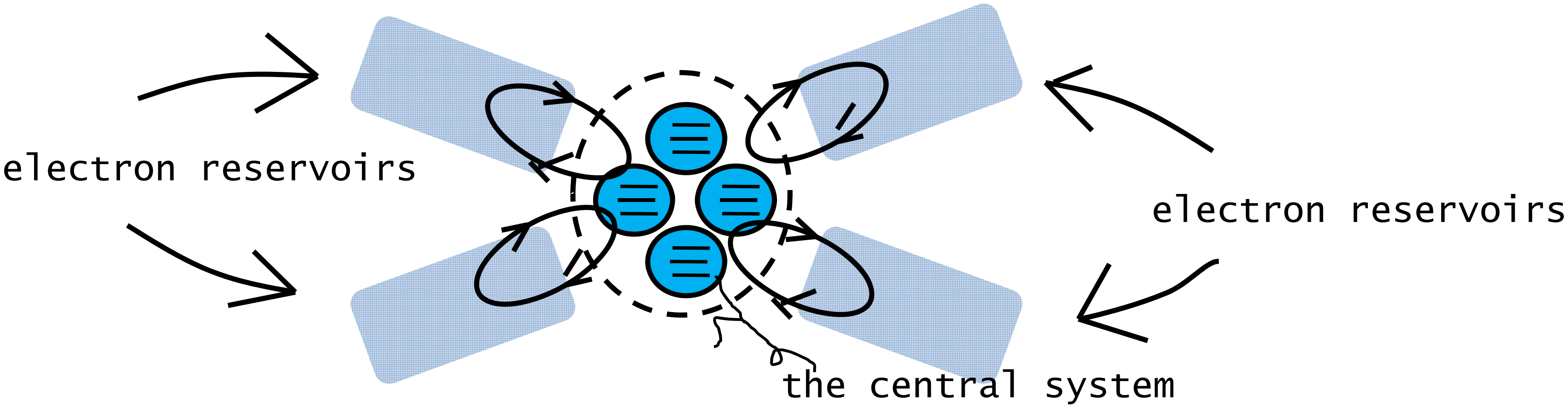
--in terms of the reduced density matrix

--targeting at the quantum state of open systems

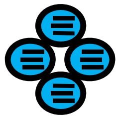
--fully characterizing the state of the central system

# I. Introduction and motivation

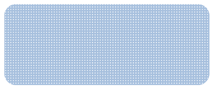
*modeling of quantum transport devices*



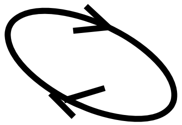

$$H(t) \;=\; H_{\rm dq}(t) + H_{\rm rev}(t) + H_T(t)$$



$$H_{qd}(t) = \sum_{ij} \epsilon_{ij}(t) d_i^\dagger d_j$$ the central system



$$H_{rev}(t) = \sum_{\alpha k} \epsilon_{\alpha k}(t) c_{\alpha k}^\dagger c_{\alpha k}$$ electron reservoirs



$$H_T(t) = \sum_{i\alpha k} [V_{i\alpha k}(t) d_i^\dagger c_{\alpha k} + V_{i\alpha k}^*(t) c_{\alpha k}^\dagger d_i]$$ electron exchange

# I. Introduction and motivation

*exact master equation for a class of nanoelectronic systems*

- **equation of motion for the reduced density operator**

$$\frac{d}{dt}\hat{\rho}(t) = -i[H_{\rm dq}(t), \hat{\rho}(t)] + \sum_{\alpha}[\mathcal{L}^{+}_{\alpha}(t) + \mathcal{L}^{-}_{\alpha}(t)]\hat{\rho}(t)$$

- **transport currents**

$$I_{\alpha}(t) = \frac{e}{2\hbar}\mathrm{tr}_s[(\mathcal{L}^{+}_{\alpha}(t) - \mathcal{L}^{-}_{\alpha}(t))\hat{\rho}(t)]$$

non-unitary processes due to electron exchanges

***Starting theory:***

M.W.Y. Tu and W.M. Zhang, PRB **78**, 235311 (2008);
M.W.Y. Tu, M.T. Lee, and W.M. Zhang, QIP (Springer) **8**, 631 (2009).
J.S. Jin, M.W.Y. Tu, W. M. Zhang, and Y.J. Yan, NJP, **12**, 083013 (2010).

***Applications:***

M.W.Y. Tu, W.M. Zhang, and J.S. Jin, Phys. Rev. B **83**, 115318 (2011)
H.N. Xiong, W. M. Zhang, M.W.Y. Tu, and D. Braun, PRA **86**, 032107(2012).
W.M. Zhang, L.P. Yuan, H.N. Xiong, M.W.Y. Tu, and F. Nori, PRL **109**, 170402(2012).
M.W.Y. Tu, W.M. Zhang, J.S. Jin, O. Entin-Wohlman, and A. Aharony, PRB **86**, 115453(2012).
M.W.Y. Tu, W. M. Zhang, and F. Nori, PRB **86**, 195403(2012).
J.S. Jin, M.W.Y. Tu, N.E. Wang and W.M. Zhang, J. Chem. Phys. **139**, 064706 (2013).
M.W.Y. Tu, A. Aharony, W.M. Zhang, O. Entin-Wohlman, PRB **90**, 165422 (2014).

↳ applied only using initial empty state, **not full use** of this master equation

*numerically solving master equation is difficult, limited to small dimension*

**general analytical solution ??**

**useful for other more applications**

# II. Quantum states of open electronic systems

*general analytical solution to exact master equation*

$$\langle P\boldsymbol{l}^{(n)}|\hat{\rho}(t)|P\boldsymbol{r}^{(n)}\rangle = \det\left[\mathbf{1}_D - \boldsymbol{v}(t)\right]\sum_{m=0}^{D}\sum_{P\boldsymbol{a}^{(m)}}\sum_{P\boldsymbol{b}^{(m)}}\left[\mathcal{J}^{\boldsymbol{l}^{(n)},\boldsymbol{r}^{(n)}}_{\boldsymbol{a}^{(m)},\boldsymbol{b}^{(m)}}(t)\langle P\boldsymbol{a}^{(m)}|\hat{\rho}(t_0)|P\boldsymbol{b}^{(m)}\rangle\right]$$

later state

**non-unitary evolutions**

initial state

environments initially at thermal equilibria

$\boldsymbol{l}^{(n)}$, $\boldsymbol{r}^{(n)}$: n-electron configurations

$\boldsymbol{a}^{(m)}$, $\boldsymbol{b}^{(m)}$: m-electron configurations

*notations for configurations*

$D$ : number of available orbitals in the system

$\mathrm{S} = \{1, 2, \cdots, D\}$ : set of available orbitals in the system

$\boldsymbol{i}^{(n)} = \{i_1, \cdots, i_n\}$: set of $n$ occupied orbitals as a configuration

*notations for multi-electron states*

$|P\boldsymbol{i}^{(n)}\rangle = d^{\dagger}_{P\boldsymbol{i}_n^{(n)}} \cdots d^{\dagger}_{P\boldsymbol{i}_1^{(n)}}|0\rangle$: an $n$ -electron state

$P\boldsymbol{i}_n^{(n)} > \cdots > P\boldsymbol{i}_2^{(n)} > P\boldsymbol{i}_1^{(n)} \in \boldsymbol{i}^{(n)}$

↑ fixing ordering to avoid fermion exchange sign problem

# II. Quantum states of open electronic systems

*elementary processes behind the open system evolutions*

- **single-particle propagations**

$$\frac{\partial}{\partial t}\boldsymbol{u}(t,\tau)+i\boldsymbol{\epsilon}(t)\boldsymbol{u}(t,\tau)+\int_{\tau}^{t}ds\sum_{\alpha}\boldsymbol{g}_{\alpha}(t,s)\boldsymbol{u}(s,\tau)=0$$

- **statistical actions from reservoirs on filling the central system**

$$\boldsymbol{v}(t)=\int_{t_0}^{t}d\tau\int_{t_0}^{t}d\tau'\boldsymbol{u}(t,\tau)\sum_{\alpha}\tilde{\boldsymbol{g}}_{\alpha}(\tau,\tau')[\boldsymbol{u}(t,\tau')]^{\dagger}=\langle d_j^{\dagger}(t)d_i(t)\rangle\Big|_{\text{initial empty state}}$$

initial empty state

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$$\boldsymbol{g}_{\alpha}(t_1,t_2)=\int\frac{d\omega}{2\pi}\Gamma_{\alpha}(\omega,t_1,t_2)\,e^{-i\omega(t_1-t_2)}$$

dissipation kernel

$$\tilde{\boldsymbol{g}}_{\alpha}(t_1,t_2)=\int\frac{d\omega}{2\pi}f_{\alpha}(\omega)\Gamma_{\alpha}(\omega,t_1,t_2)\,e^{-i\omega(t_1-t_2)}$$

fluctuation kernel

fermi function

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$$[\Gamma_{\alpha}(\omega,t_1,t_2)]_{ij}=2\pi\sum_{\boldsymbol{k}\in\alpha}V_{i\alpha\boldsymbol{k}}(t_1)\exp\left[-i\int_{t_2}^{t_1}ds\Delta_{\alpha\boldsymbol{k}}(s)\right]V_{\alpha\boldsymbol{k}j}(t_2)\,\delta\left(\omega-\epsilon_{\alpha\boldsymbol{k}}^{0}\right)$$

spectral density

tunneling amplitudes

$$\epsilon_{\alpha\boldsymbol{k}}(t)=\epsilon_{\alpha\boldsymbol{k}}^{0}+\Delta_{\alpha\boldsymbol{k}}(t)$$

: time-dependent energies of reservoir states

# II. Quantum states of open electronic systems

*propagating function in Fock space*

$$\mathcal{J}^{\boldsymbol{l}^{(n)},\boldsymbol{r}^{(n)}}_{\boldsymbol{a}^{(m)},\boldsymbol{b}^{(m)}}(t)=(-1)^{m}\det\begin{pmatrix}[\boldsymbol{J}_{00}(t)]^{\boldsymbol{a}^{(m)}}_{\boldsymbol{b}^{(m)}} & [\boldsymbol{J}_{0f}(t)]^{\boldsymbol{r}^{(n)}}_{\boldsymbol{b}^{(m)}}\\ [\boldsymbol{J}_{f0}(t)]^{\boldsymbol{a}^{(m)}}_{\boldsymbol{l}^{(n)}} & [\boldsymbol{J}_{ff}(t)]^{\boldsymbol{r}^{(n)}}_{\boldsymbol{l}^{(n)}}\end{pmatrix}$$

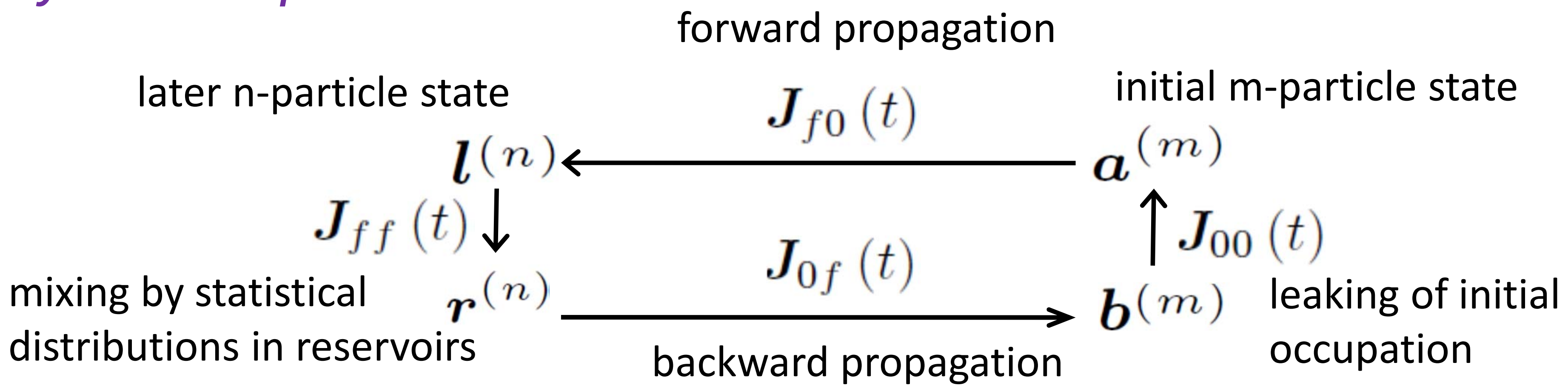
$$\left([\boldsymbol{J}_{00}(t)]^{\boldsymbol{a}^{(m)}}_{\boldsymbol{b}^{(m)}}\right)_{ij}=[\boldsymbol{J}_{00}(t)]_{P\boldsymbol{b}^{(m)}_{i}P\boldsymbol{a}^{(m)}_{j}} \qquad \left([\boldsymbol{J}_{0f}(t)]^{\boldsymbol{r}^{(n)}}_{\boldsymbol{b}^{(m)}}\right)_{ij}=[\boldsymbol{J}_{0f}(t)]_{P\boldsymbol{b}^{(m)}_{i}P\boldsymbol{r}^{(n)}_{j}}$$

$$\left([\boldsymbol{J}_{f0}(t)]^{\boldsymbol{a}^{(m)}}_{\boldsymbol{l}^{(n)}}\right)_{ij}=[\boldsymbol{J}_{f0}(t)]_{P\boldsymbol{r}^{(n)}_{i}P\boldsymbol{b}^{(m)}_{j}} \qquad \left([\boldsymbol{J}_{ff}(t)]^{\boldsymbol{r}^{(n)}}_{\boldsymbol{l}^{(n)}}\right)_{ij}=[\boldsymbol{J}_{ff}(t)]_{P\boldsymbol{l}^{(n)}_{i}P\boldsymbol{r}^{(n)}_{j}}$$

$$\boldsymbol{J}_{f0}(t)=[\boldsymbol{J}_{0f}(t)]^{\dagger}=(\mathbf{1}_{D}-\boldsymbol{v}(t))^{-1}\boldsymbol{u}(t) \qquad \boldsymbol{J}_{ff}(t)=(\mathbf{1}_{D}-\boldsymbol{v}(t))^{-1}-\mathbf{1}_{D}$$

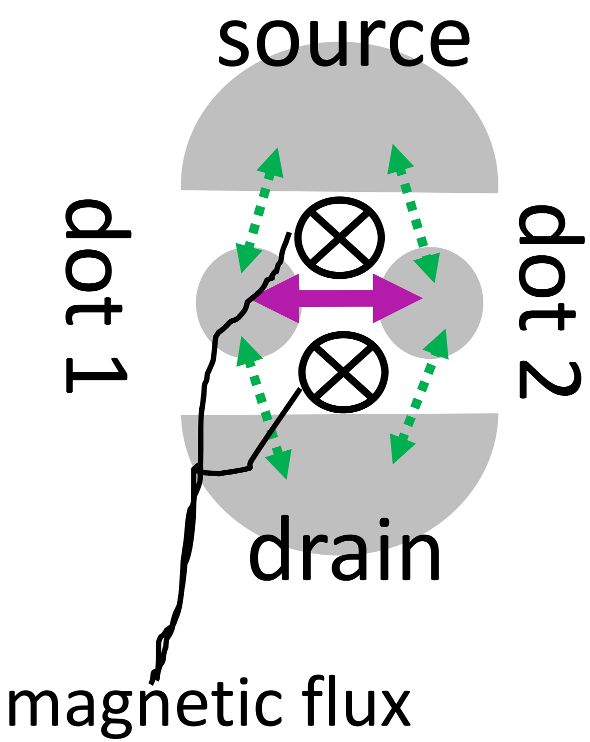
$$\boldsymbol{J}_{00}(t)=\boldsymbol{u}^{\dagger}(t)(\mathbf{1}_{D}-\boldsymbol{v}(t))^{-1}\boldsymbol{u}(t)-\mathbf{1}_{D} \qquad \boldsymbol{u}(t)=\boldsymbol{u}(t,t_{0})$$

*physical interpretation of the solution*



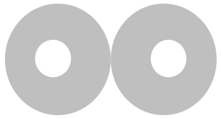
# III. Example of application

*Aharonov-Bohm interferometer with double-quantum-dot molecule*



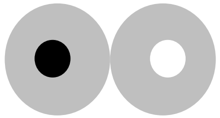
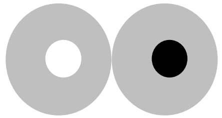

$$H_{qd} = \epsilon_{11} d_1^\dagger d_1 + \epsilon_{22} d_2^\dagger d_2 - t_c (d_1^\dagger d_2 + d_2^\dagger d_1)$$

**zero-electron state: emtpy**

 $|0,0\rangle = |0\rangle$

**one-electron states**

-- local charge states

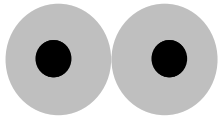
 $|1,0\rangle = |1\rangle$  $|0,1\rangle = |2\rangle$

-- molecular states

$|b\rangle = \sqrt{1/2}[|1\rangle + |2\rangle]$ $|a\rangle = \sqrt{1/2}[|1\rangle - |2\rangle]$

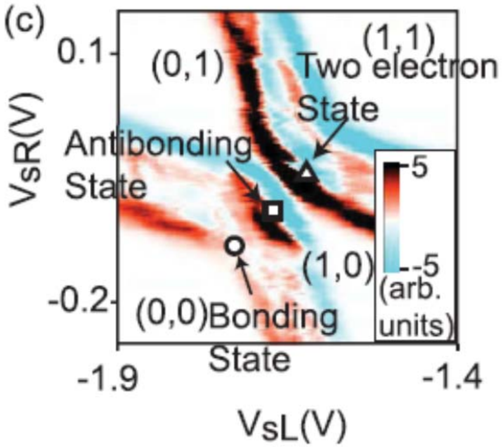
bonding state (**BS**) anti-bonding state (**AS**)

**two-electron states**

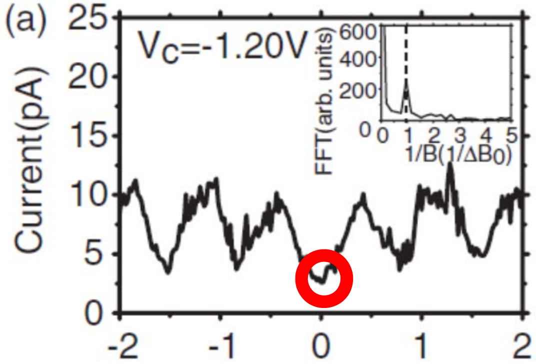
 $|1,1\rangle = |3\rangle$

# III. Example of application

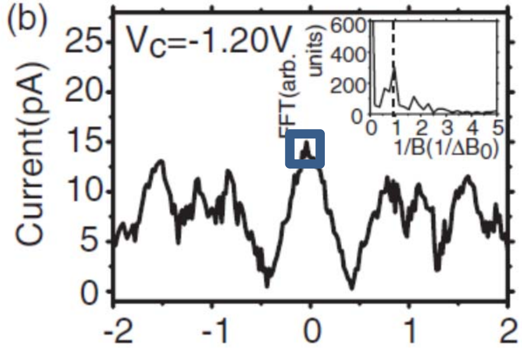
*--verifying working regimes*



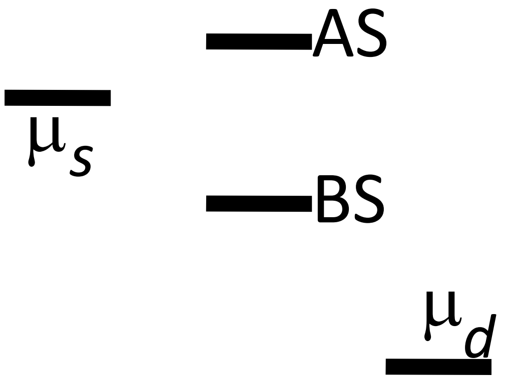

current through BS



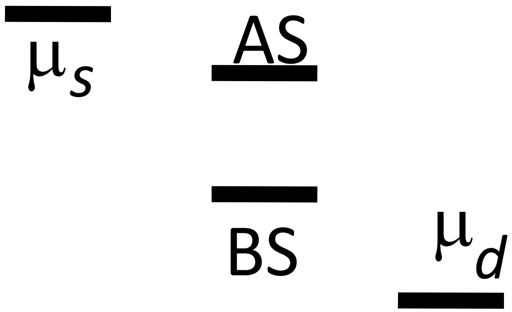

current through AS



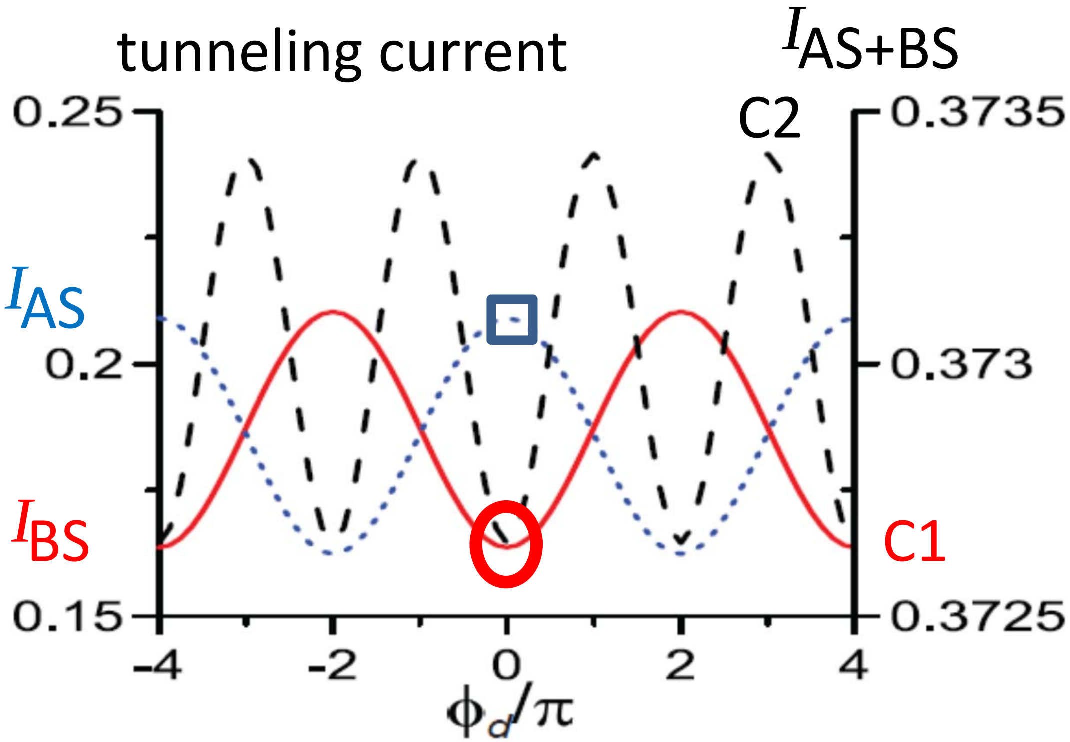

T. Hatano, T. Kubo, Y. Tokura, S. Amaha, S. Teraoka, and S. Tarucha, PRL (2011).




C1 access BS only



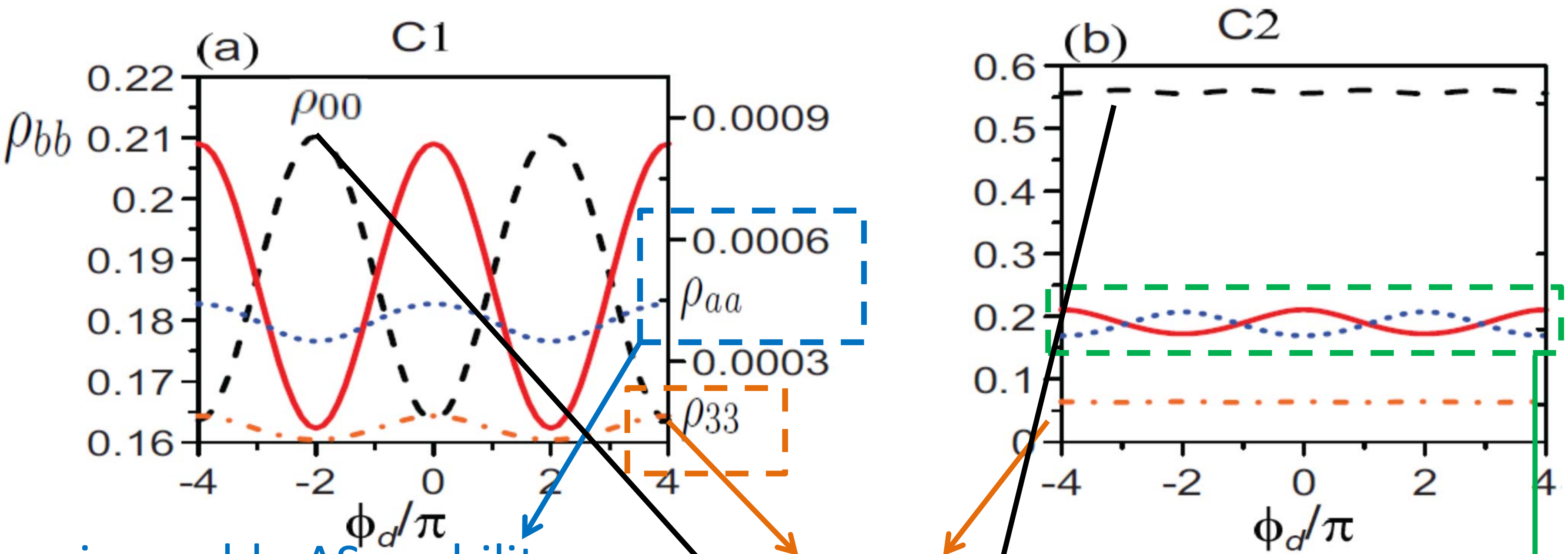

C2 access BS & AS



# III. Example of application

*quantum states under nonequilibrium transports*

*flux response  at steady-state limit*




ignorable AS probility

**ignorable two-e probability**

comparable BS and AS probabilities

considerable empty probability

$\rho_{00}$ : empty state probability

$\rho_{bb}$ : one-electron BS probability

$\rho_{aa}$ : one-electron AS probability

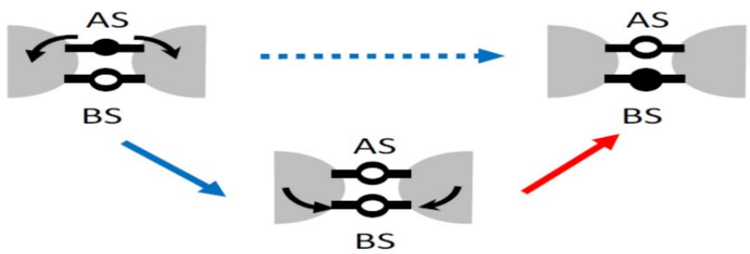
$\rho_{33}$ : two-electron state probability

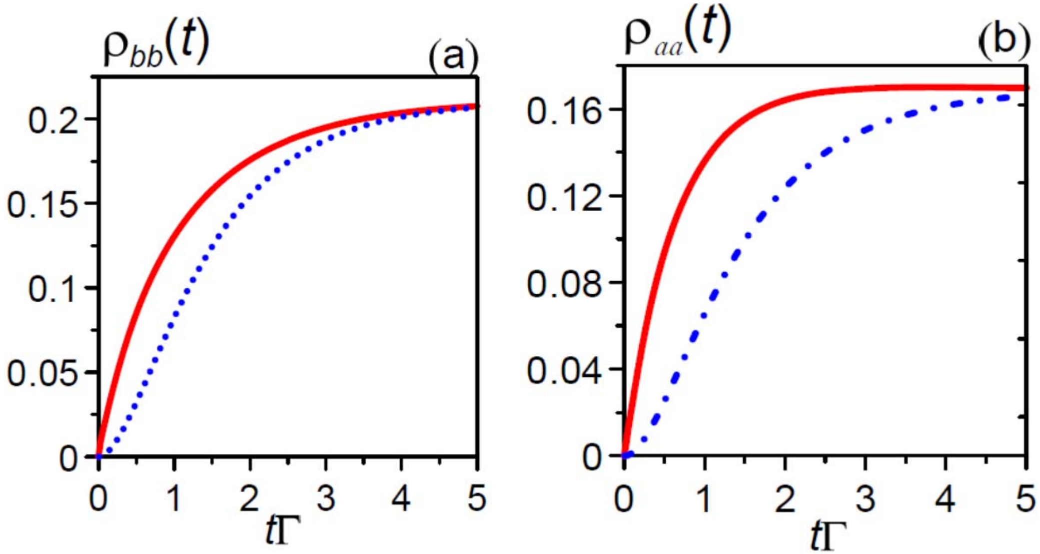
# III. Example of application

*quantum states under nonequilibrium transports*

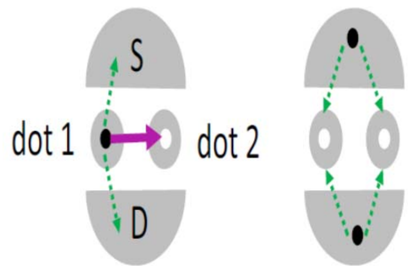
*real-time quantum state transitions*

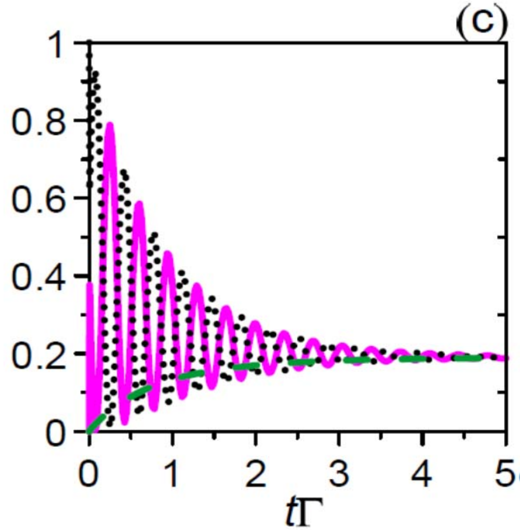
**external pathways**




**internal pathway**




*start from empty state*

*start from AS*　　　　*start from BS*

$\rho_{22}(t)$ *start from empty state*

$\rho_{22}(t)$ *start from dot 1*

$\rho_{11}(t)$ *start from dot 1*

# VI. Summary

Methodological side:

- General analytical solution, applicable to arbitrary number of orbitals and initial preparations for a class of open nanoelectronic systems

Application example :

- Connection between orbital occupation and transport through certain orbitals in DQD AB interferometer
- Distinguishing pathways for quantum state transitions from intermediate evolution processes

**Thank you for your attentions**