Wide-band approximation and beyound with applicaction of electron transport phenomena

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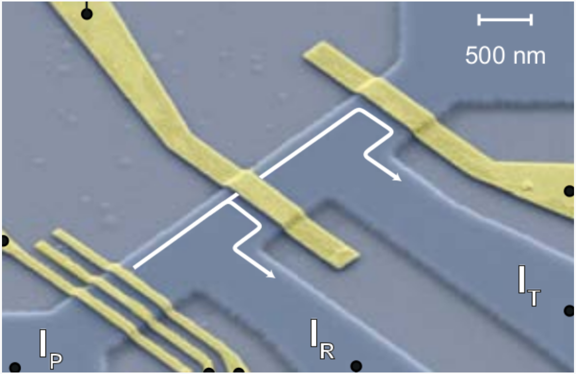
Example of physical system

- Semiconductor device
- Quantum wires where electron gas sits on (grayed pattern)
- Barrier leads (yellow)

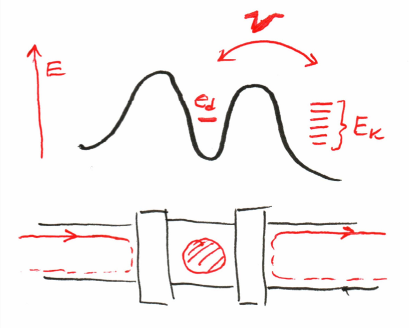


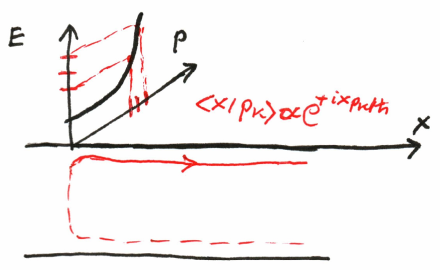
How the currents I_T and I_R depend on a way we emit electron?

The physical model

We are going to consider electron emission of quantum dot to the lead

- quantum dot state
- lead states (right part of quantum wire)
- barrier (interaction)





The outline of presentation

- General quantum problem and it's relation to system of differential equations
- How to apply Wide-Band approximation
  - Getting exact form of interaction term by using experimental evidence
  - What it allows us to conclude about dynamics of emission?
- Beyond WBA, coupling dependent on geometry of QD trapping potential
  - Adiabatic approximation
  - Analytical treatment with Demkov-Osherov model and comparission with WBA.
  - Numerical challenge

The formulation of problem

If we have given Hamiltonian, what we should do to obtain the solution of Schrodinger equation?

The Schrodinger equation in Dirac notation

$$i\hbar\frac{d}{dt}\left|\Psi\right\rangle = \hat{H}\left|\Psi\right\rangle$$

The general Hamiltonian

$$\hat{H} = \epsilon_d(t)\left|d\right\rangle\left\langle d\right| + \sum_k E_k\left|k\right\rangle\left\langle k\right| + \sum_k V_k(t)\left|d\right\rangle\left\langle k\right| + V_k(t)\left|k\right\rangle\left\langle d\right|$$

Usual approach to look for solution

$$\left|\Psi\right\rangle = c_d(t)\left|d\right\rangle + \sum_k c_k(t)\left|k\right\rangle$$

So what's the problem?

- After we put the these last block's together we obtain system of differerntial equations
- At the best for specific cases we get solution as integrals (Laplace method)
- Numerical integration tend's to fail if input $\epsilon_d(t)$ and $V_k(t)$ changes with time too fast and too differently. => Stiffness
  - Matrix exponential $\frac{d}{dt}\vec{X} = A\vec{X}$ for time independent problems gives $\vec{X} = e^{At}\vec{X}(0)$ is suggested for stiff problems.

Conclusion

We need a way to make our Hamiltonian for physiscal problem simpler!

Wide-Band approximation

The rules

- The coupling to the lead is assumed energy independent

$$V_k = V_j$$

- The energy levels in the lead is equidistant

$$\sum_k \ldots = \rho \int \ldots dE_k$$

where $\rho = 1/\Delta E_k$

Returning to Hamiltonian

The Wide-band approximation Hamiltonian

$$\hat{H} = \epsilon_d(t)\left|d\right\rangle\left\langle d\right| + \sum_k E_k \left|k\right\rangle\left\langle k\right| + \sum_k V(t)\left|d\right\rangle\left\langle k\right| + V(t)\left|k\right\rangle\left\langle d\right|$$

A nice thing that solution $c_d(t), c_k(t)$ expressed in quadratures exist for any time dependence of $\epsilon_d(t)$ an $V(t)$.

Relation to experimental data

- Experiment suggests that probability for electron to be in the dot:
$$P_d(t) = \exp\left[-const \cdot e^{t/\tau}\right]$$
- Since we now that $|c_d(t)|^2 = P_d(t)$ we get possible candidate for $V(t)$ as:
$$V(t) = \sqrt{\frac{\Gamma}{2\pi\rho}} e^{t/2\tau}$$
- But if we express $t = t(\epsilon_d)$ then for linear dependence we get:
$$V(t) = \sqrt{\frac{\Gamma}{2\pi\rho}} e^{-\frac{E_b(t)-\epsilon_d(t)}{2\Delta_b}}$$

So how the emission looks like

What happens when electron is int the lead:

- Group velocity $v_g = \frac{d\omega}{dk} = \frac{dE}{dp}$
- Dispersion relation (Hall edge channel) gives us charecteristic velocity v_F with which emited electron leaves the dot
- We can relate $E_k \approx v_F k$ so energy states becomes also momentum states
- If we assume noninteracting lead states then electron propogates as free paricle

And in this case following expression for Wigner function is valid:

$$W^t(x, \hbar k) = \frac{L}{2\pi h} \int c_{k+k'/2}(t) c_{k-k'/2}(t) e^{+ixk'} dk'$$

Time for animation ...

Coupling from geometric arguments

The general Hamiltonian

$$\hat{H} = \epsilon_d(t)\left|d\right\rangle\left\langle d\right| + \sum_k E_k \left|k\right\rangle\left\langle k\right| + \sum_k V_k(t)\left|d\right\rangle\left\langle k\right| + V_k(t)\left|k\right\rangle\left\langle d\right|$$

If we assume the barrier to be a shape of parabolic then it's possible to show that mixing coeficents are proportional to:

$$e^{-\frac{E_b(t)-E_k}{2\Delta_b}}$$

where Δ_b charectirizes the width of potential. Multiplying it with coefficient $\sqrt{\Gamma/2\pi\rho}$ (just to keep up with single notation) we get:

$$V_k(t) = \sqrt{\frac{\Gamma}{2\pi\rho}}e^{-\frac{E_b(t)-E_k}{2\Delta_b}}$$

Adiabatic approximation

- If the state $|\Psi\rangle$ changes slowly in time
- => Well defined energy in the dot for electron
- But electron does not change energy after tuneling
- => we are safe to write $E_k = \epsilon_d(t)$ and obtain:

$$\sqrt{\rho}V_k(t) = \sqrt{\Gamma_b}e^{-\frac{E_b(t)-\epsilon_d(t)}{2\Delta_b}}$$

Which is the same result as with Wide-band approximation!

Analytical treatment with Demkov-Osherov model

General Hamiltonian for Demkov-Osherov

$\hat{H} = \dot{\epsilon}_d t \left|d\right\rangle \left\langle d\right| + \sum_k E_k \left|k\right\rangle \left\langle k\right| + \sum_k V_k \left|d\right\rangle \left\langle k\right| + V_k(t) \left|k\right\rangle \left\langle d\right|$
where $\dot{\epsilon}_d$ is constant.

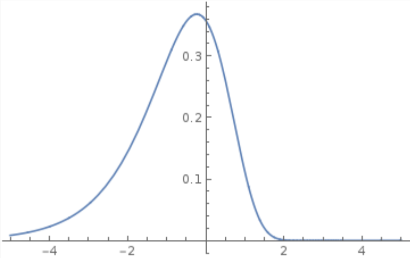
Asymtotic solution

$$P_k^{+\infty} = (1 - p_k) \prod_i^{E_i<E_k} p_i, \qquad p_k = \exp\left[-\frac{2\pi|V_k|^2}{\dot{\epsilon}_d}\right]$$

For considered problem it allows to obtain:

$$P_k^{+\infty}(E_k) = \frac{2\pi\Gamma_b\Delta_b}{\hbar\dot{\epsilon}_d} \exp\left[\frac{E_k}{\Delta_b} - \frac{2\pi\Delta_b\Gamma_b}{\hbar\dot{\epsilon}_d} e^{E_k/\Delta_b}\right]$$

Comparission with AWBA



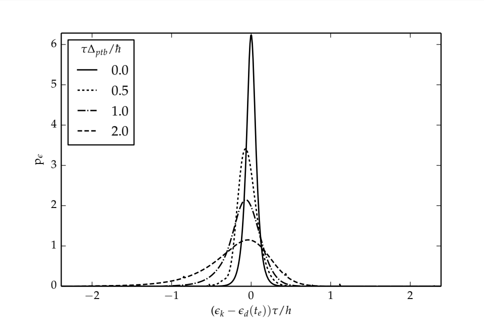


Figure : At the left Demkov-Osherov and on the right WBA solution for electron energy spectrum. (Only for qualitative comparission)

Comparission with Wigner functions

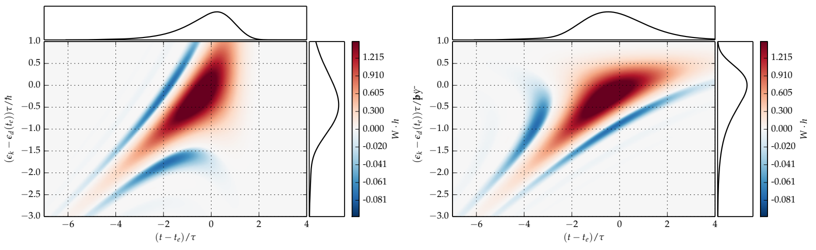


Figure : On the left WBA while on the right Demkov assymptotic state

Nummerical chalenge

With continuations lead levels:

$$\frac{dc_d}{dt} = -\int_{t_0}^{t} K(t,t')c_d(t')dt'$$

$c_d(t_0) = 1 \quad K(t,t') = f(t)f(t') \cdot \frac{1}{1+i(t-t')}$

My approach

- With discrete Fourier transform: $\frac{1}{1+ix} = \sum_j c_j e^{i\omega_j x}$
- So $K(t,t') = \sum_j c_j e^{i\omega_j t} f(t) \cdot f(t') e^{-i\omega_j t'}$
- Introduce new functions $\gamma_j(t) = \int_{t_0}^{t} f(t') e^{-i\omega_j t'} c_d(t') dt'$ and reformulate it as differential equation system.

Some nummerical results

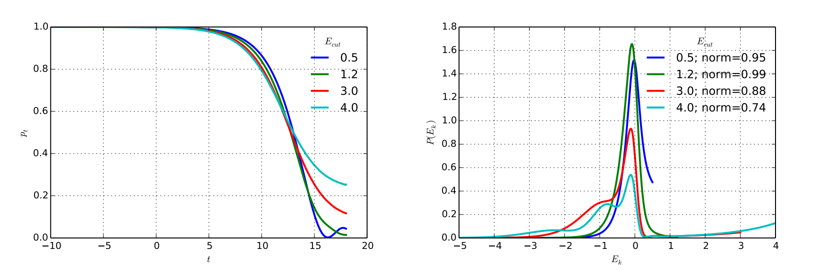


Figure : Some nummerical results with technique discussed. Should be looked with caution since solution should be independent of E_{cut} (the upper bound of considered energy states in the lead)

Conclusion and future developments

- We have seen that in certain cases adiabatic approximation overlaps with wide-band approximation. So wee see motivation for abbreviation AWBA.
- AWBA Hamiltonian is checked with help of Demkov-Osherov if coupling is time independent and has showed reasonable agreement.

Future:

- Analyse more deeply why electron states calculated with WBA and with exact approach differs
- What happens when $E_b(t) \neq const$?