Check on validity of adiabatic approximation

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We have already obtained conditions which should be satisfied if we consider adiabatic approximation. There is however uncertainty how well these conditions must be satisfied. In order to answer this question the Demkov-Osherov analytical results are used for frozen barrier, which clearly shows correspondence with adiabatic solution as the dot energy changes with time more rapidly. Also numerical technique is developed to compare asymptotic time spectrum with probability time density in the quantum dot, where dependence of cutoff energy is especially studied.

I. FORMULATION OF THE PROBLEM

Our Hamiltonian as it stands in [1] is:

$$H(t) = \epsilon_d(t) |d\rangle \langle d| + \sum_k E_k |k\rangle \langle k| + \sum_k [V_k(t) |k\rangle \langle d| + V_k(t) |d\rangle \langle k|] \tag{1}$$

where we consider [2] mixing of dot and lead states as:

$$\sqrt{\rho} V_k = \sqrt{\Gamma_b} e^{-(E_b(t)-E_k)/2\Delta_b} \tag{2}$$

A. Picking out time reference

In the case of adiabatic approximation we have Fermi Golden rule which states:

$$\Gamma(t) = 2\pi\rho |V_k|^2_{E_k=\epsilon_d(t)} = 2\pi\Gamma_b e^{\frac{E_b(t)-\epsilon_d(t)}{\Delta_b}} \tag{3}$$

on the other hand from my bachelor thesis I have used [3]:

$$\Gamma(t) = \frac{\hbar}{\tau} e^{(t-t_e)/\tau} \tag{4}$$

Picking out time reference when dot energy reaches barrier energy or:

$$E_b(0) = \epsilon_d(0) \tag{5}$$

we get that emission time (defined as event when $\Gamma(t)$ grows exponentially) is given as:

$$2\pi\Gamma_b e^{0/\Delta_b} = \frac{\hbar}{\tau} e^{(0-t_e)/\tau} \qquad \Rightarrow \qquad t_e = \tau \log\left[\frac{\hbar}{2\pi\Gamma_b\tau}\right] \tag{6}$$

B. Linearizion of the problem

For simplicity we introduce energy reference as energy in the quantum dot at $t = 0$ or $\epsilon_d(0) = 0$. Considering only linear time dependence of barrier an QD energy we get:

$$\epsilon_d(t) = \dot{\epsilon}_d t = \frac{\Delta_{ptb}}{\tau} t \tag{7}$$

$$E_b(t) = \dot{E}_b t = -|\dot{E}_b| t \tag{8}$$

where we consider only the case where $\dot{E}_b < 0$.[1] Comparing again (3) with (4) we see that characteristic time is expressed as:

$$\tau = \frac{\Delta_b}{\dot{\epsilon}_d + |\dot{E}_b|} \tag{9}$$

[1] Now we can easily state that we had an event with barrier energy E_{b0} from dot energy when $E_{b0} = E_b(t_b) - \epsilon_d(t_b) = (\dot{\epsilon}_d + \dot{E}_b)t_b$

It must be mentioned that when $\dot{E}_b = 0$ (Considered with Demkov-Osherov model) from above we obtain following restriction:

$$\Delta_b = \Delta_{ptb} \tag{10}$$

Eventually we are able to set $t_e = 0$ by restricting Γ_b from (6) as:

$$\Gamma_b = \frac{\hbar}{2\pi\tau} = \frac{\hbar(\dot{\epsilon}_d + |\dot{E}_b|)}{2\pi\Delta_b} \tag{11}$$

C. Validity of adiabatic approximation (error: both conditions must be satisfied in order for adiabatic approximation to be valid)

For Linear time dependence we have obtained Two conditions where adiabatic approximation is valid [4]. One when dot energy is raised fast $\sqrt{\hbar\dot{\epsilon}_d} \ll \Delta_b$ which in case where $\dot{E}_b = 0$ can be expressed from parameters used in [3] as:

$$1 \ll \frac{\Delta_b^2}{\hbar\dot{\epsilon}_d} = \frac{\Delta_{ptb}\tau}{\hbar} \tag{12}$$

In order to check this condition for adiabatic approximation and to obtain solution for $\dot{\epsilon}_d \to 0$ we are solving the problem exactly with Demkov-Osherov.

On the other hand we have adiabatic condition for slow rise of tunneling barrier $\sqrt{\hbar|\dot{E}_b|} \ll \Delta_b$ from which in case where $\dot{\epsilon}_d \to 0$ or $\Delta_{ptb} = 0$ we get:

$$1 \ll \frac{\Delta_b^2}{\hbar|\dot{E}_b|} = \frac{\Delta_b\tau}{\hbar} \tag{13}$$

As expected we can conclude that when $\tau \to +\infty$ adiabatic approximation is valid.

II. DEMKOV-OSHEROV SOLUTION WHEN BARRIER IS STATIC

In case where mixing of states is independent of time there exists an analytical solution [5] which in our case means non-moving barrier or $\dot{E}_b = 0$. Setting $t_e = 0$ with (11) the mixing amplitudes according to (2) are:

$$V_k = \sqrt{\Gamma_b/\rho}e^{+E_k/2\Delta_b} = \sqrt{\frac{\hbar\dot{\epsilon}_d}{2\pi\Delta_b\rho}}e^{+E_k/2\Delta_b} \tag{14}$$

The Demkov-Osherov solution in [5] is using Atomic units which transforms Schrodinger equation to:

$$i\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle \tag{15}$$

which can be obtained also with other systems of time and energy units. Considering energy units where $\Delta_b = 1$, time units with $\hbar/\Delta_b = 1$ and putting energy time dependences in Hamiltonian we obtain:

$$H(t) = \dot{\epsilon}_d t |d\rangle\langle d| + \sum_k E_k |k\rangle\langle k| + \sqrt{\frac{\dot{\epsilon}_d}{2\pi\rho}} \sum_k e^{E_k/2} [|k\rangle\langle d| + |d\rangle\langle k|] \tag{16}$$

A. Asymptotic probabilities

From analytical solution we take:

1. Probability that electron stays in the dot after emission [5, eq (79)]

$$P_d^{+\infty} = |S_{00}|^2 = \prod_i p_i \tag{17}$$

2. Electron spectrum after emission [5, eq (87)]

$$P_k^{+\infty} = |S_{0k}|^2 = (1 - p_k) \prod_i^{E_i<E_k} p_i \tag{18}$$

where p_k from our introduced parameters:

$$p_k = \exp\left[-\frac{2\pi|V_k|^2}{\dot{\epsilon}_d}\right] \tag{19}$$

Since we have many energy states in the lead we can apply wide band approximation to it which for product states the following:

$$\prod_i \ldots = \exp\left[\sum_i \log(\ldots)\right] = \exp\left[\rho \int \log(\ldots) dE_i\right] \tag{20}$$

Putting it in (17) we the probability that electron remains in the dot after emission:

$$P_d^{+\infty} = \exp\left[\rho \int_{-\infty}^{E_{cut}} \log(p_i) dE_i\right] = \exp\left[-\frac{2\pi}{\dot{\epsilon}_d} \int_{-\infty}^{E_{cut}} |\sqrt{\rho} V_i|^2 dE_i\right] \overset{SI}{=} \exp\left[-e^{E_{cut}/\Delta_b}\right] \tag{21}$$

Also we can obtain probabilities for electron to be in state $|k\rangle$ by putting (19) in (18) and using (20) for getting rid of product:

$$P_k^{+\infty} = \left(1 - \exp\left[-\frac{2\pi|V_k|^2}{\dot{\epsilon}_d}\right]\right) \exp\left[-\frac{-2\pi\rho}{\dot{\epsilon}_d} \int_{-\infty}^{E_k} |V_i| dE_i\right] \overset{\rho\to+\infty}{=} \frac{2\pi|V_k|^2}{\dot{\epsilon}_d} \exp\left[-\frac{-2\pi\rho}{\dot{\epsilon}_d} \int_{-\infty}^{E_k} |V_i|^2 dE_i\right] \tag{22}$$

where in last step I assumed that as $\rho \to +\infty$ mixing amplitudes $|V_k| \to 0$ since overall we have finite tunneling rate. In order to interpret it as probability density distribution we need to normalize it[2]:

$$\sum_k P_k = \int \rho P_k dE_k \overset{def}{=} \int P(E_k) dE_k \tag{23}$$

from which we obtain probability density distribution in the lead:

$$P_k^{+\infty}(E_k) = \frac{2\pi|\sqrt{\rho}V_k|^2}{\dot{\epsilon}_d} \exp\left[-\frac{-2\pi}{\dot{\epsilon}_d} \int_{-\infty}^{E_k} |\sqrt{\rho} V_i| dE_i\right] \overset{(14),SI}{=} \frac{1}{\Delta_b} \exp\left[\frac{E_k}{\Delta_b} - e^{E_k/\Delta_b}\right] = -\frac{d}{dE_k} \exp\left[-e^{E_k/\Delta_b}\right] \tag{24}$$

B. Comparing with adiabatic approximation's energy spectrum

From [3, eq (7)] we can get following expression for asymptotic state:

$$c_k(t) = \frac{-i}{\sqrt{2\pi\rho\hbar\tau}} e^{-iE_k t_1/\hbar} \int \exp\left[\frac{t_1}{2\tau} - \frac{i\Delta_{ptb}}{\hbar\tau}(t_1 - t_0) - \frac{1}{2} e^{t/\tau}\right] e^{+iE_k t_1} dt_1 \tag{25}$$

Which gives us following expression for Energy spectrum:

$$P_k(E_k) = \rho |c_k|^2 = \frac{1}{2\pi\hbar\tau} \left| \int \exp\left[\frac{t_1}{2\tau} - \frac{i\Delta_{ptb}}{\hbar\tau} t_1 - \frac{1}{2} e^{t_1/\tau}\right] e^{+iE_k t_1} dt_1 \right|^2 \tag{26}$$

We can also obtain energy spectrum from (24) by using relation (10):

$$P_k^{+\infty}(E_k) = \frac{1}{\Delta_{ptb}} \exp\left[E_k/\Delta_{ptb} - e^{E_k/\Delta_{ptb}}\right] \tag{27}$$

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[2] The procedure probably is called differently

C. Asymptotic states

The expressions [5, eq (85),(86)] also gives us a way of expressing asymptotic state of electron:

$$c_k = S_{k0} = -i\sqrt{\frac{2\pi}{i\dot{\epsilon}_d}}\frac{V_k^* e^{i\delta_k}}{\sqrt{a_k}\Gamma(1+i|V_k|^2/\dot{\epsilon}_d)}\prod_j^{E_j\le E_k} a_j \tag{28}$$

$$\delta_k = \frac{E_k^2}{2\dot{\epsilon}_d} - \frac{\log\dot{\epsilon}_d}{\dot{\epsilon}_d}\sum_j |V_j|^2 - \frac{1}{\dot{\epsilon}_d}\sum_{j\neq k}|V_j|^2\log|E_k-E_j| \tag{29}$$

$$a_k = \sqrt{p_k} = \exp\left[-\frac{\pi|V_k|^2}{\dot{\epsilon}_d}\right] \tag{30}$$

Before we use it for calculating the asymptotic state lets check it with (18):

$$\begin{aligned}
|c_k|^2 &= \left|-i\sqrt{\frac{2\pi}{i\dot{\epsilon}_d}}\frac{V_k^* e^{i\delta_k}}{\sqrt{a_k}\Gamma(1+i|V_k|^2/\dot{\epsilon}_d)}\prod_j^{E_j\le E_k} a_j\right|^2 = \frac{2\pi|V_k|^2}{\dot{\epsilon}_d\sqrt{p_k}}\frac{1}{|\Gamma(1+i|V_k|^2/\dot{\epsilon}_d)|^2}\prod_j^{E_j\le E_k} p_j \\
&= \frac{2\pi|V_k|^2}{\dot{\epsilon}_d\sqrt{p_k}}\frac{\sinh(\pi|V_k|^2/\dot{\epsilon}_d)}{\pi|V_k|^2/\dot{\epsilon}_d}\prod_j^{E_j\le E_k} p_j = \frac{1}{\sqrt{p_k}}\left[e^{\pi|V_k|^2/\dot{\epsilon}_d} - e^{-\pi|V_k|^2/\dot{\epsilon}_d}\right]\prod_j^{E_j\le E_k} p_j \\
&= \frac{1}{\sqrt{p_k}}\left[1/\sqrt{p_k} - \sqrt{p_k}\right]\prod_j^{E_j\le E_k} p_j = (1-p_k)\prod_j^{E_j<E_k} p_j
\end{aligned} \tag{31}$$

where in the first line I have applied $|\Gamma(1+ix)|^2 = \pi x/\sinh(\pi x)$ for $x>0$.

III. WIGNER FUNCTION IN QUASI-CONTINUOUS APPROXIMATION

For obtaining the Wigner function we must take the expression for c_k from (28) and we should put it according to [3] in:

$$W(x,\hbar k) = \frac{L}{2\pi h}\int c_{k+\xi/2}c^*_{k-\xi/2}e^{ix\xi}d\xi \tag{32}$$

where $L = v_F h\rho$. Since the asymptotic states for c_k from Demkov model ar given in interaction picture then coordinate x are given on the moving (with v_F) frame of reference. The momentum now also is given in this frame of reference.[3].

In order to get the Wigner function in time-energy axes we are setting $E_k = \hbar v_F k$, and since we are in interaction picture $x = -v_F t$:

$$W_b(t,E_k) = W(-v_F t, E_k/v_F) = \frac{\rho}{2\pi\hbar}\int c(E_k+E_\xi/2)c^*(E_k-E_\xi/2)e^{-itE_\xi/\hbar}dE_\xi \tag{33}$$

A. Quasi-continuity approximation

The main difficulty to evaluate states in quasi-continuous limit of lead states comes from logarithm present in sum of phase δ_k or $\frac{1}{\dot{\epsilon}_d}\sum_{j\neq k}|V_j|^2\log|E_k-E_j|$ which depends largely on upper bound of summation. By putting (14) in it we observe that we need a way to approximate a following sum:

$$\tilde{g}(E_k) = \frac{1}{\rho}\sum_{j\neq k} e^{E_j}\log|E_k-E_j| \tag{34}$$

[3] Which in my preference is more natural choice of coordinates

As I have shown it in next subsection it's value with quasi-continuous approximation is given as:

$$\tilde{g}(E_k) = e^{E_{cut}} \log(E_{cut} - E_k) - e^{E_k} Ei(E_{cut} - E_k) \tag{35}$$

where one sees that it goes to 0 as $E_{cut}, E_k \to -\infty$. The quasi-continuous approximation then gives us:

$$\prod_j^{E_j \le E_k} a_j = \exp\left[\rho \int_{-\infty}^{E_k} \log(a_j) dE_j\right] = \exp\left[-\frac{1}{2} e^{+E_k}\right] \tag{36}$$

$$a_k = \exp\left[-\frac{\pi |V_k|^2}{\dot{\epsilon}_d}\right] = \exp\left[-\frac{1}{2\rho} e^{E_k}\right] \overset{\rho \to +\infty}{=} 1 \tag{37}$$

$$\Gamma(1 + \frac{i}{2\pi\rho} e^{E_k}) \overset{\rho \to +\infty}{=} \Gamma(1) = 1 \tag{38}$$

$$\tag{39}$$

So the asymptotic state is simplified to:

$$c_k = \frac{-i}{\sqrt{i\rho}} \exp\left[\frac{E_k}{2} - \frac{1}{2} e^{E_k}\right] e^{i\delta_k} \tag{40}$$

The phase factor is given as:

$$\delta_k = C + \frac{E_k^2}{2\dot{\epsilon}_d} + \frac{1}{2\pi} \tilde{g}(E_k) = C + \frac{E_k^2}{2\dot{\epsilon}_d} + \frac{1}{2\pi} e^{E_{cut}} \log(E_{cut} - E_k) - \frac{1}{2\pi} e^{E_k} Ei(E_{cut} - E_k)$$
$$\overset{(47)}{\approx} C + \frac{E_k^2}{2\dot{\epsilon}_d} + \frac{1}{2\pi} e^{E_{cut}} \log(E_{cut} - E_k) - \frac{1}{2\pi} \frac{e^{E_{cut}}}{E_{cut} - E_k} \tag{41}$$

where C is constant phase term which is not needed for calculation of Wigner function.

B. Analytical treatment of sum

Here we are going to derive an analytical form of sum in quasi-continuous limit. Since in the sum we skip value where $E_k = E_j$ we take care of it by introducing $\delta \to 0$:

$$\tilde{g}(E_k) = \frac{1}{\rho} \sum_{j \ne k} e^{E_j} \log|E_k - E_j| = \int_{-\infty}^{E_k - \delta} + \int_{E_k + \delta}^{E_{cut}} \overset{x = E_j - E_k}{=} e^{E_k} \left[\int_{-\infty}^{-\delta} + \int_{+\delta}^{E_{cut} - E_k}\right] e^x \log|x| dx \tag{42}$$

Let's introduce integration along complex variable where line goes along x axis but at 0 goes along with infinite small circle of radius δ then the integration along this contour is expressed as:

$$\int_L = \int_{-\infty}^{-\delta} + \int_{L_\delta} + \int_{+\delta}^{E_{cut} - E_k} \tag{43}$$

The integration along this small circle is expressed as follows:

$$\int_{L_\delta} = \int_{L_\delta} e^z \log|z| dz = i \int_0^{+\pi} e^{\delta e^{i\phi} + i\phi} \delta \log|\delta| d\phi = 0 \tag{44}$$

So we are allowed to rewrite our sum as integration in the upper half of complex plane:

$$\tilde{g}(E_k) = e^{E_k} \int_{-\infty}^{E_{cut} - E_k} e^z \log|z| dz = e^{E_k} \Re\left[\int_{-\infty}^{E_{cut} - E_k} e^z \log(z) dz\right]$$
$$= e^{E_k} \Re\left[e^z \log(z)|_{-\infty}^{E_{cut} - E_k} - \int_{-\infty}^{E_{cut} - E_k} \frac{e^z}{z} dz\right] = e^{E_{cut}} \log(E_{cut} - E_k) - e^{E_k} Ei(E_{cut} - E_k) \tag{45}$$

where $Ei(x)$ is exponential integral $Ei(x) = -\int_{-x}^{+\infty} \frac{e^{-t}}{t} dt = \int_{-\infty}^{x} \frac{e^{t}}{t} dt$. For large arguments of Ei the following expansion at $x \gg 1$ can be used(checked numerically)[4]:

$$Ei(x) = \frac{e^x}{x} + O\left(\frac{e^x}{x^2}\right) \tag{46}$$

So in case if $E_{cut} - E_k \gg 1$ we have:

$$\tilde{g}(E_k) = e^{E_{cut}} \log(E_{cut} - E_k) - \frac{e^{E_{cut}}}{E_{cut} - E_k} \tag{47}$$

We can also expand this expression in Taylor series when $E_k/E_{cut} \ll 1$ is small to the second order:

$$\log(E_{cut} - E_k) = \log E_{cut} + \log(1 - E_k/E_{cut}) = \log(E_{cut}) - \frac{E_k}{E_{cut}} - \frac{1}{2}\left(\frac{E_k}{E_{cut}}\right)^2 + O(E_k^3/E_{cut}^3) \tag{48}$$

$$\frac{1}{E_{cut} - E_k} = \frac{1}{E_{cut}} \frac{1}{1 - E_k/E_{cut}} = \frac{1}{E_{cut}}\left(1 + \frac{E_k}{E_{cut}} + \frac{E_k^2}{E_{cut}^2} + O(E_k^3/E_{cut}^3)\right) \tag{49}$$

After putting it inside the (47) and dropping $\log(E_{cut})$, $1/E_{cut}$ as constant phase term:

$$\tilde{g}(E_k)/e^{E_{cut}} = -\frac{E_k}{E_{cut}}\left(1 - \frac{1}{E_{cut}}\right) - \frac{E_k^2}{E_{cut}^2}\left(\frac{1}{2} - \frac{1}{E_{cut}}\right) + O(E_k^3/E_{cut}^3) \tag{50}$$

where the linear term (as we are going to see) is responsible for latter (because of sign) emission as E_{cut} becomes larger. The linear approximation however should be looked with caution since this sum is argument for complex exponent so there is possibility that higher terms makes mess. Simple measure for how many terms must be taken in Taylor expansion can be estimated:

$$e^{E_{cut}}\left(\frac{E_k}{E_{cut}}\right)^n \ll 2\pi \tag{51}$$

where n is order of Taylor expansion needed.

C. Wigner function (without approximations)

In (40) and (41) we have obtained the asymptotic state for electron in the lead. To obtain Wigner function representation we need to put this state in (33), where we see that phase factor $\delta_{k+\xi/2} - \delta_{k-\xi/2}$ needs to be expressed:

$$\begin{aligned}\delta_{k+\xi/2} - \delta_{k-\xi/2} &\overset{(41)}{=} \frac{(E_k + E_\xi/2)}{2\dot{\epsilon}_d} + \frac{e^{E_{cut}}}{2\pi}\log(E_{cut} - E_k - E_\xi/2) - \frac{e^{E_k + E_\xi/2}}{2\pi} Ei(E_{cut} - E_k - E_\xi/2) \\ &\quad - \frac{(E_k - E_\xi/2)}{2\dot{\epsilon}_d} - \frac{e^{E_{cut}}}{2\pi}\log(E_{cut} - E_k + E_\xi/2) + \frac{e^{E_k - E_\xi/2}}{2\pi} Ei(E_{cut} - E_k + E_\xi/2) \\ &= \frac{E_k E_\xi}{\dot{\epsilon}_d} + \frac{e^{E_{cut}}}{2\pi}\log\left(\frac{E_{cut} - E_k - E_\xi/2}{E_{cut} - E_k + E_\xi/2}\right) - \frac{e^{E_k}}{2\pi}\left(e^{E_\xi/2} Ei(E_{cut} - E_k - E_\xi/2) - e^{-E_\xi/2} Ei(E_{cut} - E_k + E_\xi/2)\right)\end{aligned} \tag{52}$$

The correlation function however is written as:

$$\begin{aligned}c_{k+\xi/2} c^*_{k-\xi/2} &= \frac{1}{\rho}\exp\left[\frac{E_k + E_\xi/2}{2} - \frac{1}{2}e^{E_k + E_\xi/2} + \frac{E_k - E_\xi/2}{2} - \frac{1}{2}e^{E_k - E_\xi/2}\right] e^{i(\delta_{k+\xi/2} - \delta_{k-\xi/2})} \\ &= \frac{1}{\rho}\exp\left[E_k - e^{E_k}\cosh(E_\xi/2)\right] e^{i(\delta_{k+\xi/2} - \delta_{k-\xi/2})}\end{aligned} \tag{53}$$

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[4] http://en.wikipedia.org/wiki/Exponential_integral

So the Wigner function after (33) is:

$$W_b(t,E_k) = \frac{1}{2\pi}\int dE_\xi e^{-itE_\xi}\exp\left[\frac{E_k}{2} - e^{E_k}\cosh(E_\xi/2) + i\frac{E_k E_\xi}{\dot{\epsilon}_d}\right]$$
$$\times\exp\left[i\frac{e^{E_{cut}}}{2\pi}\log\left(\frac{E_{cut}-E_k-E_\xi/2}{E_{cut}-E_k+E_\xi/2}\right) - i\frac{e^{E_k}}{2\pi}\left(e^{E_\xi/2}Ei(E_{cut}-E_k-E_\xi/2) - e^{-E_\xi/2}Ei(E_{cut}-E_k+E_\xi/2)\right)\right] \tag{54}$$

D. Wigner function (with asymptotic expansion of Ei(x))

In (40) and (41) we have obtained the asymptotic state for electron in the lead. To obtain Wigner function representation we need to put this state in (33), where we see that phase factor $\delta_{k+\xi/2} - \delta_{k-\xi/2}$ needs to be expressed:

$$\begin{aligned}
\delta_{k+\xi/2} - \delta_{k-\xi/2} &\overset{(41)}{=} \frac{(E_k+E_\xi/2)}{2\dot{\epsilon}_d} + \frac{e^{E_{cut}}}{2\pi}\left(\log(E_{cut}-E_k-E_\xi/2) - \frac{1}{E_{cut}}\frac{1}{1-(E_k+E_\xi/2)/E_{cut}}\right) \\
&\quad - \frac{(E_k-E_\xi/2)}{2\dot{\epsilon}_d} - \frac{e^{E_{cut}}}{2\pi}\left(\log(E_{cut}-E_k+E_\xi/2) - \frac{1}{E_{cut}}\frac{1}{1-(E_k-E_\xi/2)/E_{cut}}\right) \\
&= \frac{E_k E_\xi}{\dot{\epsilon}_d} + \frac{e^{E_{cut}}}{2\pi}\log\left(\frac{E_{cut}-E_k-E_\xi/2}{E_{cut}-E_k+E_\xi/2}\right) - \frac{e^{E_{cut}}}{2\pi}\left(\frac{1}{E_{cut}-E_k-E_\xi/2} - \frac{1}{E_{cut}-E_k+E_\xi/2}\right)
\end{aligned} \tag{55}$$

Now we are ready to write out correlation function[5]:

$$\begin{aligned}
c_{k+\xi/2}c^*_{k-\xi/2} &= \frac{1}{\rho}\exp\left[\frac{E_k+E_\xi/2}{2} - \frac{1}{2}e^{E_k+E_\xi/2} + \frac{E_k-E_\xi/2}{2} - \frac{1}{2}e^{E_k-E_\xi/2}\right]e^{i(\delta_{k+\xi/2}-\delta_{k-\xi/2})} \\
&= \frac{1}{\rho}\exp\left[E_k - e^{E_k}\cosh(E_\xi/2)\right]e^{i(\delta_{k+\xi/2}-\delta_{k-\xi/2})}
\end{aligned} \tag{56}$$

So the Wigner function after (33) is:

$$W_b(t,E_k) = \frac{1}{2\pi}\int dE_\xi e^{-itE_\xi}\exp\left[\frac{E_k}{2} - e^{E_k}\cosh(E_\xi/2) + i\frac{E_k E_\xi}{\dot{\epsilon}_d}\right]$$
$$\times\exp\left[i\frac{e^{E_{cut}}}{2\pi}\log\left(\frac{E_{cut}-E_k-E_\xi/2}{E_{cut}-E_k+E_\xi/2}\right) - i\frac{e^{E_{cut}}}{2\pi}\left(\frac{1}{E_{cut}-E_k-E_\xi/2} - \frac{1}{E_{cut}-E_k+E_\xi/2}\right)\right] \tag{57}$$

where I used that $|c(E_{cut})|^2 \to 0$ so the integration can be streched up to infinity.

E. Comparing the solution with Wide-band approximation (Here I do drop phase term which depends on E_{cut} without justification)

If we drop the E_{cut} dependent phase term for expression of Wigner function we get:

$$W_b(t,E_k) = \frac{1}{2\pi}\int \exp\left[E_k - e^{E_k}\cosh(E_\xi/2) + iE_kE_\xi/\dot{\epsilon}_d\right]e^{-itE_\xi}dE_\xi \tag{58}$$

The energy units of [3] were chosen as $\hbar/\tau$ while time units as τ. Also in the summary instead of $\dot{\epsilon}_d$ the Δ_{ptb} where relation between them is:

$$\frac{\Delta_{ptb}\tau}{\hbar} = \frac{\Delta_{ptb}\Delta_b}{\hbar\dot{\epsilon}_d} \overset{\Delta_b=\Delta_{ptb}}{=} \frac{\Delta_b^2}{\hbar\dot{\epsilon}_d} \tag{59}$$

[5] Not sure about terminology

which in dimensionless units of $\dot\epsilon_d$ means $\Delta_{ptb}\tau/\hbar = 1/\dot\epsilon_d$. Transforming the Wigner function to these units for energy and time we get (where $\bar W = h \cdot W_b$ as in [3]):

$$\bar W(t, E_k) = \int \exp\left[\frac{E_k}{\bar\Delta_{ptb}} - e^{E_k/\bar\Delta_{ptb}}\cosh(E_\xi/2) + iE_\xi t\bar\Delta_{ptb}\right] e^{-iE_kE_\xi} dE_\xi \qquad \bar\Delta_{ptb} = \Delta_{ptb}\tau/\hbar \tag{60}$$

The expression has quite striking similarities with [3, eq (74)]especially if we approximate $E_k = \Delta_{ptb}t$:

$$\exp\left[\frac{E_k}{\bar\Delta_{ptb}} - e^{E_k/\bar\Delta_{ptb}}\cosh(\xi/2)\right] = \exp\left[t - e^t\cosh(\xi/2)\right] \tag{61}$$

F. Drawings of Wigner function

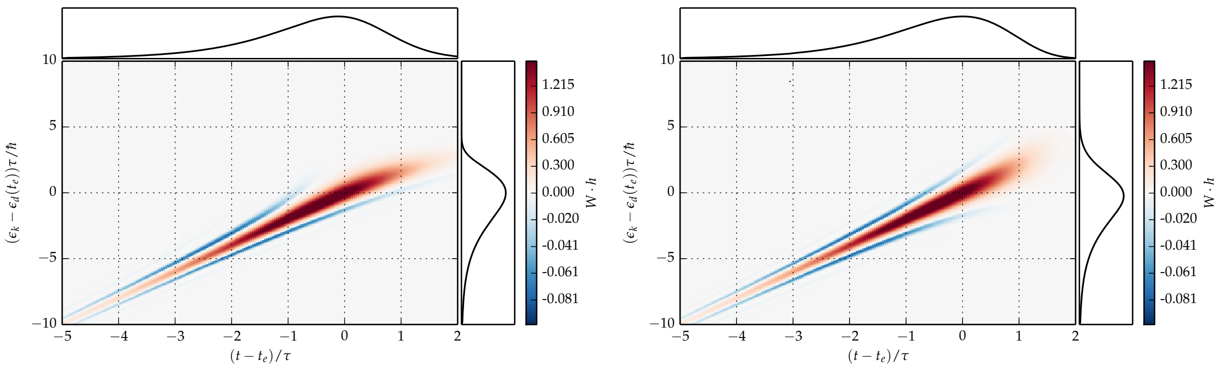

FIG. 1: Wigner functions for $\Delta_{ptb}\tau/\hbar = 2$. On the left we have quantum state obtained from (60) where on the right I have quantum state obtained in [3] with adiabatic Hamiltonian.

IV. PROBABILITY DENSITY IN THE LEAD FROM DOT AMPLITUDE

From [1, eq (7)] we see that amplitudes in the lead when we have linear drive for dot and barrier energy[6] are obtained after solving (with units where $\hbar = 1$):

$$i\frac{dc_k}{dt} = \exp\left[iE_kt - \int_{t_0}^{t}\epsilon_d(\tilde t)d\tilde t\right]V_kc_d(t) = \sqrt{\frac{\Gamma_b}{\rho}}\exp\left[iE_kt - \dot\epsilon_d(t^2 - t_0^2)/2 + |\dot E_b|t/2 + E_k/2\right]c_d(t) \tag{62}$$

Since for now we only want the emission spectrum at the time when system have became stationary t_f then probability that electron is on state $|k\rangle$ is given as:

$$P_k = \frac{\Gamma_b}{\rho}e^{E_k}\left|\int_{t0}^{tf}\exp\left[iE_kt - \dot\epsilon_dt^2/2 + |\dot E_b|t/2\right]c_d(t)dt\right|^2 \tag{63}$$

Similar as before if we want to represent it as probability density distribution when number of states in the lead are large we need to normalize it. According to (23) the probability density distribution is given as:

$$P(E_k) = \rho P_k = \Gamma_b e^{E_k}\left|\int_{t0}^{tf}\exp\left[iE_kt - \dot\epsilon_dt^2/2 + |\dot E_b|t/2\right]c_d(t)dt\right|^2 \tag{64}$$

which must coincide with (24) when $\dot E_b = 0$ if the amplitude $c_d(t)$ is calculated correctly and $t_0 \to -\infty$, $t_f \to +\infty$.

[6] We are working in the interaction picture

V. NUMERICAL METHOD FOR CALCULATING DOT AMPLITUDE

A. Method which is now used

From [4] the dot amplitude can be obtained after solving integro-differential equation:

$$\frac{dc_d}{dt} = -\int_{t_0}^{t} dt' K(t,t') c_d(t') dt', \; c_d(t_0) = 1 \qquad c_d(t_0) = 1 \tag{65}$$

where kernel $K(t,t')$ is given:

$$K(t,t') = \frac{\Gamma_b}{1 - i(t-t')} \exp\left[i\dot{\epsilon}_d (t^2 - t'^2)/2 - iE_{cut}(t-t') + |\dot{E}_b|(t+t')/2 + E_{cut} \right] \tag{66}$$

In order to obtain numerical algorithm for this equation I am approximating complex Lorentzian with sum of decaying exponentials:

$$\frac{1}{1-ix} \approx \sum_{k}^{n} A_k e^{-s_k x} \tag{67}$$

where number of terms in the sum are n. I am restricting s_k to be real, while A_k can also be complex quantities. To obtain the best correspondence with complex Lorentzian I introduce the distance between functions:

$$\|f(x)\| = \int_0^{L_{max}} |f(x)|^2 dx \tag{68}$$

where L_{max} is estimated as interval length on which we want the integro-differential equation to be solved. Now the s_k and A_k is given as solution of minimization problem.

By putting the factorized complex Lorentzian in the kernel expression one obtains:

$$K(t,t') = \sum_{k}^{n} \Gamma_b A_k e^{E_{cut}} \exp\left[i\dot{\epsilon}_d t^2/2 - iE_{cut} t + |\dot{E}_b| t/2 - s_k t \right] \times \exp\left[-i\dot{\epsilon}_d t'^2/2 + iE_{cut} t' + |\dot{E}_b| t'/2 + s_k t' \right] \tag{69}$$

If we are introducing the functions:

$$\gamma_k(t) = \int_{t_0}^{t} \exp\left[-i\dot{\epsilon}_d t'^2/2 + iE_{cut} t' + |\dot{E}_b| t'/2 + s_k t' \right] c_d(t') dt' \tag{70}$$

then we can rewrite integro-differential equation as:

$$\frac{dc_d}{dt} = -\sum_{k}^{n} \Gamma_b A_k e^{E_{cut}} \exp\left[i\dot{\epsilon}_d t^2/2 - iE_{cut} t + |\dot{E}_b| t/2 - s_k t \right] \gamma_k(t) \tag{71}$$

By taking time derivative of $\gamma_k(t)$ we obtain:

$$\frac{d\gamma_k}{dt} = \exp\left[-i\dot{\epsilon}_d t^2/2 + iE_{cut} t + |\dot{E}_b| t/2 + s_k t \right] c_d(t) \tag{72}$$

which with initial conditions $\gamma_k(t_0) = 0$ defines the differential equation system and therefore can be solved numerically:

$$\frac{dc_d}{dt} = -\sum_{k}^{n} \Gamma_b A_k e^{E_{cut}} \exp\left[i\dot{\epsilon}_d t^2/2 - iE_{cut} t + |\dot{E}_b| t/2 - s_k t \right] \gamma_k(t) \qquad c_d(t_0) = 1 \tag{73}$$

$$\frac{d\gamma_k}{dt} = \exp\left[-i\dot{\epsilon}_d t^2/2 + iE_{cut} t + |\dot{E}_b| t/2 + s_k t \right] c_d(t) \qquad \gamma_k(t_0) = 0 \qquad k = 1, 2, \ldots, n \tag{74}$$

In my numerics I do solve a bit different system[7] which is related with:

$$\tilde{\gamma_k} = \exp\left[-s_k t + i\dot{\epsilon}_d t^2/2 - iE_{cut} t - |\dot{E}_b| t/2 \right] \gamma_k(t) \tag{75}$$

---

[7] Well I am inexperienced. There are no logical arguments why I have done so except I am getting rid of some exponents in the system. However I would like to now if the system gets better or worse for numerical calculations with this transformation. Both systems have been programmed and no visual differences in solutions were not present.

which transforms the differential equation system (74) to:

$$\frac{dc_d}{dt} = -\Gamma_b \exp\left[E_{cut} + |\dot{E}_b|t\right] \sum_k^n A_k \tilde{\gamma}_k \qquad c_d(t_0) = 1 \tag{76}$$

$$\frac{d\tilde{\gamma}_k}{dt} = (-s_k + i\dot{\epsilon}_d t - iE_{cut} - \dot{E}_b/2)\tilde{\gamma}_k(t) + c_d(t) \qquad \tilde{\gamma}_k(t_0) = 0 \qquad k = 1, 2, \ldots, n \tag{77}$$

B. Factorization with discrete Fourier transform (old method)

The numerical solution which I have used sits on the fact that our kernel can be factorized as $K(t, t') = \sum_k h_k(t) g_k(t')$[8] . To obtain this factorization trigonometric interpolation is used where discrete Fourier transform is applied. It allows to represent complex Lorentzian with trigonometric series:

$$\frac{1}{1 - ix} = \sum_{k=0}^{n-1} \tilde{A}_k e^{i\omega_k x} \tag{78}$$

where n is sample size, L is symmetric interval of approximation[9] and $\tilde{A}_k$ are given from DFT coefficients A_k but frequencies ω_k:

$$\tilde{A}_k = \frac{A_k}{n} e^{\pi i k(1-1/n)} \tag{79}$$

$$\omega_k = 2\pi(n-1)k/nL \tag{80}$$

To support this kind of interpolation I tested it for some specific parameters L and n shown in Figure 2.

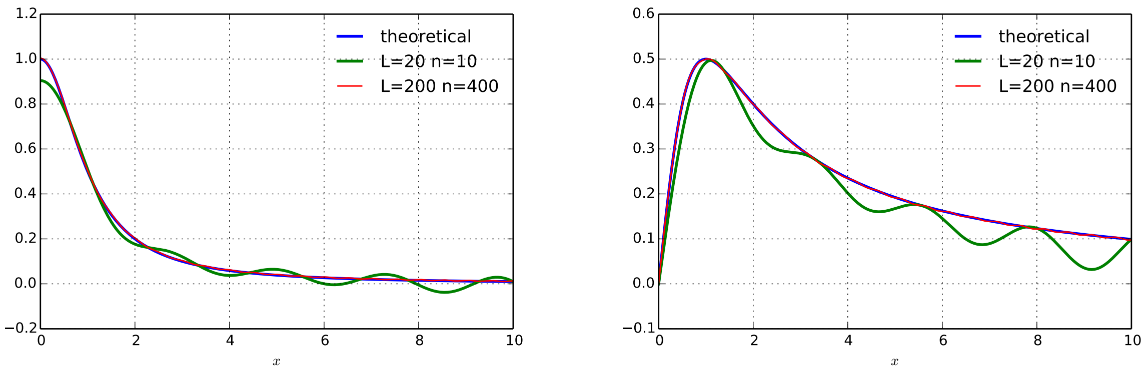

FIG. 2: Interpolation of complex Lorentzian with DFT. At the left is show real part of $1/(1 - ix)$ while on the right imaginary.

Using (78) allows us to factorize kernel due to exponential function properties:

$$K(t, t') = \sum_k \Gamma_b \tilde{A}_k \exp[i\omega_k t + i\dot{\epsilon}_d t + iE_{cut} t + |\dot{E}_b|t + E_{cut}] \exp[-i\omega_k t' - i\dot{\epsilon}_d t' - iE_{cut} t' + |\dot{E}_b|t'/2] \tag{81}$$

Now putting it in the (65) we obtain:

$$\frac{dc_d}{dt} = -\sum_k \Gamma_b \tilde{A}_k \exp[i\omega_k t + i\dot{\epsilon}_d t + iE_{cut} t + |\dot{E}_b|t + E_{cut}] \int_{t_0}^{t} \exp[-i\omega_k t' - i\dot{\epsilon}_d t' - iE_{cut} t' + |\dot{E}_b|t'/2] c_d(t') dt' \tag{82}$$

[8] Taylor series methods (for example [6]) also uses assumption of factorizable kernel therefore it could be worth to try. The difficulties would come to represent $c_d(t)$ with Taylor series as modulus $|c_d|$ approximately is double exponential which does not seems to converge fast enough by increasing number of terms.

[9] The fact that real part of complex Lorentzian is even and imaginary part odd is used.

where one sees that it is possible to transform it to differential equation system by introducing new function $\gamma_k(t)$:

$$\frac{dc_d}{dt} = -\Gamma_b e^{i\dot{\epsilon}_d t + |\dot{E}_b| t + E_{cut}} \sum_k \tilde{A}_k \gamma_k(t) \tag{83}$$

$$\frac{d\gamma_k}{dt} = \exp[-i\omega_k t - i\dot{\epsilon}_d t - iE_{cut} t + |\dot{E}_b| t/2] c_d(t) \tag{84}$$

with subject to initial conditions:

$$c_d(t_0) = 1 \qquad\qquad \gamma_k(t_0) = 0 \tag{85}$$

VI. NUMERICAL RESULTS

Warning: In the plots $\dot{E}_b = |\dot{E}_b|$

A. Comparison with Demkov-Osherov when $E_b(t) = 0$

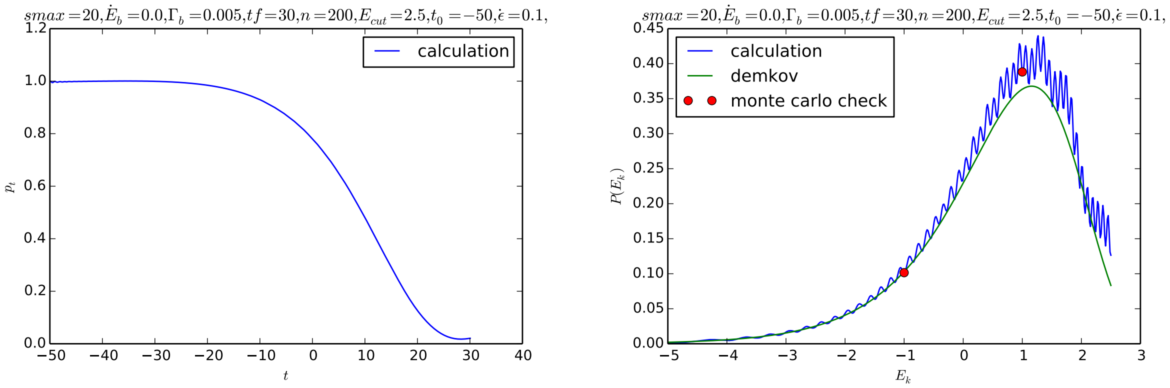

FIG. 3: Comparison of numerical calculation and analytical solution (24). Numerical method where (78) is substituted with $\frac{1}{1+ix} = \sum_k \tilde{A}_k e^{-s_k x}$ was used.

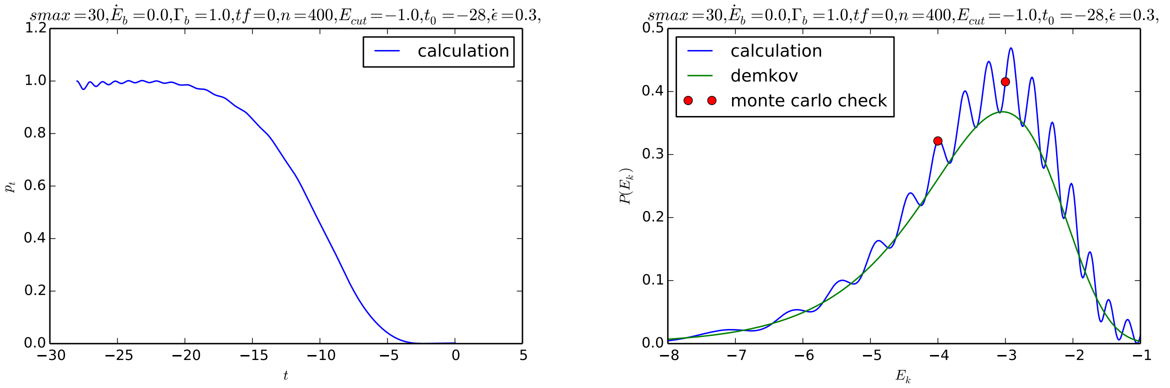

FIG. 4: Numerical results suggests that if we have Γ_b large then E_{cut} can be chosen even negative!

B. Comparison with First orders of Markov approximation when $\epsilon_d(t) = 0$

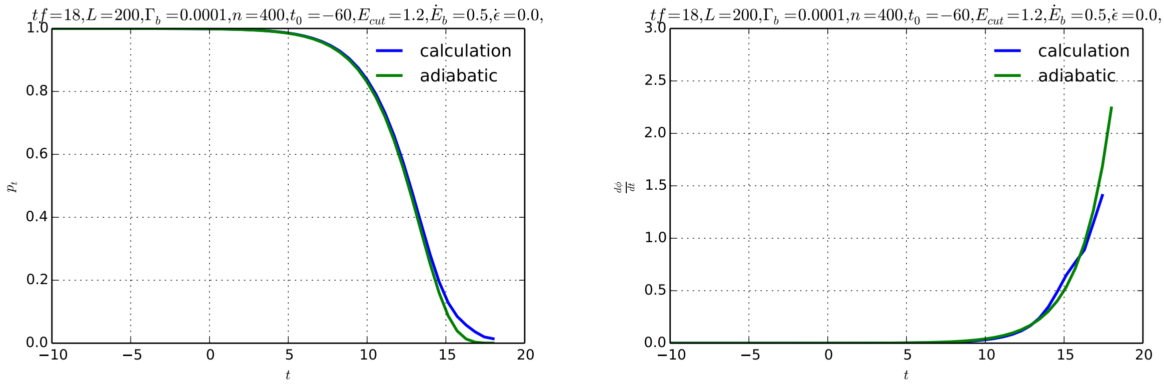

FIG. 5: Comparison of numerical solution with the adiabatic approximation [4]. At the left we see time probability distribution of electron to be in the dot for which adiabatic approximation [4, eq (18)] gives us $p_t(t) = \exp\left[-\frac{2\pi\Gamma_b}{\dot{E}_b} e^{(\dot{E}_b+\dot{\epsilon}_d)t}\right]$ which as we see is quite consistent. On the right side however the phase derivative of amplitude is shown which according to adiabatic approximation[a] is $\frac{d\phi}{dt} = \tilde{\epsilon}(t) = \Gamma_b \frac{e^{+\dot{E}_b t + E_{cut}}}{E_{cut} - \dot{\epsilon}_d t}$

[a] With assumption that $-$ sign is lost

C. Comparison with Markov approximation

In [4] we have obtained $\tilde{\Gamma}(t)$ and $\tilde{\epsilon}(t)$ for frozen dot energy or $\dot{\epsilon}_d = 0$ as:

$$\tilde{\Gamma}(t) + i\tilde{\epsilon}(t) = -i\Gamma_b e^{i\dot{E}_b/2} E_1(-(E_{cut} - i\dot{E}_b/2))e^{-\dot{E}_b t} \tag{86}$$

where $\tilde{\Gamma}(t)$ gives us probability for electron to be in the dot at time t as $P_d(t) = \exp\left[-2\int_{-\infty}^{t} \tilde{\Gamma}(t')dt'\right]$. Since the real part of expression above is:

$$\tilde{\Gamma}(t) = \Gamma_b \Re\left\{-ie^{\dot{E}_b/2} E_1(-(E_{cut} - i\dot{E}_b/2))\right\} e^{-\dot{E}_b t} \tag{87}$$

one concludes that we can obtain the same solution for $P_d(t)$ by keeping $\Gamma_b\Re\{\ldots\}$ constant. First thing to notice that expression in parenthesis grows with E_{cut} so we should notice the same tendency in numerical solution of $P_d(t)$ as Γ_b which I have shown in Figure 6. For large negative times we see that this tendency is true, however from the order of emission lines one can verify that dependence on E_{cut} in (87) must be different since confidence on numerical solution is gained. [10]

[10] Firstly I used numerical method given in V B which for this time region does not show any unexpected behavior (oscillations) even in exponential scales $|\log(P_d) - 1|$. The results were checked with different t_0 where dependence diminishes as $t_0 \to -\infty$.
To support numerical results in Figure 6 even more different numerical method were used and the same results obtained. The main idea remains the same however instead of (78) I have used decaying exponentials to represent complex Lorentzian:

$$\frac{1}{1+ix} = \sum_k \tilde{A}_k e^{-s_k x}$$

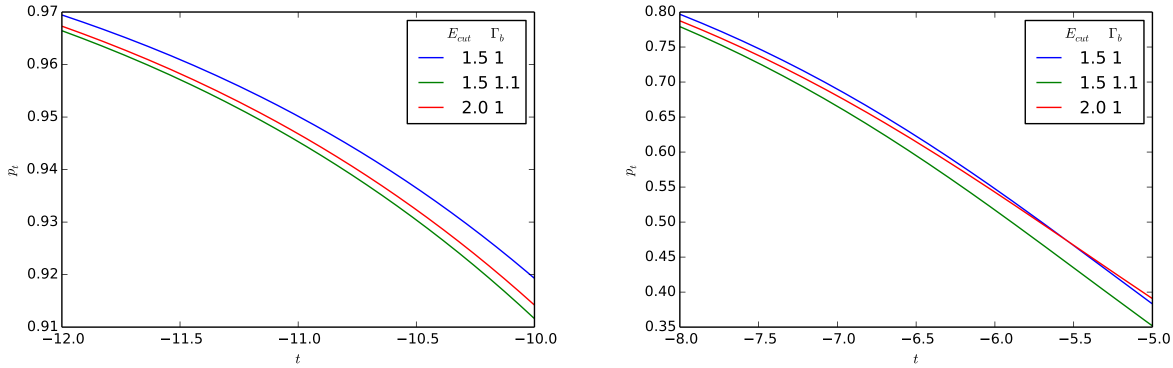

FIG. 6: Time probability density distribution for different E_{cut} and Γ_b with fixed $\dot{E}_b = 0.5$, $\dot{\epsilon}_d = 0$, $t_0 = -60$. On the left one observes that either by increasing E_{cut} or Γ_b we obtain earlier emission which was expected from Markov approximation. However at latter times this tendency fails so it rises doubts either for numerical solution or Markov approximation.

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