CLOSE-COUPLING: GENERATING FUNCTION AND FOKKER-PLANCK FOR COHERENT MULTILEVEL CASCADES (QUANTUM WALKS)

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Close-coupling in quantum systems induces cascade transitions that are not captured by simple perturbation theories and hence more relevant and complex methods are needed. However, the analytic tractability of the latter is limited to just a few highly stylized models, e.g. equidistant infinite systems. Showing that properly adjusted key modeling parameters enable an extension of analytic solutions across more realistic cases (e.g. non-uniform level spacing and finite and asymmetric boundary conditions) arising in various experimental set-ups. Also demonstrating that the Fokker-Planck approach applied to probability amplitudes rather than to probabilities themselves – the latter being a traditional kinetics approach – produces coarse-grained amplitudes "smoothed" over the fine structure of an exact solution and driven by lower order terms in the generating function. Models and results presented here naturally overlap with algorithms of Quantum Walks related to quantum computing studies.

1. Introduction

Close-coupling (CC) in its general sense emerges whenever an external perturbation ties together a large number (in the limit – infinite) of states (levels), thereby inducing chains of multilevel cascades not amenable to some form of the perturbation theory. Studies of the multilevel systems reveal what are those specific and critical aspects of exact solutions that are beyond the reach of perturbation methods (e.g. normalized or extended two-level approximations). In particular, these studies provide an insight into what fraction of distant levels (distant from the initial population point) is affected, how soon these levels are getting involved, and what is their final cumulative impact. In that context, excessive details of the perturbation potential prove insignificant and it turns out possible to formulate a relevant and analytically tractable models with outcomes extendable across models, specific experiments and even scientific disciplines. The subject is vast and covers not only traditional applications in atomic, molecular, optical (AMO) and solid state physics, but also in biological and social systems, and quite recently, in quantum computing.

Technically the problem implements via a system incorporating many linear (quasi-linear) first order differential equations for amplitudes that under certain modeling assumptions can be

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further reduced to a single equation for a so called generating function (GF, see, for instance, Olver [O1974]). The GF moments directly produce either state populations or population/ probability amplitudes (as in quantum systems). Of a special interest obviously are models where GF can be obtained in a closed analytic form. Since even that latter relatively narrow aspect includes numerous references, we'll mention just a few of them from AMO, laser and solid state physics. For instance, Fedorov [F1967] used the GF methodology for the Kapitza-Dirac effect in a strong radiation field. Presnyakov and Urnov [PU1970] gave an analytic solution via GF approach for transitions in an equidistant and infinite quantum spectrum. The same result for equidistant systems also follows from a quasi-classical action technique (see, for instance, Beigman and Lebedev [BL1995]). Alternatively, sometimes GFs are bypassed and transition amplitudes are found by matching CC equations directly to recurrent relations between special functions (polynomials) (Makarov [M1977] and Shore [S1990]). Further examples, applications and extensive discussions can be found in Akulin and Karlov [AK1992] and more recently in Akulin [A2014].

For the sake of completeness and reader convenience we preface new results with the review of some well-known ground-breaking publications. In what follows we begin with a highly-stylized yet quite insightful model of equally spaced levels (Sec. 2), and then show (Sec. 3 and 4) how key limitations of that model can be relaxed to accommodate more realistic features of multilevel systems yet preserving an analytic tractability. Sec. 5 develops Fokker-Planck motivated approach to close-coupled cascades, which is somewhat non-traditional view on quantum amplitudes. Sec. 6 contains final remarks

2. Base case scenario: equal spacing, infinite in both directions system

In this section we recall a most stylized case - the system with equal spacing and infinite in both directions, so called infinite equidistant systems [PU1970]. Despite an extremely "idealistic" character of the model, it returns surprisingly productive insight.

We begin with a standard Schrodinger equation for amplitudes:

$$i\hbar\dot{a}_n(t) = \sum_m V_{nm}(t)e^{i\varpi_{nm}t}a_m(t), \quad \varpi_{nm} = (\varepsilon_m - \varepsilon_n)/\hbar \tag{2.1}$$

where V is an environment induced potential. Consider now an evolution of a multilevel system instantaneously populated to a single level, i.e. an evolution of a Green function in n – space, where n – is an energy quantum number. If an initial population level is far enough from both lower and upper spectrum boundaries, the system is effectively infinite in both directions. To ease an analytic tractability and targeting relatively higher atomic levels we suppose that 1) energy intervals between levels are constant, denote it $\omega > 0$, and 2) matrix elements V_{nm} coupling levels n and m depend appreciably only on the difference |m-n|, but not individually

on m or n. This produces an infinite equidistant system (atomic units $\hbar = m_e = e^2 = 1$ are used below throughout):

$$i\dot{a}_n(t) = \sum_k^{\infty} V_k(t) e^{-ik\varpi t} a_{n+k}(t) + \sum_k^{\infty} V_{-k}(t) e^{ik\varpi t} a_{n-k}(t) \qquad (2.2)$$

For Hermitian potentials $V_k = V^*_{-k}$, where $k = |m-n|$ indicates the difference between level numbers and ω – as above - is a constant inter-level splitting. The system (2.2) solves in a closed integral form for any number of terms in a sum over k. However, to simplify technicalities below we limit ourselves to the closest neighbor coupling, i.e. V_k vanish for all k except k = 1 (an extension to broader coupling k > 1 is straightforward and does not cause additional complications, see, for instance [PU1970, BL1995]). Setting $V = V_1 = V^*_{-1}$, the Schrodinger equation for amplitudes $a_n(t)$ simplifies then to (for brevity we omit time dependence of t in V)

$$i\dot{a}_n(t) = Ve^{-i\varpi t} a_{n+1} + V^* e^{i\varpi t} a_{n-1}, \quad a_n(-\infty) = \delta_{n,n_0} \qquad (2.3)$$

We note in passing that initial conditions in (2.3) mean that amplitudes $a_n(t)$ are merely S-matrix elements in n-space, and, in turn, directly relate to the Green function G $(n\text{-}n_o, t)$. There are two basic ways to obtain the solution. For the first we note that the system (2.3) formally can be written in vector notations with the transition matrix M in the RHS, having non-zero elements only via two main sub-diagonals +1 and -1. Because of this exceptional simplicity, the matrix easily diagonalizes and the formal solution comes out immediately [NU1984]. However, for the purposes of the exposition transparency and extension to less stylized spectra the most convenient approach to (2.3) is a classic method of generating function GF. Namely, recast amplitudes $a_n(t)$ as Fourier- components of some function (i.e. generating function GF)

$$G(\varphi,t) = \sum_{k=-\infty}^{k=\infty} e^{ik\varphi} a_k(t), \quad a_k(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\varphi\ e^{-ik\varphi} G(\varphi,t) \qquad (2.4)$$

with a normalization in virtue of the Parseval's equality:

$$\sum_{k=-\infty}^{\infty} |a_k(t)|^2 = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\varphi\ |G(\varphi,t)|^2 \qquad (2.5)$$

We note in passing, that the Fourier form of GF is especially convenient for quantum mechanical applications because the normalization (2.5) is met automatically. In other words, (2.4) maps all amplitudes from n space to a circular φ interval $[-\pi,\pi]$ (below we use more general GF forms as well). Multiplying each equation by $e^{ik\varphi}$ and summing over k we have

$$\dot{G}(\varphi,t) = -iG(\varphi,t)[Ve^{-i\varpi t}e^{-i\varphi} + V^* e^{i\varpi t} e^{i\varphi}] \qquad (2.6)$$

Integrating (2.6) and introducing

$$A = \int_{-\infty}^{t} d\tau \; V(\tau) e^{-i\varpi\tau} = re^{i\theta} \tag{2.7}$$

r and θ being respectively module and phase of the first order amplitude A, we obtain

$$G = G_0 e^{-i(e^{-i\varphi}A + e^{i\varphi}A^*)} = G_0 e^{-i\cos(\theta-\varphi)2r}, \quad G_0 = e^{-in_0\varphi} \tag{2.8}$$

with

$$r = |A|, \quad \theta = (2i)^{-1} \ln(A / A^*) \tag{2.9}$$

Finally, employing an expansion

$$e^{ir\cos\varphi} = \sum_{k=-\infty}^{\infty} e^{ik\varphi} i^k J_k(r) \tag{2.10}$$

we find transition amplitudes $a_k(t)$ in the form

$$a_k(t) = (-i)^k e^{-ik\theta} J_k(2r) \tag{2.11}$$

This benchmarking representation was obtained in [PU1970] and we discuss its implications shortly. We also note how (2.11) solves the normalization issue: the module of first order amplitude enters as an argument of Bessel functions, the latter being always smaller than 1. This way the first order amplitude leaves its traces in the exact solution and provides a smooth transition between close coupling and perturbation theory.

The solution (2.11) facilitates another useful insight. Because of the exponential drop of Bessel functions for k = 2r, (2.11) produces a pronounced demarcation line k ~ r, which serves as a population effective upper boundary ("front") at $k = \Delta n_{eff} = [\sum_{k=1}^{\infty} k^2 J_k{}^2(2r)]^{1/2} = r$. The front kinematics varies with the amplitude r dependence on time. We estimate the latter for the simplest case of a rectangular perturbation pulse V being constant within the time interval [0, t] and vanishing outside of it. Consider first the degenerate spectrum ω = 0. Then $r \sim \int V(t)dt$ and scales as ~ t, i.e. the population front moves with a constant "speed". For a non-degenerate system ω ≠ 0 and we have $r \sim |(1 - 2\cos\omega t)|$ and the range of occupied levels can expand and contract within a single pulse of external field. One way or the other, the extent of a coherent excitation is critically wider than in the incoherent diffusive kinetics where it scales as $\sim t^{1/2}$.

3. Impact of decreasing spacing (infinite non-equidistant)

In this section we modify an equidistant model to bring it closer to the reality. Namely, we wish to capture the very simple fact that a typical atomic system spectrum becomes tighter as we move closer to the continuum, i.e. the level spacing progressively shrinks. If we denote spacing

correction as $\Delta\omega_n$ then $\omega_{n->n+1}$ changes to $\omega - \Delta\omega_n$, and $\omega_{n->n-1}$ to $\omega + \Delta\omega_n$, and, accordingly, (2.3) modifies to

$$i\dot{a}_n(t) = Ve^{i(-\varpi+\Delta\varpi_n)t}a_{n+1} + V^*e^{-i(\varpi-\Delta\varpi_n)t}a_{n-1} \tag{3.13}$$

Apparently, that makes a coupling of any given level with its upper neighbor (upper means the higher quantum number) stronger than with a lower one, and, therefore, the up-transitions are more likely than down-transitions. Indeed, if the time scale τ of a potential V change is longer than a time τ_ω associated with level spacing ω, then A in (2.7) scales as $\exp(-\tau/\tau_\omega)$, as in a so called an adiabatic regime. For instance, in terms of atomic collision theory, $\tau \sim s/v$, where s is an atomic system size, and v is a projectile speed, and $\tau_\omega \sim 1/\Delta\omega$. For higher (Rydberg) states, s scales as $\sim a_0n^2$, $v \sim v_0/n$, a_0 and v_0 being Bohr radius and velocity, $\Delta\omega_n \sim \delta/n^3$ ($\delta \leq 1$ aka a quantum defect), and so $\exp(-\tau/\tau_\omega)$ is approximately $\cong e^{-\delta}$. Therefore, it makes sense to split a universal coupling V approximately to a uniform upward coupling $V_u = V_{n->n+1} = V{\cdot}u$, ($u = e^{\delta}$), and uniform downward coupling $V_d = V_{n->n-1} = V{\cdot}d$, ($d = e^{-\delta}$). This modifies an equidistant system (2.3) to an asymmetric two-constant coupling system

$$i\dot{a}_n(t) = V_ue^{-i\varpi t}a_{n+1} + V_d^*e^{i\varpi t}a_{n-1} \tag{3.14}$$

The GF for (3.14) is

$$G = G_0e^{-i(e^{-i\varphi}A\bullet u + e^{i\varphi}A^*\bullet d)} = G_0e^{-i(e^{i(\theta-\varphi)}u + e^{-i(\theta-\varphi)}d)r} \tag{3.15}$$

The "price" of this approximation is that the normalization fails, i.e. the condition (2.5) no longer holds and $\sum_{k=-\infty}^{\infty}|a_k(t)|^2 < 1$, and technically the real phase Φ of the generating function G $\sim e^{-i\Phi}$ gets an imaginary add-on (in other words, our potential is no longer Hermitian). Below, we show how this difficulty can be side-stepped.

First, we recast the GF formulation in a more general form. Setting $t = \exp[i(\theta-\varphi)]$ in (3.14) we have

$$G = G_0e^{-i\Phi}, \quad \Phi = (e^{i(\theta-\varphi)}u + e^{-i(\theta-\varphi)}d)r = (ut + d/t)r \tag{3.16}$$

or, in an equivalent trigonometric representation

$$G = G_0e^{-i\Phi}, \ \Phi = [iD_-\sin(\theta-\varphi) + D_+\cos(\theta-\varphi)]r; \ \ D_\pm = e^{\delta} \pm e^{-\delta} \tag{3.17}$$

where for small $\delta << 1$ $D_+ \sim 2$ and $D_+ \sim 2\delta$ so that D_- vanishes when $\delta \to 0$, and we recover a uniform coupling case from Sec. 2. Now, recalling the expansion of exp(rt) and exp(-r/t) over t we obtain the expansion of exp(t-1/t)r via ordinary Bessel functions J_n

$$e^{(t-1/t)r} = \sum_{k=-\infty}^{\infty}t^kJ_k(2r) \tag{3.18}$$

Similarly, replacing t -> it we have the expansion of exp(t+1/t)t over Bessel functions I_n of an imaginary argument

$$e^{(t+1/t)r} = \sum_{n=-\infty}^{\infty} t^k I_k(2r) \tag{3.19}$$

From that readily follows the expansion

$$e^{-i(ut+d/t)r} = \sum_{k=-\infty}^{\infty} t^k (-i)^k (\sqrt{u/d})^k J_k(2r\sqrt{ud}) \tag{3.20}$$

and finally for amplitudes $a_k(t)$ (setting as before k = m – n)

$$a_k(t) = (-i)^k e^{-ik\theta} (\sqrt{u/d})^k J_k(2r\sqrt{ud}) \tag{3.21}$$

Since $(u/d)^{1/2} = e^{\delta} \doteq R_u$ and $(u/d)^{-1/2} = e^{-\delta} \doteq R_d$, our asymmetric coupling model produces a population that is expectedly skewed toward up-transitions n -> n+k. However, the solution is normalized only in the first order: the depopulation to closest levels, i.e. probability (n->n+1) + probability (n->n -1) remains normalized because first order corrections cancel each other, i.e. if δ -> 0, then $R_u^2 + R_d^2$-> 2 as in the equidistant case. However, for higher orders this cancellation does not happen. To side-step this deficiency we replace R_u and R_d with so-called "normalized" correction parameters U and D, similar to the normalized Born approximation in perturbation theory (see, for instance [BS1985]):

$$R_u^{2k} \to U_k^2 = 2\frac{R_u^{2k}}{R_u^{2k} + R_d^{2k}}, \quad R_d^{2k} \to D_k^2 = 2\frac{R_d^{2k}}{R_u^{2k} + R_d^{2k}} \tag{3.22}$$

From (3.22) it follows that $U_k^2 + D_k^2 = 2$ in all orders k regardless of the approximation used for u and d and our solution is fully normalized (albeit somewhat arbitrarily and other normalizations are possible as well).

Finally, we write

$$a_k(t) = (-i)^k e^{-ik\theta} 2^{1/2} \frac{e^{k\delta}}{(e^{2k\delta} + e^{-2k\delta})^{1/2}} J_k(2r) \tag{3.23}$$

Again, when δ -> 0, both u and d -> 1 and we recover the base case of equal spacing.

4. Impact of boundaries (semi-infinite)

Consider now the case when the initial population point n_0 is close to the lower spectrum boundary (that case occurs in a majority of applications) which we denote as $n_b = 1$. Then, truncating the initial system (2.3) we have

$$
\begin{aligned}
&i\dot{a}_1(t) = Ve^{-i\varpi t}a_2, \\
&i\dot{a}_n(t) = Ve^{-i\varpi t}a_{n+1} + V^*e^{i\varpi t}a_{n-1}, \quad a_n(-\infty) = \delta_{n,n_0}, \quad n > 1
\end{aligned}
\tag{4.23}
$$

The solution of semi-infinite system (4.23), i.e. GF, can be constructed via the reflection principle (the method of mirrored sources, see [BS1985]). Namely, using GF of the infinite system GF (n_0; φ, t) we set a new generating function as the difference GF_s = GF (n_0; φ, t) - GF (-n_0; φ, t) which fits a semi-infinite system (4.23), and has an explicit form

$$
GF_s = 2i\sin(n_0\varphi)\cdot e^{-i\cos(\theta-\varphi)2r} \tag{4.24}
$$

From (4.24) we always have $a_0(t) \equiv 0$ and the amplitudes are

$$
a_n(t) = P(k_-) - P(k_+),\ P(s) = (-i)^s e^{-is\theta}J_s(2r),\ k_\pm = n \pm n_0 \tag{4.25}
$$

In particular, for the manifold of degenerate levels (angular momentum sublevels l of n, $\omega = 0$) phase $\theta = 0$ and (4.25) simplifies to

$$
a_n(t) = Q(k_-) - Q(k_+),\ Q(s) = (-i)^s J_s(2r),\ k_\pm = n \pm n_0 \tag{4.26}
$$

It is a simple exercise in the Bessel function algebra to explicitly assure that the normalization condition for (4.26) holds. Amplitudes (4.26) become even simpler if the initial population point coincides with the lower boundary, i.e. $n_0 = n_b = 1$. In that case

$$
a_n(t) = (-i)^{n-n_0}[J_{n-1}(2r) + J_{n+1}(2r)] = (-i)^{n-1}[\frac{n}{r}J_n(2r)] \tag{4.27}
$$

and the transition probability

$$
W_{n-n_0}(t) = [\frac{n}{r}J_n(2r)]^2 \tag{4.28}
$$

is explicitly normalized.

Before closing this section we briefly mention one practically useful extensions for semi-infinite systems. Consider a semi-infinite equidistant manifold of very close or even degenerate levels interacting with an outstanding level separated from that manifold by the final energy gap (see for details [BS1985, BL1995])

The equations for amplitudes are

$$
\begin{aligned}
&i\dot{b}(t) = Ve^{-i\varpi t}a_1, \\
&i\dot{a}_1(t) = Va_2 + V^*e^{i\varpi t}b(t) \\
&i\dot{a}_n(t) = Va_{n+1} + V^*a_{n-1}, \quad a_n(-\infty) = \delta_{n,b}, \quad n > 1
\end{aligned}
\tag{4.29}
$$

Introduce new amplitudes $c_n(t) = a_n(t)/b(t)$, or equivalently, new GF as $RF(\varphi, t) = GF(\varphi, t)/b(t)$. This is a standard method in the close-coupling theory guaranteeing a proper normalization regardless of the approximation used in obtaining $a_n(t)$ (analogous, by the way, to the K-matrix method in scattering theory). Using an approximation, similar to the normalized Born approximation ([BS1985, BL1995]), the probability of transitions b -> a_n can be written as

$$W_{b\to a_n}(t) = [\frac{n}{r} J_n(2r)]^2 W_{tot}, \quad n \geq 1 \tag{4.30}$$

where W_{tot} is the total (normalized) probability of the initial level b depopulation. Practice shows that formula (4.30) works reasonably well, for instance, in the depopulation of l-sublevels in Rydberg atoms.

Finally, we note that it is straightforward to incorporate progressively reducing level spacing corrections as in (3.21 and 3.22) into semi-infinite models (4.23 and 4.29), but we do not discuss it here further.

5. Diffusion (Fokker-Planck) approach to close-coupling

In this section we convert a discrete level close coupling system (2.2, 2.3) into a differential equation of the diffusion type in n-space and, following van Kampen (1980), somewhat loosely call it the Fokker-Planck approach to close-coupling (GF-FP). The motivation comes from an obvious similarity with non-coherent master equation in kinetics, although we are still mindful of potentially material distinctions building on the imaginary factor $i\hbar$ in the LHS of the Schrodinger equation. This latter aspect is closely related to the appealing link connecting diffusion and Schrodinger equations via the Wick 90 degrees rotation of the time t-axis in the complex t-plane. An additional motivation is that the exact CC solution is known and permitting a reliable benchmarking/verification of the GF-FP approximation quality.

With that said, we first recall that in deriving (2.2) in Sec. 2 we assumed a) the level splitting to be constant and b) matrix elements V_{nm} coupling levels n and m to appreciably depend only on the difference $\Delta n = |m-n|$, but not individually on n or m. Here, in addition to that, we suppose that the V_{nm}-dependence on Δn is also slow – sufficiently to a) ignore its derivatives over Δn and b) expand amplitudes $a_{n\pm\Delta n}$ into Taylor series over Δn. We note in passing that this assumption does not look overly inappropriate, especially, for higher atomic levels. In doing so, for transparency and ease of the comparison with (2.2), we restrict ourselves to the closest neighbors $a_{n\pm1}$, but below calculations can be expanded to include close-couplings to the entire block of adjacent levels.

Based on these thoughts, we write

$$a_{n\pm1} \approx 1 \pm \frac{d}{dn} a_n + \frac{d^2}{dn^2} a_n + \ldots \tag{5.1}$$

and, retaining derivatives not exceeding 2-nd order, obtain equations for amplitudes (further below for brevity of notations k stands for Δn)

$$i\dot{a}_k(t) \approx c_+ a_k + c_- a_k' + \tfrac{1}{2} c_+ a_k'', \; c_\pm = V(e^{-i\varpi t} \pm e^{i\varpi t}) \tag{5.2}$$

where (') stands for a differentiation over k. Performing now a full Fourier transform over $a_k(t)$ as in (2.4), we arrive at the generating function equation (GF-FP):

$$i\dot{G}(\varphi,t) \approx [c_+ + c_-(-i\varphi) + \tfrac{1}{2} c_+ (-i\varphi)^2] G \tag{5.3}$$

and the generating function itself comes out as

$$G = e^{-i\Phi}, \; \Phi = [(-i\varphi)C_- + (1 - 0.5\varphi^2)C_+]; \; C_\pm = \int_{-\infty}^{t} c_\pm(t')dt \tag{5.4}$$

From Sec. 2 it follows that $C_+ = 2r\cos\theta$ and $C_- = i\,2r\sin\theta$ and

$$G = G_0 e^{-i\Phi}, \; \Phi = [(-i\varphi) i \sin\theta + (1 - 0.5\varphi^2)\cos\theta] 2r;$$
$$a_k(t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\varphi \; e^{-ik\varphi} G(\varphi, t) \tag{5.5}$$

We immediately see that GF- FP (5.4) is nothing but GF-CC in (2.8) with sin φ and cos φ replaced by their first Taylor terms, i.e. overall GF-FP approximation is GF-CC solution expanded over small phases $\varphi \sim 1/k$, corresponding to relatively large k and amplitudes r > k (otherwise, an integrand in (5.4) oscillates rapidly over φ and amplitudes are suppressed). In other words, CC-FP result is driven by small phases $\varphi \sim 1/k$, which are main contributors to transition amplitudes in a coarse-grained scale k >> 1 - and this characterizes the overall accuracy of GF-FP. Obviously, the more Taylor terms we retain when expanding $a_{n\pm1}$, the closer GF-FP is getting to GF-CC and capturing finer details of the exact solution structure.

Consider a concrete example illustrating general ideas above. For certainty, assume V(t) = V(-t), then θ in (5.5) equals zero and then it follows immediately that

$$|a_k(\infty)|^2 = \left| \frac{1}{2\pi} \int_{-\pi}^{\pi} d\varphi \; e^{-i(k\varphi + r\varphi^2)} \right|^2 \tag{5.6}$$

and, therefore,

$$|a_k(\infty)|^2 = \frac{1}{8\pi} \frac{1}{r} \left| [C(d_+) - C(d_-)] + i[S(d_+) - S(d_-)] \right|^2, \; d_\pm = \pm\pi\sqrt{r} + \frac{k}{2\sqrt{r}} \tag{5.7}$$

where C and S are Fresnel integrals [O(1980)]. It is straightforward to establish a consistency of (5.7) with (2.11) in the limit of r >> 1 and k << r. Indeed, asymptotically

$$C(d_+)-C(d_-)=S(d_+)-S(d_-)=1 \text{ and } |a_k(\infty)|^2=\frac{1}{2\pi}\frac{1}{r} \quad (5.8)$$

On the other hand, an expansion for Bessel functions $J_k(x)\approx\sqrt{2/\pi x}\cos(x-0.5k\pi-0.25k)$ for r >> k > 1 after averaging over oscillations in k produces the result identical to (5.8):

$$|a_k(\infty)|^2=\frac{1}{\pi}\frac{1}{r}\left\langle\cos^2(2r-0.5k\pi-0.25k)\right\rangle_k=\frac{1}{2\pi}\frac{1}{r} \quad (5.9)$$

Overall, two important distinctions between GF-CC and GF-FP solutions stemming from (5.7) are worth noting. Firstly, in the former the r and k dependences are separated and assigned respectively to Bessel function arguments and indices, while in the latter they both are combined into the argument of Fresnel integrals. Secondly, in the major domain of k < r Bessel amplitudes (2.11) behave as $\sim r^{-1/2}\cos(2r-0.5k\pi-0.25k)$ exhibiting largely harmonic oscillation over k, while FP amplitudes (5.5) remain, roughly speaking, constant around $r^{-1/2}$ for small k << r - but self-obviously, they both remain automatically normalized. Heuristically, we can say that while GF-CC captures the oscillatory structure with k, the GF-FP amplitudes are somewhat averaged over these oscillations in exact accordance with its spirit of a coarse-grained approximation.

Despite these two key distinctions, GF-FP displays a fair amount of similarity with the exact GF-CC solution: for both GF-CC and GF-FP a) the excitation front linearly depends on the first order amplitude r (and, respectively, the first and second moments $\bar{k}$ and $\overline{k^2}$ scale as r and r^2) and b) population amplitudes are neither constant nor monotonic in k behind the front, but rather oscillate in k which is quite typical for coherent processes. The remaining (and more subtle) distinction though is that while in GF-CC these oscillations are approximately harmonic in k (i.e. slow change in the amplitude and frequency) as in $J_k(2r)$, in GF-FP they are negligible for small k and grow noticeably anharmonic for larger k, up to k ~ r. The latter trend is clearly an imprint (artefact) of the GF-FP approximation and, in reality, the true behavior of amplitudes for larger k is in between pure harmonic and anharmonic cases. Additionally and relatedly, amplitudes in GF-FP show longer tails into larger k than in GF-CC, specifically, they reduce twice only around k ~2πr (see (4.7)), while in GF-CC they drop exponentially beyond k ~ r (the property of Bessel functions).

6. Some final remarks

Here we reiterate and summarize some key insights.

1. Exact GF-CC probabilities demonstrate an oscillatory structure over Δn < r. This is an unmistaken signature of quantum coherency linked to the cooperative behavior of closely-coupled levels. Relatedly, it can be heuristically viewed as an interference of perturbations propagating in n-space.

2. As was shown in Sec.2, the extent of the population in the coherent process is fundamentally wider than in the in-coherent (diffusive) excitation. The former scales as t, while the latter only as $t^{1/2}$, where t is typical time. As it became apparent recently, this distinction is of a particular importance in relation to quantum computing, information processing and communications (referred collectively to as quantum information technology – QIT), where one of the basic paradigms is a continuous Quantum Walk often implemented via closely-coupled cascades in quantum systems. The corrrsponding literature is vast and continuously expanding, see, for instance [QIT] and references therein.

3. In adjusting the equal spacing model closer to realistic systems, the impact of reducing level spacing can be modeled via an asymmetric two-constant coupling. The attending non-hermitian effects are alleviated by means of the normalizing techniques. The result is that equal spacing amplitudes are modulated asymmetrically thereby skewing the population towards higher n-levels.

4. Effects of finite boundaries can be quite effectively treated by standard reflection techniques based on results for infinite systems.

5. The GF-FP population, while generally agreeing with an exact solution, also shows some expectable quantitative differences (e.g. anharmonic amplitude oscillations, wider expansion into higher levels, etc). Yet, GF-FP can be a handy utility for more realistic models (e.g. non-equidistant systems, or models with a non-flat coupling dependence on the level number n) where an exact solution is feasible only numerically and FP approximation may be the only analytic option. Of note, quantum FP applies to amplitudes (and as such is still a coherent approximation) and the corresponding spreading of occupancy across levels Δn_{eff} progresses as $\sim r \sim t$ in contrast to the diffusive scaling $\sim t^{1/2}$ typical of the classic (incoherent) FP approximation in kinetics.

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