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Green function solution of quantum decay (the Fano and Lifshitz cases)

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Abstract. A Green function procedure is presented by means of which exact decay integrals can be derived without recourse to the eigenvalue problem. General solutions are given for Fano and Lifshitz type decay setups. Specific versions of these models are discussed. In particular the Bixon-Jortner model and generalisations thereof, and the excitonic transfer problem, are discussed in more detail. Novel decay features are found, such as multiple decay channels, some of which are of non-golden-rule character, and a 'crossover' phenomenon from complete to incomplete decay, which is accompanied by alterations in the damping features.

1. Introduction

In recent years many involved theoretical techniques, such as Green function and density matrix methods, projector and path integral techniques and others have been introduced or used to describe quantum decay processes. As basic and standard references we cite the papers of Kubo (1957), Nakajima (1958), Zubarev (1960), Zwanzig (1964), Argyres and Kelley (1964), Mori (1965) and Caldeira and Leggett (1983). In all of these procedures approximative or semiphenomenological assumptions have to be introduced at some stage, or even at several stages, which cannot be easily judged in their effect on the result. Very often the question seems justified, whether these assumptions do not produce artefacts in the results. It is for this reason why there is a need for exact decay laws.

The most widely used decay description is by means of Fermi's golden rule, which is the oldest and most elementary decay law in quantum physics. In many of the above-mentioned methods the final-stage calculation in fact amounts to the application of this rule. But since its derivation is based on lowest-order perturbation theory, its validity has often been disputed. It has been verified only in special exactly solvable model problems, such as that of Bixon and Jortner (1968, 1969).

There is one aspect in the quantum decay problem which, in the great majority of papers, has been carelessly handled or even forgotten. It is the fundamental fact that the very definition of the initial state already fully engenders the decay law. This is a consequence of the possibility to project any initial situation onto the exact eigenvectors of the Hamiltonian H which governs the full intrinsic dynamics. In the golden-rule case an eigenstate of some 'undisturbed' Hamiltonian H_0 is taken as the initial state, which *per se* introduces some arbitrariness and provokes further problems, if one wants to consider the decay of a symmetry-broken state. Another way of defining the initial state is by way of the Kubo formalism (Kubo 1957), which in many instances physically would seem to be a 'natural' definition. A somewhat more questionable initial-state characterisation is by way of a factorisation of the initial density matrix, or by way of the neglect of 'irrelevant' parts of the density matrix. Whatever the initial condition, the decay follows from the knowledge of the exact eigenvectors, and therefore it is these which one desires to know in the first place. But this amounts to the full solution of the eigenvalue problem, which one tries to avoid.

In the present work we present a Green function procedure which allows for the calculation of quantum decay without requiring the solution of the eigenvalue problem. This procedure is of special utility for Fano and Lifshitz type decay arrangements. The general solution of these are given in the form of decay integrals. Specific versions of the Fano and Lifshitz problems are studied in more analytical detail. For power-law coupling forms the phenomenon of 'crossover' from complete to incomplete decay is described, which gives rise to qualitative changes in the damping behaviour. The Bixon-Jortner solution is rederived and the solution of a generalised Bixon-Jortner model is also given. As a specific version of Lifshitz decay the solution of excitonic diffusion in a crystal is presented.

2. Green function preliminaries

Let us consider some Hamiltonian H with its orthonormal set of eigenvectors $\{|\mu\rangle\}$:

$$H|\mu\rangle = E_\mu|\mu\rangle. \tag{1}$$

The most general solution of the time-dependent Schrödinger equation is then

$$|\Psi(t)\rangle = \sum_\mu \langle\mu|\Psi(0)\rangle \exp(-\mathrm{i}E_\mu t)|\mu\rangle. \tag{2}$$

We now introduce an operator Green function

$$G^{(\mathrm{r,a})}(t-t') = \mp\mathrm{i}\Theta(\bullet(t-t')) \sum_\mu |\mu\rangle\langle\mu| \exp[-\mathrm{i}(E_\mu \mp \mathrm{i}\varepsilon)(t-t')] \tag{3}$$

where 'r' and 'a' (upper and lower sign) respectively indicate the 'retarded' and 'advanced' alternatives and where $\varepsilon = 0_+$. The solution (2) may then be written in the form

$$|\Psi(t)\rangle = \mathrm{i}[G^{(\mathrm{r})}(t) - G^{(\mathrm{a})}(t)]|\Psi(0)\rangle. \tag{4}$$

By definition (3) the equation of motion is found to be

$$\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} - (H \mp \mathrm{i}\varepsilon)\right) G^{(\mathrm{r,a})}(t-t') = \delta(t-t'). \tag{5}$$

We now introduce the Fourier conjugates

$$G^{(\mathrm{r,a})}(t-t') = \int_{-\infty}^{+\infty} \mathrm{d}\omega\, G^{(\mathrm{r,a})}(\omega) \exp[-\mathrm{i}\omega(t-t')] \tag{6a}$$

$$G^{(\mathrm{r,a})}(\omega) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}t}{2\pi} G^{(\mathrm{r,a})}(t-t') \exp[\mathrm{i}\omega(t-t')]. \tag{6b}$$

Inserting (3) in (6*b*) we find

$$G(E) = \frac{1}{2\pi} \sum_\mu \frac{|\mu\rangle\langle\mu|}{E - E_\mu} \qquad E = \omega \pm \mathrm{i}\varepsilon \tag{7}$$

where

$$G^{(r)}(\omega)=G(\omega+\mathrm{i}\varepsilon) \qquad G^{(a)}(\omega)=G(\omega-\mathrm{i}\varepsilon). \tag{8}$$

The Fourier-transformed equation follows as

$$[EI-H]G(E)=\frac{1}{2\pi}I \tag{9}$$

where I is the unity operator. Inserting (7) and (6a) in (4) we have

$$|\Psi(t)\rangle=\mathrm{i}\int_{-\infty}^{+\infty}\mathrm{d}\omega\,\exp(-\mathrm{i}\omega t)[G(\omega+\mathrm{i}\varepsilon)-G(\omega-\mathrm{i}\varepsilon)]|\Psi(0)\rangle \tag{10a}$$

and the basic correlation function is

$$\langle\Psi(0)|\Psi(t)\rangle=\mathrm{i}\langle\Psi(0)|\int_{-\infty}^{+\infty}\mathrm{d}\omega\,\exp(-\mathrm{i}\omega t)[G(\omega+\mathrm{i}\varepsilon)-G(\omega-\mathrm{i}\varepsilon)]|\Psi(0)\rangle. \tag{11a}$$

From (7) we observe that the poles of $G(E)$ are given by $E=E_\mu$, i.e. they are all located on the real axis in complex E space. Continuing ω to the complex plane also, the poles in ω space are given by

$$\omega_\mu=E_\mu\mp\mathrm{i}\varepsilon \qquad \varepsilon=0_+. \tag{12}$$

Hence in complex ω space the poles of $G(\omega+\mathrm{i}\varepsilon)$ will all lie below the real axis, whereas those of $G(\omega-\mathrm{i}\varepsilon)$ will be above this axis. Taking this into account, the integrals (10a) and (11a) may be handled by means of the residue theorem. For simplicity we assume all poles (eigenvalues) to be of first order. (There would be no difficulty to include higher-order poles as well.) Equations (10a) and (11a) may then be rewritten as

$$\begin{aligned}|\Psi(t)\rangle&=\mathrm{i}\oint\mathrm{d}z\,\exp(-\mathrm{i}zt)G(z+\mathrm{i}\varepsilon)|\Psi(0)\rangle &&\text{for } t>0\ (\mathrm{Im}\ \omega<0)\\&=\mathrm{i}\oint\mathrm{d}z\,\exp(-\mathrm{i}zt)G(z-\mathrm{i}\varepsilon)|\Psi(0)\rangle &&\text{for } t<0\ (\mathrm{Im}\ \omega>0)\end{aligned} \tag{10b}$$

and

$$\begin{aligned}\langle\Psi(0)|\Psi(t)\rangle&=\mathrm{i}\langle\Psi(0)|\oint\mathrm{d}z\,\exp(-\mathrm{i}zt)G(z+\mathrm{i}\varepsilon)|\Psi(0)\rangle &&\text{for } t>0\ (\mathrm{Im}\ \omega<0)\\\langle\Psi(0)|\Psi(t)\rangle&=\mathrm{i}\langle\Psi(0)|\oint\mathrm{d}z\,\exp(-\mathrm{i}zt)G(z-\mathrm{i}\varepsilon)|\Psi(0)\rangle &&\text{for } t<0\ (\mathrm{Im}\ \omega>0).\end{aligned} \tag{11b}$$

Applying the residue theorem, this yields

$$|\Psi(t)\rangle=2\pi\sum_\mu\exp(-\mathrm{i}E_\mu t)\lim_{E\to E_\mu}(E-E_\mu)G(E)|\Psi(0)\rangle \tag{10c}$$

and

$$\langle\Psi(0)|\Psi(t)\rangle=2\pi\sum_\mu\exp(-\mathrm{i}E_\mu t)\lim_{E\to E_\mu}(E-E_\mu)\langle\Psi(0)|G(E)|\Psi(0)\rangle. \tag{11c}$$

It turns out that all three different forms of (10) and (11) prove their utility in applications depending on the specific problems at stake. Their usefulness is based on the fact that they comprise a method which avoids the solution of the full eigenvalue problem. In the summation forms (10*c*) and (11*c*) it proves necessary to find only the eigenvalues E_μ and not the eigenfunctions. The integral forms (10*a*, *b*) and (11*a*, *b*) in general are even more advantageous, since the functional behaviour of $G(E)$ frequently may be found by suitable approximation methods. Moreover, in this form the effect of sequences of eigenvalues which are very close to each other (quasicontinuum or continuum) can be described by a single pole or a few poles which are located at some finite distance from the real axis. Examples will be given below. The procedures which respectively are introduced to solve the equation of motion (9) in general are developed after projecting this equation onto some suitable complete orthonormal base $\{|j\rangle\}$:

$$\langle \mu | j \rangle = \eta_j(\mu). \tag{13}$$

The coefficients $\eta_j(\mu)$ then also constitute a complete orthonormal set:

$$\sum_j \eta_j^*(\mu)\eta_j(\nu) = \delta_{\mu\nu} \tag{13a}$$

$$\sum_\mu \eta_j^*(\mu)\eta_k(\mu) = \delta_{jk} \tag{13b}$$

and the projections of the Green function operators onto the base $\{|j\rangle\}$ are found as

$$G_{jk}^{(\mathrm{r,a})}(t-t') = \mp \mathrm{i}\Theta(\pm(t-t'))\sum_\mu \eta_j^*(\mu)\eta_k(\mu)\exp[-\mathrm{i}(E_\mu \mp \mathrm{i}\varepsilon)(t-t')] \tag{14a}$$

$$G_{jk}(E) = \frac{1}{2\pi}\sum_\mu \frac{\eta_j^*(\mu)\eta_k(\mu)}{E-E_\mu} \qquad E = \omega \pm \mathrm{i}\varepsilon. \tag{14b}$$

The projected equation of motion (9) becomes

$$\sum_k (E\delta_{jk} - H_{jk})G_{kl}(E) = \frac{1}{2\pi}\delta_{jl} \qquad E = \omega \pm \mathrm{i}\varepsilon. \tag{15}$$

It is this equation which, in our calculation of decay laws, will play the crucial role.

3. Fano decay

In the Fano problem (Fano 1961) a singular state $|s\rangle$ is distinguished from the others $|k\rangle$, such that only this state is coupled to the others, whereas states $|k\rangle$ are not mutually coupled:

$$H = E_s^{(0)}|s\rangle\langle s| + \sum_{k(\neq s)} E_k^{(0)}|k\rangle\langle k| + \sum_{k(\neq s)} [V_k|s\rangle\langle k| + V_k^*|k\rangle\langle s|]. \tag{16}$$

In fact this problem is the most general version of the Bixon-Jortner model (Bixon and Jortner 1968, 1969). In the notation of the preceding section we have

$$H_{ss} = E_s^{(0)} \qquad H_{sk} = V_k \qquad H_{kk} = E_k^{(0)} \tag{17}$$

and the equation of motion (15) comes to be explicitly

$$(E - E_s^{(0)})G_{ss}(E) - \sum_{k(\neq s)} V_k G_{ks}(E) = \frac{1}{2\pi} \tag{18a}$$

$$(E - E_k^{(0)})G_{ks}(E) - V_k^* G_{ss}(E) = 0 \tag{18b}$$

$$(E - E_s^{(0)})G_{sk}(E) - \sum_{k'(\neq s)} V_{k'} G_{k'k}(E) = 0 \tag{18c}$$

$$(E - E_k^{(0)})G_{kk'}(E) - V_k^* G_{sk'}(E) = \frac{1}{2\pi}\delta_{kk'} \tag{18d}$$

which can be solved completely. Inserting (18b) in (18a) and similarly (18d) in (18c) we find

$$G_{ss}(E)=\frac{1}{2\pi}\left(E-E_s^{(0)}-\sum_{k(\neq s)}\frac{|V_k|^2}{E-E_k^{(0)}}\right)^{-1} \qquad E=\omega\pm\mathrm{i}\varepsilon \tag{19a}$$

$$G_{sk}(E)=\frac{1}{2\pi}\frac{V_k}{E-E_k^{(0)}}\left(E-E_s^{(0)}-\sum_{k'(\neq s)}\frac{|V_{k'}|^2}{E-E_{k'}^{(0)}}\right)^{-1} \qquad E=\omega\pm\mathrm{i}\varepsilon \tag{19b}$$

which respectively may be inserted in (18b) and (18d) to yield ($E=\omega\pm\mathrm{i}\varepsilon$)

$$G_{ks}(E)=\frac{1}{2\pi}\frac{V_k^*}{E-E_k^{(0)}}\left(E-E_s^{(0)}-\sum_{k'(\neq s)}\frac{|V_{k'}|^2}{E-E_{k'}^{(0)}}\right)^{-1} \tag{19c}$$

$$G_{kk'}(E)=\frac{1}{2\pi}\frac{1}{E-E_k^{(0)}}\delta_{kk'}+\frac{1}{2\pi}\frac{V_k^*V_{k'}}{(E-E_k^{(0)})(E-E_{k'}^{(0)})}\left(E-E_s^{(0)}-\sum_{k''(\neq s)}\frac{|V_{k''}|^2}{E-E_{k''}^{(0)}}\right)^{-1}. \tag{19d}$$

In passing it is worth noting two equations which establish the antiresonance nature of the Fano problem. Since from results (19b) and (19c) we have

$$V_kG_{ks}=V_k^*G_{sk} \tag{20}$$

we may insert (18c) in (18a). This yields

$$(E-E_s^{(0)})G_{ss}(E)=\frac{1}{2\pi}+\frac{1}{E-E_s^{(0)}}\sum_{kk'}V_kV_{k'}^*G_{kk'}(E) \tag{21}$$

which directly relates the singular Green function (GF) $G_{ss}(E)$ to the bath GF $G_{kk'}(E)$. Since $G_{ss}(E)$ in general will have a finite value at $E=E_s^{(0)}$, we conclude from (21) that the sum on the RHS must be zero for $E\to E_s^{(0)}$ (antiresonance). Similarly, again by use of (20), we may insert (18b) in (18c), which yields

$$\sum_{kk'}V_kV_{k'}^*G_{kk'}(E)=(E-E_s^{(0)})G_{ss}(E)\sum_{k''}\frac{|V_{k''}|^2}{E-E_{k''}^{(0)}} \tag{22}$$

which gives direct evidence of the antiresonance behaviour of the bath GF on the LHS.

Equations (19a–d), in view of relations (4) or (10), establish the general solution of the time-dependent Schrödinger equation. Hence, the decay of any arbitrary initial state may be written down in the form of a single decay integral. For illustration we have a look at the physically most interesting situation, which is the initial occupation of the singular state $|s\rangle$

$$|\Psi(0)\rangle=|s\rangle. \tag{23}$$

Then, by means of (10a)

$$|\Psi(t)\rangle=\mathrm{i}|s\rangle\int_{-\infty}^{\infty}\mathrm{d}\omega\,\exp(-\mathrm{i}\omega t)[G_{ss}(\omega+\mathrm{i}\varepsilon)-G_{ss}(\omega-\mathrm{i}\varepsilon)]$$
$$+\sum_k|k\rangle\int_{-\infty}^{\infty}\mathrm{d}\omega\,\exp(-\mathrm{i}\omega t)[G_{ks}(\omega+\mathrm{i}\varepsilon)-G_{ks}(\omega-\mathrm{i}\varepsilon)]. \tag{24}$$

Employing the Plemelj formula $(x+\mathrm{i}\varepsilon)^{-1}=P(1/x)-\mathrm{i}\pi\delta(x)$, we can write

$$\sum_k\frac{|V_k|^2}{(\omega\pm\mathrm{i}\varepsilon)-E_k^{(0)}}=\Pi(\omega)\mp\mathrm{i}\Gamma(\omega) \tag{25}$$

where

$$\Pi(\omega) = P \sum_k \frac{|V_k|^2}{\omega - E_k^{(0)}} \tag{26}$$

$$\Gamma(\omega) = \pi \sum_k |V_k|^2 \delta(\omega - E_k^{(0)}) \tag{27}$$

by means of which we have, for example,

$$G_{ss}(\omega \pm \mathrm{i}\varepsilon) = \frac{1}{2\pi} [(\omega \pm \mathrm{i}\varepsilon) - E_s^{(0)} - \Pi(\omega) \pm \mathrm{i}\Gamma(\omega)]^{-1} \tag{28a}$$

and

$$\begin{aligned} G_{ss}(\omega + \mathrm{i}\varepsilon) - G_{ss}(\omega - \mathrm{i}\varepsilon) &= 2\mathrm{i}\,\mathrm{Im}\, G(\omega + \mathrm{i}\varepsilon) \\ &= -\frac{\mathrm{i}}{\pi} \frac{\Gamma(\omega) + \varepsilon\omega}{(\omega - E_s^{(0)} - \Pi(\omega))^2 + (\Gamma(\omega) + \varepsilon)^2} \qquad \varepsilon = 0_+ \end{aligned} \tag{28b}$$

where $\varepsilon = 0_+$ has been preserved to also include the singular poles of this expression in regions where $\Gamma(\omega) = 0$. Inserting result (28) in (24) the basic correlation function turns out to be

$$\langle \Psi(0) | \Psi(t) \rangle = \frac{1}{\pi} \int_{-\infty}^{+\infty} \mathrm{d}\omega \frac{(\Gamma(\omega) + \varepsilon) \exp(-\mathrm{i}\omega t)}{[\omega - (E_s^{(0)} + \Pi(\omega))]^2 + (\Gamma(\omega) + \varepsilon)^2}. \tag{29}$$

If the bath eigenvalues $E_k^{(0)}$ constitute a quasicontinuous sequence in a spectral region R and if there are none outside ($\Gamma(\omega) = 0$ if $\omega \notin R$), we may rewrite (29) in the form

$$\begin{aligned} \langle \Psi(0) | \Psi(t) \rangle = &\frac{1}{\pi} \int_{\omega \in R} \mathrm{d}\omega \frac{\Gamma(\omega) \exp(-\mathrm{i}\omega t)}{[\omega - E_s^{(0)} - \Pi(\omega)]^2 + (\Gamma(\omega))^2} \\ &+ \frac{1}{\pi} \int_{\omega \notin R} \mathrm{d}\omega \frac{\varepsilon \exp(-\mathrm{i}\omega t)}{[\omega - E^{(0)} - \Pi(\omega)]^2 + \varepsilon^2} \qquad \varepsilon = 0_+. \end{aligned} \tag{30}$$

The second term on the RHS acquires a finite value if the denominator of the integrand turns zero at some $\omega_r \notin R$:

$$\omega_r - E_s^{(0)} - \Pi(\omega_r) = 0 \qquad \omega_r \notin R. \tag{31}$$

Expression (30) then takes on the form

$$\begin{aligned} \langle \Psi(0) | \Psi(t) \rangle = &\frac{1}{\pi} \int_{\omega \in R} \mathrm{d}\omega \frac{\Gamma(\omega) \exp(-\mathrm{i}\omega t)}{[\omega - E_s^{(0)} - \Pi(\omega)]^2 + (\Gamma(\omega))^2} \\ &+ \sum_r \left[1 - \left(\frac{\mathrm{d}\Pi(\omega)}{\mathrm{d}\omega} \right)_{\omega = \omega_r} \right]^{-1} \exp(-\mathrm{i}\omega_r t) \end{aligned} \tag{32}$$

where we have used the formula

$$\frac{1}{\pi} \frac{\varepsilon}{g(x)^2 + \varepsilon^2} = \sum_r \left(\frac{\mathrm{d}}{\mathrm{d}x} g(x) \right)_{x = x_r}^{-1} \delta(x - x_r) \qquad g(x_r) = 0. \tag{33}$$

From result (32) we note that the decay of a singular state $|s\rangle$ may be incomplete even if its position $E_s^{(0)}$ is located within the region of bath states. The decay term is then supplemented by monochromatic additions which are characterised by the solutions of (31). In the trivial case $V_k = 0$ ($\Pi(\omega) = 0, \Gamma(\omega) = 0$)) equation (31) has the single solution $\omega_r = E^{(0)}$ and the monochromatic evolution is the only remaining term. On the other hand, if the coupling V_k is switched on and gradually increased, there may be a critical coupling strength, for which (31) starts to have a solution outside the region R of band states $E^{(0)}$. This 'crossover' is considered in § 4.

In the small-coupling regime, and provided that there is a quasicontinuous $E_k^{(0)}$ sequence such that $\Gamma(E_s^{(0)}) \neq 0$, our result (32) merges into the golden-rule result

$$\langle\Psi(0)|\Psi(t)\rangle = \exp(-\mathrm{i}E_s t - \Gamma(E_s)t) \tag{34}$$

where

$$E_s = E_s^{(0)} + \Pi(E_s^{(0)}) \tag{35}$$

$$\Gamma(E_s) = \pi \sum_k |V_k|^2 \delta(E_s - E_k^{(0)}) = \pi |V_k(E_s)|^2 \rho(E_s) \tag{36}$$

and where $\rho(\omega)$ is the frequency density of the states $|k\rangle$.

4. Crossover behaviour in the Fano decay

As explained following (29), the decay of a singular state $|s\rangle$ turns incomplete if (31) has a solution outside the region of bath states $E_k^{(0)}$. By changing the coupling constants V_k we may change the magnitude of the quantity $\Pi(\omega)$, and in doing so we may cross the borderline of creating a solution of (31) where previously there was none. This crossover on the one hand establishes a monochromatic contribution to the correlation function $\langle\Psi(0)|\Psi(t)\rangle$ as already noted. But, in addition it also changes the qualitative character of the decay behaviour of the band part of $\langle\Psi(0)|\Psi(t)\rangle$. To make this more explicit, let us consider a power law coupling of the form

$$\Gamma_m(\omega) = \pi|V(\omega)|^2\rho(\omega) = \alpha\Omega(\omega/\Omega)^m \qquad \text{for } 0 \leqslant \omega \leqslant \Omega \tag{37}$$

$$= 0 \qquad \text{otherwise}$$

where $m = 0, 1, 2, 3, \ldots$. Then, from (26)

$$\begin{aligned} \Pi_m(\omega) \equiv \Omega p_m(x) &= -\frac{\alpha\Omega}{\pi} P \int_0^1 \mathrm{d}y \frac{y^m}{(y-x)} && x = (\omega/\Omega) \\ &= -\frac{\alpha\Omega}{\pi} \ln\frac{|1-x|}{|x|} && \text{for } m = 0 \\ &= -\frac{\alpha\Omega}{\pi}\left(1 + x\ln\frac{|1-x|}{|x|}\right) && \text{for } m = 1 \\ &= -\frac{\alpha\Omega}{\pi}\left(\tfrac{1}{2} + x + x^2\ln\frac{|1-x|}{|x|}\right) && \text{for } m = 2 \\ &= -\frac{\alpha\Omega}{\pi}\left(\tfrac{1}{3} + \tfrac{1}{2}x + x^2 + x^3\ln\frac{|1-x|}{|x|}\right) && \text{for } m = 3 \end{aligned} \tag{38}$$

where dimensionless quantities α and $x = \omega/\Omega$ have been introduced, and we will further use $x_s = E_s^{(0)}/\Omega$, $0 < x_s < 1$. Then, inserting (38) in (31), we have

$$x - x_s - p_m(x) = 0 \qquad x \notin (0, 1). \tag{39}$$

For $x = x_N > 1$ ($\omega = \omega_N = \Omega x_N$) it turns out that there is always a singular solution. We show this by first assuming α to be such that $x_N = 1 + \delta$, $0 < \delta \ll x_s < 1$. Then (39), by using (38), becomes

$$\begin{aligned} 1 + \delta &= x_s - \frac{\alpha}{\pi} \ln \delta + \frac{\alpha}{\pi} \delta + \mathrm{O}(\alpha\delta^2) \qquad &\text{for } m = 0 \\ &= x_s - \frac{\alpha}{\pi} - \frac{\alpha}{\pi} \ln \delta + \mathrm{O}(\alpha\delta \ln \delta) \qquad &\text{for } m = 1, \text{etc} \end{aligned} \tag{40}$$

or

$$\begin{aligned} \delta &= \exp\left(-\frac{\pi}{\alpha}(1 - x_s) \right) + \mathrm{O}(\delta^2/\alpha) \qquad &\text{for } m = 0 \\ &= \exp\left(-\frac{\pi}{\alpha}(1 - x_s) - 1 \right) + \mathrm{O}(\delta^2/\alpha) \qquad &\text{for } m = 1, \text{etc.} \end{aligned} \tag{41}$$

Hence, for $\alpha \to 0$ we have $\delta \to 0$, in agreement with the presupposition $\delta \ll 1$. For increasing α values δ also increases, but we refrain from discussing its analytic form in the large coupling limit.

Below the band region there is also always a solution $x = x_0 < 0$ in the case $m = 0$. To show this we first assume α to be such that $x_0 = -\eta$, $0 < \eta \ll x_s < 1$. Then from (39) employing (38) for $m = 0$, we find

$$\frac{\alpha}{\pi} \ln \frac{1}{\eta} = x_s + \eta - \frac{\alpha}{\pi} \eta + \mathrm{O}(\eta^2) \tag{42}$$

or

$$\eta = \exp(-\pi x_s/\alpha) + \mathrm{O}(\eta^2/\alpha) \tag{43}$$

which is seen to be consistent with the presupposition $\eta \ll 1$ for small α. For increasing α values the singular solution gradually moves away from the lower band edge (increasing η values), but we do not pursue this further. In the other power cases ($m > 0$) there is only a solution below the lower band edge ($x_0 < 0$) if α exceeds a crossover coupling value α_c which is given by

$$\alpha_c = \pi m x_s \qquad \text{for } m > 0. \tag{44}$$

This can be seen once more if we presume $x_0 = -\eta$, $\eta \ll 1$. Then we find from (39), employing (38) for $m > 0$, that $\eta \to 0$ for $\alpha = \alpha_c + 0_+$, whereas there is no solution $x_0 < 0$ for $\alpha < \alpha_c$. But we refrain from discussing this in detail.

To sum up, the overall situation therefore is as follows. The total correlation function (32) consists of three constituents:

$$\langle \Psi(0) | \Psi(t) \rangle = \langle \Psi(0) | \Psi(t) \rangle_{\mathrm{dec}} + A_0 \exp(-\mathrm{i}\Omega x_0 t) + A_N \exp(-\mathrm{i}\Omega x_N t). \tag{45}$$

Two of these are of a purely oscillatory character with frequencies $\Omega_0 = \Omega x_0$ and $\Omega_N = \Omega x_N$, respectively, which represent the singular solutions outside the continuous band. The amplitudes A_0 and A_N are given by (see (32))

$$A_r = \left[1 - \left(\frac{\mathrm{d}\Pi(\omega)}{\mathrm{d}\omega} \right)_{\omega = \Omega_r} \right]^{-1} \qquad r = 0, N. \tag{46}$$

If the coupling law is governed by the power $m=0$, both singular solutions exist for any coupling value α. For $m=1, 2, 3$, however, there is a crossover coupling strength α_c, below which the lower singular solution $\Omega_0<0$ does not exist. The amplitudes A_0 and A_N are drawn in figure 1 for $m=1$. The decaying part $\langle\Psi(0)|\Psi(t)\rangle_{\mathrm{dec}}$ of the correlation function is given by (see (32))

$$\langle\Psi(0)|\Psi(t)\rangle_{\mathrm{dec}}=\frac{\alpha}{\pi}\int_0^1 \mathrm{d}x\frac{x^m\exp(-\mathrm{i}\Omega xt)}{(x-x_s-p_m(x))^2+(\alpha x^m)^2}. \tag{47}$$

The time behaviour of this constituent is drawn in figure 2 for four different α values below the crossover value α_c and in figure 3 for two different α values above α_c. From

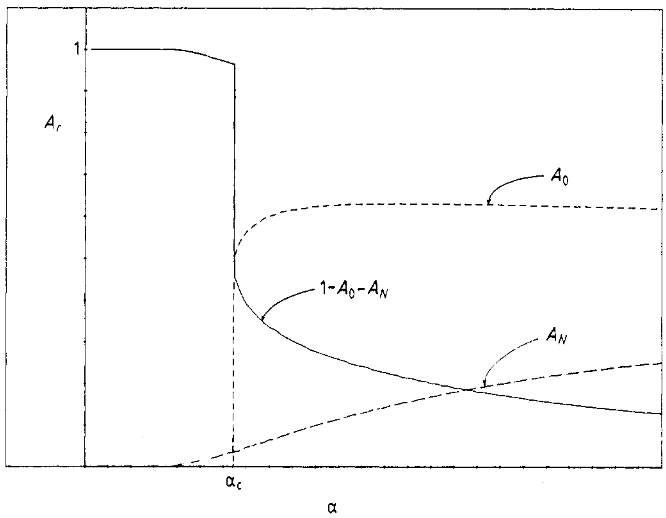

Figure 1. Amplitudes of the decaying and non-decaying parts in a Fano problem with a spectrally restricted bath ($0<E_k^{(0)}<E^{(0)}<\Omega$) and a power law coupling $\pi V^2(\omega)\rho(\omega)=\alpha\omega$. α_c indicates the 'crossover' coupling (see text).

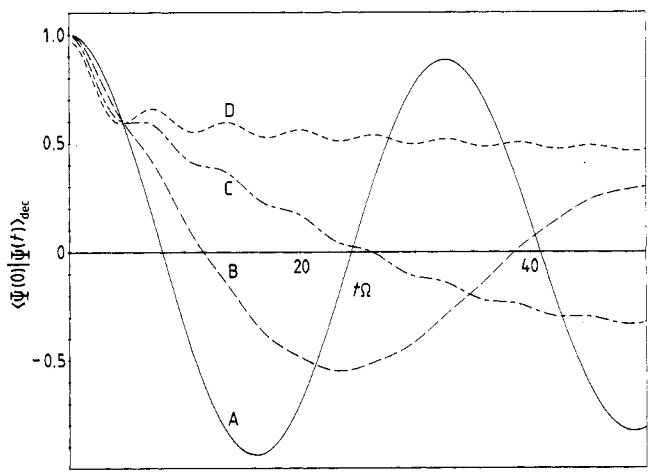

Figure 2. Decay in a Fano system evolution below the 'crossover' coupling strength ($\alpha_c=0.628$). Spectrally restricted bath and a power law coupling $\pi V(\omega)^2\rho(\omega)=\alpha\omega$. $\alpha_c=0.628$. $\alpha_1=0.002$ (A), $\alpha_2=0.2$ (B), $\alpha_3=0.4$ (C), $\alpha_4=0.61$ (D). $m=1$, $x_s=0.2\Omega$.

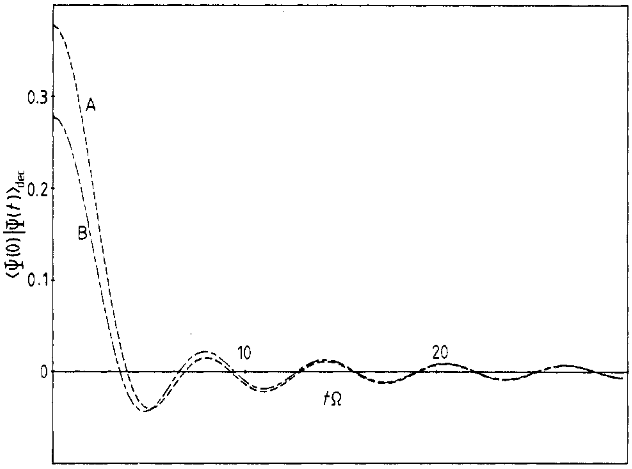

Figure 3. Decay in a Fano system. Evolution above the 'crossover' coupling strength (α_c). Only the decaying part is drawn. Spectrally restricted bath and a power law coupling $\pi V(\omega)^2\rho(\omega)=\alpha\omega$. $\alpha_1=0.65$ (A), $\alpha_2=1.0$ (B). $m=1$, $x_s=0.2\Omega$.

figure 2 we note that the decay preserves some oscillatory character, which gradually fades away when α approaches α_c. For $\alpha>\alpha_c$ there is a sharp short-time decay of $\langle\Psi(0)|\Psi(t)\rangle$ which is followed by an extended long-time tail. This tail again displays some oscillatory character, which is governed by the cutoff frequency Ω.

5. Bixon–Jortner model and modifications thereof

In the Bixon-Jortner model (Bixon and Jortner 1968, 1969) it is assumed that the singular states of a Fano system are contrasted to a sequence of 'band' states with equal spacing which spread out over $(-\infty,\infty)$:

$$E_k^{(0)}=k\Delta \qquad k=0,\pm1,\pm2,\ldots,\pm\infty. \tag{48}$$

It is further assumed that all coupling constants are equal:

$$V_k=v. \tag{49}$$

Then the crucial summation of (19a–d) can be exactly performed via the method of residues (see, e.g., Korn and Korn 1968, p 202)

$$\sum_{k=-\infty}^{+\infty}\frac{|V_k|^2}{E-E_k^{(0)}}=-\frac{v^2}{\Delta}\sum_{k=-\infty}^{+\infty}\frac{1}{k-(E/\Delta)}=\pi\frac{v^2}{\Delta}\cot(\pi E/\Delta). \tag{50}$$

The GF of (19a) is then given by

$$G_{ss}(E)=\frac{1}{2\pi}[E-E_s^{(0)}-(\pi v^2/\Delta)\cot(\pi E/\Delta)]^{-1} \tag{51}$$

with its poles E_ν given by the solution of the eigenvalue equation

$$N(E_\nu)\equiv E_\nu-E_s^{(0)}-(\pi v^2/\Delta)\cot(\pi E_\nu/\Delta)=0. \tag{52}$$

Near each pole the denominator $N(E)$ of $G_{ss}(E)$ may be expanded:

$$N(E)=(E-E_\nu)[1+(\pi v/\Delta)^2(\sin(\pi E_\nu/\Delta))^{-2}]+\mathrm{O}((E-E_\nu)^2). \tag{53}$$

This, by employing (52), may be rewritten as

$$N(E)=(E-E_\nu)\left[1+\left(\frac{\pi v}{\Delta}\right)^2+\frac{1}{v^2}(E_\nu-E_s^{(0)})^2\right]+\mathrm{O}((E-E_\nu)^2). \tag{54}$$

The residues of $G_{ss}(E)$ then become

$$\begin{aligned}\operatorname{Res} G_{ss}(E_\nu)&\equiv\frac{1}{2\pi}\lim_{E\to E_\nu}(E-E_\nu)\frac{1}{N(E)}\\ &=\frac{1}{2\pi}v^2[(E_\nu-E_s^{(0)})^2+v^2+(\pi v^2/\Delta)^2]^{-1}.\end{aligned} \tag{55}$$

Inserting this in (11c) we find for $\Psi(0)=|s\rangle$

$$\begin{aligned}\langle\Psi(0)|\Psi(t)\rangle&=2\pi\sum_\mu\exp(-\mathrm{i}E_\mu t)\lim_{E\to E_\mu}(E-E_\mu)G_{ss}(E)\\ &=\sum_\mu\frac{v^2\exp(-\mathrm{i}E_\mu t)}{[(E_\mu-E_s^{(0)})^2+v^2+(\pi v^2/\Delta)^2]}.\end{aligned} \tag{56}$$

This is the result derived by Bixon and Jortner (1968, 1969) via the solution of the eigenvalue problem, employing not only the eigenvalues E_μ but also the eigenfunctions. Since, by discussing (50), each of the eigenvalues is seen to lie between two adjacent undisturbed values, $E_{k+1}>E_\mu>E_k$, (56) approximately constitutes a Lorentzian form, and for $v\gg\Delta$ we may replace the sum by an integral, whence

$$\langle\Psi(0)|\Psi(t)\rangle=\frac{\pi v^2}{\Gamma_{\mathrm{BJ}}\Delta}\exp(-\mathrm{i}E_s^{(0)}t-\Gamma_{\mathrm{BJ}}|t|) \tag{57}$$

where

$$\Gamma_{\mathrm{BJ}}=[v^2+(\pi v^2/\Delta)^2]^{1/2}\qquad\text{for } v\gg\Delta. \tag{58}$$

We now want to exemplify the solution of the same problem by use of formulae (26)-(28). Replacing the summations in (26) and (27) by integrals we get

$$\Pi(\omega)=\frac{1}{\Delta}P\int_{-\infty}^{\infty}\frac{v^2}{\omega-\Delta k}\,\mathrm{d}k=0 \tag{59}$$

$$\Gamma(\omega)=\pi v^2/\Delta\qquad\text{for } v\gg\Delta \tag{60}$$

and upon inserting in (29)

$$\begin{aligned}\langle\Psi(0)|\Psi(t)\rangle&=\frac{v^2}{\Delta}\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{\exp(-\mathrm{i}\omega t)}{(\omega-E_s^{(0)})^2+(\pi v^2/\Delta)^2}\\ &=\exp[-\mathrm{i}E_s^{(0)}t-(\pi v^2/\Delta)|t|]\qquad\text{for } v\gg\Delta.\end{aligned} \tag{61}$$

This coincides with the Bixon-Jortner result (57) within the presupposition made ($v\gg\Delta$) in both cases to replace the summations by integrals. From both calculations given here we become aware of the practical suitability of the GF method. A rather general natural extension of the Bixon-Jortner model is given by

$$|V_k|^2=W(E_k^{(0)})\qquad E_k^{(0)}=\Delta k\qquad k=0,\pm1,\ldots,\pm\infty \tag{62}$$

where the analytic continuation of $W(E_k^{(0)})$ is denoted by $W(E)$. We assume $W(E)$ to have a sequence of poles at sites $E=S_r$, $r=\pm1,\pm2,\ldots$, such that $\mathrm{Im}\, S_r>0$ for $r>0$ and $S_{-r}=S_r^*$. To be more specific, we introduce

$$W(E)=\sum_r \frac{A_r}{E-S_r} \qquad S_{-r}=S_r^* \qquad A_{-r}=A_r^* \qquad r=\pm1,\pm2,\ldots \tag{63}$$

which is still a rather flexible extension of the Bixon-Jortner model. The summation (50) then takes on the form

$$\sum_{k=-\infty}^{\infty}\frac{|V_k|^2}{E-E_k^{(0)}}=-\frac{1}{\Delta}\sum_{k=-\infty}^{\infty}\frac{W(\Delta k)}{k-(E/\Delta)}. \tag{64}$$

This, by again employing the method of residues (see Korn and Korn 1968, p 202), can be summed up to yield

$$\sum_{k=-\infty}^{\infty}\frac{|V_k|^2}{E-E_k^{(0)}}=-\frac{\Delta}{2\pi\mathrm{i}}\oint_C \pi\,\mathrm{d}E'\,\frac{W(E')}{E'-E}\cot(\pi E'/\Delta)+\frac{\pi}{\Delta}W(E)\cot(\pi E/\Delta)$$
$$+\frac{\pi}{\Delta}\sum_r^{(C)}\frac{\cot(\pi S_r/\Delta)}{S_r-E'}\lim_{E'\to S_r}(E'-S_r)W(E'). \tag{65}$$

We choose the contour C as a circle at infinity. Then, by means of (63) the integrand turns to zero sufficiently fast, whence the contour integral dissapears. By inserting (63) we then find

$$\sum_{k=-\infty}^{\infty}\frac{|V_k|^2}{E-E_k^{(0)}}=\frac{\pi}{\Delta}\sum_r\frac{A_r}{E-S_r}[\cot(\pi E/\Delta)-\cot(\pi S_r/\Delta)]. \tag{66}$$

This expression constitutes the analogue of (50) and the further calculation completely parallels the one given by (50)–(61). The details of this calculation will be given elsewhere. At this point we only note the results for the most simple version of an extension of the Bixon-Jortner model, which is given by choosing $r=\pm1$, $S_1=\mathrm{i}a$, $A_1=-\mathrm{i}av^2/2$. Then the denominator of the GF (19a) is given by

$$\begin{aligned}N(E)&\equiv E-E_s^{(0)}-\sum_{k=-\infty}^{\infty}\frac{|V_k|^2}{E-E_k^{(0)}}\\ &=E-E_s^{(0)}-\frac{\pi}{\Delta}\frac{v^2a}{E^2+a^2}\left[a\cot\left(\frac{\pi E}{\Delta}\right)+E\,\mathrm{cotanh}\left(\frac{\pi a}{\Delta}\right)\right]\\ &=[2\pi G_{ss}(E)]^{-1}.\end{aligned} \tag{67}$$

Since $\cot(\pi E/\Delta)$ runs over all values in $(-\infty,+\infty)$, if E moves from one $E_k^{(0)}$ value $(=\Delta k)$ to a neighbouring one, whereas all other quantities (67) almost remain unchanged in the same interval, there must be a solution of (67) in this interval. Hence the eigenvalues E_μ are again respectively located in between two adjacent undisturbed eigenvalues $E_k^{(0)}$. The analogue of (56) is

$$\begin{aligned}\langle\Psi(0)|\Psi(t)\rangle=v^2\sum_\mu\exp(-\mathrm{i}E_\mu t)\Bigg\{&v^2+v^2\frac{2E_\mu(E_\mu-E_s^{(0)})}{E_\mu^2+a^2}\\ &+\left(\frac{\pi v^2}{\Delta}\right)^2\frac{a^2}{E_\mu^2+a^2}\left[1-\frac{\Delta}{\pi a}\mathrm{cotanh}\left(\frac{\pi a}{\Delta}\right)\right]\\ &+\frac{E_\mu^2+a^2}{a^2}\left[E_\mu-E_s^{(0)}-\frac{\pi}{\Delta}\frac{av^2E_\mu}{E_\mu^2+a^2}\mathrm{cotanh}\left(\frac{\pi a}{\Delta}\right)\right]^2\Bigg\}^{-1}.\end{aligned} \tag{68}$$

Similarly, the analogues of (59)-(61) are found to be

$$\Pi(\omega)-\mathrm{i}\Gamma(\omega)=\frac{\pi a}{\Delta}v^2\frac{1}{\omega+\mathrm{i}a} \qquad \text{for } v\gg\Delta \tag{69}$$

$$\begin{aligned}\langle\Psi(0)|\Psi(t)\rangle &= \frac{v^2}{a^2}\int_{-\infty}^{+\infty}\mathrm{d}\omega\,\exp(-\mathrm{i}\omega t)\,\frac{a^2}{a^2+\omega^2}\\ &\quad\times\frac{1}{[\omega-E_s^{(0)}-(\pi a/\Delta)v^2(\omega+\mathrm{i}a)^{-1}][\omega-E_s^{(0)}-(\pi a/\Delta)v^2(\omega-\mathrm{i}a)^{-1}]}\\ &= \frac{v^2}{a^2}\int_{-\infty}^{+\infty}\mathrm{d}\omega\,\exp(-\mathrm{i}\omega t)\\ &\quad\times\frac{a^2}{[(\omega-E_s^{(0)})(\omega+\mathrm{i}a)-(\pi a/\Delta)v^2][(\omega-E_s^{(0)})(\omega-\mathrm{i}a)-(\pi a/\Delta)v^2]}\\ &\quad\text{for } v\gg\Delta.\end{aligned} \tag{70}$$

The two expressions (68) and (70) coincide again under the premise $(v/\Delta)\gg 1$, if $\operatorname{cotanh}(\pi a/\Delta)\approx 1$ is taken. We note that the integrand is no longer of a simple Lorentzian form. Rather, there is now a competition of two decay channels, which are given by the four poles of the integrand

$$\omega_{1/2}=\tfrac{1}{2}(E_s^{(0)}-\mathrm{i}a)\pm\frac{1}{2}\left((E_s^{(0)}+\mathrm{i}a)^2+\frac{4\pi a}{\Delta}v^2\right)^{1/2} \tag{71a}$$

and

$$\omega_{3,4}=(\omega_{1,2})^*=\tfrac{1}{2}(E_s^{(0)}+\mathrm{i}a)\pm\frac{1}{2}\left((E_s^{(0)}-\mathrm{i}a)^2+\frac{4\pi a}{\Delta}v^2\right)^{1/2}. \tag{71b}$$

For $|E_s^{(0)}+\mathrm{i}a|^2\gg(4\pi a v^2/\Delta)$ we find

$$\begin{aligned}\langle\Psi(0)|\Psi(t)\rangle &= \left[1-\left(\frac{\pi a v^2}{\Delta}\right)\frac{1}{(E_s^{(0)}+\mathrm{i}a)^2}\right]\\ &\quad\times\exp\left[-\mathrm{i}E_s^{(0)}\left(1+\frac{\pi a v^2}{\Delta}\frac{1}{E_s^{(0)2}+a^2}\right)t-\frac{\pi v^2}{\Delta}\frac{a^2}{E_s^{(0)2}+a^2}t\right]\\ &\quad+\frac{\pi a v^2}{\Delta}\frac{1}{(E_s^{(0)}+\mathrm{i}a)^2}\exp\left[\mathrm{i}E_s^{(0)}\frac{\pi a v^2}{\Delta}\frac{1}{E_s^{(0)2}+a^2}t\right.\\ &\quad\left.-a\left(1-\frac{\pi a v^2}{\Delta}\frac{a}{E_s^{(0)2}+a^2}\right)t\right]\end{aligned} \tag{72}$$

which merges into the BJ result for $a\to\infty$. On the other hand, for $|E^{(0)}+\mathrm{i}a|^2\ll(4\pi a v^2/\Delta)$ the result is

$$\langle\Psi(0)|\Psi(t)\rangle=\cos\left[\left(\frac{\pi a v^2}{\Delta}\right)^{1/2}t\right]\exp\left(-\tfrac{1}{2}\mathrm{i}E_s^{(0)}t-\tfrac{1}{2}at\right) \tag{73}$$

which is the opposite extremal case. This result displays a rather remarkable feature. The coupling strength v, which conventionally dominates the decay constant, has now lost this influence, but establishes a monochromatic modulation of the decay. The decay constant now is given by the spectral breadth a of the coupling function.

6. Lifshitz decay

We use the term 'Lifshitz decay' in analogy to a notation in disturbed lattice dynamics (see, e.g., Maradudin *et al* 1971) where a Lifshitz problem is one for which only a singular degree of freedom is involved in the disturbed Hamiltonian. Similarly, we characterise the quantum Lifshitz problem as one where the disturbance can be characterised by a single base vector $|r\rangle$ in Hilbert space and we assume that $|r\rangle$ is a number of the complete ON set $\{|j\rangle\}$, onto which the Hamiltonian is projected:

$$H=\sum_{jk} H_{jk}^{(0)}|j\rangle\langle k| + V|r\rangle\langle r|. \tag{74}$$

The eigenvectors $|\varphi^{(0)}\rangle$ of $H^{(0)}$ are assumed to be known:

$$H^{(0)}|\varphi_\mu^{(0)}\rangle = E_\mu^{(0)}|\varphi_\mu^{(0)}\rangle \tag{75}$$

such that the zero-order Green function is known:

$$G_{jk}^{(0)}(E)=\frac{1}{2\pi}\sum_\mu \frac{\langle j|\varphi_\mu^{(0)}\rangle\langle\varphi_\mu^{(0)}|k\rangle}{E-E_\mu^{(0)}} \qquad E=\omega\pm \mathrm{i}\varepsilon \tag{76}$$

(see (14*b*)). The equation of motion (15) may then be partially inverted (multiplication by $2\pi G^{(0)}$ from the left) to become

$$G_{jk}(E)=G_{jk}^{(0)}(E)+2\pi V G_{jr}^{(0)}(E)G_{rk}(E) \tag{77}$$

which has the solution

$$G_{rk}(E)=G_{rk}^{(0)}(E)[1-2\pi V G_{rr}^{(0)}(E)]^{-1} \tag{78}$$

$$G_{jk}(E)=G_{jk}^{(0)}(E)+2\pi V G_{jr}^{(0)}(E)G_{rk}^{(0)}(E)[1-2\pi V G_{rr}^{(0)}(E)]^{-1} \qquad \text{for } j\neq r \tag{79}$$

and specifically

$$G_{rr}(E)=G_{rr}^{(0)}(E)[1-2\pi V G_{rr}^{(0)}(E)]^{-1}. \tag{80}$$

The preceding solution technique is intimately related to the one invented in the old sequence of Lifshitz papers (Lifshitz 1947, 1956).

The Green functions being known, again by way of (10) and (11), all decay situations can be calculated. In particular we may consider the evolution of the initial state

$$|\Psi(0)\rangle=|r\rangle \tag{81}$$

for which, by means of (11*a*), (76) and (79), we get

$$\begin{aligned}\langle\Psi(0)|\Psi(t)\rangle &= \mathrm{i}\int_{-\infty}^{\infty} \mathrm{d}\omega\ \exp(-\mathrm{i}\omega t)[G_{rr}(\omega+\mathrm{i}\varepsilon)-G_{rr}(\omega-\mathrm{i}\varepsilon)] \\ &= \mathrm{i}\int_{-\infty}^{\infty} \mathrm{d}\omega\ \exp(-\mathrm{i}\omega t)\{G_{rr}^{(0)}(\omega+\mathrm{i}\varepsilon)[1-2\pi V G_{rr}(\omega+\mathrm{i}\varepsilon)]^{-1}-\mathrm{cc}\}.\end{aligned} \tag{82}$$

7. Excitonic dissipation

To illustrate the Lifshitz type of decay problem we consider a chain $\{j\}$ of excitonic states $\{|j\rangle\}$, $j=0, \pm 1, \ldots, \pm N/2$, with periodic boundary conditions, $j+N\equiv j$, and assume the chain to be disturbed at site $j=0$:

$$H=-\tfrac{1}{2}\sum_{j=-N/2}^{+N/2} T_\delta(|j\rangle\langle j+\delta|+\text{HC})+V|0\rangle\langle 0| \tag{83}$$

where $\delta(=1,2,\ldots,g)$ denotes the g neighbour sites of j. The undisturbed part of H is diagonalised by a Bloch ansatz:

$$|\varphi^{(0)}\rangle=N^{-1/2}\sum_j \exp\left(\mathrm{i}\frac{2\pi}{N}kj\right)|j\rangle \qquad k=0,\pm 1,\ldots,\pm N/2 \tag{84}$$

and the undisturbed eigenvalues $E_k^{(0)}$ are given by

$$E_k^{(0)}=-\sum_\delta T_\delta \cos\left(\frac{2\pi}{N}k\delta\right). \tag{85}$$

By (76) we then find

$$G_{00}^{(0)}\equiv\frac{1}{2\pi}\sum_k\frac{\langle 0|\varphi_k^{(0)}\rangle\langle\varphi_k^{(0)}|0\rangle}{E-E_k^{(0)}}=\frac{1}{2\pi N}\sum_k\frac{1}{E-E_k^{(0)}}. \tag{86}$$

Assuming now that initially the exciton at site $j=0$ is created, $\Psi(0)=|0\rangle$, (82) becomes

$$\langle\Psi(0)|\Psi(t)\rangle=\mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\exp(-\mathrm{i}\omega t)\{G_{00}^{(0)}(\omega+\mathrm{i}\varepsilon)[1-2\pi VG_{00}^{(0)}(\omega+\mathrm{i}\varepsilon)]^{-1}-\text{CC}\} \tag{87}$$

for the evolution at $t>0$. The sequence of eigenvalues $E_k^{(0)}$ (see (85)) are densely spaced and cover a region $R\equiv\{E_{\min}^{(0)}, E_{\max}^{(0)}\}$. It is crucial to take notice of this fact when calculating $G_{00}^{(0)}(\omega+\mathrm{i}\varepsilon)$. If ω is located in the region R, we may apply the Plemelj formula $(x\pm\mathrm{i}\varepsilon)^{-1}=P(1/x)\mp\mathrm{i}\pi\delta(x)$ by way of the dense distribution of $E_k^{(0)}$ values ($N\gg 1$). However, outside this region the Plemelj formula no longer applies since all $(\omega-E_k^{(0)})$ values are finite, and therefore we have to keep ε in its place. We therefore write

$$G_{00}^{(0)}(\omega\pm\mathrm{i}\varepsilon)=A(\omega)\mp\mathrm{i}B(\omega) \qquad \text{for } \omega\in R \tag{88a}$$

$$=C(\omega)\mp\mathrm{i}\varepsilon D(\omega) \qquad \text{for } \omega\notin R \tag{88b}$$

where

$$A(\omega)=\frac{1}{2\pi N}P\sum_k\frac{1}{\omega-E_k^{(0)}} \qquad (\omega\in R) \tag{89}$$

$$B(\omega)=\frac{1}{2N}\sum_k\delta(\omega-E_k^{(0)}) \qquad (\omega\in R) \tag{90}$$

$$C(\omega)=\frac{1}{2\pi N}\sum_k\frac{1}{\omega-E_k^{(0)}} \qquad (\omega\notin R) \tag{91}$$

$$D(\omega)=\frac{1}{2\pi N}\sum_k\frac{1}{(\omega-E_k^{(0)})^2}=-\frac{\mathrm{d}}{\mathrm{d}\omega}C(\omega) \qquad (\omega\notin R). \tag{92}$$

Inserting (89)-(92) in (87) we have

$$\langle\Psi(0)|\Psi(t)\rangle = \mathrm{i}\int_{\omega\in R} \mathrm{d}\omega\, \exp(-\mathrm{i}\omega t)$$
$$\times\left(\frac{A(\omega)-\mathrm{i}B(\omega)}{1-2\pi V[A(\omega)-\mathrm{i}B(\omega)]}-\frac{A(\omega)+\mathrm{i}B(\omega)}{1-2\pi V[A(\omega)+\mathrm{i}B(\omega)]}\right)$$
$$+\mathrm{i}\int_{\omega\notin R} \mathrm{d}\omega\, \exp(-\mathrm{i}\omega t)$$
$$\times\left(\frac{C(\omega)-\mathrm{i}\varepsilon D(\omega)}{1-2\pi V[C(\omega)-\mathrm{i}\varepsilon D(\omega)]}-\frac{C(\omega)+\mathrm{i}\varepsilon D(\omega)}{1-2\pi V[C(\omega)+\mathrm{i}\varepsilon D(\omega)]}\right)$$
$$=2\int_{\omega\in R} \mathrm{d}\omega\, \exp(-\mathrm{i}\omega t)\frac{B(\omega)}{[1-2\pi VA(\omega)]^2+(2\pi VB(\omega))^2}$$
$$+2\int_{\omega\notin R} \mathrm{d}\omega\, \exp(-\mathrm{i}\omega t)\frac{\varepsilon D(\omega)}{[1-2\pi VC(\omega)]^2+(2\pi VD(\omega))^2\varepsilon^2}. \tag{93}$$

Now for $\varepsilon \to 0_+$ the integral over the region ($\omega \notin R$) remains finite only if $1-2\pi VC(\omega) = 0$ has a solution $\omega_s \notin R$:

$$1-2\pi VC(\omega_s)=0 \qquad \omega_s \notin R. \tag{94}$$

Then we may expand $C(\omega)$ around ω_s and find

$$1-2\pi VC(\omega)$$
$$=-2\pi V\left(\frac{\mathrm{d}C}{\mathrm{d}\omega}\right)_{\omega=\omega_s}(\omega-\omega_s)+\mathrm{O}((\omega-\omega_s)^2) \qquad \omega_s\notin R \tag{95}$$

and since (see (92) $D=-\mathrm{d}C/\mathrm{d}\omega$, the last integral of (93) transmutes into the form

$$-2\varepsilon\int_{\omega\notin R} \mathrm{d}\omega\, \exp(-\mathrm{i}\omega t)\frac{D(\omega)}{[1-2\pi VC(\omega)]^2+\varepsilon^2(2\pi VD(\omega))^2}$$
$$=-\frac{1}{2\pi V^2(\mathrm{d}C/\mathrm{d}\omega)_{\omega_s}}\int_{\omega\notin R} \mathrm{d}\omega\, \exp(-\mathrm{i}\omega t)\frac{(\varepsilon/\pi)}{(\omega-\omega_s)^2+\varepsilon^2}$$
$$=-\left[2\pi V^2\left(\frac{\mathrm{d}C}{\mathrm{d}\omega}\right)_{\omega_s}\right]^{-1}\exp(-\mathrm{i}\omega_s t) \tag{96}$$

where $\delta(x)=\varepsilon/\pi(x^2+\varepsilon^2)$ has been used. Upon inserting in (93) we finally have

$$\langle\Psi(0)|\Psi(t)\rangle = 2\int_{\omega\in R} \mathrm{d}\omega\, \exp(-\mathrm{i}\omega t)\frac{B(\omega)}{[1-2\pi VA(\omega)]^2+(2\pi VB(\omega))^2}$$
$$-\left[2\pi V^2\left(\frac{\mathrm{d}C}{\mathrm{d}\omega}\right)_{\omega=\omega_s}\right]^{-1}\exp(-\mathrm{i}\omega_s t) \qquad \omega_s\notin R. \tag{97}$$

Hence, by way of the last term, the decay will be incomplete if a singular state $E=\omega_s$ shows up outside R. Expression (97) still constitutes an exact result, and explicit final computations can be administered if the functions $A(\omega)$, $B(\omega)$ and $C(\omega)$ are known. In this manner the decay problem has reached its most economic formulation. In this formulation the feasibility of approximations is particularly lucid. We show this by giving a simple example. From (85) we observe that $E_k^{(0)}$ is an even distribution in

$k(E^{(0)}_{-k}=E^{(0)}_k)$. This implies that $A(\omega)$ and $C(\omega)$ (see (89) and (90)) are odd and $B(\omega)$ and $D(\omega)$ (see (91) and (92)) are even functions of ω. For $\omega \in R \equiv \{-\omega_0, \omega_0\}$ we therefore make the crudest possible approximation $A(\omega)=\omega/2\pi\omega_0^2$, $B(\omega)=(4\omega_0)^{-1}$ and for $\omega \notin R$:

$$C(\omega) = -(1/4\pi\omega_0)\ln\left(\frac{|1-\omega_0/\omega|}{|1+\omega_0/\omega|}\right) \qquad D(\omega) = -\frac{\mathrm{d}C}{\mathrm{d}\omega} = -(1/2\pi)(\omega^2-\omega_0^2)^{-1}.$$

This approximation is somewhat appropriate for $\omega_0 \gg V > 0$. The solution of (95) is then $\omega_s = \omega_0[1+2\exp(-1/2\pi V)]$ and the decay is given by

$$\begin{aligned}
\langle\Psi(0)|\Psi(t)\rangle &= \frac{1}{2\omega_0}\int_{-\omega_0}^{\omega_0}\mathrm{d}\omega\,\frac{\exp(-\mathrm{i}\omega t)}{(1-V\omega/\omega_0^2)^2+(\pi V/2\omega_0)^2} \\
&\quad + \left(\frac{V^2}{2\omega_0^2}\exp(2\omega_0/V)\right)^{-1}\exp(-\mathrm{i}\omega_s t) \\
&= \frac{1}{\omega_0}\frac{\sin\omega_0 t}{t} + \mathrm{i}\,\frac{2V}{\omega_0^3}\left(\frac{\omega_0\cos\omega_0 t}{t} - \frac{\sin\omega_0 t}{t^2}\right) \\
&\quad + \left(\frac{2\omega_0}{V}\right)^2[1+\exp(-\tfrac{1}{2}\pi V)]\exp(-1/2\pi V)\exp(-\mathrm{i}\omega_s t).
\end{aligned} \tag{98}$$

On the other hand, the decay setup given by the Hamiltonian (83) makes it very suggestive to have a look at the oldest microscopic decay law of physics which was found by Hamilton (1839) in the course of investigating the dynamics of a chain of coupled oscillators. This problem is a kind of classical analogue to the excitonic chain considered here. If we only allow for a nearest-neighbour transfer coupling in (85), $\delta = \pm 1$, $T_\delta \equiv T$, we find

$$E^{(0)}_k = -T\cos\frac{2\pi}{N}k \qquad k = 0, \pm 1, \ldots, \pm N/2. \tag{99}$$

The Fourier transform of the undisturbed GF (86) is then

$$\begin{aligned}
G^{(0)}_{00}(t) &= \mp\frac{\mathrm{i}}{N}\Theta(\pm t)\sum_{k=-N/2}^{N/2}\exp(-\mathrm{i}E^{(0)}_k t) \\
&= \mp\frac{\mathrm{i}}{2\pi}\Theta(\pm t)\int_{-\pi}^{+\pi}\mathrm{d}x\,\exp(\mathrm{i}Tt\cos x)
\end{aligned} \tag{100}$$

where the summation of $\{k\}$ has been transmuted into an integral (N large). Involving the definition of Bessel function $J_0(z)$ (see, e.g., Gradshteyn and Ryzhik 1965, p 953) we arrive at

$$G^{(0)}_{00}(t) = \mp\mathrm{i}\Theta(\pm t)J_0(Tt). \tag{101}$$

For $V=0$ we therefore get from (82)

$$\langle\Psi(0)|\Psi(t)\rangle = J_0(Tt). \tag{102}$$

It is this result which corresponds to the one of Hamilton (1839), Havelock (1910) and Schrödinger (1914). As regards the disturbed problem ($V \neq 0$) itself the Fourier transform of (101) becomes effective:

$$
\begin{aligned}
G_{00}^{(0)}(\omega \pm \mathrm{i}\varepsilon) &= \int_{-\infty}^{\infty} \frac{\mathrm{d}t}{2\pi} G_{00}^{(0)}(t) \exp(\mathrm{i}\omega t) \\
&= \mp \frac{\mathrm{i}}{2\pi} \frac{1}{(T^2-\omega^2)^{1/2}} \qquad \text{for } T^2 > \omega^2 > 0,\ \omega \gtrless 0 \\
&= \pm \frac{1}{2\pi} \frac{1}{(\omega^2-T^2)^{1/2}} \qquad \text{for } \omega^2 > T^2 > 0,\ \omega \gtrless 0
\end{aligned} \tag{103}
$$

(see Gradshteyn and Ryzhik 1965, p 731) from which, by (89) and (90),

$$
A(\omega) = \pm \frac{1}{2\pi} \frac{1}{(\omega^2-T^2)^{1/2}} \qquad \text{for } \omega^2 > T^2 > 0,\ \omega \gtrless 0 \tag{104}
$$

$$
B(\omega) = \frac{1}{2\pi} \frac{1}{(T^2-\omega^2)^{1/2}} \qquad \text{for } \omega^2 < T^2 > 0 \tag{105}
$$

whereas $A(\omega)=0$ for ω in $(-T, T)$ and $B(\omega)=0$ for ω outside $(-T, T)$. Then (95) yields the singular solution

$$
\omega_s = \pm (T^2+V^2)^{1/2} \qquad \text{for } V \gtrless 0 \tag{106}
$$

and

$$
\left(\frac{\mathrm{d}C}{\mathrm{d}\omega}\right)_{\omega=\omega_s} = \mp \frac{(T^2+V^2)^{1/2}}{2\pi V^3} \qquad \text{for } V \gtrless 0. \tag{107}
$$

Hence (see (97)), the decay law is of the form

$$
\begin{aligned}
\langle \Psi(0) | \Psi(t) \rangle &= \frac{1}{\pi} \int_{-T}^{+T} \mathrm{d}\omega \frac{(T^2-\omega^2)^{1/2}}{T^2-\omega^2+(2\pi V)^2} \exp(-\mathrm{i}\omega t) \\
&\quad \pm \frac{V}{(T^2+V^2)^{1/2}} \exp[\pm \mathrm{i}(T^2+V^2)^{1/2} t] \qquad \text{for } V \gtrless 0.
\end{aligned} \tag{108}
$$

8. Summary and further perspectives

We have presented a Green function method by means of which quantum decay functions can be written in the form of decay integrals. They do not require the full solution of the eigenvalue problem, provided the equation of motion for the Green function is solved. We have explicitly derived the decay formulae for Fano and Lifshitz decay arrangements. In particular the decay integral for the Fano case applies to any arbitrary coupling function and is of practical utility for an analytical discussion of specific coupling scenarios.

We have done this analysis for the Bixon–Jortner model and generalisations thereof. We have regained the BJ result itself, as well as the explicit decay law for a modified BJ model, where the coupling strength $V(E)$ is peaked at the same energy and has a spectral distribution characterised by a breadth. The novel feature of the latter decay problem is the fact that the decay function now displays two channels, one of which may be denoted as the 'Bixon–Jortner' channel, showing a golden-rule type of behaviour, and another one, where the coupling strength no longer denominates the decay constant but establishes a monochromatic modulation of the decay constant, whereas the decay constant is given by the breadth of the coupling function. Depending on the intrinsic model parameters, either of the two channels may adopt the primary role.

If the quasicontinuous region of the energy distribution is bounded, there may be non-decaying monochromatic contributions both in the Fano and Lifshitz scenarios ('localised states'). The amplitude and the frequency of these contributions is also handled within our GF treatment without the need to calculate the localised eigenvectors. The specific novel feature in this model disposition is the existence of a critical coupling strength α_c which marks the 'crossover' from complete to incomplete decay. This phenomenon is accompanied by modifications in the damping features of the decaying part.

The presented method seems to have applicability in several physical problems, such as quantum diffusion and the analysis of non-radiative decay. This will be described elsewhere.

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