Physique statistique, thermodynamique/Statistical physics, thermodynamics

## **Electronically induced nuclear transitions – temperature dependence and Rabi oscillations**

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Abstract This paper deals with a nucleus electromagnetically coupled with the bound states of its electronic surroundings. It describes the temperature dependence of its dynamics and the onset of potential Rabi oscillations by means of a Master Equation. The latter is generalized in order to account for possible strong resonances. Throughout the paper the approximation schemes are discussed and tested. *To cite this article: J.-J. Niez, C. R. Physique 3 (2002)* 1255–1261.

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electromagnetic decay / nuclear physics / quantum statistical mechanics

# Transitions nucleaires induites par le cortège électronique – dépendance en température et oscillations de Rabi

Résumé On s'intéresse ici à un système nucléaire couplé électromagnétiquement aux états liés de son environnement électronique. On décrit, en fonction de la température, sa dynamique et le début d'éventuelles oscillations de Rabi en utilisant une équation maîtresse issue d'une technique de projection. On montre comment généraliser l'approche précédente dans le cas de résonances fortes. Tout au long du papier les schémas d'approximation sont discutés et testés. *Pour citer cet article : J.-J. Niez, C. R. Physique 3 (2002) 1255–1261.* © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

décroissance électromagnétique / physique nucléaire / mécanique statistique quantique

### Version française abrégée

Dans de récentes publications [1,2] il a été proposé qu'une transition électronique entre états liés pouvait être le processus dominant la décroissance électromagnétique de l'état excité du noyau <sup>125</sup>Te\* ( $\hbar\omega_N = 35.5$  keV) d'un ion Tellure très fortement ionisé. C'est l'effet BIC (Bound Internal Conversion). Par ailleurs l'examen [3] de l'excitation de l'état isomérique <sup>235m</sup>U ( $\hbar\omega_N = 76.8$  eV) de l'Uranium dans un plasma ( $T \sim 20-100$  eV) semble, lui aussi, relever de la même origine. Les situations envisagées impliquant l'apparition d'éventuelles résonances de Rabi *dans un contexte thermodynamique*, il est apparu nécessaire de traiter l'évolution dynamique d'un petit système, dont on peut isoler deux états pertinents *e* et *g* ( $\omega_{eg} \equiv \omega_N$ ), en contact avec un réservoir à température *T* pouvant présenter des résonances proches de  $\omega_N$ .

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Pour ce faire, on écrit l'équation d'évolution (1) de la matrice densité  $\sigma(t)$  du petit système dans l'espace de Liouville, le superopérateur L (agissant dans l'espace des opérateurs standards de la Mécanique Quantique et défini par  $L * \cdot \equiv \frac{1}{h}[H, \cdot]$ ) gouvernant la dynamique. Ce dernier contient la dynamique  $L_N$  du noyau (habillé du champ statique moyen induit par le réservoir), la dynamique  $L_R$  du réservoir (dont les états propres sont notés  $\mu$ ,  $\nu$ ), et l'interaction  $L_{RN}$  (privée du champ moyen). Focalisant l'analyse sur les éléments diagonaux de  $\sigma(t)$ , qui représentent les populations des états nucléaires, ceux-ci sont extraits par une technique de projecteurs ((2)–(6)), et on obtient l'équation (7) ci dessous, avec dans le cas particulier d'un système à deux états (a, b) = (e, g). Dans les noyaux  $K_a^b(\omega)$  qui la caractérisent on note  $|\nu a\rangle$  l'opérateur (ket  $\otimes$  bra) $|\nu a\rangle\langle\nu a|$  et, le produit scalaire utilisé étant défini par (2), le superopérateur  $\Pi_D$  est un projecteur sur l'espace vectoriel sous-tendu par  $\sum_{\mu} |\mu e\rangle\langle\mu e| \oplus \sum_{\mu} |\mu g\rangle\langle\mu g|$ . Cette équation (7), exacte car déduite de seules manipulations algébriques, ne contient rien de plus que l'équation de Liouville dont elle est issue. Aussi les noyaux  $K_a^b(\omega)$  sont-ils inaccessibles hors d'un schéma d'approximations qui se doit bien sûr d'être testé. Pour ce faire on se donne trois contraintes fortes que les résultats obtenus doivent vérifier, à savoir :

- (a) positivité des populations, soit  $\sigma_e(t)$ ,  $\sigma_g(t) > 0$ ,
- (b) conservation de la norme, soit  $\sigma_e(t) + \sigma_g(t) = 1$ ,
- (c) thermalisation du système aux temps longs, soit  $\sigma_e(t \to \infty)/\sigma_g(t \to \infty) = \exp(-\beta \hbar \omega_N)$ , avec  $\beta = 1/kT$ .

Le calcul des noyaux  $K_a^b(\omega)$  conduit naturellement à faire l'approximation qui consiste à ne retenir dans leur dynamique que la partie  $L_0 \equiv L_N + L_R$  (négligeant  $L_{RN}$ ). On montre dans l'article que la pertinence de cette approximation repose sur l'analyse de l'espace vectoriel W des opérateurs (ket  $\otimes$  bra) $|\mu a\rangle\langle vb|$ pour lesquels est réalisée la condition  $||L_0 * |\mu a\rangle\langle vb|| \le 0$ , et ce *pour une forte densité d'états*  $\mu$  et v. Si le superopérateur  $1 - \Pi_D$  projette en dehors de cet espace W, alors l'approximation est licite. Sinon il faut modifier  $\Pi_D$  de telle sorte que son espace de projection recouvre l'intégralité de W. Ceci conduit bien sûr à augmenter le nombre des variables à traiter explicitement.

Ces considérations sont illustrées par l'analyse de l'effet BIC. Dans ce cas, si on écrit l'équation (7) pour les populations, en lui adjoignant l'approximation proposée, il apparaît que l'on perd la contrainte (a) lorsque l'on se rapproche d'une résonance entre états nucléaires et états électroniques. On redéfinit donc le réservoir en particularisant les deux états électroniques liés (1, 2) pertinents (avec  $\omega_{21} \simeq \omega_N$ ), lesquels sont regardés comme en contact avec un bain à température *T*, le nouveau réservoir (dont les états propres sont maintenant notés  $\mu_R$ ). Ici l'espace W est formé des 4 opérateurs de forme générique  $|\mu_R \alpha a\rangle \langle \mu_R \alpha a|$ , avec  $\alpha = (1, 2)$  et a = (e, g), auxquels il faut ajouter, puisque  $\omega_{21} \simeq \omega_N$ , les 2 opérateurs  $|\mu_R 2g\rangle \langle \mu_R 1e|$  et  $|\mu_R 1e\rangle \langle \mu_R 2g|$ . On est ainsi conduit à définir un nouveau jeu de 6 variables (cf. équation (11)), duquel on peut extraire linéairement la matrice densité du système nucléaire cherchée.

On montre que les contraintes imposées sont vérifiées, et on met en évidence les fréquences de Rabi du système (13), et leur variation au premier ordre en  $e^{-\beta\hbar\omega_N}$  (14). Notons pour finir que les calculs permettant d'arriver à ces résultats ne sont qu'esquissés dans la note, seul le principe est présenté.

In recent papers [1,2] it has been proposed that the excited state <sup>125</sup>Te\* ( $\hbar\omega_N = 35.5$  keV) of the nucleus of a highly ionized (stripped) ion of Tellurium can decay through an electronic excitation between two bound states of the atomic cloud. This is the so-called Bound Internal Conversion (BIC) effect. Moreover, although the experimental data are sparse, the analysis [3] of the Nuclear Excitation of <sup>235</sup>U into its isomeric state <sup>235m</sup>U ( $\hbar\omega_N = 76.8$  eV) in a plasma ( $T \sim 20-100$  eV) points also to a process induced by an Electronic Transition between two atomic bound states, an example of the so called NEET effect (the inverse of the BIC effect). It turns out that the theoretical estimates given in these papers rely on the Fermi Golden Rule [4]; consequently they may be questionable when the aforementioned transitions are near a

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resonance, or when the temperature of the surroundings becomes of the order of the transition frequency. Since these situations are met in the quoted works [1-3], we sketch here a more appropriate description of these effects in order to improve further estimates. To simplify we restrict the presentation to the BIC effect.

Addressing this problem let us first derive a dynamic equation for the density matrix,  $\sigma(t)$ , of the nucleus. Since in the treatment of the BIC effect the low frequency range of the dynamics is the only one which is of relevance, and since the off-diagonal elements of  $\sigma(t)$  have essentially a high frequency behavior, we will focus on the diagonal elements of  $\sigma(t)$ , the so-called populations  $\sigma_a(t)$ . Let us stress that any attempt aiming to reach these populations must satisfy the following three constraints:

- (a) the positivity of the density matrix,  $\forall a, \sigma_a(t) > 0$ ;
- (b) the normalization of the density,  $\sum_{a} \sigma_{a}(t) = 1$ ;
- (c) the nuclear long time thermalization condition with the reservoir,  $\sigma_a(t \to \infty)/\sigma_b(t \to \infty) = \exp(-\beta\hbar\omega_{ab})$ , with  $\beta = 1/kT$ .

As a consequence these three conditions will serve as validity tests for the approximations which will be proposed in the paper.

To be specific, let us consider the simple situation where only two nuclear eigenstates (e, g) are involved, their transition frequency (greater than the expected transition rate) being  $\omega_{eg} \equiv \omega_N > 0$ . We then call  $h_N^0$  the Hamiltonian of the nucleus,  $h_R$  the Hamiltonian of the reservoir, and  $h_{RN}^0$  the electromagnetic coupling between them, the latter having its standard form [5] including Coulomb and transverse couplings. Furthermore, at time t = 0, the bath is supposed to be described by the thermodynamical equilibrium density matrix  $D_R^0 = \sum_{\mu} p_{\mu} |\mu\rangle \langle \mu|$ , ' $\mu$ ' labelling the bath eigenstates. Dressing  $h_N^0$  with the effective static mean field induced by the reservoir on the nucleus, we define a new Hamiltonian for the nucleus, namely  $h_N \equiv$  $h_N^0 + \text{Tr}_R \{D_R^0 h_{RN}^0\}$ , where the notation  $\text{Tr}_R$  stands for the trace over the states of the reservoir. Meanwhile the coupling term must be redefined such that  $h_{RN} \equiv h_{RN}^0 - \text{Tr}_R \{D_R^0 h_{RN}^0\}$ , thus  $\text{Tr}_R \{D_R^0 h_{RN}^0\} = 0$ .

If D(t) is the density matrix of the whole system, the density matrix of the nucleus is given [6] by

$$\sigma(t) = \operatorname{Tr}_{R} \left\{ D(t) \right\},\tag{1}$$

where the time evolution of D(t) can be written  $D(t) = e^{iLt} * \{D_R^0 \otimes \sigma(0)\}$ , *L* standing for the Liouville superoperator [7] associated with the total Hamiltonian  $H \equiv h_N + h_R + h_{RN}$ . In this algebraic framework, *L* operates on a space  $\mathcal{V}$  of vectors which are the direct product of a ket and a bra. If *a* and *a'* are nuclear eigenstates, the corresponding vectors read  $|\mu a\rangle\langle \mu' a'|$ , and  $L * |\mu a\rangle\langle \mu' a'| \equiv \frac{1}{h}[H, |\mu a\rangle\langle \mu' a'|]$ . In the following we write  $|\mu a\rangle\langle \mu' a'| \equiv |\mu a, \mu' a'\rangle$ , or  $|\mu a\rangle$  whenever  $(\mu, a) = (\mu', a')$ . Let us now define on  $\mathcal{V}$  the Hermitian product

$$(A|B) \equiv \operatorname{Tr}\{(D_{0R} \otimes I_N) A^+ B\},\tag{2}$$

where  $I_N$  is the unit density matrix in the space of the nuclear states. Then, using Eqs. (1) and (2), the populations of  $\sigma(t)$ , can be written:

$$\sigma_a(t) = \sum_{\mu\nu}^b \sigma_b \left( \mu b | \theta(t) \, \mathrm{e}^{\mathrm{i}Lt} * |\nu a \right),\tag{3}$$

the initial condition being characterized by  $\sigma_{aa'}(t=0) = \delta_{aa'}\sigma_a$ .

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The above formulation suggests the introduction of a set of projection superoperators, acting on  $\mathcal{V}$ , according to  $\Pi_a = \sum_{\mu\mu'} |\mu'a\rangle(\mu a|$ . It is an easy task to check that  $\Pi_a$  is indeed a projection such that  $\Pi_a \Pi_{a'} = \delta_{aa'} \Pi_a$  and that one has

$$[L_0, \Pi_a] = 0, \quad \text{and} \quad \Pi_{a'} L_{RN} \Pi_a = 0, \tag{4}$$

where  $L_0$  and  $L_{RN}$  are the Liouville operators associated with  $h_N + h_R$  and  $h_{RN}$ , respectively.

Aiming to write a Master Equation for  $\sigma(t)$ , one now uses the trivial equality

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma_a(t) - \delta(t)\sigma_a - \theta(t)\sum_{\mu\nu}^b \sigma_b\left(\mu b | \mathrm{e}^{\mathrm{i}Lt}\Pi_a \mathrm{i}L * |\nu a\right) = \theta(t)\sum_{\mu\nu}^b \sigma_b\left(\mu b | \mathrm{e}^{\mathrm{i}Lt}(1 - \Pi_a) \mathrm{i}L * |\nu a\right), \quad (5)$$

then, in the right-hand side of (5), the easily stated relation

$$e^{iLt} = e^{i(1-\Pi_D)Lt} + \int_0^t ds \, e^{iL(t-s)} \Pi_D \, iL \, e^{i(1-\Pi_D)Ls},\tag{6}$$

where  $\Pi_D$  is a new projection. If one now chooses  $\Pi_D = \sum_a \Pi_a$ , one gets a *complete set of equations* which read in the frequency domain ( $\omega_+ = \omega + i0$ ):

$$\omega_{+} \sigma_{a}(\omega) - \mathrm{i}\sigma_{a} = \sum_{b} K_{a}^{b}(\omega)\sigma_{b}(\omega), \qquad (7)$$

where the kernels  $K_a^b(\omega)$  are given by  $K_a^b(\omega) = \sum_{\mu\nu} \left( \mu b \left| L_{RN} \frac{1}{\omega_+ + (1 - \Pi_D)(L_0 + L_{RN})(1 - \Pi_D)} L_{RN} * \right| \nu a \right).$ 

Being established along the procedure used for standard Quantum Langevin Equations [8,9], Eqs. (7) are rigorous, and bear a formal similarity with the theory of irreversible processes [10,11]. In (7) the kernels  $K_a^b(\omega)$  carry all the coupling between the nucleus and the bath. Being memory terms in the time domain, they are at least of second order in  $h_{RN}$ , as expected  $(h_N^0 \rightarrow h_N)$ . Note the presence inside these kernels of an implicit  $1 - \sum_a \prod_a$  operator on each side of the 'Green's operator' (see (4)). Thus, when like in (7)  $\prod_D = \sum_a \prod_a$ , the latter must be calculated on the space  $\mathcal{E}(1 - \prod_D) \equiv (1 - \prod_D)\mathcal{V}$ .

Although Eqs. (7) are the cornerstone of what follows they cannot be used as such, and one needs to make an approximation to evaluate the kernels  $K_a^b(\omega)$ . Calling it ' $L_0$  approximation', we here decide to replace  $L_0 + L_{RN}$  by  $L_0$  in the calculation of the 'Green's operator', the dynamics of the new kernels,  $\tilde{K}_a^b(t)$ , being now ruled by  $L_0$  [6,9]. But it turns out that this approximation must be handled with care. And, for example, in the case of the BIC effect it would fail if a strong resonance is present, since one then encounters a *violation of the constraint* (a). This occurs when the width  $\eta$  of the electronic resonance is smaller than the square root of the nuclear-electronic coupling, *and* if the offset of resonance between the electronic and the nuclear lines is smaller than  $\eta$  (see below).

However, in the framework of the BIC effect, this last pathological situation rarely occurs. Thus, in the majority of the physical situations all three constraints are fulfilled and one can describe, through the solution of the system (7), the dynamics of  $\sigma_e(t)$  using the explicit  $\omega$  dependence for its associated kernel namely,

$$\widetilde{K}_{e}^{e}(\omega) + \widetilde{K}_{g}^{g}(\omega) = \left(\frac{1}{\pi\hbar}\right) \int_{-\infty}^{+\infty} d\nu \left(n_{B}(\nu) - n_{B}(-\nu)\right) \times \Phi(\nu) \left(\frac{\omega_{+}}{(\nu - \omega_{a\bar{a}})^{2} - \omega_{+}^{2}}\right), \tag{8}$$

where, using standard quantum mechanical notations,  $\Phi(v) = 2 \langle \mathbf{j}_{ge} | \operatorname{Im} \frac{\mathcal{G}^+(v)}{v} | \mathbf{j}_{ge} \rangle$ . In this expression,  $\mathbf{j}$  is the nuclear current operator, and  $\mathcal{G}^+$  is the retarded solution of Maxwell's equation characterizing the bath

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electric response through its electronic susceptibility  $\chi^+$ . Note that the latter, associated with the atomic cloud, can be evaluated at its lowest order (one loop calculation [12]). In the Markovian framework, where the kernels are evaluated at zero frequency, Eq. (8) yields, at least at zero temperature, previously known results [13,1–3], however from a completely different viewpoint. But let us stress that Eq. (8) go further since the  $\omega$  dependence of the kernels allows us to describe *the onset of Rabi oscillations*.

Returning now to the situation of strong resonance, we have just said that our first attempt, which lead to write the system (7), dressed with the ' $L_0$ ' approximation and consequently Eq. (8), fails. To cure this problem one must extend the set of projections in  $\Pi_D$ . As a consequence, one inverts ( $\omega_+ + L_0$ ) on a new (smaller) space from which all the low frequency free (driven by  $L_0$ ) dynamics have been expelled. But, in order to recover a complete system, we end up adding new variables to the explicitly treated set { $\sigma_a$ }. However, one still must check all three constraints on the final results.

More precisely, let us recall that the resonant BIC effect addresses the case where, within the reservoir, one has an electronic transition between two bound states (here (1, 2)) such that  $\omega_{21} \simeq \omega_N$ . And in order to characterize the correlation part of their coulomb coupling with the other electrons (*the new bath*), we associate to each of them a phenomenological life time  $(\xi_1^C, \xi_2^C \text{ with } \eta^C \equiv \xi_1^C + \xi_2^C)$ . As a consequence, labelling the electronic states of the (new) bath by  $\mu_R$ , the entire electronic vector space is now described by  $(\alpha \otimes \mu_R)$  with  $\alpha = 1 \oplus 2$ , such that the total Hamiltonian reads  $H = h_N + h_\alpha + h_R + h_{R,N\otimes\alpha}$ . Then, following the above requirements, we now have to look for the vectors  $\mathcal{W}$  such that  $||(L_N + L_\alpha + L_R) * \mathcal{W}|| \sim 0$ . Here we find them to be

$$\mathcal{W} = \{ |\mu_R \alpha \, a), |\mu_R 2g, \mu_R 1e), |\mu_R 1e, \mu_R 2g) \}.$$
(9)

Indeed, one has  $||L_0 * |\mu_R \alpha a|| = 0$ , as usual for the set associated with the populations; and moreover  $||L_0 * |\mu_R 2g, \mu_R 1e\rangle|| = ||L_0 * |\mu_R 1e, \mu_R 2g\rangle|| = |\omega_{21} - \omega_N|, \ 0$  when approaching the resonance. In order to lump these states into one single notation one will write in the following:  $|\mu_R \alpha a| \equiv |0; \mu_R \alpha a|$  and,  $|\mu_R \alpha a, \mu_R \overline{\alpha} \overline{a}\rangle \equiv |1; \mu_R \alpha a\rangle$ .

From  $\mathcal{W}$ , one now introduces two sets of projections,  $\Pi_{(0;\alpha a)}$  and  $\Pi_{(1;\alpha a)}$  according to:

$$\Pi_{(s;\alpha a)} \equiv \sum_{\mu_R, \mu'_R} |s; \mu'_R \alpha a) (s; \mu_R \alpha a|,$$
(10)

with s = (0, 1), and the convention  $(1; \alpha a) = (1; 2g)$  or (1; 1e). Moreover, as earlier, one chooses  $\Pi_D \equiv \sum_{(s;\alpha a)} \Pi_{s;\alpha a}$ . Then, *in order to end up with a complete system*, we associate with  $\Pi_D$  the following 6 relevant variables,

$$\sigma_{(s;\alpha a)}(t) = \sum_{\mu_R,\mu_R'}^{\beta b} \sigma_{(\beta b)} \left(0; \mu_R \beta b \left| \theta(t) \, \mathrm{e}^{\mathrm{i}Lt} * \left| s; \mu_R' \alpha \, a \right| \right),$$
(11)

with  $\sigma_{(0;\alpha a)}(t = 0) \equiv \sigma_{(\alpha a)}$ . From (11) one can extract the desired nuclear populations through  $\sigma(t) = \text{Tr}_{\alpha} \{\sigma_0(t)\}$ . Now,  $h_{R,N\otimes\alpha}$  having its usual form (coupling the electronic and nuclear currents with the electromagnetic field), one recovers equations such as (4), in particular  $\Pi_{(s;\alpha a)} L_{R,N\otimes\alpha} \Pi_{(s';\alpha'a')} = 0$ . Also, following (4)–(7), one gets the Master Equation for  $\sigma_{(s;\alpha a)}(\omega)$  which is solved for  $\sigma_{(0;\alpha a)}(\omega)$  into:

$$\omega_{+}\sigma_{(0;\alpha a)}(\omega) - \mathrm{i}\sigma_{(\alpha a)} = \sum_{\beta b} \left[ \widetilde{K}_{0;\alpha a}^{0;\beta b} + \sum_{(1;\gamma c)} \widetilde{K}_{0;\alpha a}^{1;\gamma c} \frac{1}{\omega_{+} + \Delta_{\gamma c}} \widetilde{K}_{1;\gamma c}^{0;\beta b} \right] \sigma_{(0;\beta b)}(\omega), \tag{12}$$

where the new kernels  $\widetilde{K}$  are calculated within the ' $L_0$  approximation', and in the Markovian limit ( $\omega \sim 0$ ). In (12)  $\Delta_{\gamma c} \simeq \omega_{c\overline{c}} + \omega_{\gamma \overline{\gamma}} + i[\eta^C + (1/2)\eta^R (1 + e^{-\beta \hbar \omega_N})]$ , with  $\eta^R \equiv \tau_e^R + \tau_2^R$ , where  $\tau_e^R$  (resp.  $\tau_2^R$ ) is

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the temperature dependent *radiative* lifetime of the nuclear (resp. atomic) level *e* (resp. 2). Note that  $\Delta_{\gamma c}$  is small in case of strong resonance. Indeed, the denominator  $(\omega_+ + \Delta_{\gamma c})$  in (12) describes the effect, on the populations, of the resonant behavior of the states  $|1; \mu_R \alpha a|$ .

From (12) one finds that in general  $\sigma_{(0;\alpha a)}(\omega)$  has 6 poles, one in  $\omega = 0$  giving the constraint (c), the other five lying in the lower half part of the  $\omega$ -plane. In the particular case where  $e^{-\beta \hbar \omega_N} \sim 0$  and  $\sigma_{(1e)} = 1$ , then  $\sigma_{(0;2e)}(t) = 0$  and the number of poles reduces to 4. Let us add that the complete study of Eq. (12), which will be published elsewhere, yields as a first outcome the other two constraints (a) and (b).

Here, in order to illustrate our findings, we select two specific results subject to the conditions  $\eta^C$ ,  $\eta^R \ll \sqrt{\widetilde{\Gamma}}$ , where  $\widetilde{\Gamma}$  is the *strictly positive* coupling parameter. Using the nuclear and electronic current operators  $\mathbf{j}^N$  and  $\mathbf{j}^e$ , it is defined at zero temperature by

$$\widetilde{\Gamma} \equiv \frac{4}{\hbar^2} \operatorname{Re}\left\{ \left\langle \mathbf{j}_{21}^{e} \middle| \frac{\mathcal{G}^{+}(\omega_N)}{\omega_N} \middle| \mathbf{j}_{eg}^{N} \right\rangle \left\langle \mathbf{j}_{12}^{e} \middle| \frac{\mathcal{G}^{+}(\omega_N)}{\omega_N} \middle| \mathbf{j}_{ge}^{N} \right\rangle \right\} + 2 \tau_e^R \tau_2^R.$$

Then:

(i) If  $e^{-\beta\hbar\omega_N} \sim 0$  and  $\sigma_{(1e)} = 1$ , one finds that  $\sigma_e(\omega) (= \sigma_{(0;1e)}(\omega))$  has 4 poles,  $\Omega_{1,2}$  and  $\Omega_{3,4}$ , given by:

$$\Omega_1 \simeq \Omega_2 \simeq -\frac{i}{2} \left( \eta^C + \eta^R \right), \quad \text{and} \quad \Omega_{3,4} \simeq -\frac{i}{2} \left( \eta^C + \eta^R \right) \pm \sqrt{\widetilde{\Gamma} + (\omega_N - \omega_{21})^2}. \tag{13}$$

Each of these poles having a weight  $\simeq 1/4$ , one recognizes a dynamics driven by a Rabi frequency  $\Omega_R = \sqrt{\widetilde{\Gamma} + (\omega_N - \omega_{21})^2}$ .

(ii) Finally, focusing on the Rabi frequency when  $\omega_N = \omega_{21}$ , one finds that its temperature dependence is given to first order in  $e^{-\beta \hbar \omega_N}$  by:

$$\frac{\Omega_R}{\sqrt{\widetilde{\Gamma}}} \simeq 1 - \left(\frac{16 \,\mathrm{e}^{-\beta \hbar \omega_N}}{\hbar^2 \widetilde{\Gamma}}\right) \left| \left\langle \mathbf{j}_{21}^e | \frac{\mathrm{Im} \,\mathcal{G}^+(\omega_N)}{\omega_N} | \mathbf{j}_{eg}^N \right\rangle \right|^2. \tag{14}$$

Let us now sum up. The analysis of our original BIC problem led us to the following conclusions: If the nucleus, in contact with a reservoir, is far from any strong resonant behavior, one needs to write a Master Equation for the whole set of populations in order to properly describe the influence of the temperature on the low frequency part of its dynamics. The kernels of this equation are then calculated within the approximation of free dynamics, governed by the Liouville superoperator  $L_0$ . If the system undergoes a resonance, although one can still describe its onset in the previous framework, the procedure fails when the resonance dominates. In order to describe the latter it has been shown that one must extend the set of the explicitly treated variables. This goes through the analysis of the vectorial subspace W defined by  $||L_0W|| \leq 0$ . Let us stress that the range of application of this work is much wider that the initial BIC/NEET problems. For any small system in contact with a thermostat, it exhibits the relevant response functions of the bath in a natural way, and provides a sound approximation scheme.

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