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Exactly solvable 3D model of resonance energy transfer

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Abstract. The dynamics of two atoms coupled to the vacuum radiation field is investigated within the framework of the resonance dipole approximation. The exact solution of the resonance energy transfer problem is obtained.

1. Introduction

In a previous article [1], we presented a solution of a 1D quantum model describing a system of two identical atoms coupled to a vacuum radiation field based on a generalization of the standard Wigner–Weisskopf renormalization procedure. In particular, we had found explicit expressions for the spectral density of radiation and the time behaviour of the atoms plus quantized field system, provided that, in the initial state of the system, only one of the atoms were excited, while the other and the field were in their ground state (the Fermi problem).

In this article we study the dynamics of the atoms plus quantized field system in three-dimensional (3D) space, when all the field harmonics are available for spontaneous decay of an atomic excitation. This canonical problem of the quantum theory of radiation has been investigated in numerous works employing various different approximations and approaches [2–16].

In the same manner as in [1], we use a novel approach based on an exact diagonalization of the model Hamiltonian, in conjunction with a generalization of the standard Wigner–Weisskopf renormalization procedure, which allows us to obtain the solution of the dynamical problem in a trivial way. One of the characteristic features of our approach will be the use of the spherical harmonic representation in the description of the field. In this representation, the field operators depend on one continuous variable (a frequency) and two discrete variables (an angular momentum and a projection thereof on an axis of quantization). Therefore, within the framework of the resonance approximation, the model can be reduced to a one-dimensional (1D) model in which a continuous variable (corresponding to the radius of the 'wave front') plays a role as the 1D coordinate.

Our results confirm the approach of Milonni and Knight [9], however we are able to show that the time evolution of the atomic wavefunctions is such that causality is indeed preserved. The approach developed here can be seen to have application in the study of dispersive media or photonic bandgap materials [17], which have been doped with two-level atoms. In particular, the use of the spherical harmonic representation leads to a simple set

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of equations describing a photon-impurity band for an ordered system of two-level atoms, which have been placed within dispersive media or photonic bandgaps [18]. We also anticipate that this approach could be also be applied to studies of many-particle eigenstates of the two-impurity Kondo and Anderson models, as well as those of a two-atom optical system.

As a physical example of what our result implies, consider any solid matrix with an impurity uniformly distributed in it. Then causality would demand that if one excited only one impurity atom, then no other impurity atom would become excited faster than the time required for a light signal to travel from the excited atom to that atom. This is exactly what our result demonstrates.

2. Atom–field coupling

It is convenient to choose the system of coordinates where the atoms are located on the z axis, with the origin positioned midway between the atoms. Then, in Cartesian coordinates, the atoms have the coordinates $\boldsymbol{r}_1 = \boldsymbol{a} = (0, 0, a)$ and $\boldsymbol{r}_2 = -\boldsymbol{a} = (0, 0, -a)$ where $2a$ is the atomic separation.

In what follows, an atom is regarded as a quantum system which has a ground state of angular momentum $J_1 = 0$ and an excited state of angular momentum $J_2 = 1$. The latter state is triply degenerate with three possible values for the z-component of angular momentum, $M_2 = -1, 0, 1$. Then, for the transition $M_2 = 0 \leftrightarrow M_1 = 0$, the only non-zero matrix element of the atomic dipole operator is the z-component, while for two other transitions, $M_2 = \pm 1 \leftrightarrow M_1 = 0$, the non-zero matrix elements lie in the xy plane.

As usual, the atomic dipole operator is expressed in terms of the spin operators $\sigma_a^i = (\sigma_a^x, \sigma_a^y, \sigma_a^z)$; $\sigma_a^{\pm} = \sigma_a^x \pm \mathrm{i}\sigma_a^y$ which satisfy the commutator

$$[\sigma_a^i, \sigma_b^j] = \mathrm{i}\delta_{ab}\,\mathrm{e}^{ijk}\sigma_a^k \tag{2.1}$$

(where e^{ijk} is the unit antisymmetric tensor and the index $a = 1, 2$ numbers the atoms) as follows:

$$\boldsymbol{d}_a = d\,\boldsymbol{e}_z(\sigma_a^+ + \sigma_a^-) \tag{2.2}$$

for the transition $0 \leftrightarrow 0$, and

$$\boldsymbol{d}_a = d\left(\frac{1+\mathrm{i}}{2}\boldsymbol{e}_-\sigma_a^+ + \frac{1-\mathrm{i}}{2}\boldsymbol{e}_+\sigma_a^-\right) \tag{2.3}$$

for the transition $1 \leftrightarrow 0$, where $\boldsymbol{e}_{\pm} = \boldsymbol{e}_x \pm \mathrm{i}\boldsymbol{e}_y$ and d is the reduced matrix element of the dipole operator [19].

It should be emphasized that if the ground state of the transition under consideration is also degenerate ($J_1 \neq 0$) then the dipole operator cannot be expressed in terms of the Pauli spin matrices and instead the full Lie algebra $gl(4)$ would have to be considered [20].

The electric–dipole interaction between the two-level atoms and quantized electromagnetic field is given by the operator

$$V = -[\boldsymbol{d}_1\boldsymbol{E}(\boldsymbol{a}) + \boldsymbol{d}_2\boldsymbol{E}(-\boldsymbol{a})] \tag{2.4}$$

where $\boldsymbol{E}(\boldsymbol{a})$ and $\boldsymbol{E}(-\boldsymbol{a})$ are the operators of the electric field at the points $\boldsymbol{r} = \pm\boldsymbol{a}$. In what follows, it is convenient to use the spherical harmonic representation [21] for the electric field operators. In this representation the operators of the electric field are expanded in terms of the spherical harmonic vectors

$$\boldsymbol{E}(\boldsymbol{r}) = \sum_{\alpha=e,m}\sum_{j=1}^{\infty}\sum_{m=-j}^{j}\int_0^{\infty}\frac{\mathrm{d}\omega}{2\pi}\{\boldsymbol{E}_{\omega jm}^{(\alpha)}(\boldsymbol{r})c_{\omega jm}^{(\alpha)} + \boldsymbol{E}_{\omega jm}^{(\alpha)*}(\boldsymbol{r})c_{\omega jm}^{(\alpha)+}\} \tag{2.5}$$

where the operators $c^{(\alpha)+}_{\omega jm}$ ($c^{(\alpha)}_{\omega jm}$), obeying the commutation rules

$$[c^{(\alpha)}_{\omega jm}, c^{(\alpha')+}_{\omega' j'm'}] = 2\pi\delta(\omega-\omega')\delta_{\alpha\alpha'}\delta_{jj'}\delta_{mm'} \tag{2.6}$$

create (annihilate) a photon of an electric ($\alpha = e$) or a magnetic ($\alpha = m$) type with a frequency ω, an angular momentum j and projection thereof m. The Fourier component

$$\boldsymbol{E}^{(\alpha)}_{\omega jm}(\boldsymbol{k}) = \int \mathrm{d}^3 r\ \boldsymbol{E}^{(\alpha)}_{\omega jm}(\boldsymbol{r})\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \tag{2.7}$$

of the function $\boldsymbol{E}^{(\alpha)}_{\omega jm}(\boldsymbol{r})$ is given by ($\boldsymbol{n}$ is a unit vector in the direction of $\boldsymbol{k}$)

$$\boldsymbol{E}^{(\alpha)}_{\omega jm}(\boldsymbol{k}) = 4\pi^2\mathrm{i}\left(\frac{2\pi}{\omega}\right)^{1/2}\delta(|\boldsymbol{k}|-\omega)\boldsymbol{Y}^{(\alpha)}_{jm}(\boldsymbol{n})\,. \tag{2.8}$$

The spherical harmonic vectors $\boldsymbol{Y}^{(\alpha)}_{jm}(\boldsymbol{n})$ are also defined in [21].

Since only the photon states with a frequency ω lying near the transition frequency ω_{12} (and within the width $\Gamma \ll \omega_{12}$) interact effectively with an atom, we can ignore the photon states further out (the resonance approximation). In our formalism this means, first of all, that the terms $\sigma^+ c^+_{\omega jm}$ and $\sigma^- c_{\omega jm}$ in the operator V can be omitted. Then, the model Hamiltonian takes the initial form

$$H = H_0 + V \tag{2.9}$$

$$H_0 = \omega_{12}(\sigma^z_1 + \sigma^z_2 + 1) + \sum_{\alpha jm}\int_0^\infty \frac{\mathrm{d}\omega}{2\pi}\,\omega\, c^{(\alpha)+}_{\omega jm}\, c^{(\alpha)}_{\omega jm} \tag{2.10}$$

$$V = \sum_{\alpha jm}\int_0^\infty \frac{\mathrm{d}\omega}{2\pi}\sqrt{\gamma(\omega)}\int \mathrm{d}o_{\boldsymbol{n}}\ \Big[\pi^{(\alpha)}_{jm}(\boldsymbol{n})\, c^{(\alpha)}_{\omega jm}\,(\sigma^+_1\mathrm{e}^{\mathrm{i}\omega\boldsymbol{a}\cdot\boldsymbol{n}} + \sigma^+_2\mathrm{e}^{-\mathrm{i}\omega\boldsymbol{a}\cdot\boldsymbol{n}})$$
$$+ \pi^{(\alpha)*}_{jm}(\boldsymbol{n})\, c^{(\alpha)+}_{\omega jm}\,(\sigma^-_1\mathrm{e}^{-\mathrm{i}\omega\boldsymbol{a}\cdot\boldsymbol{n}} + \sigma^-_2\mathrm{e}^{\mathrm{i}\omega\boldsymbol{a}\cdot\boldsymbol{n}})\Big] \tag{2.11}$$

where $\gamma(\omega) = 4\omega^3 d^2/3$. The functions $\pi^{(\alpha)}_{jm}(\boldsymbol{n})$ are different for different transitions. For the transition $1 \leftrightarrow 0$

$$\pi^{(\alpha)}_{jm}(\boldsymbol{n}) = -\mathrm{i}\frac{1+\mathrm{i}}{2}\left(\frac{3}{8\pi}\right)^{1/2}\boldsymbol{e}_-\cdot\boldsymbol{Y}^{(\alpha)}_{jm}(\boldsymbol{n}) \tag{2.12}$$

and it contains both electric and magnetic components, while for the transition $0 \leftrightarrow 0$

$$\pi^{(e)}_{jm}(\boldsymbol{n}) = -\mathrm{i}\left(\frac{3}{8\pi}\right)^{1/2}\boldsymbol{e}_z\cdot\boldsymbol{Y}^{(e)}_{jm}(\boldsymbol{n}) \tag{2.13}$$

but $\pi^{(m)}_{jm}(\boldsymbol{n}) = 0$, because the electric field of a magnetic photon is perpendicular to the dipole moment of the transition.

3. Renormalization procedure

The 'particle' number operator of the model

$$N = \sum_{a=1,2}\left(\sigma^z_a + \frac{1}{2}\right) + \sum_{\alpha jm}\int_0^\infty \frac{\mathrm{d}\omega}{2\pi}c^{(\alpha)+}_{\omega jm}c^{(\alpha)}_{\omega jm} \tag{3.1}$$

commutes with the Hamiltonian (2.9)–(2.11), therefore, all the model eigenstates can be classified with respect to the number of 'particles', or eigenvalues of the operator N.

The vacuum state of the model $|0\rangle$

$$c^{(\alpha)}_{\omega jm}|0\rangle = \sigma^-_a|0\rangle = 0 \tag{3.2}$$

contains no particle, $N|0\rangle = H|0\rangle = 0$. The subject of our interest in this article is one-particle eigenstates,

$$N|\Psi_1\rangle = 1\cdot|\Psi_1\rangle \qquad H|\Psi_1\rangle = \lambda\cdot|\Psi_1\rangle \tag{3.3}$$

where λ is eigenenergy, which we look for in the form

$$|\Psi\rangle = \left[\xi_1\sigma_1^+ + \xi_2\sigma_2^+ + \sum_{\alpha jm}\int_0^\infty \frac{\mathrm{d}\omega}{2\pi} f^{(\alpha)}_{\omega jm} c^{(\alpha)+}_{\omega jm}\right]|0\rangle\,. \tag{3.4}$$

Then, the Schrödinger equation $(H-\lambda)|\Psi\rangle = 0$ takes the form

$$(\omega-\lambda) f^{(\alpha)}_{\omega jm}(\lambda) + \sqrt{\gamma(\omega)}\int \mathrm{d}o_{\boldsymbol{n}}\, \pi^{(\alpha)*}_{jm}(\boldsymbol{n})[\xi_1(\lambda)\mathrm{e}^{-\mathrm{i}\omega\boldsymbol{a}\cdot\boldsymbol{n}} + \xi_2(\lambda)\mathrm{e}^{\mathrm{i}\omega\boldsymbol{a}\cdot\boldsymbol{n}}] = 0 \tag{3.5}$$

$$(\omega_{12}-\lambda)\xi_1(\lambda) + \sum_{\alpha jm}\int_0^\infty \frac{\mathrm{d}\omega}{2\pi}\sqrt{\gamma(\omega)}\int \mathrm{d}o_{\boldsymbol{n}}\, \pi^{(\alpha)}_{jm}(\boldsymbol{n})\mathrm{e}^{\mathrm{i}\omega\boldsymbol{a}\cdot\boldsymbol{n}} f^{(\alpha)}_{\omega jm}(\lambda) = 0 \tag{3.6}$$

$$(\omega_{12}-\lambda)\xi_2(\lambda) + \sum_{\alpha jm}\int_0^\infty \frac{\mathrm{d}\omega}{2\pi}\sqrt{\gamma(\omega)}\int \mathrm{d}o_{\boldsymbol{n}}\, \pi^{(\alpha)}_{jm}(\boldsymbol{n})\mathrm{e}^{-\mathrm{i}\omega\boldsymbol{a}\cdot\boldsymbol{n}} f^{(\alpha)}_{\omega jm}(\lambda) = 0. \tag{3.7}$$

The general solution of (3.5) is given by

$$f^{(\alpha)}_{\omega jm}(\lambda) = 2\pi\delta(\omega-\lambda)\psi^{(\alpha)}_{\omega jm} + \frac{\sqrt{\gamma(\omega)}}{\lambda-\omega+\mathrm{i}0}\xi_1(\lambda)\int \mathrm{d}o_{\boldsymbol{n}}\, \pi^{(\alpha)*}_{jm}(\boldsymbol{n})\mathrm{e}^{-\mathrm{i}\omega\boldsymbol{a}\cdot\boldsymbol{n}}$$
$$+\frac{\sqrt{\gamma(\omega)}}{\lambda-\omega+\mathrm{i}0}\xi_2(\lambda)\int \mathrm{d}o_{\boldsymbol{n}}\, \pi^{(\alpha)*}_{jm}(\boldsymbol{n})\mathrm{e}^{\mathrm{i}\omega\boldsymbol{a}\cdot\boldsymbol{n}} \tag{3.8}$$

where $\psi^{(\alpha)}_{\omega jm}$ is an arbitrary function. Substituting equation (3.8) into (3.6), (3.7) and making use of equations (A.5), (A.6) from the appendix, we find

$$(\lambda-\omega_{12}+\mathrm{i}g_{11}(\lambda))\xi_1(\lambda) + \mathrm{i}g_{12}(\lambda)\xi_2(\lambda) = C_1(\lambda) \tag{3.9}$$

$$(\lambda-\omega_{12}+\mathrm{i}g_{22}(\lambda))\xi_2(\lambda) + \mathrm{i}g_{21}(\lambda)\xi_1(\lambda) = C_2(\lambda) \tag{3.10}$$

where

$$C_1(\lambda) = \sqrt{\gamma(\lambda)}\sum_{\alpha jm}\psi^{(\alpha)}_{\lambda jm}\int \mathrm{d}o_{\boldsymbol{n}}\, \pi^{(\alpha)}_{jm}(\boldsymbol{n})\mathrm{e}^{\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} \tag{3.11}$$

$$C_2(\lambda) = \sqrt{\gamma(\lambda)}\sum_{\alpha jm}\psi^{(\alpha)}_{\lambda jm}\int \mathrm{d}o_{\boldsymbol{n}}\, \pi^{(\alpha)}_{jm}(\boldsymbol{n})\mathrm{e}^{-\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}}\,. \tag{3.12}$$

The functions

$$g_{11} = g_{22} = \int_0^\infty \frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\frac{\gamma(\omega)}{\omega-\lambda-\mathrm{i}0} \tag{3.13}$$

$$g_{12} = g_{21} = \int_0^\infty \frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\frac{\gamma(\omega)}{\omega-\lambda-\mathrm{i}0}\int \mathrm{d}o_{\boldsymbol{n}}\left(\frac{3}{8\pi}\sin^2\theta\right)\mathrm{e}^{2\mathrm{i}\omega\boldsymbol{a}\cdot\boldsymbol{n}} \tag{3.14}$$

for the transition $0\leftrightarrow 0$, and

$$g_{12} = g_{21} = \int_0^\infty \frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\frac{\gamma(\omega)}{\omega-\lambda-\mathrm{i}0}\int \mathrm{d}o_{\boldsymbol{n}}\left[\frac{3}{8\pi}\left(1-\frac{1}{2}\sin^2\theta\right)\right]\mathrm{e}^{2\mathrm{i}\omega\boldsymbol{a}\cdot\boldsymbol{n}} \tag{3.15}$$

in the case of the transitions $\pm 1 \leftrightarrow 0$, contain the contributions of the atom–field interaction (the effective interatomic coupling) to the atomic wavefunctions.

The integrals over frequency in (3.13)–(3.15) diverge and have to be renormalized. Let us first analyse the expression (3.13), which could be rewritten in the form

$$\mathrm{g}_{11}(\lambda) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi \mathrm{i}} \frac{\gamma(\omega)}{\omega - \lambda - \mathrm{i}0} - \int_{0}^{\infty} \frac{\mathrm{d}\omega}{2\pi \mathrm{i}} \frac{\gamma(\omega)}{\omega + \lambda}\,. \tag{3.16}$$

In accordance with the standard Wigner–Weisskopf renormalization procedure, we replace

$$\gamma(\omega) \to \gamma = \tfrac{4}{3} d^2 \omega_{12}^3 = \text{constant} \tag{3.17}$$

and omit the second integral, because this integral describes the purely real correction to the atomic transition frequency (Lamb shift), which cannot be properly treated within the framework of our semi-relativistic model, since it is not relativistic. Then the first integral yields the standard Wigner–Weisskopf expression

$$\mathrm{g}_{11} = \mathrm{g}_{22} = \tfrac{1}{2}\gamma \tag{3.18}$$

that leads to the Lorentzian shape of a radiation spectrum for a single atom in empty space.

Turning to equation (3.14), after the integration over solid angles, it takes on the form

$$\mathrm{g}_{12} = \mathrm{g}_{21} = \int_{0}^{\infty} \frac{\mathrm{d}\omega}{2\pi \mathrm{i}} \frac{\gamma(\omega)}{\omega - \lambda - \mathrm{i}0} \frac{3}{(\omega l)^2} \left(\frac{\sin \omega l}{\omega l} - \cos \omega l \right) \tag{3.19}$$

or upon using the WW renormalization procedure

$$\mathrm{g}_{12} = \mathrm{g}_{21} = I_1 - I_2 \tag{3.20}$$

$$I_1 = \frac{3\gamma}{(\omega_{12} l)^2} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi \mathrm{i}} \frac{1}{\omega - \lambda - \mathrm{i}0} \left(\frac{\sin \omega l}{\omega_{12} l} - \cos \omega l \right)$$

$$= -\frac{3}{2} \frac{\gamma}{(\omega_{12} l)^2} \left(1 + \frac{\mathrm{i}}{\omega_{12} l} \right) \mathrm{e}^{\mathrm{i}\lambda l} \tag{3.21}$$

$$I_2 = \frac{3\gamma}{(\omega_{12} l)^2} \int_{0}^{\infty} \frac{\mathrm{d}\omega}{2\pi \mathrm{i}} \frac{1}{\omega + \lambda} \left(\frac{\sin \omega l}{\omega_{12} l} - \cos \omega l \right) \tag{3.22}$$

where $l = 2a$ is the interatomic separation. The resonance approximation for the one-atom problem assumes that the main contribution to the atom–field coupling comes from photon states lying in an narrow vicinity, $\Delta \approx \gamma \ll \omega_{12}$, near the transition frequency ω_{12}. However, in our two-atom problem, there is a new parameter, $\omega_{12} l$, involving the interatomic separation l, which appears. This is because photon states with frequencies $\omega \sim l^{-1}$ can contribute to the effective interatomic coupling.

For $\omega_{12} l \gg 1$, the second integral I_2 contains an additional smallness in the parameter $(\omega_{12} l)^{-1}$ compared with the first one, I_1, and could be omitted. In what follows we confine ourselves to the case of long interatomic distances $l \gg \omega_{12}^{-1}$. Then, for the transition $0 \leftrightarrow 0$ we have

$$\mathrm{g}_{12} = \mathrm{g}_{21} = -\frac{3}{2}\gamma \left(\frac{1}{(\omega_{12} l)^2} + \frac{\mathrm{i}}{(\omega_{12} l)^3} \right) \mathrm{e}^{\mathrm{i}\lambda l}\,. \tag{3.23}$$

In an analoguous way for the transitions $\pm 1 \leftrightarrow 0$ we also find

$$\mathrm{g}_{12} = \mathrm{g}_{21} = \frac{3}{4}\gamma \left(-\frac{\mathrm{i}}{\omega_{12} l} + \frac{1}{(\omega_{12} l)^2} + \frac{\mathrm{i}}{(\omega_{12} l)^3} \right) \mathrm{e}^{\mathrm{i}\lambda l}\,. \tag{3.24}$$

Taking into account that we already omitted the integral I_2, only the leading first terms of expressions (3.23), (3.24) should be retained.

It should be emphasized that the omitted integral I_2 contributes only to the renormalization of the atomic transition frequency and does not affect the time behaviour of the system which is the main subject of our interest in the present paper. For short interatomic distances, $\omega_{12} l \leqslant 1$, the contribution of I_2 can be taken into account by means of a separation into symmetric and antisymmetric eigenstates as was done in [1]. We will return to this question in the end of the next section.

It can easily be seen that the above renormalization procedure is equivalent to putting $\gamma(\omega) \to \gamma(\omega_{12}) =$ constant with an extension of the integration over frequency in the model Hamiltonian, (2.9)–(2.11), to a lower limit of $-\infty$. Then, defining new operators

$$\epsilon_{jm}^{(\alpha)}(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} c_{\omega jm}^{(\alpha)} \mathrm{e}^{\mathrm{i}\omega x} \qquad c_{\omega jm}^{(\alpha)} = \int_{-\infty}^{\infty} \mathrm{d}x\ \epsilon_{jm}^{(\alpha)}(x) \mathrm{e}^{-\mathrm{i}\omega x} \tag{3.25}$$

which have the commutation relations

$$[\epsilon_{jm}^{(\alpha)}(x), \epsilon_{j'm'}^{(\alpha')+}(x')] = \delta(x - x')\delta_{\alpha\alpha'}\delta_{jj'}\delta_{mm'} \tag{3.26}$$

the effective Hamiltonian takes the form

$$H_0 = \omega_{12}(\sigma_1^z + \sigma_2^z + 1) - \mathrm{i} \sum_{\alpha jm} \int_{-\infty}^{\infty} \mathrm{d}x\ \epsilon_{jm}^{(\alpha)+}(x) \frac{\partial}{\partial x} \epsilon_{jm}^{(\alpha)}(x) \tag{3.27}$$

$$V = \sqrt{\gamma} \sum_{\alpha jm} \int_{-\infty}^{\infty} \mathrm{d}x\ \Big[v_{jm}^{(\alpha)}(x) \epsilon_{jm}^{(\alpha)}(x)\, \sigma_1^+ + v_{jm}^{(\alpha)*}(x) \epsilon_{jm}^{(\alpha)+}(x)\, \sigma_1^- + u_{jm}^{(\alpha)}(x) \epsilon_{jm}^{(\alpha)}(x)\, \sigma_2^+$$

$$+ u_{jm}^{(\alpha)*}(x) \epsilon_{jm}^{(\alpha)+}(x) \sigma_2^- \Big] \tag{3.28}$$

where the atomic form-factors are given by

$$v_{jm}^{(\alpha)}(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \int \mathrm{d}o_{\boldsymbol{n}}\ \mathrm{e}^{\mathrm{i}\omega(x - \boldsymbol{a}\cdot\boldsymbol{n})} \pi_{jm}^{(\alpha)}(\boldsymbol{n}) = \int \mathrm{d}o_{\boldsymbol{n}}\ \delta(x - \boldsymbol{a}\cdot\boldsymbol{n}) \pi_{jm}^{(\alpha)}(\boldsymbol{n}) \tag{3.29}$$

$$u_{jm}^{(\alpha)}(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \int \mathrm{d}o_{\boldsymbol{n}}\ \mathrm{e}^{\mathrm{i}\omega(x + \boldsymbol{a}\cdot\boldsymbol{n})} \pi_{jm}^{(\alpha)}(\boldsymbol{n}) = \int \mathrm{d}o_{\boldsymbol{n}}\ \delta(x + \boldsymbol{a}\cdot\boldsymbol{n}) \pi_{jm}^{(\alpha)}(\boldsymbol{n})\,. \tag{3.30}$$

The variable x can be viewed as a coordinate along an arbitrary ray, passing through the origin of the coordinate system. Then, the region $x < 0$ corresponds to ingoing spherical waves, while the region $x > 0$ corresponds to outgoing waves.

According to the WW renormalization procedure, the last step in (3.29) and (3.30) is incorrect. What we have done is formally to carry out the integration over frequency *before* the renormalization procedure was completed. The last integration in (3.29) and (3.30) is incorrect per the WW renormalization procedure and when done, leads to a loss of causality, because the atomic form-factors do not vanish for any $|x| < a$. The correct procedure is to first integrate over the solid angles and then, before the final integration over frequency is done, replace ω with ω_{12} everywhere except in any exponential factors. Moreover, strictly speaking, the resonance approximation cannot be applied directly to the model Hamiltonian until *after* all angular integrations have been done. This is because H contains all spherical harmonics, and, hence, the integration over a solid angle can contain high powers of the frequency, $(\omega l)^j$, when $j \gg \omega l$. In what follows, we will use only the first expressions in (3.29) and (3.30). Then we will apply the resonance approximation to all expressions for physical values only after any summation over the spherical harmonics has been evaluated.

4. One-particle eigenstates

In terms of the operators (3.25) the expression for one-particle eigenstate (3.4) is rewritten as follows:

$$|\Psi_1\rangle = \left[\xi_1\sigma_1^+ + \xi_2\sigma_2^+ + \sum_{\alpha jm}\int_{-\infty}^{\infty} \mathrm{d}x\ f_{jm}^{(\alpha)}(x)\epsilon_{jm}^{(\alpha)+}(x)\right]|0\rangle. \tag{4.1}$$

Then, the Schrödinger equation for the photon wavefunctions $f_{jm}^{(\alpha)}(x)$ and the wavefunctions of the atomic excitations ξ_a takes the form

$$\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} + \lambda\right) f_{jm}^{(\alpha)}(x) = \sqrt{\gamma}[\xi_1 v_{jm}^{(\alpha)*}(x) + \xi_2 u_{jm}^{(\alpha)*}(x)] \tag{4.2}$$

$$(\lambda - \omega_{12})\xi_1 = \sqrt{\gamma}\sum_{\alpha jm}\int_{-\infty}^{\infty} \mathrm{d}x\ f_{jm}^{(\alpha)}(x)v_{jm}^{(\alpha)}(x) \tag{4.3}$$

$$(\lambda - \omega_{12})\xi_2 = \sqrt{\gamma}\sum_{\alpha jm}\int_{-\infty}^{\infty} \mathrm{d}x\ f_{jm}^{(\alpha)}(x)u_{jm}^{(\alpha)}(x)\,. \tag{4.4}$$

The substitution

$$f_{jm}^{(\alpha)}(x) = \mathrm{e}^{\mathrm{i}\lambda x}\int \mathrm{d}o_{\boldsymbol{n}}\ \pi_{jm}^{(\alpha)*}(\boldsymbol{n})\phi_{\boldsymbol{n}}(x) \tag{4.5}$$

leads to the simple equation for $\phi_{\boldsymbol{n}}(x)$:

$$-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\phi_{\boldsymbol{n}}(x) + \sqrt{\gamma}\,[\xi_1\,\mathrm{e}^{-\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}}\delta(x - \boldsymbol{a}\cdot\boldsymbol{n}) + \xi_2\,\mathrm{e}^{\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}}\delta(x + \boldsymbol{a}\cdot\boldsymbol{n})] = 0 \tag{4.6}$$

with the general solution

$$\phi_{\boldsymbol{n}}(x) = \Phi_{\boldsymbol{n}} - i\sqrt{\gamma}\,[\xi_1\,\mathrm{e}^{-\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}}\theta(x - \boldsymbol{a}\cdot\boldsymbol{n}) + \xi_2\,\mathrm{e}^{\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}}\theta(x + \boldsymbol{a}\cdot\boldsymbol{n})] \tag{4.7}$$

where

$$\theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases}$$

and $\Phi_{\boldsymbol{n}}$ is an arbitrary function. Inserting equations (4.5), (4.6) into (4.3), (4.4) and taking into account equations (A.5), (A.6) from the appendix, for the atomic wavefunctions ξ_a one again obtains

$$(\lambda - \omega_{12} + \mathrm{i}\gamma/2)\xi_1 + \mathrm{i}\gamma\mathrm{g}\xi_2 = \sqrt{\gamma}C_1 \tag{4.8}$$

$$\mathrm{i}\gamma\mathrm{g}\xi_1 + (\lambda - \omega_{12} + \mathrm{i}\gamma/2)\xi_2 = \sqrt{\gamma}C_2 \tag{4.9}$$

where the integral $\int \mathrm{d}x\,\theta(x)\delta(x)$ is taken to be $\frac{1}{2}$, and

$$C_1 = \frac{3}{8\pi}\int \mathrm{d}o_{\boldsymbol{n}}\ \sin^2\theta\,\Phi_{\boldsymbol{n}}\mathrm{e}^{\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} \tag{4.10}$$

$$C_2 = \frac{3}{8\pi}\int \mathrm{d}o_{\boldsymbol{n}}\ \sin^2\theta\,\Phi_{\boldsymbol{n}}\mathrm{e}^{-\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} \tag{4.11}$$

$$\mathrm{g}(\lambda) = \frac{3}{8\pi}\int \mathrm{d}o_{\boldsymbol{n}}\ \sin^2\theta\,\theta(\boldsymbol{a}\cdot\boldsymbol{n})\,\mathrm{e}^{2\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} \tag{4.12}$$

for the transition $0 \leftrightarrow 0$, or

$$C_1 = \frac{3}{8\pi}\int \mathrm{d}o_{\boldsymbol{n}}\ \left(1-\frac{1}{2}\sin^2\theta\right)\Phi_{\boldsymbol{n}}\mathrm{e}^{\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} \tag{4.13}$$

$$C_2 = \frac{3}{8\pi}\int \mathrm{d}o_{\boldsymbol{n}}\ \left(1-\frac{1}{2}\sin^2\theta\right)\Phi_{\boldsymbol{n}}\mathrm{e}^{-\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} \tag{4.14}$$

$$\mathrm{g}(\lambda) = \frac{3}{8\pi}\int \mathrm{d}o_{\boldsymbol{n}}\ \left(1-\frac{1}{2}\sin^2\theta\right)\theta(\boldsymbol{a}\cdot\boldsymbol{n})\,\mathrm{e}^{2\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} \tag{4.15}$$

for the transitions $\pm 1 \leftrightarrow 0$.

In the case of two identical atoms considered here, equations (4.8), (4.9), it is convenient to rewrite for the values $\xi_\pm = \xi_1 \pm \xi_2$

$$[\lambda - \omega_{12} + \mathrm{i}\gamma(\tfrac{1}{2}+\mathrm{g})]\xi_+ = \sqrt{\gamma}C_+ \tag{4.16}$$

$$[\lambda - \omega_{12} + \mathrm{i}\gamma(\tfrac{1}{2}-\mathrm{g})]\xi_- = \sqrt{\gamma}C_- \tag{4.17}$$

where

$$C_\pm = \frac{3}{8\pi}\int \mathrm{d}o_{\boldsymbol{n}}\ \sin^2\theta\,\Phi_{\boldsymbol{n}}(\mathrm{e}^{\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} \pm \mathrm{e}^{-\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}}) \tag{4.18}$$

and

$$C_\pm = \frac{3}{8\pi}\int \mathrm{d}o_{\boldsymbol{n}}\ \left(1-\frac{1}{2}\sin^2\theta\right)\Phi_{\boldsymbol{n}}(\mathrm{e}^{\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} \pm \mathrm{e}^{-\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}}) \tag{4.19}$$

for transitions $0 \leftrightarrow 0$ and $\pm 1 \leftrightarrow 0$, respectively. Now it can easily be seen that the choice of an arbitrary function in the form

$$\Phi_{\boldsymbol{n}} = \mathrm{e}^{\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} + \mathrm{e}^{-\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} \tag{4.20}$$

yields $C_+ = 2(1+2g')$, $C_- = 0$ and, hence, leads to the symmetric solution

$$\xi_1 = \xi_2 = \xi^{(\mathrm{s})} = \frac{1}{\sqrt{\gamma}}\frac{2\Gamma^{(\mathrm{s})}}{\lambda - \Omega^{(\mathrm{s})} + \mathrm{i}\Gamma^{(\mathrm{s})}} \tag{4.21}$$

$$f_{jm}^{(\alpha)(\mathrm{s})} = \int \mathrm{d}o_{\boldsymbol{n}}\ \pi_{jm}^{(\alpha)}\left[\frac{\lambda - \Omega^{(\mathrm{s})} - \mathrm{i}\Gamma^{(\mathrm{s})}\mathrm{sgn}\,(x-\boldsymbol{a}\cdot\boldsymbol{n})}{\lambda - \Omega^{(\mathrm{s})} + \mathrm{i}\Gamma^{(\mathrm{s})}}\mathrm{e}^{\mathrm{i}\lambda(x-\boldsymbol{a}\cdot\boldsymbol{n})}\right. \tag{4.22}$$

$$\left. + \frac{\lambda - \Omega^{(\mathrm{s})} - \mathrm{i}\Gamma^{(\mathrm{s})}\mathrm{sgn}\,(x+\boldsymbol{a}\cdot\boldsymbol{n})}{\lambda - \Omega^{(\mathrm{s})} + \mathrm{i}\Gamma^{(\mathrm{s})}}\mathrm{e}^{\mathrm{i}\lambda(x+\boldsymbol{a}\cdot\boldsymbol{n})}\right] \tag{4.23}$$

where

$$\Omega^{(\mathrm{s})} = \omega_{12} + \gamma\mathrm{g}'' \qquad \Gamma^{(\mathrm{s})} = \tfrac{1}{2}\gamma(1+2\mathrm{g}') \tag{4.24}$$

and $\mathrm{g}' = \mathrm{Re}\,\mathrm{g}(\lambda)$, $\mathrm{g}'' = \mathrm{Im}\,\mathrm{g}(\lambda)$

$$\mathrm{sgn}\,(x) = \begin{cases} 1 & x > 0 \\ 0 & x = 0 \\ -1 & x < 0. \end{cases}$$

The choice

$$\Phi_{\boldsymbol{n}} = \mathrm{e}^{\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} - \mathrm{e}^{-\mathrm{i}\lambda\boldsymbol{a}\cdot\boldsymbol{n}} \tag{4.25}$$

(and, hence, $C_+ = 0$, $C_- = 2(1 - 2g')$) leads to the antisymmetric solution

$$\xi_1 = -\xi_2 = \xi^{(\mathrm{as})} = \frac{1}{\sqrt{\gamma}} \frac{2\Gamma^{(\mathrm{as})}}{\lambda - \Omega^{(\mathrm{as})} + \mathrm{i}\Gamma^{(\mathrm{as})}} \tag{4.26}$$

$$f_{jm}^{(\alpha)(\mathrm{as})} = \int \mathrm{d}o_{\boldsymbol{n}}\, \pi_{jm}^{(\alpha)} \left[\frac{\lambda - \Omega^{(\mathrm{as})} - \mathrm{i}\Gamma^{(\mathrm{as})} \mathrm{sgn}\,(x - \boldsymbol{a}\cdot\boldsymbol{n})}{\lambda - \Omega^{(\mathrm{as})} + \mathrm{i}\Gamma^{(\mathrm{as})}} \mathrm{e}^{\mathrm{i}\lambda(x - \boldsymbol{a}\cdot\boldsymbol{n})} \right. \tag{4.27}$$

$$\left. - \frac{\lambda - \Omega^{(\mathrm{as})} - \mathrm{i}\Gamma^{(\mathrm{as})} \mathrm{sgn}\,(x + \boldsymbol{a}\cdot\boldsymbol{n})}{\lambda - \Omega^{(\mathrm{as})} + \mathrm{i}\Gamma^{(\mathrm{as})}} \mathrm{e}^{\mathrm{i}\lambda(x + \boldsymbol{a}\cdot\boldsymbol{n})} \right] \tag{4.28}$$

where

$$\Omega^{(\mathrm{as})} = \omega_{12} - \gamma \mathrm{g}'' \qquad \Gamma^{(\mathrm{as})} = \tfrac{1}{2}\gamma(1 - 2\mathrm{g}')\,. \tag{4.29}$$

Thus, we find for one-particle eigenstates corresponding to the eigenenergy λ:

$$|\lambda; \mathrm{s}\rangle = \left[\xi^{(\mathrm{s})}(\lambda)(\sigma_1^+ + \sigma_2^+) + \sum_{\alpha jm} \int_{-\infty}^{\infty} \mathrm{d}x\; f_{jm}^{(\alpha)(\mathrm{s})}(x, \lambda) \epsilon_{jm}^{(\alpha)+}(x) \right] |0\rangle \tag{4.30}$$

$$|\lambda; \mathrm{as}\rangle = \left[\xi^{(\mathrm{as})}(\lambda)(\sigma_1^+ - \sigma_2^+) + \sum_{\alpha jm} \int_{-\infty}^{\infty} \mathrm{d}x\; f_{jm}^{(\alpha)(\mathrm{as})}(x, \lambda) \epsilon_{jm}^{(\alpha)+}(x) \right] |0\rangle\,. \tag{4.31}$$

These states compose the complete orthonormal set of one-particle states and will be used in what follows to study the model's dynamics. Here, omitting standard but tedious calculations, we present the expressions for the scalar products, namely

$$\langle \sigma'; \lambda' | \lambda; \sigma \rangle = 8\pi \frac{\Gamma^{(\sigma)}}{\gamma} \delta_{\sigma\sigma'} \delta(\lambda - \lambda') \sigma = \mathrm{s}, \mathrm{as}. \tag{4.32}$$

Finally, we need to evaluate the function $\mathrm{g}(\lambda)$, equations (4.12), (4.15) in an implicit form. Keeping in mind the discussion in the end of the previous section, one has to treat the factor $\theta(\boldsymbol{a}\cdot\boldsymbol{n}) \exp(\mathrm{i}\lambda \boldsymbol{a}\cdot\boldsymbol{n})$ in an integral form:

$$\theta(\boldsymbol{a}\cdot\boldsymbol{n}) \mathrm{e}^{\mathrm{i}\lambda \boldsymbol{a}\cdot\boldsymbol{n}} = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{\mathrm{e}^{\mathrm{i}\omega \boldsymbol{a}\cdot\boldsymbol{n}}}{\omega - \lambda - \mathrm{i}0} \tag{4.33}$$

and to integrate first over a solid angle, neglecting the ω-dependence in the denominator of the expression thus arising in accordance with the resonance approximation. Then, the remaining integration over the frequency yields the correct expressions (3.23) and (3.24) which have straightforwardly been derived from the model Hamiltonian (2.9)–(2.11).

To obtain the correction to the resonance transition frequency due to the effective interatomic coupling one simply needs to replace ω_{12} in expressions (4.24) and (4.29) by

$$\omega_{12}^{(\mathrm{s})} = \omega_{12} - I_2 = \omega_{12} - \frac{3\gamma}{(\omega_{12} l)^2} \int_0^{\infty} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{1}{\omega + \omega_{12}} \left(\frac{\sin \omega l}{\omega_{12} l} - \cos \omega l \right) \tag{4.34}$$

$$\omega_{12}^{(\mathrm{as})} = \omega_{12} + I_2 = \omega_{12} + \frac{3\gamma}{(\omega_{12} l)^2} \int_0^{\infty} \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{1}{\omega + \omega_{12}} \left(\frac{\sin \omega l}{\omega_{12} l} - \cos \omega l \right) \tag{4.35}$$

for the symmetric and antisymmetric eigenstates, respectively.

Thus, we have found the one-particle eigenstates of the model under consideration within the framework of the resonance approximation. In section 5 we will show that the Wigner–Weisskopf renormalization of the two-atom problem preserves causality, as must occur, in order for any renormalization procedure to be physical.

5. The Fermi problem

Further analysis of the 3D problem is obviously completely equivalent to that of the 1D model [1]. Indeed, the initial state of the atoms plus field system,

$$|\mathrm{In}\rangle = \sigma_1^+|0\rangle \tag{5.1}$$

is represented as a linear superposition of the one-particle eigenstates of the model,

$$|\mathrm{In}\rangle = \sum_{\sigma=a,as}\int_{-\infty}^{\infty}\frac{\mathrm{d}\lambda}{2\pi}A^{(\sigma)}(\lambda)|\lambda\rangle \qquad A^{(\sigma)}(\lambda) = \frac{\sqrt{\gamma}}{2}\,\frac{1}{\lambda-\Omega^{(\sigma)}-\mathrm{i}\Gamma^{(\sigma)}} \tag{5.2}$$

and, hence, the dynamics of the in-state is determined by

$$|\Phi(t)\rangle = \exp(-iHt)|\mathrm{In}\rangle = \sum_{\sigma=s,a}\int_{-\infty}^{\infty}\frac{\mathrm{d}\lambda}{2\pi}\,A^{(\sigma)}(\lambda)\mathrm{e}^{-\mathrm{i}\lambda t}|\lambda\rangle^{(\sigma)}\,. \tag{5.3}$$

Then, the probability amplitudes to find the atoms in the excited state are given by

$$\phi_1(t) \equiv \langle 0|\sigma_1^-|\Phi(t)\rangle = -\int_{-\infty}^{\infty}\frac{\mathrm{d}\lambda}{4\pi i}\left(\frac{1}{r_+(\lambda)}+\frac{1}{r_-(\lambda)}\right)\mathrm{e}^{-\mathrm{i}\lambda t} \tag{5.4}$$

$$\begin{aligned}\phi_2(t) \equiv \langle 0|\sigma_2^-|\Phi(t)\rangle &= -\int_{-\infty}^{\infty}\frac{\mathrm{d}\lambda}{4\pi i}\left(\frac{1}{r_+(\lambda)}-\frac{1}{r_-(\lambda)}\right)\mathrm{e}^{-\mathrm{i}\lambda t}\\ &= \gamma\int_{-\infty}^{\infty}\frac{\mathrm{d}\lambda}{2\pi\,\mathrm{i}}\,\frac{\mathrm{g}(\lambda)}{r_+(\lambda)r_-(\lambda)}\,\mathrm{e}^{\mathrm{i}\lambda t}\end{aligned} \tag{5.5}$$

where

$$r_+ = \lambda-\omega_{12}^{(s)}+\mathrm{i}\gamma(\tfrac{1}{2}+\mathrm{g}(\lambda)) \qquad r_- = \lambda-\omega_{12}^{(as)}+\mathrm{i}\gamma(\tfrac{1}{2}-\mathrm{g}(\lambda))\,. \tag{5.6}$$

Here we have omitted terms containing the functions $r_\pm^*(\lambda)$, because all the zeros of the functions $r_\pm(\lambda)$ lie below the real axis, and hence do not contribute to the integral for any $t > 0$.

It can now easily be seen that the probability amplitude for finding the second (initially unexcited) atom in the excited state vanishes on the interval $0 < t < l$, as it should be, in accordance with the causality principle.

The integrals in (5.4), (5.5) have the form

$$I_\pm(t) = -\mathrm{e}^{-\mathrm{i}\omega_{12}t}\int_{-\infty}^{\infty}\frac{\mathrm{d}\lambda}{4\pi i}\,\frac{\mathrm{e}^{-\mathrm{i}\lambda t}}{r_\pm(\lambda)} \tag{5.7}$$

$$r_\pm(\lambda) = \lambda+\mathrm{i}(\gamma/2)(1\pm b(l)\mathrm{e}^{\mathrm{i}(\lambda+\omega_{12})l}) \tag{5.8}$$

where

$$b(l) = -3\left(\frac{\mathrm{i}}{\omega_{12}l}+\frac{1}{(\omega_{12}l)^3}\right)$$

and

$$b(l) = -\frac{3}{2}\left(\frac{\mathrm{i}}{\omega_{12}l}-\frac{1}{(\omega_{12}l)^2}-\frac{\mathrm{i}}{(\omega_{12}l)^3}\right)$$

for the transitions $0 \Leftrightarrow 0$ and $\pm1 \Leftrightarrow 0$, respectively. It can easily be seen that these integrals are absolutely equivalent to that calculated in our previous article [1] devoted to the 1D

model of the resonance energy transfer. So, we can immediately present the following expressions for the atomic wavefunctions:

$$\phi_1^{(n)}(\tau) = \mathrm{e}^{-\mathrm{i}(\omega_{12}-\mathrm{i}\gamma/2)(t-nl)}\,\frac{1}{2n!}\left(\frac{\mathrm{d}^n}{\mathrm{d}z^n}[F_+(z)+F_-(z)]\right)\Big|_{z=0} \tag{5.9}$$

$$\phi_2^{(n)}(\tau) = \mathrm{e}^{-\mathrm{i}(\omega_{12}-\mathrm{i}\gamma/2)(t-nl)}\,\frac{1}{2n!}\left(\frac{\mathrm{d}^n}{\mathrm{d}z^n}[F_+(z)-F_-(z)]\right)\Big|_{z=0} \tag{5.10}$$

where

$$F_+(z) = \frac{\mathrm{e}^{-(\gamma/2)b\tau z}}{1 - z\mathrm{e}^{-(\gamma/2)lbz}\,\mathrm{e}^{-\mathrm{i}(\omega_{12}-\mathrm{i}\gamma/2)l}} \tag{5.11}$$

$$F_-(z) = \frac{\mathrm{e}^{(\gamma/2)b\tau z}}{1 - z\mathrm{e}^{(\gamma/2)lbz}\,\mathrm{e}^{-\mathrm{i}(\omega_{12}-\mathrm{i}\gamma/2)l}}\,. \tag{5.12}$$

Here the temporal axis $0 \leqslant t < \infty$ is divided into an infinite set of temporal zones, i.e. the temporal variable is represented as

$$t = \tau + nl \tag{5.13}$$

where $\tau \in (0, l)$ and $n = 0, 1, \ldots$. Carrying out the elementary calculations, the expressions for the atomic wavefunctions can be rewritten in the explicit form

$$\phi_1^{(n)}(\tau) = \sum_{m=0}^{n} \frac{(n-m)!}{2n!}\left(\frac{\gamma}{2}b(l)\right)^m \left[(ml-t)^m + (t-ml)^m\right]\mathrm{e}^{-\mathrm{i}(\omega_{12}-\gamma/2)(t-ml)} \tag{5.14}$$

$$\phi_2^{(n)}(\tau) = \sum_{m=0}^{n} \frac{(n-m)!}{2n!}\left(\frac{\gamma}{2}b(l)\right)^m \left[(ml-t)^m - (t-ml)^m\right]\mathrm{e}^{-\mathrm{i}(\omega_{12}-\gamma/2)(t-ml)}\,. \tag{5.15}$$

The functions $\phi_1^{(n)}$ and $\phi_2^{(n)}$ contain only even ($m = 2k$) and odd ($m = 2k+1$) terms of the sum, respectively. Therefore, the function $\phi_1^{(n)}$ is not changed at the odd points $n = 2k+1$, while the function $\phi_2^{(n)}$ is conserved at the even points $n = 2k$.

In the limiting case of large interatomic distances $l \gg \omega_{12}^{-1}$, one can restrict a consideration by the first several temporal zones. Then, we have

$$\phi_1(t) = \mathrm{e}^{-\mathrm{i}\omega_{12}t}\mathrm{e}^{-\gamma t}\begin{cases} 1 & 0 \leqslant t < 2l \\ 1 - \frac{1}{2}\left(\frac{1}{2}\gamma b(l)\right)^2 (t-2l)^2\mathrm{e}^{2\mathrm{i}(\omega_{12}-\mathrm{i}\gamma/2)l} & 2l \leqslant t < 4l \end{cases} \tag{5.16}$$

$$\phi_2(t) = \mathrm{e}^{-\mathrm{i}\omega_{12}t}\mathrm{e}^{-\gamma t}\begin{cases} 0 & 0 \leqslant t < l \\ -\frac{1}{2}\gamma b(l)(t-l)\mathrm{e}^{\mathrm{i}(\omega_{12}-\mathrm{i}\gamma/2)l} & l \leqslant t < 3l\,. \end{cases} \tag{5.17}$$

The 'retardation' effect is obvious to take place at the moment of time $t = 2l$ and to be repeated in the period $T = 2l$.

Finally, it should be noted that the results for the 3D model is distinctly different from those of the 1D model. In the 3D model, we saw the resonance transition, via the definition $\lambda_{12} = \omega_{12}^{-1}$, appearing also in the role of a characteristic interatomic separation (wavelength). On the other hand, in the case of the 1D model [1], an interatomic influence extended up to even macroscopically large interatomic distances, $l \approx \gamma^{-1}$. The difference is that in 3D waves can disperse more easily, whereas in 1D they are channelled.

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Appendix

Here we demonstrate the method of the summation over spherical harmonics which is used in this article. For instance, for the transition $0 \leftrightarrow 0$ the characteristic expression has the form

$$G = \sum_{jm} \pi^*_{jm}(\boldsymbol{n}')\pi_{jm}(\boldsymbol{n}) = \frac{3}{8\pi}(\boldsymbol{e}_z \cdot \nabla_{\boldsymbol{n}})(\boldsymbol{e}_z \cdot \nabla_{\boldsymbol{n}'})\mathcal{D}(\boldsymbol{n}, \boldsymbol{n}') \tag{A.1}$$

where the function

$$\mathcal{D}(\boldsymbol{n}, \boldsymbol{n}') = \sum_{jm} \frac{1}{j(j+1)} Y^*_{jm}(\boldsymbol{n}')Y_{jm}(\boldsymbol{n}) \tag{A.2}$$

is obviously the Green function of the angular part of the Laplace operator

$$\Delta_{\boldsymbol{n}}\mathcal{D}(\boldsymbol{n}, \boldsymbol{n}') = \delta(\boldsymbol{n} - \boldsymbol{n}') \tag{A.3}$$

and, hence, depends on $(\boldsymbol{n} - \boldsymbol{n}')$ only. Then, the differential operator in (A.1) is rewritten as follows:

$$(\boldsymbol{e}_z \cdot \nabla_{\boldsymbol{n}})(\boldsymbol{e}_z \cdot \nabla_{\boldsymbol{n}'}) = -(\boldsymbol{e}_z \cdot \nabla_{\boldsymbol{n}})(\boldsymbol{e}_z \cdot \nabla_{\boldsymbol{n}}) = \sin^2\theta\, \Delta_{\boldsymbol{n}} + \frac{\partial^2}{\partial\phi^2} \tag{A.4}$$

and we find

$$G = \frac{3}{8\pi}\left(\sin^2\theta\, \delta(\boldsymbol{n} - \boldsymbol{n}') + \frac{\partial^2}{\partial\phi^2}\mathcal{D}(\boldsymbol{n} - \boldsymbol{n}')\right) \tag{A.5}$$

where the contribution of the second term vanishes after the integration over ϕ, because in the geometry of our problem $\boldsymbol{a}||\hat{z}$.

An analoguous result can be obtained by a similar, but more tedious way for the transition $\pm 1 \leftrightarrow 0$:

$$G = \sum_{\alpha=e,m}\sum_{jm} \pi^{(\alpha)*}_{jm}(\boldsymbol{n}')\pi^{(\alpha)}_{jm}(\boldsymbol{n}) = \frac{3}{8\pi}\left(1 - \frac{1}{2}\sin^2\theta\right)\delta(\boldsymbol{n} - \boldsymbol{n}')\,. \tag{A.6}$$

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