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Erratum

Erratum for *JCMNS* **27** (2018) 97–142, "Phonon-mediated Nuclear Excitation Transfer"

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Abstract

This erratum concerns a model appearing in Appendix B, which was added hastily prior to sending in the paper. The Hamiltonian for a set of two two-level systems that are driven by an electromagnetic field, and which undergo resonant excitation transfers, is incorrect. In this erratum the Hamiltonian is corrected. The Ehrenfest theorem equations for the updated Hamiltonian are much more complicated, and it is not obvious that such a complicated model will be useful. We also provide a correction to Equation (69) of the paper.

Keywords: Coherence, Ehrenfest theorem, Resonant excitation transfer, Phonon–nuclear coupling, Quantum dynamics

1. Introduction

The Appendix B of this paper [1] was added hastily just before sending off, and was subsequently found to be in error. This was drawn to my attention by Matt Lilly, who has been interested in excitation transfer. The Hamiltonian used in this work is not correct, and leads to a relatively simple model which was thought to be of use. In this Erratum we would like to correct the Hamiltonian, and to provide some of the Ehrenfest theorem equations that result. The model that results is considerably more complicated, and it is not obvious that such a complicated model will be useful.

2. Model

The idea was to specify a simple and idealized model for resonant excitation transfer between two sites, under conditions where an incident monochromatic electromagnetic wave is incident.

2.1. Hamiltonian

The Hamiltonian used should have been

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$$\hat{H} = \Delta E \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} + U_0 \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$+V_0 \begin{bmatrix} 0 & \mathrm{e}^{-i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)} & \mathrm{e}^{-i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)} & 0 \\ \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)} & 0 & 0 & \mathrm{e}^{-i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)} \\ \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)} & 0 & 0 & \mathrm{e}^{-i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)} \\ 0 & \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)} & \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)} & 0 \end{bmatrix}. \tag{1}$$

This Hamiltonian is relevant to basis states defined according to $\{\downarrow\downarrow, \downarrow\uparrow, \uparrow\downarrow, \uparrow\uparrow\}$.

2.2. Equivalent two-level system operators

It is reasonable to define equivalent two-level system operators according to

$$\sigma_x^{(1)} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \qquad \sigma_y^{(1)} = \begin{bmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{bmatrix}, \qquad \sigma_z^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \tag{2}$$

$$\sigma_x^{(2)} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, \qquad \sigma_y^{(2)} = \begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{bmatrix}, \qquad \sigma_z^{(2)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}. \tag{3}$$

2.3. Evolution equations for two-level system operators

We make use of Ehrenfest's theorem

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{Q} \rangle = \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle + \frac{1}{i\hbar} \left\langle [\hat{Q}, \hat{H}] \right\rangle \tag{4}$$

to develop dynamical equations for expectation values associated with this model. This leads directly to

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \sigma_x^{(1)} \rangle = -\omega_0 \langle \sigma_y^{(1)} \rangle + \frac{2V_0}{\hbar} \sin(\mathbf{k}\cdot\mathbf{r}_1 - \omega t) \langle \sigma_z^{(1)} \rangle + \frac{U_0}{\hbar} \left\langle \begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{bmatrix} \right\rangle, \tag{5}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \sigma_y^{(1)} \rangle = \omega_0 \langle \sigma_x^{(1)} \rangle - \frac{2V_0}{\hbar} \cos(\mathbf{k}\cdot\mathbf{r}_1 - \omega t) \langle \sigma_z^{(1)} \rangle - \frac{U_0}{\hbar} \left\langle \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} \right\rangle, \tag{6}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\sigma_z^{(1)}\rangle = 2\frac{V_0}{\hbar}e^{-i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)}\left\langle\begin{bmatrix}0 & -i & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & -i\\ 0 & 0 & 0 & 0\end{bmatrix}\right\rangle + 2\frac{V_0}{\hbar}e^{i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)}\left\langle\begin{bmatrix}0 & 0 & 0 & 0\\ i & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & i & 0\end{bmatrix}\right\rangle$$
$$-\frac{2U_0}{\hbar}\left\langle\begin{bmatrix}0 & 0 & 0 & 0\\ 0 & 0 & -i & 0\\ 0 & i & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}\right\rangle, \tag{7}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\sigma_x^{(2)}\rangle = -\omega_0\langle\sigma_y^{(2)}\rangle + \frac{2V_0}{\hbar}\sin(\mathbf{k}\cdot\mathbf{r}_2-\omega t)\langle\sigma_z^{(2)}\rangle + \frac{U_0}{\hbar}\left\langle\begin{bmatrix}0 & -i & 0 & 0\\ i & 0 & 0 & 0\\ 0 & 0 & 0 & i\\ 0 & 0 & -i & 0\end{bmatrix}\right\rangle, \tag{8}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\sigma_y^{(2)}\rangle = \omega_0\langle\sigma_x^{(2)}\rangle - \frac{2V_0}{\hbar}\cos(\mathbf{k}\cdot\mathbf{r}_2-\omega t)\langle\sigma_z^{(2)}\rangle - \frac{U_0}{\hbar}\left\langle\begin{bmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{bmatrix}\right\rangle, \tag{9}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\sigma_z^{(2)}\rangle = 2\frac{V_0}{\hbar}e^{-i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)}\left\langle\begin{bmatrix}0 & 0 & -i & 0\\ 0 & 0 & 0 & -i\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}\right\rangle + 2\frac{V_0}{\hbar}e^{i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)}\left\langle\begin{bmatrix}0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ i & 0 & 0 & 0\\ 0 & i & 0 & 0\end{bmatrix}\right\rangle$$
$$+\frac{2U_0}{\hbar}\left\langle\begin{bmatrix}0 & 0 & 0 & 0\\ 0 & 0 & -i & 0\\ 0 & i & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}\right\rangle. \tag{10}$$

Ehrenfest theorem equations often couple to more complicated expectation values, as is the case here.

2.4. Evolution equations for some of the other operators

We can write evolution equations for some of the operators that appear in these equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\begin{bmatrix}0 & 0 & 0 & 0\\ 0 & 0 & -i & 0\\ 0 & i & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}\right\rangle = -\frac{V_0}{\hbar}\mathrm{e}^{-i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)}\left\langle\begin{bmatrix}0 & 1 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\end{bmatrix}\right\rangle - \frac{V_0}{\hbar}\mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)}\left\langle\begin{bmatrix}0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 1 & 0\end{bmatrix}\right\rangle$$
$$-2\frac{U_0}{\hbar}\left\langle\begin{bmatrix}0 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}\right\rangle, \tag{11}$$

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{bmatrix}\right\rangle \;=\; & \frac{\Delta E}{\hbar}\left\langle\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}\right\rangle - \frac{2V_0}{\hbar}\cos(\mathbf{k}\cdot\mathbf{r}_2-\omega t)\left\langle\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\right\rangle \\
& + \frac{2V_0}{\hbar}e^{-i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)}\left\langle\begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\right\rangle + \frac{2V_0}{\hbar}\mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)}\left\langle\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}\right\rangle - \frac{U_0}{\hbar}\langle\sigma_x^{(1)}\rangle,
\end{aligned}
\tag{12}
$$

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}\right\rangle \;=\; & -\frac{\Delta E}{\hbar}\left\langle\begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{bmatrix}\right\rangle + \frac{2V_0}{\hbar}\sin(\mathbf{k}\cdot\mathbf{r}_2-\omega t)\left\langle\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\right\rangle \\
& + \frac{2V_0}{\hbar}\mathrm{e}^{-i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)}\left\langle\begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\right\rangle + \frac{2V_0}{\hbar}\,\mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}_1-\omega t)}\left\langle\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}\right\rangle + \frac{U_0}{\hbar}\langle\sigma_y^{(1)}\rangle,
\end{aligned}
\tag{13}
$$

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\begin{bmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{bmatrix}\right\rangle \;=\; & -\frac{\Delta E}{\hbar}\left\langle\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{bmatrix}\right\rangle - \frac{2V_0}{\hbar}\cos(\mathbf{k}\cdot\mathbf{r}_1-\omega t)\left\langle\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\right\rangle \\
& - \frac{2V_0}{\hbar}\mathrm{e}^{-i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)}\left\langle\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\right\rangle + \frac{2V_0}{\hbar}\mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)}\left\langle\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}\right\rangle + \frac{U_0}{\hbar}\langle\sigma_x^{(2)}\rangle,
\end{aligned}
\tag{14}
$$

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{bmatrix}\right\rangle \;=\; & -\frac{\Delta E}{\hbar}\left\langle\begin{bmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{bmatrix}\right\rangle + \frac{2V_0}{\hbar}\sin(\mathbf{k}\cdot\mathbf{r}_1-\omega t)\left\langle\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\right\rangle \\
& + \frac{2V_0}{\hbar}\mathrm{e}^{-i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)}\left\langle\begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\right\rangle + \frac{2V_0}{\hbar}\mathrm{e}^{+i(\mathbf{k}\cdot\mathbf{r}_2-\omega t)}\left\langle\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}\right\rangle + \frac{U_0}{\hbar}\langle\sigma_y^{(2)}\rangle.
\end{aligned}
\tag{15}
$$

At this point we have 11 Ehrenfest theorem equations, and it is clear that many more will emerge from continued calculations.

3. Discussion

The motivation initially for this kind of model was that perhaps we might be able to gain some insight as to what happens in a simple model with a driven transition and excitation transfer. The advantage of using Ehrenfest theorem equations for this is that we can add loss terms approximately in a convenient generalization.

Only a modest number of coupled Ehrenfest theorem equations resulted from the incorrect Hamiltonian adopted in [1], and a model with only a modest number of coupled equations would have been useful. When a more suitable Hamiltonian is used it seems clear that the problem is more complicated. Consequently, it is not obvious that this approach will be useful.

A model for excitation transfer among different sites in a lattice would be very useful, and there are other approaches to develop such a model. More important is the intuition that would result from the solutions to such a model. Similarly, a model for excitation transfer that includes driving terms associated with an incident electromagnetic field for use in connection with a synchrotron experiment would be useful. We hope to report progress on such models soon.

4. Contribution to excitation transfer

We note in addition that Equation (69) in the manuscript should read

$$
\begin{aligned}
T_{s1} \;=\; & i\frac{(Mc^2)^2}{4N}\sum_{J_2}\sum_{J_2'}\left(\frac{2}{(E_{10}-E_{00})(E_{10}-E_{20})(E_{10}-E_{2'0})}-\frac{2}{(E_{10}-E_{11})(E_{10}-E_{21})(E_{10}-E_{2'1})}\right. \\
& \left.+\frac{1}{(E_{10}-E_{20})(E_{10}-E_{2'0})(E_{10}-E_{2'2})}-\frac{1}{(E_{10}-E_{21})(E_{10}-E_{2'1})(E_{10}-E_{2'2})}\right) \\
& \sum_j\sum_{j'}\sum_{m_0}\sum_{m_1}\sum_{m_2}\sum_{m_0'}\sum_{m_1'}\sum_{m_2'}\Big(|J_0m_0\rangle\langle J_1m_1|\Big)_j\Big(|J_1m_1'\rangle\langle J_0m_0'|\Big)_{j'} \\
& \sum_\alpha\sum_\beta\sum_\gamma\sum_\delta(\langle J_0m_0|\mathbf{a}_j|J_2m_2\rangle)_\alpha(\langle J_2m_2|\mathbf{a}_j|J_1m_1\rangle)_\beta(\langle J_1m_1'|\mathbf{a}_{j'}|J_2'm_2'\rangle)_\gamma(\langle J_2'm_2'|\mathbf{a}_{j'}|J_0m_0'\rangle)_\delta \\
& \left[\frac{1}{N}\sum_{\mathbf{k},\sigma}(\hbar\omega_{\mathbf{k},\sigma})^2(\mathbf{u}_{\mathbf{k},\sigma})_\alpha(\mathbf{u}_{\mathbf{k},\sigma})_\beta(\mathbf{u}_{\mathbf{k},\sigma})_\gamma(\mathbf{u}_{\mathbf{k},\sigma})_\delta\hat{n}_{\mathbf{k},\sigma}\sin\left(2\mathbf{k}(\mathbf{R}_{j'}^{(0)}-\mathbf{R}_j^{(0)})\right)\right]
\end{aligned} \tag{16}
$$

References

[1] P.L. Hagelstein, Phonon-mediated nuclear excitation transfer, *J. Condensed Matter Nucl. Sci.* **27** (2018) 97–142.