

Erratum: “Surface hopping with a manifold of electronic states. III. Transients, broadening and the Marcus picture” [J. Chem. Phys. 142, 234106 (2015)]

Wenjie Dou, Abraham Nitzan, and Joseph E. Subotnik

Citation: *The Journal of Chemical Physics* **143**, 189902 (2015); doi: 10.1063/1.4935713

View online: <http://dx.doi.org/10.1063/1.4935713>

View Table of Contents: <http://scitation.aip.org/content/aip/journal/jcp/143/18?ver=pdfcov>

Published by the [AIP Publishing](#)

Articles you may be interested in

Erratum: “Virial coefficients and demixing in the Asakura–Oosawa model” [J. Chem. Phys. 142, 014902 (2015)]

J. Chem. Phys. **143**, 029902 (2015); 10.1063/1.4926462

Surface hopping with a manifold of electronic states. III. Transients, broadening, and the Marcus picture

J. Chem. Phys. **142**, 234106 (2015); 10.1063/1.4922513

Erratum: “Velocity redistribution of excited atoms by radiative excitation transfer. II. Theory of radiation trapping in collimated beams” [J. Chem. Phys. 119, 7094 (2003)]

J. Chem. Phys. **120**, 4545 (2004); 10.1063/1.1643893

Erratum: “Fourth-order quantum master equation and its Markovian bath limit” [J. Chem. Phys. 116, 2705 (2002)]

J. Chem. Phys. **117**, 10428 (2002); 10.1063/1.1519534

Erratum: “Three-body collision contributions to recombination and collision-induced dissociation. II. Kinetics” [J. Chem. Phys. 109, 6714 (1998)]

J. Chem. Phys. **113**, 1668 (2000); 10.1063/1.481957

A promotional banner for AIP Applied Physics Reviews. On the left is a thumbnail of a journal cover for 'Applied Physics Reviews' featuring a diagram of a device. The main part of the banner has a blue background with a bright light source on the right. The text 'NEW Special Topic Sections' is prominently displayed in white. Below this, in an orange bar, it says 'NOW ONLINE' and 'Lithium Niobate Properties and Applications: Reviews of Emerging Trends'. The AIP Applied Physics Reviews logo is in the bottom right corner.

NEW Special Topic Sections

NOW ONLINE
Lithium Niobate Properties and Applications:
Reviews of Emerging Trends

AIP Applied Physics Reviews

Erratum: “Surface hopping with a manifold of electronic states. III. Transients, broadening and the Marcus picture” [J. Chem. Phys. 142, 234106 (2015)]

Wenjie Dou,¹ Abraham Nitzan,² and Joseph E. Subotnik¹

¹Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA

²School of Chemistry, The Sackler Faculty of Science, Tel Aviv University, Tel Aviv 69978, Israel

(Received 2 November 2015; accepted 2 November 2015; published online 11 November 2015)

[<http://dx.doi.org/10.1063/1.4935713>]

An error appeared in Eqs. (22) and (23) for the referenced article. As originally published, the equations of motion for the reduced density matrices are lacking their respective complex conjugates.¹ The correct nonsecular (full) quantum master equation (nQME) should read

$$\begin{aligned} \frac{d\rho_0(i,j)}{dt} = & -\frac{\mathbf{i}}{\hbar}(\epsilon_0(i) - \epsilon_0(j))\rho_0(i,j) - \frac{\Gamma}{2\hbar} \sum_{i',k} f(\epsilon_1(i') - \epsilon_0(k))F_{i \rightarrow i'}F_{k \rightarrow i'}\rho_0(k,j) \\ & - \frac{\Gamma}{2\hbar} \sum_{i',k} \rho_0(i,k)f(\epsilon_1(i') - \epsilon_0(k))F_{j \rightarrow i'}F_{k \rightarrow i'} + \frac{\Gamma}{2\hbar} \sum_{i',j'} (1 - f(\epsilon_1(j') - \epsilon_0(j)))F_{i \rightarrow i'}F_{j \rightarrow j'}\rho_1(i',j') \\ & + \frac{\Gamma}{2\hbar} \sum_{i',j'} \rho_1(i',j')(1 - f(\epsilon_1(i') - \epsilon_0(i)))F_{i \rightarrow i'}F_{j \rightarrow j'}, \end{aligned} \quad (22)$$

$$\begin{aligned} \frac{d\rho_1(i',j')}{dt} = & -\frac{\mathbf{i}}{\hbar}(\epsilon_1(i') - \epsilon_1(j'))\rho_1(i',j') - \frac{\Gamma}{2\hbar} \sum_{i,k'} (1 - f(\epsilon_1(k') - \epsilon_0(i)))F_{i \rightarrow i'}F_{i \rightarrow k'}\rho_1(k',j') \\ & - \frac{\Gamma}{2\hbar} \sum_{i,k'} \rho_1(i',k')(1 - f(\epsilon_1(k') - \epsilon_0(i)))F_{i \rightarrow j'}F_{i \rightarrow k'} + \frac{\Gamma}{2\hbar} \sum_{i,j} f(\epsilon_1(j') - \epsilon_0(j))F_{i \rightarrow i'}F_{j \rightarrow j'}\rho_0(i,j) \\ & + \frac{\Gamma}{2\hbar} \sum_{i,j} \rho_0(i,j)f(\epsilon_1(i') - \epsilon_0(i))F_{i \rightarrow i'}F_{j \rightarrow j'}. \end{aligned} \quad (23)$$

For the sake of clarity, above, we use bold \mathbf{i} to denote the imaginary unit. As a result of this error, the nQME data in Figures 1 and 2 of the reference paper are only slightly changed, as presented below. The overall conclusions of our paper are

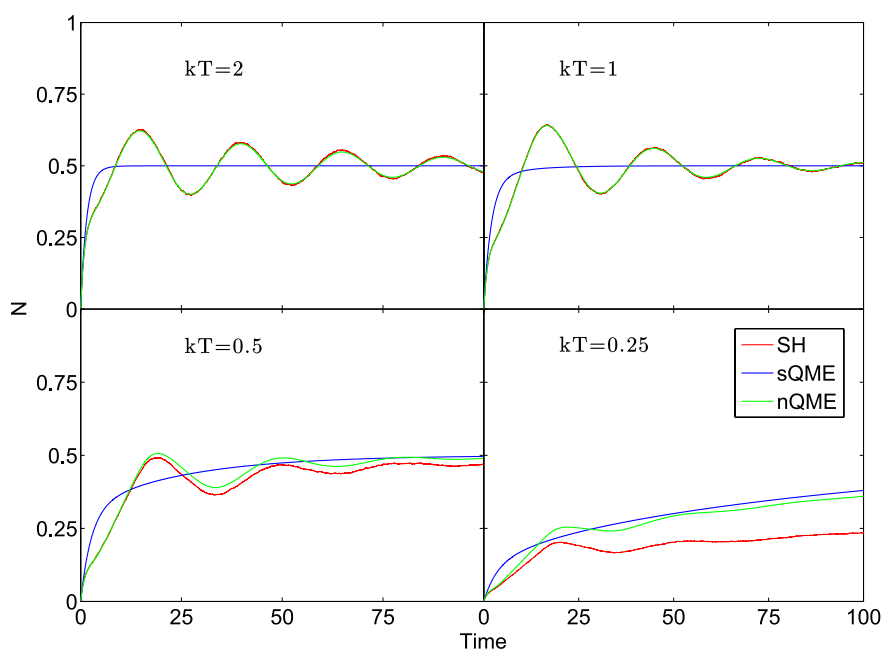


FIG. 1. Transient dynamics: the impurity electron population as a function of time. $\Gamma = 1$, $\hbar\omega = 0.3$, e-ph coupling $g = 0.75$, $\vec{E}_d = 0$. Note that SH and nQME agree at high temperatures. The sQME does not show any oscillations in electronic population, whereas the nQME shows transient oscillations which are (empirically) close to the frequency ω . At time zero, the phonon is prepared to be equilibrated thermally (assuming the impurity is unoccupied).

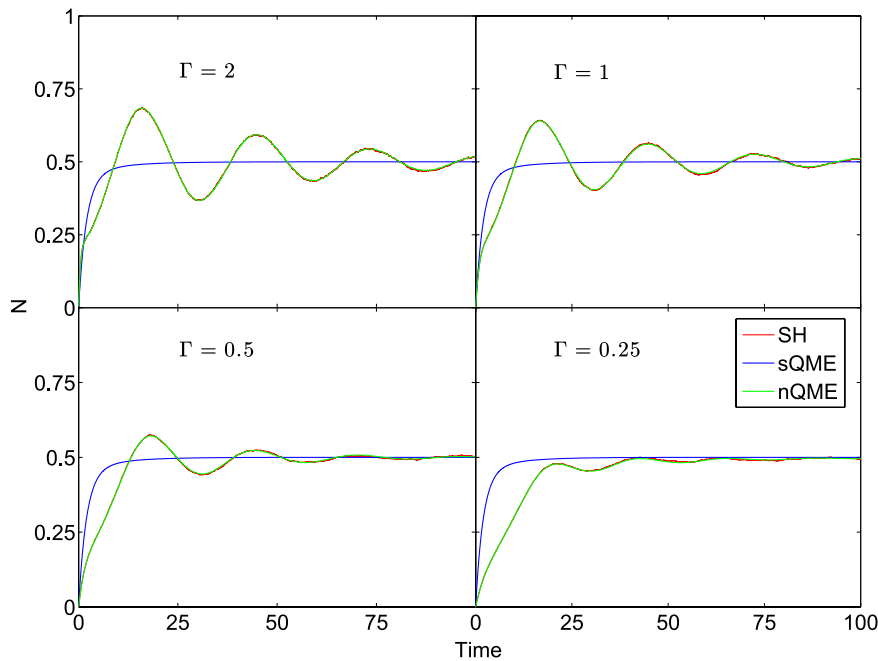


FIG. 2. Transient dynamics: the impurity electron population as a function of time. $kT = 1$, $\hbar\omega = 0.3$, e-ph coupling $g = 0.75$, $E_d = 0$. Note that SH and nQME agree over a large range of Γ . The sQME does not show any oscillations in electronic population, whereas the nQME shows transient oscillations which are (empirically) close to the frequency ω . At time zero, the phonon is prepared to be equilibrated thermally (assuming the impurity is unoccupied).

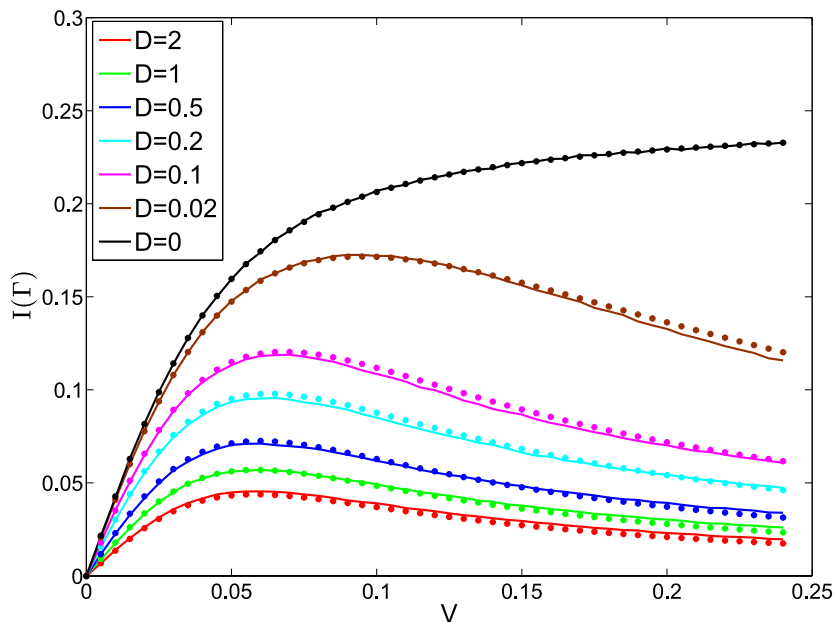


FIG. 6. I-V curves for different values of D (see Eq. (46)). Lines from SH, dots from the sQME. $g = 0.005$, $\hbar\omega = 0.003$, $kT = 0.01$, $\Gamma = 2\Gamma_0 = 0.01$, $E_d = 0$. We observe negative differential resistance when D is nonzero.

unchanged; in fact, however, it now appears that the classical master equation matches up with the nonsecular quantum master equation even better than before.

There was also a typo in Eq. (26) of the referenced article, which should read

$$F_{i \rightarrow i'} = (p!/Q!)^{1/2} \lambda^{Q-p} e^{-\lambda^2/2} L_p^{Q-p}(\lambda^2) [\text{sgn}(i' - i)]^{i-i'}. \quad (26)$$

Additionally, there was a numerical error for Figure 6 for the secular quantum master equation (sQME) data. After correction, sQME agrees with surface hopping (SH) almost exactly.

¹W. Dou, A. Nitzan, and J. E. Subotnik, "Surface hopping with a manifold of electronic states. III. Transients, broadening and the Marcus picture," *J. Chem. Phys.* **142**, 234106 (2015).