RELAXATION TIME APPROXIMATION IN THE PRESENCE OF CAPTURE PROCESSES INVOLVING REAL PROBABILITY DEPLETION

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The straightforward application of the standard relaxation time procedure is shown to lead to unacceptable results when capture processes involving an actual depletion of the density or probability of the moving particle coexist with scattering processes. It is shown through an explicit prescription how the standard approximation procedure may be modified for such situations.

The well-known relaxation-time approximation of transport theory [1,2], when applied in its standard form to cases wherein true sink processes causing real depletion of the density or probability of the moving particle coexist with the collision processes, leads to a certain absurdity. In this note we point out this problem and suggest how the relaxation-time approximation should be modified in such situations.

These situations are quite physical. A moving quasi-particle such as an electron or an exciton could undergo a capture process such as trapping at a site along with the usual scattering arising from phonon or defect interactions. The transport equation describing the evolution of the probability $f_k(t)$ that the k-state is occupied is then

$$\mathrm{d}f_k(t)/\mathrm{d}t + \alpha_k f_k(t) = \sum_{k'} [Q_{kk'} f_{k'}(t) - Q_{k'k} f_k(t)] , \tag{1}$$

where the k'-summation would be an integral if k is continuous, where α_k is the capture rate, $Q_{kk'}$ denotes the usual scattering rates and where the trap state is external to the k-band.

The standard relaxation-time procedure would replace the right-hand side of eq. (1) by a simple decay term. Specifically, eq. (1) would be approximated by

$$\mathrm{d}f_k(t)/\mathrm{d}t + \alpha_k f_k(t) = (f_k^{\mathrm{th}} - f_k(t))/\tau_k , \tag{2}$$

where τ_k is the relaxation time suitably obtained from the rates $Q_{kk'}$, and f_k^{th} is the t-independent thermal distribution. Eq. (2) is, however, quite unacceptable because it leads to the incorrect result that $f_k(t)$ tends to the non-zero value $f_k^{\mathrm{th}}/(\alpha_k\tau_k + 1)$ at long times. It is quite clear from eq. (1) or from the physics of the problem, that $f_k(t)$ should actually tend to zero since eventually the quasi-particle would go completely out of the k-band and into the trap.

It is important from a practical viewpoint to learn how to modify the standard relaxation-time prescription in the presence of real capture processes. As in the sinkless case realistic scattering rates $Q_{kk'}$ are usually complicated enough to defy exact analysis and necessitate the use of such approximation procedures. Replacing f_k^{th} by zero in eq. (2) does give the required long-time limit of $f_k(t)$ but hardly constitutes a solution of the problem because one *cannot* then recover the usual result $f_k(t) \to f_k^{\mathrm{th}}$ in the absence of sinks if we put $\alpha_k = 0$.

We arrive at our suggestion for the modified procedure (eq. (6) below) by analysing how the standard relaxation-time approximation (for $\alpha_k = 0$) is obtained. There is a simple case when that approximation is exact. This happens when the scattering rates are constant: $Q_{kk'} = \Gamma/N$, where N is the number of k-

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states in the band. Putting $\alpha_k = 0$, eqs. (1) and (2) are found to be *equivalent* to each other if the relaxation time $\tau_k = (\Sigma_{k'} Q_{k'k})^{-1} = 1/\Gamma$ since, for this case, $f_k^{\rm th} = 1/N$. Although there are generally extra factors in the usual expressions [1,2] for τ_k, let us retain the above prescription

$$1/\tau_k = \sum_{k'} Q_{k'k}, \tag{3}$$

and observe that the standard relaxation-time procedure (for $\alpha_k = 0$) for the general case involving nonconstant $Q_{kk'}$ may be said to arise from the approximation

$$\sum_{k'} Q_{kk'} f_{k'}(t) \approx f_k^{\rm th} \sum_{k'} Q_{k'k} = f_k^{\rm th}/\tau_k, \tag{4}$$

for the first term on the right-hand side of eq. (1), and eq. (3) for the second term. Alternatively, the extra factors such as $(1 - \cos\theta)$ that arise in elastic scattering [1,2], may be incorporated in *both* eqs. (4) and (3). Note that in a certain sense eq. (4) arises from detailed balance.

We now suggest that in the presence of true sinks eq. (4) should be replaced by the natural extension

$$\sum_{k'} Q_{kk'} f_{k'}(t) \approx \left(f_k^{\rm th} \sum_{k'} Q_{k'k}\right) \sum_{k'} f_{k'}(t) = [f_k^{\rm th}/\tau_k] F(t), \tag{5}$$

where $F(t) = \Sigma_k f_k(t)$ is the total probability that the band is still excited. In the absence of capture processes $F(t) = 1$ and the standard results [1,2] are recovered. Generally, our prescription approximates eq. (1) not by eq. (2) but by

$$\mathrm{d}f_k(t)/\mathrm{d}t + \alpha_k f_k(t) = (f_k^{\rm th} F(t) - f_k(t))/\tau_k. \tag{6}$$

The τ_k may be obtained from more general standard approximations [1,2] and not necessarily from eq. (3).

Eq. (6) has the solution

$$f_k(t) = f_k(0) \exp\{-t(\alpha_k + 1/\tau_k)\} + (f_k^{\rm th}/\tau_k) \int_0^t \mathrm{d}t \exp\{-(t-t')(\alpha_k + 1/\tau_k)\} F(t'). \tag{7}$$

The total probability that the particle has not yet been captured, i.e. $F(t)$, may be either approximated by a suitable average exponential $\mathrm{e}^{-t\alpha}$ which would lead to

$$f_k(t) = [f_k(0) - f_k^{\rm th}/(\tau_k(\alpha_k - \alpha) + 1] \times \exp\{-t(\alpha_k + 1/\tau_k)\} + [f_k^{\rm th}/(\tau_k(\alpha_k - \alpha) + 1)] \exp\{-t\alpha\}, \tag{8}$$

or it may be obtained exactly from

$$F(t) = \int_0^t \mathrm{d}t'\, g(t - t') \times \sum_k f_k(0) \exp\{-t'(\alpha_k + 1/\tau_k)\}, \tag{9}$$

wherein $g(t)$ is given by

$$g(t) = \mathcal{L}^{-1}\left[1 - \mathcal{L} \sum_k (f_k^{\rm th}/\tau_k) \times \exp\{-t(\alpha_k + 1/\tau_k)\}\right]^{-1}, \tag{10}$$

the symbols $\mathcal{L}$ and $\mathcal{L}^{-1}$ denoting, respectively, the Laplace and the Laplace inverse transforms.

Exact evaluation of eqs. (10), (9) and (8) is possible for certain cases, and for others perturbative and nonperturbative approximation schemes for the calculation of $F(t)$ can be used. An application of some of that material will be reported elsewhere [3] in the context of exciton capture.

References

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