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Energetic consequences of decoherence at small times for coupled systems

B Gaveau[1] and L S Schulman[2,3]

[1] Laboratoire analyse et physique mathématique, 14 avenue Félix Faure, 75015 Paris, France
[2] Physics Department, Clarkson University, Potsdam, NY 13699-5820, USA
[3] Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, D-01187 Dresden, Germany

E-mail: gaveau@ccr.jussieu.fr and schulman@clarkson.edu

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Abstract

Disentangling two systems can cause an increase in energy, as discussed in Schulman and Gaveau (2006 *Phys. Rev. Lett.* **97** 240405). We here prove a critical inequality used in that letter. Let A and B be two systems and suppose that the initial density matrix for the combined system is a product. Let them have coupling V and let them evolve for a time t under the full Hamiltonian (including V). For the now-entangled full density matrix, the energy is unchanged. Next, disentangle, obtaining the new density matrix for A by tracing over the B variables, and similarly for B. We show that for a large class of V's the expected energy obtained using the product of the disentangled density matrices exceeds the original energy.

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1. Introduction

In [1] we explored the effect of decoherence and entanglement on energy conservation. Specifically, it appeared that the mere fact that two particles separated after an elastic collision could cause an increase in their total energy. Of course further examination showed that this was not the case; nevertheless, certain kinds of decoherence that one might have considered harmless did in fact change a system's energy.

In our previous study [1] we made use of an inequality with the following content: let there be two systems, A and B, interacting with a potential V, of a particular form. Let the system initially have a density matrix that is a product of A and B density matrices, i.e. it is of the form $\rho_A(0) \otimes \rho_B(0)$ (using standard notation). Now let it evolve under the full Hamiltonian for a time t. The time-t density matrix is not in general a product, since the

Hamiltonian entangles the two systems. But now we take a partial trace over each subsystem. Thus we define e.g., $\rho_A(t) \equiv \mathrm{Tr}_B \rho(t)$, with Tr_B the trace over the B-variables. If we evaluate the energy using the untraced $\rho(t)$, it will be unchanged from its time-0 value. However, if $\rho(t)$ is replaced by $\rho_A(t) \otimes \rho_B(t)$, then the energy could change, and with the form of V used in [1] and for short periods of time, it always increases.

In the present paper we present a detailed derivation of the inequality used in [1]. In particular, we will indicate the conditions on V, the interaction, necessary for the result to hold. Although the result is more general than was indicated in [1], it does not hold universally. In particular, as mentioned in [1], while the spin-boson model does have the indicated energy increase, the Jaynes–Cummings model does not.

The result of [1] suggests that operations that seem quite innocent, in particular the erasure of certain correlations, can have significant effects. The Boltzmann H-theorem [2] may be the most well-known example of this, but other discussions, such as van Kampen's criticism of the Green–Kubo formula, may well hinge on similar issues [3–5]. Another situation with surprising survival of entanglement effects is studied in [6, 7].

The calculation we are about to present does not have shortcuts and involves quite a bit of attention to detail. Its structure is similar to that of a calculation of measurement-induced dissipation [8] related to the Lindblad equation. It would be of great interest if a simpler demonstration could be found.

2. Coupled systems: definitions

Consider two quantum systems A and B. The Hamiltonian of A is H_A and similarly for B. The full system A+B has the Hamiltonian

$$H = H_A + H_B + \sum_{i=1}^{N} A_i \otimes B_i. \tag{1}$$

Here A_i (resp. B_i) are operators acting on A (resp. B) only. In the following, definitions are understood to apply to both A and B, and 'resp.' will be omitted. In general, the index A means an operator acting only on system A. In equation (1), H_A is an abbreviation for $H_A \otimes I_B$ where I_B is the identity operator on B. A_i and B_i are assumed to be Hermitian. We also require that the A_i's, as well as the B_i's, commute with one another:

$$[A_i, A_j] = 0 \qquad (\forall\, i, j), \qquad [B_i, B_j] = 0 \qquad (\forall\, i, j). \tag{2}$$

(That the A's commute with the B's holds by virtue of their acting on different spaces.)

Remark. The commutativity and Hermiticity conditions distinguish the spin-boson model, for which the result of this paper holds, from the Jaynes–Cummings model, for which it does not.

Remark. These conditions are in fact used only near the end of the proof. See equations (54) and (57). All formulas prior to those equations are true with neither commutativity or Hermiticity.

At time $t = 0$, the system A+B is taken to have a density matrix ρ that is a tensor product:

$$\rho(0) = \rho_A^{(0)} \otimes \rho_B^{(0)}, \tag{3}$$

where $\rho_A^{(0)}$ is a density matrix for A and $\rho_B^{(0)}$ for B. At time t, the density matrix of A+B is $\rho(t)$ where

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = -\mathrm{i}[H, \rho] \tag{4}$$

with

$$\rho|_{t=0} = \rho(0). \tag{5}$$

For any operator Q on A+B, we define the partial traces

$$Q_A = \mathrm{Tr}_B Q \qquad \text{and} \qquad Q_B = \mathrm{Tr}_A Q, \tag{6}$$

where Tr_B is the trace over B's degrees of freedom, so that $\mathrm{Tr}_B Q$ is an operator on A and is denoted by Q_A. In particular, we define the 'marginal' density matrices at time t for A and B, namely

$$\rho_A(t) = \mathrm{Tr}_B \rho(t) \qquad \text{and} \qquad \rho_B = \mathrm{Tr}_A \rho(t). \tag{7}$$

The trace of each of these operators is 1. We then consider

$$\delta_E(t) = \mathrm{Tr}[(\rho_A(t) \otimes \rho_B(t))H] - \mathrm{Tr}[\rho(t)H], \tag{8}$$

and we want to calculate the difference of average energy for small time t.

The quantity $\delta_E(t)$ is the central object of the present paper, and we will show that for short times and for the AB interaction taken above, it is positive.

3. Evaluation of $\delta_E(t) > 0$ to second order in t

3.1. A simplification

The first remark is that

$$\delta_E(t) = \sum_{i=1}^{N} \{\mathrm{Tr}_A[\rho_A(t)A_i]\,\mathrm{Tr}_B[\rho_B(t)B_i] - \mathrm{Tr}[\rho(t)(A_i \otimes B_i)]\}. \tag{9}$$

This follows immediately from the definitions of the partial traces and of the operators H_A and H_B. Using those definitions, the traces over H_A and H_B cancel. There remains only the trace over the interaction energy, $\sum A_i \otimes B_i$, which yields equation (9).

3.2. Short time evolution of $\rho(t)$ and energy

3.2.1. First step. From equation (4), we obtain for small t

$$\rho(t) = \rho(0) - \mathrm{i}t[H, \rho(0)] - \frac{t^2}{2}[H, [H, \rho(0)]] + \mathrm{O}(t^3). \tag{10}$$

The first commutator gives

$$[H, \rho(0)] = \left[H_A, \rho_A^{(0)}\right] \otimes \rho_B^{(0)} + \rho_A^{(0)} \otimes \left[H_B, \rho_B^{(0)}\right] + \sum_i \left[A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\right]. \tag{11}$$

Iterating, one gets

$$\begin{aligned}[H, [H, \rho(0)]] = {} & \left[H_A, \left[H_A, \rho_A^{(0)}\right]\right] \otimes \rho_B^{(0)} \\ & + \rho_A^{(0)} \otimes \left[H_B, \left[H_B, \rho_B^{(0)}\right]\right] + 2\left[H_A, \rho_A^{(0)}\right] \otimes \left[H_B, \rho_B^{(0)}\right] \\ & + \sum_i \left(\left[A_i \otimes B_i, \left[H_A, \rho_A^{(0)}\right] \otimes \rho_B^{(0)}\right] + \left[A_i \otimes B_i, \rho_A^{(0)} \otimes \left[H_B, \rho_B^{(0)}\right]\right]\right) \\ & + \left\{ \sum_i \left(\left[H_A, \left[A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\right]\right] + \left[H_B, \left[A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\right]\right]\right) \right\}_1 \\ & + \sum_{i,j} \left[A_j \otimes B_j, \left[A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\right]\right]. \end{aligned} \tag{12}$$

As stated earlier, H_A stands for $H_A \otimes I_B$, etc, and we have grouped together similar terms. We have also used the identity

$$[U_A \otimes I_B, X_A \otimes Y_B] = [U_A, X_A] \otimes Y_B, \tag{13}$$

(where U_A, X_A refer to A only, etc). Use the Jacobi identity for the terms in the expression enclosed by the curly bracket subscripted with a '1' in equation (12):

$$\big[H_A, \big[A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\big]\big] = \big[A_i \otimes B_i, \big[H_A, \rho_A^{(0)}\big] \otimes \rho_B^{(0)}\big] + \big[[H_A, A_i] \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\big], \tag{14}$$

so that equation (12) becomes

$$\begin{aligned}[H, [H, \rho^{(0)}]] = {} & \big[H_A, \big[H_A, \rho_A^{(0)}\big]\big] \otimes \rho_B^{(0)} + \rho_A^{(0)} \otimes \big[H_B, \big[H_B, \rho_B^{(0)}\big]\big] \\ & + 2\big[H_A, \rho_A^{(0)}\big] \otimes \big[H_B, \rho_B^{(0)}\big] + \Bigg\{ 2\Bigg[\sum_i A_i \otimes B_i, \big[H_A, \rho_A^{(0)}\big] \otimes \rho_B^{(0)}\Bigg] \\ & + 2\Bigg[\sum_i A_i \otimes B_i, \rho_A^{(0)} \otimes \big[H_B, \rho_B^{(0)}\big]\Bigg]\Bigg\}_1 \\ & + \sum_i \big[[H_A, A_i] \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\big] + \big[A_i \otimes [H_B, B_i], \rho_A^{(0)} \otimes \rho_B^{(0)}\big] \\ & + \Bigg\{\Bigg[\sum_i A_j \otimes B_j, \Bigg[\sum_i A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\Bigg]\Bigg]\Bigg\}_2. \end{aligned} \tag{15}$$

3.2.2. The trace of the energy of interaction, calculated from equation (10).

$$\begin{aligned}\mathrm{Tr}\Bigg[\Bigg(\sum_k A_k \otimes B_k\Bigg)\rho(t)\Bigg] = {} & \sum_k \mathrm{Tr}_A\big(A_k \rho_A^{(0)}\big)\,\mathrm{Tr}_B\big(B_k \rho_B^{(0)}\big) \\ & - \mathrm{i}t\,\mathrm{Tr}\Bigg([H, \rho^{(0)}] \sum_k A_k \otimes B_k\Bigg) - \frac{t^2}{2}\mathrm{Tr}\Bigg([H, [H, \rho^{(0)}]] \sum_k A_k \otimes B_k\Bigg). \end{aligned} \tag{16}$$

For any operators V and U, one has $\mathrm{Tr}(V[V, U]) = 0$. From equation (11) and this identity, it follows that

$$\begin{aligned}\mathrm{Tr}\Bigg(\Bigg(\sum_k A_k \otimes B_k\Bigg)[H, \rho^{(0)}]\Bigg) = {} & \sum_k \mathrm{Tr}_A\big(A_k\big[H_A, \rho_A^{(0)}\big]\big)\,\mathrm{Tr}_B\big(B_k \rho_B^{(0)}\big) \\ & + \sum_k \mathrm{Tr}_A\big(A_k \rho_A^{(0)}\big)\mathrm{Tr}_B\big(B_k\big[H_B, \rho_B^{(0)}\big]\big). \end{aligned} \tag{17}$$

In the same way, when we calculate $\mathrm{Tr}\big(\big(\sum_k A_k \otimes B_k\big)[H, [H, \rho^{(0)}]]\big)$ and we use equation (15) for the double bracket, the contributions of the curly-bracketed expressions with subscripts '1' and '2' of equation (15) give 0:

$$\begin{aligned}\mathrm{Tr}\Bigg(\sum_k (A_k \otimes B_k)[H, [H, \rho^{(0)}]]\Bigg) = {} & \sum_k \big(\mathrm{Tr}_A\big(A_k\big[H_A, \big[H_A, \rho_A^{(0)}\big]\big]\big)\,\mathrm{Tr}_B\big(B_k \rho_B^{(0)}\big) + [A \leftrightarrow B]\big) \\ & + 2\sum_k \mathrm{Tr}_A\big(A_k\big[H_A, \rho_A^{(0)}\big]\big)\mathrm{Tr}_B\big(B_k\big[H_B, \rho_B^{(0)}\big]\big) \\ & + \sum_{k,i} \big\{\mathrm{Tr}\big((A_k \otimes B_k)\big[[H_A, A_i] \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\big]\big) \\ & + \mathrm{Tr}\big((A_k \otimes B_k)\big[A_i \otimes [H_B, B_i], \rho_A^{(0)} \otimes \rho_B^{(0)}\big]\big)\big\}. \end{aligned} \tag{18}$$

We rearrange the last sum in equation (18),

$$\mathrm{Tr}\big((A_k \otimes B_k)\big[[H_A, A_i] \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\big]\big) = \mathrm{Tr}_A\big(A_k[H_A, A_i]\rho_A^{(0)}\big)\mathrm{Tr}_B\big(B_k B_i \rho_B^{(0)}\big) \\ - \mathrm{Tr}_A\big(A_k\rho_A^{(0)}[H_A, A_i]\big)\mathrm{Tr}_B\big(B_k\rho_B^{(0)} B_i\big), \tag{19}$$

and we sum by renaming the indices

$$\sum_{k,i} \mathrm{Tr}\big((A_k \otimes B_k)\big[[H_A, A_i] \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\big]\big) \\ = \sum_{i,k} \mathrm{Tr}_B\big(B_k B_i \rho_B^{(0)}\big)\mathrm{Tr}_A\big(A_k[H_A, A_i]\rho_A^{(0)} - A_i\rho_A^{(0)}[H_A, A_k]\big) \\ = \sum_{k,i} \mathrm{Tr}_B\big(B_k B_i \rho_B^{(0)}\big)\big[\mathrm{Tr}_A\big(A_k H_A A_i \rho_A^{(0)} - A_k A_i H_A \rho_A^{(0)} \\ - A_i\rho_A^{(0)} H_A A_k + A_i\rho_A^{(0)} A_k H_A\big)\big] \\ = \sum_{k,i} \mathrm{Tr}_B\big(B_k B_i \rho_B^{(0)}\big)\mathrm{Tr}_A\big((2A_k H_A A_i - A_k A_i H_A - H_A A_k A_i)\rho_A^{(0)}\big). \tag{20}$$

The expressions in the last line of equation (20) are reminiscent of the Lindblad equation, and in fact guided us in this calculation [8]. Using this expression, equation (18) becomes

$$\mathrm{Tr}\bigg(\sum_k (A_k \otimes B_k)[H, [H, \rho^{(0)}]]\bigg) \\ = \sum_k \big(\mathrm{Tr}_A\big(A_k\big[H_A, \big[H_A, \rho_A^{(0)}\big]\big]\big)\,\mathrm{Tr}_B\big(B_k\rho_B^{(0)}\big) + [A \leftrightarrow B]\big) \\ + 2\sum_k \mathrm{Tr}_A\big(A_k\big[H_A, \rho_A^{(0)}\big]\big)\mathrm{Tr}_B\big(B_k\big[H_B, \rho_B^{(0)}\big]\big) \\ + \sum_{k,i} \big(\mathrm{Tr}_B\big(B_k B_i \rho_B^{(0)}\big)\,\mathrm{Tr}_A\big((2A_k H_A A_i - A_k A_i H_A - H_A A_k A_i)\rho_A^{(0)}\big) \\ + [A \leftrightarrow B]\big). \tag{21}$$

Note also

$$2A_k H_A A_i - A_k A_i H_A - H_A A_k A_i = A_k[H_A, A_i] + [A_k, H_A]A_i. \tag{22}$$

Finally, we use equations (17) and (21) to rewrite equation (16) for small t as

$$\mathrm{Tr}\bigg(\bigg(\sum_k A_k \otimes B_k\bigg)\rho(t)\bigg) = \sum_k \mathrm{Tr}_A\big(A_k\rho_A^{(0)}\big)\mathrm{Tr}_B\big(B_k\rho_B^{(0)}\big) \\ - \mathrm{i}t\bigg\{\sum_k \mathrm{Tr}_A\big(A_k\big[H_A, \rho_A^{(0)}\big]\big)\,\mathrm{Tr}_B\big(B_k\rho_B^{(0)}\big) + [A \leftrightarrow B]\bigg\} \\ - \frac{t^2}{2}\bigg\{\sum_k \big(\mathrm{Tr}_A\big(A_k\big[H_A, \big[H_A, \rho_A^{(0)}\big]\big]\big)\mathrm{Tr}_B\big(B_k\rho_B^{(0)}\big) + [A \leftrightarrow B]\big) \\ + 2\sum_k \mathrm{Tr}_A\big(A_k\big[H_A, \rho_A^{(0)}\big]\big)\,\mathrm{Tr}_B\big(B_k\big[H_B, \rho_B^{(0)}\big]\big) \\ + \sum_{k,i} \big(\mathrm{Tr}_B\big(B_k B_i \rho_B^{(0)}\big)\,\mathrm{Tr}_A\big((A_k[H_A, A_i] + [A_k, H_A]A_i)\rho_A^{(0)}\big) + [A \leftrightarrow B]\big)\bigg\}. \tag{23}$$

3.3. Partial traces and product of the partial traces

3.3.1. Calculation of $\rho_A(t)$. We take the trace over B of $\rho(t)$ in equation (10)

$$\rho_A(t) = \mathrm{Tr}_B\rho(t) = \rho_A^{(0)} - \mathrm{i}t\mathrm{Tr}_B[H, \rho^{(0)}] - \frac{t^2}{2}\mathrm{Tr}_B[H, [H, \rho^{(0)}]] + \cdots . \tag{24}$$

We use equation (11), noticing that

$$\mathrm{Tr}_B[U_B, V_B] = 0, \qquad \mathrm{Tr}_B\rho_B^{(0)} = 1, \tag{25}$$

and we obtain

$$\mathrm{Tr}_B[H, \rho^{(0)}] = \left[H_A, \rho_A^{(0)}\right] + \mathrm{Tr}_B\left[\sum_i A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\right], \tag{26}$$

and then, we use equation (15) to get

$$\begin{aligned}\mathrm{Tr}_B[H, [H, \rho^{(0)}]] = {} & \left[H_A, \left[H_A, \rho_A^{(0)}\right]\right] \\ & + 2\mathrm{Tr}_B\left[\sum_i (A_i \otimes B_i), \left[H_A, \rho_A^{(0)}\right] \otimes \rho_B^{(0)}\right] \\ & + 2\mathrm{Tr}_B\left[\sum_i (A_i \otimes B_i), \rho_A^{(0)} \otimes \left[H_B, \rho_B^{(0)}\right]\right] \\ & + \mathrm{Tr}_B\left[\sum_i ([H_A, A_i] \otimes B_i + A_i \otimes [H_B, B_i]), \rho_A^{(0)} \otimes \rho_B^{(0)}\right] \\ & + \mathrm{Tr}_B\left[\sum_j A_j \otimes B_j, \left[\sum_i A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\right]\right].\end{aligned} \tag{27}$$

3.3.2. Calculation of $\mathrm{Tr}_A(A_k\rho_A(t))$. From equation (24), equation (26) and equation (27), using the fact that

$$\mathrm{Tr}_A(A_k\, Tr_B\, X) = \mathrm{Tr}(A_k X) \tag{28}$$

we obtain

$$\begin{aligned}\mathrm{Tr}_A(A_k\rho_A(t)) = {} & \mathrm{Tr}_A\left(A_k\rho_A^{(0)}\right) - \mathrm{i}t\left\{\mathrm{Tr}_A A_k\left[H_A, \rho_A^{(0)}\right]\right. \\ & \left. + \mathrm{Tr}\left(A_k\left[\sum_i A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\right]\right)\right\} - \frac{t^2}{2}\left\{\mathrm{Tr}_A\left(A_k\left[H_A, \left[H_A, \rho_A^{(0)}\right]\right]\right)\right. \\ & + 2\mathrm{Tr}\left(A_k\left[\sum_i A_i \otimes B_i, \left[H_A, \rho_A^{(0)}\right] \otimes \rho_B^{(0)}\right]\right) \\ & + 2\mathrm{Tr}\left(A_k\left[\sum_i A_i \otimes B_i, \rho_A^{(0)} \otimes \left[H_B, \rho_B^{(0)}\right]\right]\right) \\ & + \mathrm{Tr}_A\left(A_k\left[\sum_i ([H_A, A_i] \otimes B_i + [A_i \otimes H_B, B_i]), \rho_A^{(0)} \otimes \rho_B^{(0)}\right]\right) \\ & \left. + \mathrm{Tr}_A\left(A_k\left[\sum_j A_j \otimes B_j, \left[\sum_i A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\right]\right]\right)\right\}.\end{aligned} \tag{29}$$

We have an analogous formula for $\mathrm{Tr}_B(B_k\rho_B(t))$ obtained by exchanging A and B in equation (29).

3.3.3. Sum of the product of traces. To calculate $\delta_E(t)$ we also need to calculate

$$\sum \equiv \sum_k \mathrm{Tr}_A(A_k \rho_A(t))\mathrm{Tr}_B(B_k \rho_A(t)). \tag{30}$$

Term of order 0 in t. This term is the product of the terms of order 0 in equation (29) and the terms in the corresponding equation for B_k. So it is

$$\sum\nolimits_0 \equiv \sum_k \mathrm{Tr}_A\left(A_k \rho_k^{(0)}\right)\mathrm{Tr}_B\left(B_k \rho_k^{(0)}\right). \tag{31}$$

Terms of order 1 in t. This is the product of the term of order 0 of equation (29) and the term of order 1 of the corresponding equation for B and the exchange term A↔B. So

$$\sum_1 = -\mathrm{i}t \left\{ \sum_k \mathrm{Tr}_A\left(A_k \rho_A^{(0)}\right)\left(\mathrm{Tr}_B\left(B_k\left[H_A, \rho_A^{(0)}\right]\right) \right.\right.$$
$$\left.\left. + \mathrm{Tr}\left(B_k \left[\sum_i A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\right]\right) + [A \leftrightarrow B]\right\}. \tag{32}$$

Now, consider in equation (32) the terms

$$\sum_{k,i} \mathrm{Tr}_A\left(A_k \rho_A^{(0)}\right) \mathrm{Tr}\left(B_k\left[A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\right]\right)$$
$$= \sum_{k,i} \mathrm{Tr}_A\left(A_k \rho_A^{(0)}\right)\left\{\mathrm{Tr}\left(A_i \rho_A^{(0)} \otimes B_k B_i \rho_B^{(0)}\right) - \mathrm{Tr}\left(\rho_A^{(0)} A_i \otimes B_k \rho_B^{(0)} B_i\right)\right\}$$
$$= \sum_{k,i} \left(\mathrm{Tr}_A\left(A_k \rho_A^{(0)}\right)\mathrm{Tr}_A\left(A_i \rho_A^{(0)}\right)\right)\left\{\mathrm{Tr}_B\left(B_k B_i \rho_B^{(0)}\right) - \mathrm{Tr}_B\left(B_i B_k \rho_B^{(0)}\right)\right\} \equiv 0 \tag{33}$$

(recall that here B_k is $I_A \otimes B_k$). This is zero because the first bracket is symmetric in A_k, A_i and the curly bracket is skew symmetric in B_i, B_k. Thus, $\sum_1$ reduces to

$$\sum\nolimits_1 \equiv -\mathrm{i}t \left\{\sum \mathrm{Tr}_A\left(A_k \rho_A^{(0)}\right) \mathrm{Tr}_B\left(B_k\left[H_A, \rho_A^{(0)}\right]\right) + [A \leftrightarrow B]\right\}. \tag{34}$$

Conclusion: *The terms of orders 0 and 1 in t of*

$$\sum_k \mathrm{Tr}_A(A_k \rho_A(t))\mathrm{Tr}_B(B_k \rho_B(t)) \tag{35}$$

are identical to the corresponding term of $\mathrm{Tr}\left(\sum_k (A_k \otimes B_k)\rho(t)\right)$ *in equation (23).*

Terms of order 2 with respect to t in $\sum$ *of equation (30).* These terms, $\sum_2$, are the product of the terms of order 2 in t in equation (29) and the term of order 0 in the B equation, the exchange term in A↔B, and the product of the terms of order 1 in t in equation (29) and the term of order 1 in t in the B equation. Thus, we write

$$\sum\nolimits_2 = -\frac{t^2}{2}\widehat{\sum}_2 \tag{36}$$

with $\widehat{\sum}_2$ given by

$$\widehat{\sum}_2 \equiv \sum_k \mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right)\Bigg[\ \mathrm{Tr}_A\left(A_k\left[H_A,\left[H_A,\rho_A^{(0)}\right]\right]\right)$$
$$+\left\{2\sum_i\left(\mathrm{Tr}\left(A_k\left[A_i\otimes B_i,\left[H_A,\rho_A^{(0)}\right]\otimes\rho_B^{(0)}\right]\right)+\mathrm{Tr}\left(A_k\left[A_i\otimes B_i,\rho_A^{(0)}\otimes\left[H_B,\rho_B^{(0)}\right]\right]\right)\right\}_3$$
$$+\left\{\sum_i\left(\mathrm{Tr}\left(A_k\left([H_A,A_i]\otimes B_i,\rho_A^{(0)}\otimes\rho_B^{(0)}\right)\right)+\mathrm{Tr}\left(A_k[A_i\otimes[H_B,B_i]],\rho_A^{(0)}\otimes\rho_B^{(0)}\right)\right)\right\}_4$$
$$+\left\{+\sum_{i,j}\mathrm{Tr}\left(A_k\left[A_j\otimes B_j,\left[A_i\otimes B_i,\rho_A^{(0)}\otimes\rho_B^{(0)}\right]\right]\right)\right\}_5\Bigg]+[A\leftrightarrow B]$$
$$+2\sum_k\left\{\mathrm{Tr}_A\left(A_k\left[H_A,\rho_A^{(0)}\right]\right)+\sum_i\mathrm{Tr}_A\left([A_k,A_i]\rho_A^{(0)}\right)\mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right)\right\}$$
$$\times\left\{\mathrm{Tr}_B\left(B_k\left[H_B,\rho_B^{(0)}\right]\right)+\sum_i\mathrm{Tr}_A\left(A_i\rho_A^{(0)}\right)\mathrm{Tr}_B\left([B_k,B_i]\rho_B^{(0)}\right)\right\}. \tag{37}$$

Here we have used the fact that in the first order terms of equation (29), one has

$$\begin{aligned}\mathrm{Tr}\left(A_k\left[A_i\otimes B_i,\rho_A^{(0)}\otimes\rho_B^{(0)}\right]\right) &= \mathrm{Tr}\left((A_k\otimes I_B)\left[A_i\otimes B_i,\rho_A^{(0)}\otimes\rho_B^{(0)}\right]\right)\\ &= \mathrm{Tr}_A\left(A_kA_i\rho_A^{(0)}\right)\mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right)-\mathrm{Tr}_A\left(A_k\rho_A^{(0)}A_i\right)\mathrm{Tr}_B\left(\rho_B^{(0)}B_i\right)\\ &= \mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right)\mathrm{Tr}_A\left((A_kA_i-A_iA_k)\rho_A^{(0)}\right)\\ &= \mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right)\mathrm{Tr}_A\left([A_k,A_i]\rho_A^{(0)}\right).\end{aligned} \tag{38}$$

We next simplify equation (37).

(a) Terms in the first sum and curly bracket no. 3 in equation (37):

$$\begin{aligned}&2\sum_{i,k}\mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right)\mathrm{Tr}\left(A_k\left[A_i\otimes B_i,\left[H_A,\rho_A^{(0)}\right]\otimes\rho_B^{(0)}\right]\right)\\ &\quad= 2\sum_{i,k}\mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right)\mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right)\mathrm{Tr}_A\left(A_kA_i\left[H_A,\rho_A^{(0)}\right]-A_k\left[H_A,\rho_A^{(0)}\right]A_i\right)\\ &\quad= 2\sum_{i,k}\mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right)\mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right)\mathrm{Tr}_A\left(\left[H_A,\rho_A^{(0)}\right][A_k,A_i]\right)\equiv 0,\end{aligned} \tag{39}$$

because the B terms are symmetric in i,k and the A terms are skew symmetric,

$$\begin{aligned}&2\sum_{i,k}\mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right)\mathrm{Tr}\left(A_k\left[A_i\otimes B_i,\rho_A^{(0)}\otimes\left[H_B,\rho_B^{(0)}\right]\right]\right)\\ &\quad= 2\sum_{i,k}\mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right)\mathrm{Tr}_B\left(B_i\left[H_B,\rho_B^{(0)}\right]\right)\mathrm{Tr}_A\left([A_k,A_i]\rho_A^{(0)}\right).\end{aligned} \tag{40}$$

(b) Terms in the first sum and curly bracket no. 4 in equation (37):

$$\begin{aligned}&\sum_{k,i}\mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right)\mathrm{Tr}\left(A_k\left[[H_A,A_i]\otimes B_i,\rho_A^{(0)}\otimes\rho_B^{(0)}\right]\right)\\ &\quad= \sum_{k,i}\mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right)\mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right)\mathrm{Tr}_A\left([A_k,[H_A,A_i]]\rho_A^{(0)}\right)\\ &\qquad\times\sum_{k,i}\mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right)\mathrm{Tr}\left(A_k\left[A_i\otimes[H_B,B_i],\rho_A^{(0)}\otimes\rho_B^{(0)}\right]\right)\\ &\quad= \sum_{k,i}\mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right)\mathrm{Tr}_B\left([H_B,B_i]\rho_B^{(0)}\right)\mathrm{Tr}_A\left([A_k,A_i]\rho_A^{(0)}\right).\end{aligned} \tag{41}$$

But $\mathrm{Tr}([X,Y]Z) = \mathrm{Tr}(XYZ - YXZ) = \mathrm{Tr}(Y[Z,X])$. Thus,

$$\sum_{k,i} \mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right) \mathrm{Tr}\left(A_k \underline{\mathrm{i}}g[A_i \otimes [H_B, B_i], \rho_A^{(0)} \otimes \rho_B^{(0)}]\right)$$
$$= -\sum_{k,i} \mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right) \mathrm{Tr}_B\left(B_i\left[H_B, \rho_B^{(0)}\right]\right) \mathrm{Tr}_A[A_k, A_i]\rho_A^{(0)}. \tag{42}$$

Thus, this term cancels partially the term of equation (40) (recall that there is a 2 in (40))

(c) Terms of the last sum over k of equation (37):

$$2\sum_k \left[\mathrm{Tr}_A\left(A_k\left[H_A, \rho_A^{(0)}\right]\right) + \sum_k \mathrm{Tr}_A\left([A_k, A_i]\rho_A^{(0)}\right) \mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right)\right]$$
$$\times \left[\mathrm{Tr}_B B_k\left[H_B, \rho_B^{(0)}\right] + \sum_k \mathrm{Tr}_A\left(A_i\rho_A^{(0)}\right) \mathrm{Tr}_B\left([B_k, B_i]\rho_B^{(0)}\right)\right]$$
$$= 2\sum_k \mathrm{Tr}_A\left(A_k\left[H_A, \rho_A^{(0)}\right]\right) \mathrm{Tr}_B\left(B_k\left[H_B, \rho_B^{(0)}\right]\right)$$
$$+2\sum_{k,i} \mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right) \mathrm{Tr}_B\left(B_k\left[H_B, \rho_B^{(0)}\right]\right) \mathrm{Tr}_A\left([A_k, A_i]\rho_A^{(0)}\right) + [A \leftrightarrow B]$$
$$+2\sum_{k,i,j} \mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right) \mathrm{Tr}_A\left(A_j\rho_A^{(0)}\right) \mathrm{Tr}_A\left([A_k, A_i]\rho_A^{(0)}\right) \mathrm{Tr}_B[B_k, B_j]\rho_B^{(0)}. \tag{43}$$

In equation (43), the term

$$2\sum_{k,i} \mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right) \mathrm{Tr}_B B_k\left[H_B, \rho_B^{(0)}\right] \mathrm{Tr}_A\left([A_k, A_i]\rho_A^{(0)}\right) \tag{44}$$

also combines with equation (40) and equation (42).

(d) Terms in the first sum and curly bracket no. 5 of equation (37). Indeed, by the cyclic property of the trace

$$\sum_{i,j} \mathrm{Tr}\left(A_k\left[A_j \otimes B_j, \left[A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\right]\right]\right)$$
$$= \sum_{i,j} \left[\mathrm{Tr}_A\left(A_kA_jA_i\rho_A^{(0)}\right) \mathrm{Tr}_B\left(B_jB_i\rho_B^{(0)}\right) - \mathrm{Tr}_A\left(A_iA_kA_j\rho_A^{(0)}\right) \mathrm{Tr}_B\left(B_iB_j\rho_B^{(0)}\right)\right.$$
$$\left. - \mathrm{Tr}_A\left(A_jA_kA_i\rho_A^{(0)}\right) \mathrm{Tr}_B\left(B_jB_i\rho_B^{(0)}\right) + \mathrm{Tr}_A\left(A_iA_jA_k\rho_A^{(0)}\right) \mathrm{Tr}_B\left(B_iB_j\rho_B^{(0)}\right)\right]$$
$$= \sum_{i,j} \left[\mathrm{Tr}_A\left([A_k, A_j]A_i\rho_A^{(0)}\right) \mathrm{Tr}_B\left(B_jB_i\rho_B^{(0)}\right)\right.$$
$$\left. + \mathrm{Tr}_A\left(A_i[A_j, A_k]\rho_A^{(0)}\right) \mathrm{Tr}_B\left(B_iB_j\rho_B^{(0)}\right)\right]$$
$$= \sum_{i,j} \left(\mathrm{Tr}_A\left([A_i, [A_j, A_k]]\rho_A^{(0)}\right) \mathrm{Tr}_B\left(B_iB_j\rho_B^{(0)}\right)\right.$$
$$\left. + \mathrm{Tr}_A\left([A_j, A_k]A_i\rho_A^{(0)}\right) \mathrm{Tr}_B\left(B_i, B_j\rho_B^{(0)}\right)\right). \tag{45}$$

Now the last sum in equation (45) contains $\mathrm{Tr}_B\left([B_i, B_j]\rho_B^{(0)}\right)$, which is skew symmetric in i, j. So in this last sum, one can replace $[A_j, A_k]A_i$ by $\frac{1}{2}[[A_j, A_k], A_i]$ without changing the sum. Then, we deduce

$$\sum_{i,j} \mathrm{Tr}\left(A_k\left[A_j \otimes B_j, \left[A_i \otimes B_i, \rho_A^{(0)} \otimes \rho_B^{(0)}\right]\right]\right)$$
$$= \sum_{i,j} \mathrm{Tr}_A\left([A_i, [A_j, A_k]]\rho_A^{(0)}\right) \mathrm{Tr}_B\left(\frac{(B_iB_j + B_jB_i)}{2}\rho_B^{(0)}\right). \tag{46}$$

Finally, one can collect all the terms of $\widehat{\sum}_2$ of equation (37). We use equations (39), (40), (41), (42), (43) and (46) to obtain

$$\widehat{\sum}_2 = \Bigg\{ \sum_k \mathrm{Tr}_B\big(B_k\rho_B^{(0)}\big)\,\mathrm{Tr}_A\big(A_k\big[H_A,\big[H_A,\rho_A^{(0)}\big]\big]\big) + \sum_{i,k} \mathrm{Tr}_B\big(B_k\rho_B^{(0)}\big)\,\mathrm{Tr}_B\big(B_i\big[H_B,\rho_B^{(0)}\big]\big)\,\mathrm{Tr}_A\big([A_i,A_k]\rho_A^{(0)}\big) + \sum_{i,k} \mathrm{Tr}_B\big(B_k\rho_B^{(0)}\big)\,\mathrm{Tr}_B\big(B_i\rho_B^{(0)}\big)\,\mathrm{Tr}_A\big([A_k,[H_A,A_i]]\rho_A^{(0)}\big) + \sum_{i,j,k} \mathrm{Tr}_B\big(B_k\rho_B^{(0)}\big)\,\mathrm{Tr}_B\left(\frac{(B_iB_j+B_jB_i)}{2}\rho_B^{(0)}\right)\mathrm{Tr}_A\big([A_i,[A_j,A_k]]\rho_A^{(0)}\big)\Bigg\} + [A\leftrightarrow B] + 2\sum_k \mathrm{Tr}_A\big(A_k\big[H_A,\rho_A^{(0)}\big]\big)\,\mathrm{Tr}_B\big(B_k\big[H_B,\rho_B^{(0)}\big]\big) + 2\sum_{k,i,j} \mathrm{Tr}_B\big(B_i\rho_B^{(0)}\big)\,\mathrm{Tr}_A\big(A_j\rho_A^{(0)}\big)\,\mathrm{Tr}_A\big([A_k,A_i]\rho_A^{(0)}\big)\,\mathrm{Tr}_B\big([B_k,B_j]\rho_B^{(0)}\big). \tag{47}$$

3.4. Calculation of $\delta_E(t)$

$\delta_E(t)$ is given by equation (9):

$$\delta_E(t) = \sum_{i=1}^{N}\{\mathrm{Tr}_A(\rho_A(t)A_i)\mathrm{Tr}_B(\rho_B(t)B_i) - \mathrm{Tr}(\rho(t)(A_i\otimes B_i))\}. \tag{48}$$

In this equation, the first sum is the $\sum$ of equation (30) and the second sum is given by equation (23). We have seen in equation (35) that the zeroth and first order terms in t cancel in the difference, equation (46). As a consequence, the difference $\delta_E(t)$ is the difference of terms in t^2 from equations (23) and (47) (multiplied by $-\frac{t^2}{2}$). We see immediately that in these equations there are cancellations of

$$\sum_k \mathrm{Tr}_B\big(B_k\rho_B^{(0)}\big)\,\mathrm{Tr}_A\big(A_k\big[H_A,\big[H_A,\rho_A^{(0)}\big]\big]\big) + [A\leftrightarrow B] \tag{49}$$

and of

$$2\sum_k \mathrm{Tr}_A\big(A_k\big[H_A,\rho_A^{(0)}\big]\big)\,\mathrm{Tr}_B\big(B_k\big[H_B,\rho_B^{(0)}\big]\big). \tag{50}$$

So $\delta_E(t)$ is, after rearrangements,

$$\delta_E(t) = -\frac{t^2}{2}\Bigg\{ \sum_{i,k} \mathrm{Tr}_B\big(B_k\rho_B^{(0)}\big)\,\mathrm{Tr}_B\big(B_i\rho_B^{(0)}\big)\,\mathrm{Tr}_A\big([A_k,[H_A,A_i]]\rho_A^{(0)}\big) - \sum_{i,k} \mathrm{Tr}_B\big(B_kB_i\rho_B^{(0)}\big)\,\mathrm{Tr}_A\big((A_k[H_A,A_i]+[A_k,H_A]A_i)\rho_A^{(0)}\big) + \sum_{i,k} \mathrm{Tr}_B\big(B_k\rho_B^{(0)}\big)\,\mathrm{Tr}_B\big(B_i\big[H_B,\rho_B^{(0)}\big]\big)\,\mathrm{Tr}_A\big([A_i,A_k]\rho_A^{(0)}\big) + \sum_{k,i,j} \mathrm{Tr}_B\big(B_k\rho_B^{(0)}\big)\,\mathrm{Tr}_B\left(\frac{(B_iB_j+B_jB_i)}{2}\rho_B^{(0)}\right)\mathrm{Tr}_A\big([A_i,[A_j,A_k]]\rho_A^{(0)}\big) + \sum_{k,i,j} \mathrm{Tr}_B\big(B_i\rho_B^{(0)}\big)\,\mathrm{Tr}_A\big(A_j\rho_A^{(0)}\big)\,\mathrm{Tr}_A\big([A_k,A_i]\rho_A^{(0)}\big)\,\mathrm{Tr}_B\big([B_k,B_j]\rho_B^{(0)}\big)\Bigg\} + [A\leftrightarrow B]. \tag{51}$$

(Note that the last line in equation (46) can be rewritten with a 1 instead of a 2 and $[A \leftrightarrow B]$.) Let us now rearrange the first summation in equation (51). This summation is a summation of

$$\mathrm{Tr}_A\left\{(A_k H_A A_i - A_k A_i H_A - H_A A_i A_k + A_i H_A A_k)\rho_A^{(0)}\right\} \tag{52}$$

with the coefficient $\mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right)\mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right)$, which is symmetric in i, k. So it can be written as

$$\begin{aligned}\sum_{i,k} \mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right) \mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right) \mathrm{Tr}_A\left((2A_k H_A A_i - A_k A_i H_A - H_A A_k A_i)\rho_A^{(0)}\right)\\ = \sum_{i,k} \mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right) \mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right) \mathrm{Tr}_A\left((A_k[H_A, A_i] + [A_k, H_A]A_i)\rho_A^{(0)}\right).\end{aligned} \tag{53}$$

Thus, equation (51) can be rewritten as

$$\begin{aligned}\delta_E(t) = -\frac{t^2}{2}\Bigg\{ &\sum_{i,k} \left(\mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right) \mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right)\right.\\ &\left.- \mathrm{Tr}_B\left(B_k B_i\rho_B^{(0)}\right)\right) \mathrm{Tr}_A\left((A_k[H_A, A_i] + [A_k, H_A]A_i)\rho_A^{(0)}\right)\\ &+ \sum_{i,k} \mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right) \mathrm{Tr}_B\left(B_i\left[H_B, \rho_B^{(0)}\right]\right) \mathrm{Tr}_A\left([A_i, A_k]\rho_A^{(0)}\right)\\ &+ \sum_{i,j,k} \mathrm{Tr}_B\left(B_k\rho_B^{(0)}\right) \mathrm{Tr}_B\left(\frac{(B_iB_j + B_jB_i)}{2}\rho_B^{(0)}\right) \mathrm{Tr}_A\left([A_i, [A_j, A_k]]\rho_A^{(0)}\right)\\ &+ \sum_{i,j,k} \mathrm{Tr}\left(B_k\rho_B^{(0)}\right) \mathrm{Tr}\left(A_j\rho_A^{(0)}\right) \mathrm{Tr}_A\left([A_i, A_k]\rho_A^{(0)}\right) \mathrm{Tr}_A\left([B_i, B_j]\rho_B^{(0)}\right)\Bigg\}\\ &+ [A \leftrightarrow B].\end{aligned} \tag{54}$$

Recall now our assumption, equation (2), on the operators A_i and B_i:

$$[A_i, A_j] = 0 \quad (\forall\, i, j) \qquad \text{and} \qquad [B_i, B_j] = 0 \quad (\forall\, i, j). \tag{55}$$

Then equation (54) can be simplified as follows:

$$\begin{aligned}\delta_E(t) = -\frac{t^2}{2}\sum_{i,j} &\left(\mathrm{Tr}_B\left(B_j\rho_B^{(0)}\right) \mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right) - \mathrm{Tr}_B\left(B_j B_i\rho_B^{(0)}\right)\right) \mathrm{Tr}_A\left((A_j[H_A, A_i]\right.\\ &\left.+ [A_j, H_A]A_i)\rho_A^{(0)}\right) + [A \leftrightarrow B] + \mathrm{O}(t^3).\end{aligned} \tag{56}$$

Moreover, using the fact that the B_i's are Hermitian operators, one can define a symmetric matrix M_{ij} by

$$M_{ij} \equiv \mathrm{Tr}_B\left(B_iB_j\rho_B^{(0)}\right) - \mathrm{Tr}_B\left(B_j\rho_B^{(0)}\right) \mathrm{Tr}_B\left(B_i\rho_B^{(0)}\right). \tag{57}$$

Then (M_{ij}) *is symmetric and positive.*

Proof. Indeed, it is symmetric because $B_iB_j = B_jB_i$. Let ξ_i be real numbers. Then

$$\sum \xi_i\xi_j M_{ij} = \mathrm{Tr}_B\left((\xi.B)^2\rho_B^{(0)}\right) - \left(\mathrm{Tr}_B(\xi.B)\rho_B^{(0)}\right)^2 \tag{58}$$

with $\xi \cdot B = \sum \xi_i B_i$. But if C is a Hermitian operator, with eigenvalues c_α, in a basis in which C is diagonal

$$\mathrm{Tr}(C^2\rho) - (\mathrm{Tr}C\rho)^2 = \sum \rho_{\alpha\alpha}c_\alpha^2 - \left(\sum \rho_{\alpha\alpha}c_\alpha\right)^2. \tag{59}$$

But $\rho_{\alpha\alpha} > 0$ and $\sum_\alpha \rho_{\alpha\alpha} = 1$, so that by Jensen's inequality for the convex functions x^2, one has

$$\left(\sum \rho_{\alpha\alpha} c_\alpha\right)^2 \leqslant \sum \rho_{\alpha\alpha} c_\alpha^2 \tag{60}$$

(with equality if and only if $c_\alpha = \lambda \rho_{\alpha\alpha}$).

4. Interaction of particles: sum of separable potentials

Suppose the system A is formed of quantum particles with coordinates $x = (x_1, \ldots, x_n)$ and the system B is formed of particles with coordinates $y = (y_1, \ldots, y_p)$. Take

$$\begin{aligned} H_A &= \frac{p_A^2}{2} + V_A(x), \qquad & p_{A,j} &= \frac{1}{\mathrm{i}}\frac{\partial}{\partial x_j} \\ H_B &= \frac{p_B^2}{2} + V_B(y), \qquad & p_{B,j} &= \frac{1}{\mathrm{i}}\frac{\partial}{\partial y_j} \end{aligned} \tag{61}$$

where p_A (resp. p_B) are the conjugate momenta of x (resp. y).

Suppose now that the $A_j = A_j(x)$ and $B_j = B_j(y)$ are functions of x and y, respectively, and assume that they are real functions. So the A_j, B_j are commuting Hermitian operators and equation (56) for $\delta_E(t)$ can be used.

We evaluate each term in equation (56). Clearly,

$$[H_A, A_i] = -\tfrac{1}{2}[\Delta_A, A_i] = -\tfrac{1}{2}(\Delta_A A_i) - (\overrightarrow{\nabla} A_i).\overrightarrow{\nabla}. \tag{62}$$

Here, $\Delta_A = \sum_{j=1}^n \frac{\partial^2}{\partial x_j^2}$ and $(\overrightarrow{\nabla} A_i)\overrightarrow{\nabla} = \sum_{j=1}^n \left(\frac{\partial}{\partial x_j} A_i\right)\frac{\partial}{\partial x_j}$. Thus,

$$\begin{aligned} A_k[H_A, A_i] + [A_k, H_A]A_i &= -\tfrac{1}{2}A_k(\Delta_A A_i) - A_k(\overrightarrow{\nabla} A_i).\overrightarrow{\nabla} + \tfrac{1}{2}(\Delta_A A_k)A_i + (\overrightarrow{\nabla} A_k)\overrightarrow{\nabla} A_i \\ &= \tfrac{1}{2}((\Delta_A A_k)A_i - A_k(\Delta_A A_i)) + (A_i(\overrightarrow{\nabla} A_k)\overrightarrow{\nabla} \\ &\quad - A_k(\overrightarrow{\nabla} A_i).\overrightarrow{\nabla}) + (\overrightarrow{\nabla} A_k.\overrightarrow{\nabla} A_i). \end{aligned} \tag{63}$$

Now the first two terms following the second equal sign in equation (63) are skew symmetric in k, i. But in $\delta_E(t)$ they are summed over k, i with coefficients that are symmetric in k, i, so they disappear in the summation. Then, the summation reduces to

$$\sum_{i,j} \left(\mathrm{Tr}_B\left(B_i \rho_B^{(0)}\right)\mathrm{Tr}_B\left(B_j \rho_B^{(0)}\right) - \mathrm{Tr}_B\left(B_i B_j \rho_B^{(0)}\right)\right)\mathrm{Tr}_A\left((\overrightarrow{\nabla} A_i.\overrightarrow{\nabla} A_j)\rho_A^{(0)}\right). \tag{64}$$

In equation (64), the traces can be easily written as space integrals over the x or y variables. We get

$$\begin{aligned} \delta_E(t) = \frac{t^2}{2}\sum_{i,j}\Bigg[\int & B_i(y)B_j(y)\rho_B^{(0)}(y,y)\,\mathrm{d}y \\ &- \left(\int B_i(y)\rho_B^{(0)}(y,y)\,\mathrm{d}y\right)\left(\int B_j(y)\rho_B^{(0)}(y,y)\,\mathrm{d}y\right)\Bigg] \\ &\times \left[\int (\overrightarrow{\nabla} A_i(x).\overrightarrow{\nabla} A_j(x))\rho_A^{(0)}(x,x)\,\mathrm{d}x\right] + [A \leftrightarrow B] + \mathrm{O}(t^3). \end{aligned} \tag{65}$$

In equation (65), the summation of the second member is of the type

$$\sum_{i,j} M_{ij} N_{ji} \tag{66}$$

with

$$M_{ij} = \int B_i(y)B_j(y)\rho_B^{(0)}(y,y)\,\mathrm{d}y - \left(\int B_i(y)\rho_B^{(0)}(y,y)\,\mathrm{d}y\right)\left(\int B_j(y)\rho_B^{(0)}(y,y)\,\mathrm{d}y\right)$$
$$N_{ij} = \int (\overrightarrow{\nabla} A_i(x)\overrightarrow{\nabla} A_j(x))\rho_A^{(0)}(x,x)\,\mathrm{d}x. \tag{67}$$

M_{ij} and N_{ij} are symmetric matrices. We have seen above that (M_{ij}) is positive. Now, (N_{ij}) is also positive because $\sum \xi_i\xi_j N_{ij} = \int \|\overrightarrow{\nabla}(\xi.A)\|^2\rho_A^{(0)}(y,y)\,\mathrm{d}y > 0$.

So the summation of equation (66) is also positive because it is $\mathrm{Tr}(MN)$ which can be evaluated in a basis for which N is diagonal with eigenvalues ν_i, and thus it is $\sum M_{ii}\nu_i$. But here $\nu_i \geqslant 0$, because N is positive and $M_{ii} > 0$ because M is also positive.

This completes the proof that $\delta_E(t) \geqslant 0$.

5. Interaction of particles: two-body potentials

Until now we have considered separable potentials. We now show how this includes more common kinds of coupling.

One has two systems, A and B, of degrees of freedom x and y, respectively:

$$H_A = \frac{p_A^2}{2} + V_A(x), \qquad p_A \text{ conjugate to the } x$$
$$H_B = \frac{p_B^2}{2} + V_B(y), \qquad p_B \text{ conjugate to the } y \tag{68}$$

and the interaction between x and y is

$$\sum_\alpha W_\alpha(x^{(\alpha)} - y^{(\alpha)}), \tag{69}$$

where $x^{(\alpha)}$ is a subset of the x and $y^{(\alpha)}$ is a subset of the y with same indices.

Functions of a difference of coordinates, as in equation (69), can be approximated by sums of separable potentials. Restricting to the case of a single even potential, W, one writes

$$W(x-y) = \int \cos\left(p(x-y)\right) W(p)\frac{\mathrm{d}p}{(2\pi)^n}$$
$$= \int [\cos(px)\cos(py) + \sin(px)\sin(py)]\,\frac{\mathrm{d}p}{(2\pi)^n} \tag{70}$$

and one has

$$W(x-y) = \lim \sum_\mu (A'_\mu B'_\mu + A''_\mu B''_\mu), \tag{71}$$

with

$$A'_\mu = \cos(p_\mu x), \qquad B'_\mu = \cos(p_\mu y)W(p_\mu)\frac{\Delta p_\mu}{(2\pi)^n},$$
$$A''_\mu = \sin(p_\mu x), \qquad B''_\mu = \sin(p_\mu y)W(p_\mu)\frac{\Delta p_\mu}{(2\pi)^n}. \tag{72}$$

In this expression the p_μ are discretized values of p, and the limit in equation (71) refers to decreasing the mesh in this discretization. Note that the A_μ and B_μ are real functions, hence Hermitian operators.

The foregoing demonstration considered a single even potential W. For odd potentials, one replaces the trigonometric identity for the cosine by that for the sine. Furthermore, any potential can be written as a sum of even and odd potentials. Finally, there is no difficulty extending this result to a sum of potentials, as in equation (69).

It follows that the results of our previous sections apply, and we deduce that for any potential interaction of the form (69), $\delta(t) > 0$ for small time.

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