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Laser Physics Letters doi:10.1088/1612-2011/13/5/055203

Invalidity of the quantitative adiabatic condition and general conditions for adiabatic approximations

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Received 23 March 2016 Accepted for publication 23 March 2016 Published 12 April 2016

Abstract

The adiabatic theorem was proposed about 90 years ago and has played an important role in quantum physics. The quantitative adiabatic condition constructed from eigenstates and eigenvalues of a Hamiltonian is a traditional tool to estimate adiabaticity and has proven to be the necessary and sufficient condition for adiabaticity. However, recently the condition has become a controversial subject. In this paper, we list some expressions to estimate the validity of the adiabatic approximation. We show that the quantitative adiabatic condition is invalid for the adiabatic approximation via the Euclidean distance between the adiabatic state and the evolution state. Furthermore, we deduce general necessary and sufficient conditions for the validity of the adiabatic approximation by different definitions.

Keywords: quantum adiabatic computing, adiabatic theorem, adiabatic approximation

1. Introduction

The adiabatic theorem was first presented about 90 years ago [1], which is described as follows. A system that is initially in an eigenstate of the Hamiltonian will remain in this eigenstate up to a multiplicative phase factor if the Hamiltonian varies sufficiently slowly. The adiabatic theorem plays a key role in adiabatic quantum processes, the adiabatic approximation, geometric phase [2], and quantum adiabatic computing [3]. The following quantitative adiabatic condition (QAC) is traditionally considered as the necessary and sufficient condition for the adiabaticity of quantum evolutions

$$\left|\frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_m(t) - E_n(t)}\right| \ll 1, t \in [0, T], m \neq n,$$
(1)

where *T* is the total evolution time.

Marzlin and Sanders first suggested the inconsistency of the adiabatic theorem [4]. After that, many efforts were devoted to the investigation of the new conditions for adiabaticity [5–25].

A counterexample to the sufficiency of QAC was given [7]. Via the perturbation theory, the conditions for adiabaticity were derived [10, 13]. By experimental study, it was shown that QAC is neither sufficient nor necessary [6]. After that a sufficient condition for adiabaticity was deduced [11] and general criteria and exact bounds for quantum adiabatic evolution were derived [14]. Then, adiabaticity with exponential accuracy for adiabatic quantum computation was discussed [15]. Recently, adiabaticity conditions were investigated for a class of Hamiltonians which are differential three times [23] and for the requirement $\langle E_k | \dot{E}_k \rangle = 0$ [24]. It is noted that recently, the necessity of QAC for adiabaticity becomes controversial [22].

In this paper, we give two different definitions for the adiabatic approximation to investigate adiabaticity. We show the invalidity of QAC for adiabaticity by definition 2 via the Euclidean distance between the adiabatic state and the evolution state. Furthermore, we investigate the general necessary and sufficient conditions for adiabaticity by different definitions.



In this paper, in section 2 we use two different definitions for adiabaticity and discuss the relation among them. In section 3, we exemplify the invalidity of QAC by definition 2. In sections 4 and 5, we propose general necessary and sufficient conditions for adiabaticity by definitions 1 and 2, respectively.

2. Two definitions for the validity of the adiabatic approximation

Consider a time-dependent Hamiltonian H(t) over an N dimensional quantum system. Let $E_n(t)$ and $|E_n(t)\rangle$ be the eigenvalues and orthonormal eigenstates of H(t), i.e.

$$H(t)|E_n(t)\rangle = E_n(t)|E_n(t)\rangle, n = 1, \cdots, N.$$
(2)

The evolution state $|\psi(t)\rangle$ of the system at time *t* satisfies the Schrödinger equation

$$\mathbf{i}|\dot{\psi}(t)\rangle = H(t)|\psi(t)\rangle,\tag{3}$$

where $|\psi(0)\rangle = |E_n(0)\rangle$. $|\psi(t)\rangle$ can be expanded as

$$|\psi(t)\rangle = \sum_{i} c_{i}(t) |E_{i}(t)\rangle, \qquad (4)$$

where $\sum_{j} |c_{j}(t)|^{2} = 1$ since $|||\psi(t)\rangle|| = 1$. Let the adiabatic state

$$|\psi_n^{\text{adi}}(t)\rangle = e^{i\beta_n(t)}|E_n(t)\rangle, \qquad (5)$$

where

$$\beta_n(t) = -\int_0^t E_n(x) \mathrm{d}x + \mathrm{i} \int_0^t \langle E_n(x) | \dot{E}_n(x) \rangle \mathrm{d}x.$$
 (6)

 $|\psi_n^{adi}(t)\rangle$ is proposed to describe the evolution process of the quantum system instead of the evolution state $|\psi(t)\rangle$ when the Hamiltonian H(t) varies slowly enough.

We give the following definitions for adiabaticity.

2.1. Definition 1

The definition has three equivalent versions.

1(a). The adiabatic state $|\psi_n^{adi}(t)\rangle$ is the adiabatic approximation for the evolution state $|\psi(t)\rangle$ if and only if $|\langle \psi_n^{adi}(t)|\psi(t)\rangle| \approx 1.$

The fidelity is usually used to define adiabaticity in previous literature, for example in [7, 6].

1(b). The adiabatic state $|\psi_n^{adi}(t)\rangle$ is the adiabatic approximation for the evolution state $|\psi(t)\rangle$ if and only if $1 - |c_n(t)| \ll 1$.

The definition is often used in previous literature, for example in [16, 8, 10, 14]. It is easy to know that the fidelity $|\langle \psi_n^{adi}(t) | \psi(t) \rangle| = |c_n(t)|$. So, versions 1(a) and (b) are equivalent.

Note that

$$1 - |c_n(t)|^2 \le 2(1 - |c_n(t)|) \tag{7}$$

and

$$(1 - |c_n(t)|) \leq 1 - |c_n(t)|^2.$$
(8)

From equations (7) and (8), clearly, $1 - |c_n(t)|^2 \ll 1$ if and only if $1 - |c_n(t)| \ll 1$. Thus, version 1(b) can be rewritten as follows.

1(c). The adiabatic state $|\psi_n^{adi}(t)\rangle$ is the adiabatic approximation if and only if $1 - |c_n(t)|^2 \ll 1$.

2.2. Definition 2

The definition has two equivalent versions.

2(a). Let $|D^{adi}(t)\rangle$ be the difference between the evolution state $|\psi(t)\rangle$ and the adiabatic state $|\psi_n^{adi}(t)\rangle$. That is,

$$|D^{\mathrm{adi}}(t)\rangle = |\psi(t)\rangle - |\psi_n^{\mathrm{adi}}(t)\rangle.$$
(9)

Then the adiabatic state $|\psi_n^{\text{adi}}(t)\rangle$ is the adiabatic approximation for the evolution state $|\psi(t)\rangle$ if and only if

$$\||D^{\mathrm{adi}}(t)\rangle\| \ll 1. \tag{10}$$

 $|||D^{adi}(t)\rangle||$ means the Euclidean distance between the adiabatic state and the evolution state. The Euclidean distance is also used to define adiabaticity but with the different adiabatic states [11].

A calculation yields

$$|||D^{\mathrm{adi}}(t)\rangle||^{2} = 2(1 - \operatorname{Re}(\mathrm{e}^{-\mathrm{i}\beta_{n}}c_{n}(t))).$$
(11)

Via equation (11) version 2(a) for the definition can be rephrased as follows.

2(b). The adiabatic state $|\psi_n^{adi}(t)\rangle$ is the adiabatic approximation if and only if

$$1 - \operatorname{Re}(\mathrm{e}^{-\mathrm{i}\beta_n}c_n(t)) \ll 1. \tag{12}$$

2.3. The relation between two definitions

We can show that definitions 1 and 2 are inequivalent below. Since $\text{Re}z \leq |z|$, it is easy to see

$$1 - |c_n(t)| \le 1 - \operatorname{Re}(e^{-i\beta_n}c_n(t)).$$
(13)

Equation (13) means that definition 2 implies definition 1. However, the converse is not true. Therefore, definitions 1 and 2 are inequivalent.

3. Exemplifying the invalidity of QAC by definition 2

In previous literature, definition 1 is used to discuss the validity of QAC for adiabaticity. So far no one has investigated the validity of QAC by definition 2. We use the example [26] to exemplify the invalidity of QAC by version 2(a) of definition 2. For readability, we list the example in table 1.

(insufficient) Let $\lambda = \omega/\omega_0$ and $\theta = \pi/2$. Then, when $\lambda = 0.001$, from equation (A.4) in appendix A, we obtain

$$\left|\frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_m(t) - E_n(t)}\right| = 0.0005 \tag{14}$$

Table 1. The example.

 $H(t) = \frac{\omega_0}{2} (\sigma_x \sin \theta \cos \omega t + \sigma_y \sin \theta \sin \omega t + \sigma_z \cos \theta),$

$$E_{\rm I}(t) = -\frac{\omega_0}{2}, |E_{\rm I}(t)\rangle = \begin{pmatrix} e^{-i\omega t/2} \sin \frac{\theta}{2} \\ -e^{i\omega t/2} \cos \frac{\theta}{2} \end{pmatrix},$$

$$E_{\rm 2}(t) = \frac{\omega_0}{2}, |E_{\rm 2}(t)\rangle = \begin{pmatrix} e^{-i\omega t/2} \cos \frac{\theta}{2} \\ e^{i\omega t/2} \sin \frac{\theta}{2} \end{pmatrix},$$

$$|\psi(t)\rangle = a(t)|E_{\rm I}\rangle + b(t)|E_{\rm 2}\rangle,$$

$$a(t) = \cos(\tilde{\omega}t/2) + i\sin(\tilde{\omega}t/2)(\omega_0 - \omega\cos\theta)/\tilde{\omega},$$

$$b(t) = i(\omega/\tilde{\omega})\sin\theta\sin(\tilde{\omega}t/2),$$

$$\tilde{\omega} = \sqrt{\omega_0^2 + \omega^2 - 2\omega_0\omega\cos\theta},$$

$$|\psi_1^{\rm adi}(t)\rangle = e^{i(\omega_0 - \omega\cos\theta)t/2}|E_{\rm I}\rangle$$

and from equation (A.5) in appendix A, $|||D^{adi}(t)\rangle||^2 = 1.3694$ for $\omega_0 = 10^7$ and t = 0.5. Thus, QAC is satisfied but the adiabatic approximation is invalid.

(unnecessary) Clearly $|||D^{adi}(0)\rangle||= 0$. While for $\theta = \frac{\pi}{2}$ and $\frac{\omega}{\omega_0} = 200$, from equation (A.1) in appendix A $\left|\frac{\langle E_m(t) \mid \dot{E}_n(t) \rangle}{E_m(t) - E_n(t)}\right| = 100$ for any time *t*. It means that QAC is not necessary for adiabaticity.

4. The adiabatic approximation by definition 1

Here we explore the general conditions for adiabaticity for the adiabatic state $|\psi_n^{\text{adi}}(t)\rangle$ by version 1(c) of definition 1. First we evaluate $1 - |c_n(t)|^2$ in appendix **B**.

4.1. A necessary and sufficient condition

By version 1(c) of definition 1, from equation (B.3) in appendix B we obtain a necessary and sufficient condition for adiabaticity.

Theorem 1. The adiabatic state $|\psi_n^{adi}(t)\rangle$ is the adiabatic approximation by definition 1 if and only if

$$\int_0^{t_n} \operatorname{Re} \sum_k c_n^*(t') c_k(t') \langle E_n(t') | \dot{E}_k(t') \rangle dt' \ll 1.$$
(15)

But it is not practical to calculate the left-hand side of equation (15) because $c_n^*(t)$ and $c_k(t)$ are unknown.

4.2. Upper bounds of $1 - |c_n(t)|^2$

Next we derive the upper bounds of $1 - |c_n(t)|^2$ to give sufficient conditions via the eigenvalues and eigenstates of the Hamiltonian. Note that $\text{Re}z \leq |z|$. Then, from equation (B.3)

$$1 - |c_n(t)|^2 \leqslant 2\Pi,\tag{16}$$

where

$$\Pi = \int_0^t \left| \sum_k c_n^*(t') c_k(t') \langle E_n(t') | \dot{E}_k(t') \rangle \right| \mathrm{d}t'.$$
(17)

Table 2. The upper bounds of
$$\Pi$$
.

$$B_{1} = \sum_{k} \int_{0}^{t} |\langle E_{n}(t') | \dot{E}_{k}(t') \rangle| dt'$$

$$2B_{2} = 2 \sum_{k} |\int_{0}^{t} \langle E_{n}(t') | \dot{E}_{k}(t') \rangle dt'|$$

$$B_{3} = \int_{0}^{t} \sqrt{\sum_{k} |\langle E_{n}(t') | \dot{E}_{k}(t') \rangle|^{2}} dt'$$

$$B_{4} = \sqrt{\sum_{k} (\int_{0}^{t} |\langle E_{n}(t') | \dot{E}_{k}(t') \rangle| dt'})^{2}$$

We majorize Π below. First we can obtain the upper bound B_1 of Π in table 2. Assume that the imaginary part and the real part of $c_n^*(t)c_k(t)$ are continuous and the imaginary part and the real part of $\langle E_n(t) | \dot{E}_k(t) \rangle$ are integrable and do not change sign in the interval [0, t]. Then applying the second mean value theorem for integrals for real functions, we obtain the upper bound $2B_2$ of Π in table 2.

Via equation (17), we also obtain

$$\Pi \leqslant \int_0^t \sum_k |c_k(t')\langle E_n(t')|\dot{E}_k(t')\rangle| \mathrm{d}t'$$
(18)

Via equation (18) and noting $\sum_k |c_k(t)|^2 = 1$, by applying Caushy–Schwarz inequality we obtain the upper bounds B_3 and B_4 in table 2 and give a detailed derivation for the upper bound B_4 as follows.

$$\Pi \leq \sum_{k} \int_{0}^{t} |c_{k}(t')\langle E_{n}(t')|\dot{E}_{k}(t')\rangle|dt'$$

$$= \sum_{k} |c_{k}(\xi)| \int_{0}^{t} |\langle E_{n}(t')|\dot{E}_{k}(t')\rangle|dt'$$

$$\leq \sqrt{\sum_{k} (\int_{0}^{t} |\langle E_{n}(t')|\dot{E}_{k}(t')\rangle|dt'})^{2}.$$
(19)

It is not difficult to show that

$$B_i \leq B_1, i = 2, 3, 4.$$
 (20)

4.3. Sufficient conditions

By definition 1 and equation (16), we obtain four sufficient conditions $B_i \ll 1$ (i = 1, 2, 3, 4) for adiabaticity.

Theorem 2. The adiabatic state $|\psi_n^{adi}(t)\rangle$ is the adiabatic approximation by definition 1 if one of $B_i \ll 1$ (i = 1, 2, 3, 4) is fulfilled.

We list these conditions in table 3. Via equation (20), clearly if $B_1 \ll 1$ then $B_i \ll 1$, i = 2, 3, 4. However, the converse is not true. It means that the sufficient conditions $B_i \ll 1$ (i = 2, 3, 4) are more powerful than the sufficient condition $B_1 \ll 1$ for adiabaticity.

For the example in table 1, the general sufficient conditions $B_i \ll 1$, i = 1, 2, 3, 4, reduce to the ones in the right column of table 3. Next we demonstrate the validity of the reduced conditions for the example in table 1.

For the example, a calculation yields

$$|b(t)| = \frac{\omega t \sin \theta}{2} \frac{\sin(\tilde{\omega}t/2)}{(\tilde{\omega}t/2)} \leqslant \frac{\omega t \sin \theta}{2}.$$
 (21)

Table 3. The four sufficient conditions for the validity of the adiabatic approximation by definition 1.

Sufficient conditions	For the example in table 1
$B_1 \ll 1$	$\omega t(\sin\theta + \cos\theta)/2 \ll 1$
$B_2 \ll 1$	$\omega t(\sin\theta + \cos\theta)/2 \ll 1$
$B_3 \ll 1$	$\omega t/2 \ll 1$
$B_4 \ll 1$	$\omega t/2 \ll 1$

From table 3 and equation (21), it is easy to see that the conditions in the right column of table 3 guarantee that $|b(t)| \ll 1$. Therefore, for the example, the conditions in the right column of table 3 are sufficient for adiabaticity by definition 1.

5. The adiabatic approximation by definition 2

By version 2(b) of definition 2, we explore the conditions for adiabaticity for the adiabatic state $|\psi_n^{adi}(t)\rangle$. First we calculate $1 - \text{Re}(e^{-i\beta_n}c_n(t))$ in appendix C.

5.1. A necessary and sufficient condition

By version 2(b) of definition 2, from equation (C.4) in appendix C we obtain a necessary and sufficient condition for adiabaticity.

Theorem 3. The adiabatic state $|\psi_n^{adi}(t)\rangle$ is the adiabatic approximation by version 2(b) of definition 2 if and only if

$$\operatorname{Re} \int_0^t e^{-i\beta_n(t')} \sum_{k \neq n} c_k(t') \langle E_n(t') | \dot{E}_k(t') \rangle dt' \ll 1.$$
(22)

Note that $c_k(t)$ in equation (22) are unknown. Therefore, it is not practical to calculate the left-hand side of equation (22).

5.2. Upper bounds of $1 - \text{Re}(e^{-i\beta_n}c_n(t))$

Via eigenvalues and eigenstates of the Hamiltonian, we construct practical sufficient conditions below. Note that $\text{Re}z \leq |z|$. Then, from equation (C.4)

$$1 - \operatorname{Re}(\mathrm{e}^{-\mathrm{i}\beta_n}c_n(t)) \leq \left| \int_0^t \, \mathrm{e}^{-\mathrm{i}\beta_n(t')} \sum_{k \neq n} c_k(t') \langle E_n(t') | \dot{E}_k(t') \rangle \mathrm{d}t' \right|$$
(23)

$$\leq \int_0^t \sum_{k \neq n} |c_k(t') \langle E_n(t') | \dot{E}_k(t') \rangle | \mathrm{d}t'.$$
(24)

By using the same methods for the upper bounds of Π , we obtain four upper bounds $B'_i(i = 1, 2, 3, 4)$ of $1 - \text{Re}(e^{-i\beta_n}c_n(t))$ in table 4. The four upper bounds B'_i in table 4 correspond to the four upper bounds B_i of Π . The only difference is that we need to change the subscript 'k' in B_i as ' $k \neq n$ '. For the upper bound B'_2 , we require the same limitation as the one for Π_2 . We can argue that $B'_i \leq B'_1$, i = 2, 3, 4. It means that B'_i (i = 3, 4), are tighter upper bounds than B'_1 .

Table 4. The upper bounds of
$$1 - \text{Re}(e^{-i\beta_n}c_n(t))$$
.

$$B'_{1} = \sum_{k \neq n} \int_{0}^{t} |\langle E_{n}(t') | \dot{E}_{k}(t') \rangle| dt'$$

$$2B'_{2} = 2 \sum_{k \neq n} \left| \int_{0}^{t} \langle E_{n}(t') | \dot{E}_{k}(t') \rangle dt' \right|$$

$$B'_{3} = \int_{0}^{t} \sqrt{\sum_{k \neq n} |\langle E_{n}(t') | \dot{E}_{k}(t') \rangle|^{2}} dt'$$

$$B'_{4} = \sqrt{\sum_{k \neq n} (\int_{0}^{t} |\langle E_{n}(t') | \dot{E}_{k}(t') \rangle| dt')^{2}}$$

5.3. Sufficient conditions

From the four upper bounds in table 4, we obtain four sufficient conditions.

Theorem 4. The adiabatic state $|\psi_n^{adi}(t)\rangle$ is the adiabatic approximation by version (b) of definition 2 if one of $B'_i \ll 1$ (i = 1, 2, 3, 4) is fulfilled.

For the example in table 1, the four general sufficient conditions $B'_i \ll 1$, i = 1, 2, 3, 4, reduce to $(\omega t \sin \theta)/2 \ll 1$.

6. Summary

In this paper, we have listed two different definitions for adiabaticity and have clarified the relation among different definitions. We have deduced the invalidity of QAC for the adiabatic approximation via the Euclidean distance between the adiabatic state and the evolution state, and we have proposed general necessary and sufficient conditions for adiabaticity by definition 1 with the fidelity and definition 2 with the Euclidean distance.

Acknowledgments

The paper was supported by NSFC (Grant No. 10875061).

Appendix A. Calculation of example 1

For the example in table 1, a tedious calculation yields

$$\frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_m(t) - E_n(t)} = (\omega\sin\theta)/(2\omega_0), \tag{A.1}$$

$$\psi_1^{\text{adi}}(t)\rangle = e^{i(\omega_0 - \omega\cos\theta)t/2} |E_l(t)\rangle,$$
 (A.2)

and

$$||D^{\mathrm{adi}}(t)\rangle||^{2} = 2 + \frac{\omega_{0} - \omega\cos\theta - \bar{\omega}}{\bar{\omega}}\cos\frac{(\bar{\omega} + \omega_{0} - \omega\cos\theta)t}{2} - \frac{\omega_{0} - \omega\cos\theta + \bar{\omega}}{\bar{\omega}}\cos\frac{(\bar{\omega} - \omega_{0} + \omega\cos\theta)t}{2}.$$
(A.3)

Let $\lambda = \omega/\omega_0$ and $\theta = \pi/2$. Then, from equation (A.1), we obtain

$$\left|\frac{\langle E_m(t)|E_n(t)\rangle}{E_m(t)-E_n(t)}\right| = \lambda/2 \tag{A.4}$$

and from equation (A.3), we obtain

$$\||D^{\mathrm{adi}}(t)\rangle\|^{2} = 2 + \left(\frac{1}{\sqrt{1+\lambda^{2}}} - 1\right)\cos\frac{t\omega_{0}(\sqrt{1+\lambda^{2}}+1)}{2} - \left(\frac{1}{\sqrt{1+\lambda^{2}}} + 1\right)\cos\frac{t\omega_{0}(\sqrt{1+\lambda^{2}}-1)}{2}.$$
(A.5)

Appendix B. Calculation of $1-|c_n(t)|^2$

First we evaluate $1-|c_n(t)|^2$. By substituting equation (4) into equation (3), we can obtain

$$\dot{c}_{\ell}(t) = -\mathbf{i}E_{\ell}(t)c_{\ell}(t) - \sum_{k} c_{k}(t)\langle E_{\ell}(t)|\dot{E}_{k}(t)\rangle.$$
(B.1)

It is known that

$$\frac{\mathrm{d}}{\mathrm{d}t}|c_{\ell}(t)| = \frac{\mathrm{Re}(c_{\ell}^{*}(t)\dot{c}_{\ell}(t))}{|c_{\ell}(t)|},\tag{B.2}$$

where $c_{\ell}^{*}(t)$ is the complex conjugate of $c_{\ell}(t)$. By integrating equation (B.2), we obtain

$$1 - |c_n(t)|^2 = 2 \int_0^t \operatorname{Re} \sum_k c_n^*(t') c_k(t') \langle E_n(t') | \dot{E}_k(t') \rangle dt'. \quad (B.3)$$

Appendix C. Calculation of $1 - \text{Re}(e^{-i\beta_n}c_n(t))$

Let us calculate $1 - \text{Re}(e^{-i\beta_n}c_n(t))$ below. First we calculate $c_n(t)$. From equation (B.1), we obtain

$$\dot{c}_n(t) + c_n(t)(\mathbf{i}E_n(t) + \langle E_n(t)|\dot{E}_n(t)) = -\sum_{k\neq n} c_k(t)\langle E_n(t)|\dot{E}_k(t)\rangle.$$
(C.1)

It is not hard to solve the first-order ODE in equation (C.1). Then, we obtain the analytic expression of $c_n(t)$

$$c_{n}(t) = e^{i\beta_{n}(t)} [1 - \int_{0}^{t} e^{-i\beta_{n}(t')} \sum_{k \neq n} c_{k}(t') \langle E_{n}(t') | \dot{E}_{k}(t') \rangle dt'],$$
(C.2)

where $e^{i\beta_n(t)} = e^{-\int_0^t [iE_n(z) + \langle E_n(z) | \dot{E}_n(z)] dz}$.

Then,

$$e^{-i\beta_n}c_n(t) = 1 - \int_0^t e^{-i\beta_n(t')} \sum_{k \neq n} c_k(t') \langle E_n(t') | \dot{E}_k(t') \rangle dt'. \quad (C.3)$$

Then,

$$1 - \operatorname{Re}(\mathrm{e}^{-\mathrm{i}\beta_n}c_n(t)) = \operatorname{Re}\int_0^t \mathrm{e}^{-\mathrm{i}\beta_n(t')} \sum_{k\neq n} c_k(t') \langle E_n(t') | \dot{E}_k(t') \rangle \mathrm{d}t'.$$
(C.4)

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