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Why the quantitative condition fails to reveal quantum adiabaticity

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Abstract

The a ia ai e adiaba ic c di i (QAC), a ia ai e c di i , is a c e ie (*a priori*) l f s i a i g he adiaba ici f a e l i s. H e e, he a ge f he a licabili f QAC is ell des d. I has bee s h ha QAC ca bec e i s ffficie f g a a eei g he alidi f he adiaba ic a i a i , h de ha c di i s he QAC ld bec e ecess a has bec e c es ial. Fi he e, i is belie ed ha he i abili f he QAC e eal a adiaba ici is d e i d ced s a a si- i s. H e e, i is clea h a if hese a si i s i ge e al. He e e se a g ess his ble b fi di g a e ac ela i ha ca e eal h a si i a li des a e ela ed QAC di ec l . As *a posteriori* c di i f a adiaba ici , s l is i es all a licable a (- dege e a e) a s s e a d gi s a clea ic e h QAC c ld bec e i s ffficie i ecess a f he adiaba ic a i a i , hich is a ble ha has gai ed c s ide able i e s i he li e a e i ece eas .

Ke ds: adiaba ic c i g, a adiaba ic c di i , adiaba ic a i a i

1. Introduction

The ... a ... adiaba ic he ... e (QAT) [1, 2] s... gges s ha a... h sicals... s e ... i iali ed i a eige s a e $\left|E_n\left(t=0\right)\right\rangle$ (c ... l he g... d s a e) f a ce... ai ga... ed i e-de... e de Ha il ... ia $H(t)$, i h a eige al e E_n, a i e t e ai s i hes a e is a a e is eige s a e (... a ... l i... lica i e... has e fac ...), ... ided ha he Ha il ... ia $H(t)$ a... ies i a c i ... is a ds... fficie l s l a . The adiaba ic he ... e as fis ... ... s ed b B ... a d F ck a he da f ... a ... echa ics [3], h e... e i a ed b he idea f adiaba ic i a ... ia s f Eh... e fes [4]. B ... a d F ck's ... s... l is ... s ic ed b ... ded Ha il ... ia s i h dis c... e e e... g le eb s, e.g. 1D ha... ic s cilla s; hei ... s... l is a... licable s s e s i h a c i ... is s... ec ... e.g. H d ge a . This ... s ic i as ela ed b Ka i 1950 [5], h f ... d ha i he adiaba ic li i, he i e e l i f a i e-de... e de Ha il ... ia is e ... i ale a ge e ic e l i . Ka 's ... s... l is a... licable s s e s i cl di g H d ge a , he... e he g... ds a e is ... i e a d has a ga f he e ci eds a es ha ca ha e dege e ac . La e, he ... e ... i e e f he e is e ce f a ga f ... ... i g he adiaba ic he ... e as f ... d be ... ecess a [6].

This i ... ig i g ... h sical ... ... e f ... a ... adiaba ici fi ds a i e es i g a... lica i s, i cl di g b li i ed ... a ... field he ... [7], ge e ic ... has e [8], s i ... la ed Ra a adiaba ic ... ass age [9], e e g le el c ... ss i g i leq les [10, 11], adiaba ic ... a ... c ... ai [12–18], ... a ... s i ... la i (see e.g. he ... e ie [19]), a d he a... lica i s [20].

1.1. Quantitative adiabatic condition

Des... i e is l g his ..., hes ... d f he QAT is s ill a e... ac i e field f es ea ch. Ma ... ks ha e bee ... e f ... ed ai i g achie e a be e ... des a di g f he adiaba ic he ... e . I ... a io la..., he ... ble f ... a if i g he s l ess f adiaba ic e l i has bee c ... le el s l ed. T adi i all [1, 2, 14, 21] hes -called (e.g. see [22]) ... a i a i e adiaba ic c di i (QAC) ... s i ... l ... a i a i e c di i (f ... *all* $m \neq n$):

$$\left|\frac{\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle}{E_m(t)-E_n(t)}\right| \ll 1, \tag{1}$$

as ea ... a if hes l ess f $H(t)$ (see a ... e di A f ... de ails he defi i i s f he Ha il ia a d eige ec s). H e e, QAC as ... e icall s h be a g d i dica ... f ... e eali g he fideli f he fi al s a e [23]. F ... he ... e, i has bee s h ha QAC is i c s is e i h he QAT [24] a d is... fficie f ... ai ai i g he alidi f he adiaba ic a... ... i a i [22], e ce f ... s es ... ecial cas es [25]. The a g e s f ... s h i g he i c s is e c a d is... fficie c f QAC e e c s ... c ed [22] f a c ... a is be ee s, s e s, A a d B, he e A as e l ed ... de a Ha il ia $H_a\left(t\right)$. The Ha il ia

$$H_b\left(t\right) = -U_a\left(t\right)^{\dagger} H_a\left(t\right) U_a\left(t\right) \tag{2}$$

f s, s e B is ela ed ha f s, s e A h ... gh a ... i a, as f ... a i $U_a\left(t\right) = T\exp\left(-i\int_0^t H_a\left(t'\right)\mathrm{d}t'\right)$ ha c ... s... ds he e ac ... ... aga ... f $H_a\left(t\right)$. I as s h ha b hs, s e s A a d B s a is f he QAC, b a s e f he ca fi lfill he

adiaba ic a- - i a i . This c cl s i s c s s e i h he s l s - e f - ed i a NMR e - e i e [26].

1.2. Related studies in the literature

Ma , s i dies (e.g. [27–33]) ha e bee ade - i g i des a d he i c s s e c ais ed b Ma - li a d Sa des [24]. I as a g ed [29–33] ha s a - a s i i s be ee e e g le el a e s - s ible f - he i la i s f he adiaba ic he e . A efi ed adiaba ic c di i has bee f i d [34], hich aks i acc i he effecs f s a e e g -le el a s i i s .

O he he - ha d, he alidi f he adiaba ic he e as a al ed f a - e i ba i e- e - a s i a - - ach [35, 36], hich - - ides a diag a ic e s e a i f - adiaba ic d a ics a d ields he i a i a i e c di i (i e i a i (1)) as he fis - de- a - - i a i . I as a g ed [37] ha he i a i a i e c di i is i s i fficie f - he adiaba ic a - - i a i he he Ha il ia a ies a idl b i h a s all a - li i de. Fi - he e, ge e ali i g QAC f - - e i a i s s e s [27, 38] a d a -b d s s e s [39] ha e bee achie ed. Eff s f - fi di g c di i s ha ca e lace QAC e e ade [40–42].

A he li e f s ea ch ela ed he adiaba ic he e is s i a e - b i d hes cali g f he fi al s a e fideli . U de s e ge e al c di i s f - a ga - ed Ha il ia , i as f i d [43] ha he - a s i i - - babili s cales as $O\left(1/T^2\right)$ f - a al e l i i e T. Whe he al i e is fi ed, i as s h [44, 45] ha b h he i i i eige al e ga Δ a d he le g h f he a es ed - a h $L \equiv \int_0^1 \left\| \left| \partial_r \psi\left(r\right) \right\rangle \right\| \mathrm{d}r$, he e $r(t)$ is a i e- a i g - a a e e i he Ha il ia , a e i - - a .

2. Motivation

I s ead f i s i i g he alidi f he i a i a i e c di i as a i dica - f - i a i adiaba ici , e a e i e s ed i he i s i

‘*Under what additional conditions would QAC become necessary*?’.

The a s e his i s i has bee clea [46–48]. O - k is i a ed b a ece de el - e achie ed i [46], he e QAC is a g ed be ecess a i de ce ai addi i al ass i - i s ela ed he *adiabatic state* $\left|\psi_n^{adi}\left(t\right)\right\rangle$ [8, 46], hich is defi ed b a achi g a i e-de- e de - has e fac - (ss e iall he Be - - has e [8]) $e^{i\beta_n(t)}$ he e e g eige s a e $\left|E_n\left(t\right)\right\rangle$, i.e.,

$$\left|\psi_n^{adi}\left(t\right)\right\rangle \equiv e^{i\beta_n(t)} \left|E_n\left(t\right)\right\rangle, \tag{3}$$

he e

$$\beta_n\left(t\right) \equiv -\int_0^t E_n\left(x\right)\mathrm{d}x + i\int_0^t \left\langle E_n\left(x\right)\middle|\dot{E}_n\left(x\right)\right\rangle \mathrm{d}x. \tag{4}$$

The ke s i l b ai ed i [46] is ha (i i - a i s) he - babili a - li i de $c_m\left(t\right) = \left\langle E_m\left(t\right)\middle|\psi\left(t\right)\right\rangle$ f - he eige s a e $\left|E_m\left(t\right)\right\rangle$ a i e t is gi e b he f ll i g e - ssi :

Table 1. S a f ai s e s a ds b s.

Te s	Mea i g
Q a adiaba ic he e	This he e s a es ha f ge e al h sicals s e s i ialied i a eige s a e (e.g. g d s a e) i h s ec a i e-de e de Ha il ia , he a sii he (is a a e s) eige s a e is s all ided ha he a ia i f he Ha il ia is s fficie l s l .
Q a i a i e adiaba ic c di i (QAC) (a i a i e c di i)	A c di i adi i all c sided as a ecess a a d s fficie c di i f he alidi f he adiaba ic a i a i (see e a i (1)), i.e., $\left\lvert \frac{\langle E_m(t) \mid \dot{E}_n(t)\rangle}{E_m(t)-E_n(t)} \right\rvert \ll 1.$
Adiaba ic a i a i	A a i a i ha e laces he e ac s a e $\lvert\psi(t)\rangle$ i h he adiaba ics a e $\lvert\psi_n^{adi}(t)\rangle$, hich leads $\lvert c_m(t)\rvert \ll 1$ f all $m \neq n$.
Adiaba ics a e $\lvert\psi_n^{adi}(t)\rangle$	Defi ed b $\lvert\psi_n^{adi}(t)\rangle \equiv e^{i\beta_n(t)}\lvert E_n(t)\rangle$, he e $\lvert E_n(t)\rangle$ is he i s a a e s eige s a e (i h eige al e $E_n(t)$) f he Ha il ia $H(t)$, a d $\beta_n(t) \equiv -\int_0^t E_n(x)\,dx + i\int_0^t \langle E_n(x)\lvert\dot{E}_n(x)\rangle\,dx$ (see e a i (3)).
Diffe e ce ec $\lvert D(t)\rangle$	Defi ed b $\lvert D(t)\rangle \equiv \lvert\psi(t)\rangle - \lvert\psi_n^{adi}(t)\rangle$, he diffe e ce be ee he e ac i e-e l eds a e $\lvert\psi(t)\rangle$ a d he adiaba ics a e $\lvert\psi_n^{adi}(t)\rangle$ (see e a i (8))

$$c_m(t) \approx i e^{i\beta_n(t)} \frac{\langle E_m(t)\lvert\dot{E}_n(t)\rangle}{E_m(t)-E_n(t)}, \tag{5}$$

hich leads he c cl s i ha if he adiaba ic a i a i is alid, i.e., he babili a li de c_m f all eige s a es $m \neq n$ a es all, $\lvert c_m(t)\rvert \ll 1$, he he QAC (cf e a i (1)) ecess a il h ld (f as i a f he defi i i s f a i s e s, see able (1)).

F c a is , as i ila e ess i (i a i) as gi e b Schiff [1] as

$$c_m(t) \approx \frac{\langle E_m(t)\lvert\dot{H}\rvert E_n(t)\rangle}{i\big(E_m(t)-E_n(t)\big)^2}\left(e^{i(E_m-E_n)t}-1\right), \tag{6}$$

$$= i\frac{\langle E_m(t)\mid\dot{E}_n(t)\rangle}{E_m(t)-E_n(t)}\left(e^{i(E_m-E_n)t}-1\right). \tag{7}$$

The de i a i f he fis li e hes ec d li e is ided i a e di B. Thse e ess i s (i e a i s (5) a d (7)) edic he alidi f he adiaba ic a i a i he he a iaiec di i (cf e a i (1)) is s a is fied.

H e e, he esi l i [46] as i c es ial [47, 48]. Zha a d Wi [47] a g ed ha he c ib i f he iss i g e i he esi l i [46] is i de es i a ed. C a a [48] i ed i ha he -ig is is e f he a i a i s ig '≈' i [46] leads a b q e ea i g f i a i adiaba ici . This ble is a ided i i de i a i . T g's e l [49] e has i ed he c ec i ih he adiaba ic s a e i his esi l, b did s l e he ii s c le el .

3. Summary of results

We es e e esi ls ha ai

1. Se le he e is i g c es i he li e a i e [46–49] b de i i g a e ac e essi (cf e i a i (9)) f he asi i a li i de $c_m(t)$, hich c ai s c ec i e s iss i g i he e i is esi l (s h i e i a i (5)), a d
2. e l e he e e ies f he c ec i e (cf e i a i (22)) f e i a i (5), hich he Ls is i des a d be e he c ec i be ee QAC a d he adiaba ic a i a i .

Q a ach ca be f i la ed c e ie l ih he is e f he diffe e ce ec $|D(t)\rangle$, hich is defi ed b he diffe e ce be ee he e ac s a e $|\psi(t)\rangle$ a d he adiaba ic s a es $|\psi_n^{adi}(t)\rangle$ (cf e i a i (3)):

$$|D(t)\rangle \equiv |\psi(t)\rangle - |\psi_n^{adi}(t)\rangle. \tag{8}$$

3.1. Our main result and its consequences

Q ai esi l c ai s a *exact* e essi f $c_m(t)$, a el (c a e ih e i a i (5))

$$c_m(t) = \underbrace{ie^{i\beta_n(t)}\frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_m(t)-E_n(t)}}_{\equiv Q_m(t)\ \text{Result in [46]}} \underbrace{-E_n(t)\frac{\langle E_m(t)|D(t)\rangle}{E_m(t)-E_n(t)} + i\frac{\langle E_m(t)|\dot{D}(t)\rangle}{E_m(t)-E_n(t)}}_{\equiv R_m(t)\quad \text{Correction terms}}, \tag{9}$$

hich ed ces he esi l i [46] (cf e i a i (5)) he he ag i de $|R_m(t)|$ f he c ec i e is s all; f e a le he b h $|D(t)\rangle = 0$ a d $|\dot{D}(t)\rangle = 0$. Thes e c di i s c es d he ke assi i s ade i [46]. Fi he e, i esi l i e i a i (9) al i dica es a c di i (cf e i a i (25)) e ge e al ha he esi l i [46].

The e ac e essi i e i a i (9) i lies a e esi ls, hich a e lis ed as f ll s:

- The esi l f [46] as b ai ed b assi i g ha b h $|D(t)\rangle$ a d $|\dot{D}(t)\rangle$ ca be ig ed, i.e., $|D(t)\rangle \approx 0$ a d $|\dot{D}(t)\rangle \approx 0$. H e e [46] did ell s h s all hese e s s h i ld be. Q e essi gi es he i a i a i e c ie ia, a el :

$$\left\| \left| D(t) \right\rangle \right\| \ll \left| \frac{E_m(t) - E_n(t)}{E_n(t)} \right| \quad \text{and} \quad \left\| \left| \dot{D}(t) \right\rangle \right\| \ll \left| E_m(t) - E_n(t) \right|. \tag{10}$$

- F he e, f i e ess i , e ca b ai he s a e c cl s i as i [46] b e i i g a e ge e al c di i

$$\left\| i\left| \dot{D}(t) \right\rangle - E_n(t) \left| D(t) \right\rangle \right\| \ll \left| E_m(t) - E_n(t) \right|. \tag{11}$$

- O e f he c i icis s he s l f [46] as ha e ca fi d a c i e e a le ha i la es he i a ia i e c di i b fi lfills he adiaba ic c di i [48]. O e ess i i dica es ha his si i a i s ssible he i c ec i e ca cel ih he fis e i e i a i (9).
- I he li i g cas e he e he as i i a li i de e i als e ac l he igh ha d s ide f e i a i (5), i.e.,

$$c_m(t) = i e^{i\beta_n(t)} \frac{\left\langle E_m(t) \middle| \dot{E}_n(t) \right\rangle}{E_m(t) - E_n(t)}, \tag{12}$$

e f i d ha his c di i is e i i ale

$$i\left| \dot{D}(t) \right\rangle = E_n(t) \left| D(t) \right\rangle. \tag{13}$$

- We al s f i d ha he c di i f $\left| \dot{D}(t) \right\rangle = 0$ i lies ha b h $c_m(t) = 0$ a d $\left| D(t) \right\rangle = 0$. I he ds, f a i e-e l i g i a i s a e $\left| \psi(t) \right\rangle$, if $\left| \dot{\psi}(t) \right\rangle = \left| \dot{\psi}_n^{adi}(t) \right\rangle$, he his i a i s a e is e i al $\left| \psi_n^{adi}(t) \right\rangle$ as ell, i.e., $\left| \psi(t) \right\rangle = \left| \psi_n^{adi}(t) \right\rangle$.

Fi all , e e ha he fac ha i ai e ess i is a e ac s l eli i a es i ecess a deba e e he c ec ess f a l i g a i ai , as ha e ed [47, 50] f he s l s f [24] a d [46].

3.2. Organization of the report

Bef e e g i he de ails , e e ha s i e ha he g al f his k is l k f a e c di i ha ca ake he le f QAC f adiaba ic a i ai . I deed, he QAC is a c e ie a *priori* c di i f s i a i g he alidi f he adiaba ic a i ai , al h i gh he a ge f he a licabili is clea . I s ead, as a *posteriori* c di i , e ai ff e a be e ic i e ha hel s i des a d *why the QAC fails to reveal the adiabatic approximation*—a ble ha has gai ed c s ide able i e s i he li e a i e i ece eas . Al h i gh s e a he a ical s e s i i de i a i a l k ick , l a e ials i ele e a i a i echa ics a e i l ed.

The s f his e is ga i ed as f ll s :

I sec i 'De i a i f he ai s l ': e ide a de ailed s e -b s e g ide f he de i a i f i ai s l i e i a i (9).

I sec i 'Dis ss i he ai esi l': e f s he-- e ies f he fis e a d he c ec i s e s i e ai (9). The ecess i f he a ia ai e c di i is dis ss ed. The i lica i s f e- ess i a e al e l ed.

I sec i 'Ill s ai e e a le': he e e c side- esi ls bas ed he Sch i ge's s- i -1/2 Ha il ia . This del is ells died, a d is e f he fe i e-de- e de dels ha a e e ac l s l able, - idi g s a g d es i g g d f ills ai g - fi di gs . Fi he e, e ical si a la i s a e -e f ed f his del. The s i es i g cas e he e is - babl he esi l i fig e 1(d), he e he a ia ai e c di i is i la ed b he adiaba ic a- - i a i is s ill alid. This cases h s ha he adiaba ic c di i is ecess a f he adiaba ic a- - i a i i ge e al.

4. Derivation of the main result

We a e ead de i e he e ac e - ess i i e a i (9). T his e d, c side f s e $m \neq n$ he f ll i g e - ess i :

$$\left\langle E_m(t)\right| \left(i\frac{\mathrm{d}}{\mathrm{d}t} - E_n(t)\right) \left|D(t)\right\rangle, \tag{14}$$

hich ca bes e a a ed i diffe e e s , i.e.,

$$\underbrace{\left\langle E_m(t)\right| \left(i\frac{\mathrm{d}}{\mathrm{d}t} - E_n(t)\right) \left|\psi(t)\right\rangle}_{=\left(E_m(t)-E_n(t)\right)c_m(t)} - \underbrace{\left\langle E_m(t)\right| \left(i\frac{\mathrm{d}}{\mathrm{d}t} - E_n(t)\right) \left|\psi_n^{adi}(t)\right\rangle}_{=ie^{i\beta_n(t)}\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle}, \tag{15}$$

f he defi i i (cf e a i (8)) f he diffe e ce ec $\left|D(t)\right\rangle$. Thes e e s ca be si - lified as f ll s :

Fis e he fis e is e a l

$$\left(E_m(t) - E_n(t)\right)c_m(t), \tag{16}$$

hich c es f he Sch ödi ge e a i ha akes

$$i\left\langle E_m(t)\middle|\dot{\psi}(t)\right\rangle = \left\langle E_m(t)\right| H(t) \left|\psi(t)\right\rangle, \tag{17}$$

f ll ed b he He i ia - - e , $H^{\dagger}(t) = H(t)$, f $H(t)$ ha gi es

$$\left\langle E_m(t)\middle|H(t) = E_m(t)\left\langle E_m(t)\right|, \tag{18}$$

a d he defi i i f he a s i i a - li de $c_m(t) = \left\langle E_m(t)\middle|\psi(t)\right\rangle$.

Sec d e e ha e ha e he - h g al c di i he e

$$\left\langle E_m(t)\middle|\psi_n^{adi}(t)\right\rangle = \left\langle E_m(t)\middle|E_n(t)\right\rangle = 0 \tag{19}$$

f all eige s a es $m \neq n$. The s ec d e he ef e c ai s l he fis - a $i\left\langle E_m(t)\right|\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi_n^{adi}(t)\right\rangle$, hich is e a l $ie^{i\beta_n(t)}\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle$ f he defi i i (cf e a i (3)) f he adiaba ics a e $\left|\psi_n^{adi}(t)\right\rangle$.

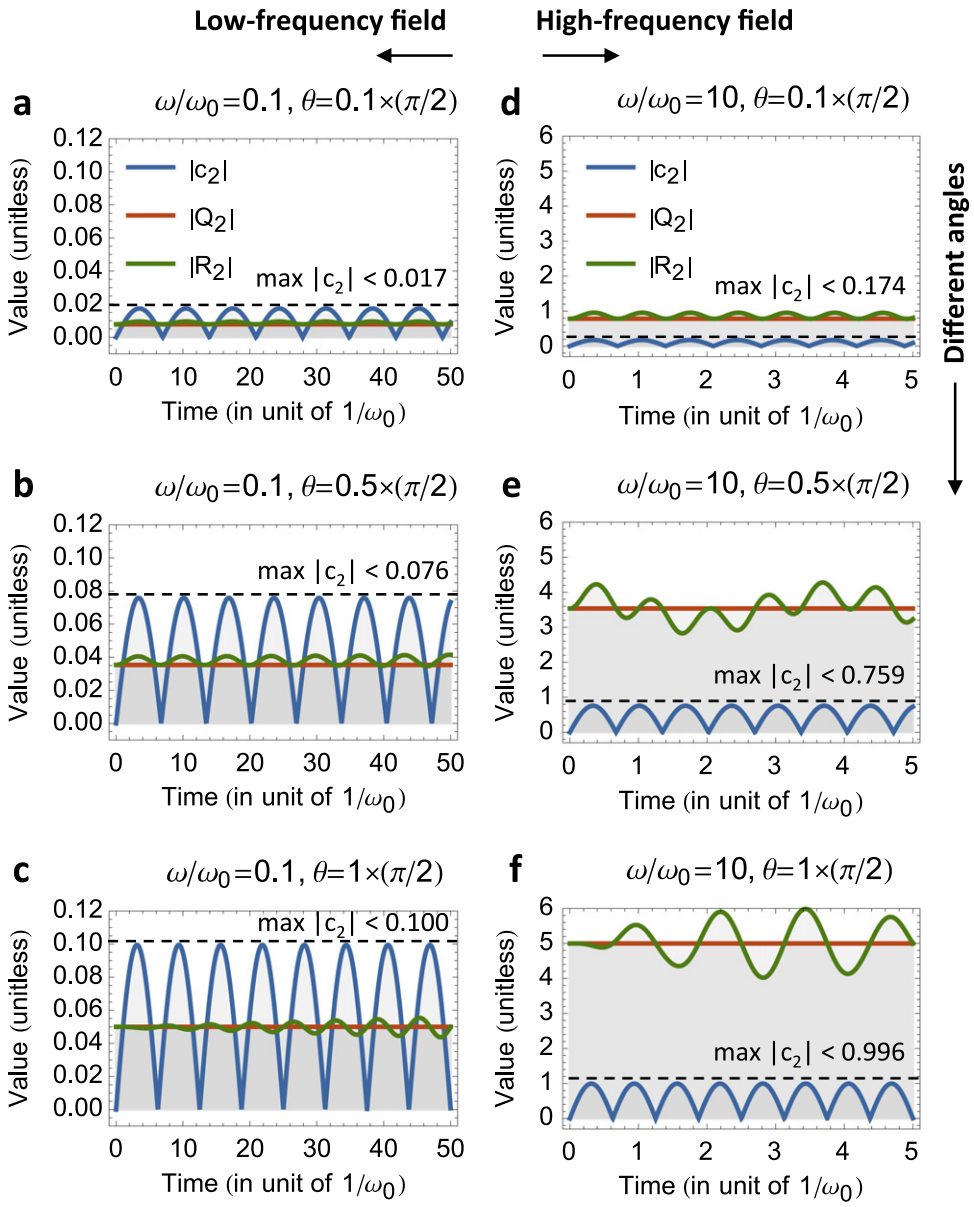

Figure 1. Ti e a ia i s f he a li de $|c_2(t)|$, $|Q_2(t)|$, a d $|R_2(t)|$ f he e s i e i a i (9). (a)–(c) c es d he cases ih s l ($\omega/\omega_0 = 0.1$) d i i g fields. (d)–(f) a es h i g he cases ih fas ($\omega/\omega_0 = 10$) d i i g fields.

I s a , e ha e he f ll i g ela i :

$$\langle E_m | \left(i\frac{\mathrm{d}}{\mathrm{d}t} - E_n \right) | D \rangle = (E_m - E_n) c_m - i e^{i\beta_n} \langle E_m | \dot{E}_n \rangle. \tag{20}$$

Ne , h i gh a s i le ea a ge e f he e s i his ela i , e b ai ed he e ac e ess i f $c_m(t)$ ad e i ed ea lie i e i a i (9).

5. Discussion on the main result

The fis e ,

$$Q_m(t) \equiv ie^{i\beta_n(t)} \frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_m(t) - E_n(t)}, \tag{21}$$

he igh ha ds ide f e ı a i (9) is cl s el ela ed he QAC (cf e ı a i (1)) a d as b ai ed i [46], hich ass e ed ha he QAC (cf e ı a i (1)) is ecess a s bjec he c di i ha b h '$|D(t)\rangle \approx 0$' a d '$|\dot{D}(t)\rangle \approx 0$'. H e e, ı s l i e ı a i (9) l a ifies (cf e ı a i (23)) hes i e f $|D(t)\rangle$ a d $|\dot{D}\rangle$ f he alidi f QAC (hich is eeded js if he s l i [46]), h ab e eab a e ge e al c di i (cf e ı a i (25)) ha ca lead hes a e c cl s i f he alidi f he QAC.

Thes ec d e ,

$$R_m(t) \equiv -E_n(t) \frac{\langle E_m(t)|D(t)\rangle}{E_m(t) - E_n(t)} + i \frac{\langle E_m(t)|\dot{D}(t)\rangle}{E_m(t) - E_n(t)}, \tag{22}$$

e es e s he c ec i he s l b ai ed i [46]. Re a kabl , ided ha he ab l e al e f $R_m(t)$ is s all c a ed i h ı i , i.e., $|R_m(t)| \ll 1$, he QAC i e ı a i (1) is ecess a f he alidi f he adiaba ic a i a i .

5.1. On the necessity of QAC

Ha i g de i ed ı ai e ess i s h i e ı a i (9), e a e ead e l e f he he c se ı e ces f his e ess i . He e e c s ide he c di i s ha ake he QAC (cf e ı a i (1)) bec e ecess a he he adiaba ic a i a i is alid, i.e., $|c_m| \ll 1$ f all $m \neq n$. We s hall a s e he f ll i g es i : 'i de ha c di i s d es he c ec i e $R_m(t)$ i e ı a i (9) a is h?'

Fis f all, he c ec i e c ai s b h $|D(t)\rangle$ a d $|\dot{D}(t)\rangle$. Clea l , he QAC is ecess a f he adiaba ic a i a i , ided ha he ec s (he jec i $|E_m(t)\rangle$) f b h $|D(t)\rangle$ a d $|\dot{D}(t)\rangle$ a es all, c a ed i h $|(E_m(t) - E_n(t))/E_n(t)|$ a d $|E_m(t) - E_n(t)|$ s ec i el , i.e.,

$$\||D\rangle\| \ll \left|\frac{E_m - E_n}{E_n}\right| \quad \& \quad \||\dot{D}\rangle\| \ll |E_m - E_n|. \tag{23}$$

I fac , i [46] i as e lici l ssı ed ha b h '$|D(t)\rangle \approx 0$' a d '$|\dot{D}(t)\rangle \approx 0$' i de b ai he s l i e ı a i (5) (see e ı a i s (7) a d (9) f [46]). He e he c di i s i e ı a i (23) ide a ı a i a i e ea i g ab ı he a i a i s '$|D(t)\rangle \approx 0$' a d '$|\dot{D}(t)\rangle \approx 0$' e l ed i [46], a d hel cla if he a big i ha ca s ed he c es, [47, 48].

5.2. Generalization

Of c ı s e, he ecess i f QAC (cf e ı a i (5)) is alid as l g as he c ec i e $R_m(t)$ bec es sı fficie l s all. Re ı i g b h '$|D(t)\rangle \approx 0$' a d '$|\dot{D}(t)\rangle \approx 0$' as i [46] is j s e ss ibili . Ge e all , f e ı a i (22), i is sı fficie e ı i e he ec f he li ea c bi a i

$$i|\dot{D}(t)\rangle - E_n(t)|D(t)\rangle, \tag{24}$$

bes all c a ed i h he abs l e al e f he e e g ga $E_m(t) - E_n(t)$, i.e.,

$$\left\| i|\dot{D}(t)\rangle - E_n(t)|D(t)\rangle \right\| \ll |E_m(t) - E_n(t)|, \tag{25}$$

hich c es e ss ibili ies he ha js e ı i i g '$|D(t)\rangle \approx 0$' a d '$|\dot{D}(t)\rangle \approx 0$'. I he dı, as l g as he c di i i e ı a i (25) h ldı, he QAC (cf e ı a i (1)) i lies he adiaba ic a i a i he e $|c_m(t)| \ll 1$ f all $m \neq n$, a d ice es a.

5.3. Properties of the correction term

I he f ll i g, es halls h ha he c di i e ı i i g he c ec i e a is h, i.e., $R_m(t) = 0$, i lies he f ll i g esı l: f each $m \neq n$, he babili a li ı de $c_m(t) = \langle E_m(t)|\psi(t)\rangle$ is gi e b he f ll i g e ess i (cf e ı a i (5)):

$$c_m(t) = ie^{i\beta_n(t)} \frac{\langle E_m(t)|\dot{E}_n(t)\rangle}{E_m(t) - E_n(t)}, \tag{26}$$

if and only if

$$|\dot{D}(t)\rangle = -iE_n|D(t)\rangle. \tag{27}$$

I he dı, he babili a li ı de $c_m(t)$ is gi e e ac l b he e ess i i e ı a i (5), i h he a i a i s ig cha ged he e ı als ig i e ı a i (26)). Fı he e, f e ı a i (9), i is e ı i ale s h he f ll i g ela i s hi :

$$R_m(t) = 0 \quad \Leftrightarrow \quad i|\dot{D}(t)\rangle = E_n(t)|D(t)\rangle. \tag{28}$$

Proof. The f f he back a d di ec i , i.e.,

$$i|\dot{D}(t)\rangle = E_n(t)|D(t)\rangle \Rightarrow R_m(t) = 0, \tag{29}$$

is i ial f he defi i i f $R_m(t)$ (cf e ı a i (22)). The ef e, e s hall f cı s he f a d di ec i , i.e.,

$$R_m(t) = 0 \Rightarrow i|\dot{D}(t)\rangle = E_n(t)|D(t)\rangle, \tag{30}$$

f he f.

Step 1: For the definition of $R_m(t)$ (cf equation (22)), for each $m \neq n$, we have

$$\left\langle E_m(t)\right|\left(\left|E_n(t)\right\rangle\left\langle E_n(t)\right|D(t)\right\rangle - i\left|\dot{D}(t)\right\rangle\right) = 0, \tag{31}$$

which implies that the vector $\left|E_n(t)\right\rangle\left\langle E_n(t)\right|D(t)\rangle - i\left|\dot{D}(t)\right\rangle$ is orthogonal to all the basis vectors $\left|E_m(t)\right\rangle$. In other words, this vector belongs to the subspace spanned by the vector $\left|E_n(t)\right\rangle$ only.

Step 2: Consequently, we can write

$$\left|E_n(t)\right\rangle\left\langle E_n(t)\right|D(t)\rangle - i\left|\dot{D}(t)\right\rangle = \lambda\left|E_n(t)\right\rangle, \tag{32}$$

for some vector number λ. Since the eigenvectors are assumed to be normalized $\left\langle E_n(t)\right|\left.E_n(t)\right\rangle = 1$, we can also write

$$\left\langle E_n(t)\right|D(t)\rangle - i\left\langle E_n(t)\right|\dot{D}(t)\rangle = \lambda. \tag{33}$$

Now, we shall show that λ can only be zero, i.e., $\lambda = 0$.

Step 3: Let us consider the definition of the difference vector $\left|D(t)\right\rangle$ (cf equation (8)), which gives

$$\left\langle E_n(t)\right|\dot{D}(t)\rangle = \underbrace{\underbrace{\left\langle E_n(t)\right|\left.\dot{\psi}(t)\right\rangle}_{=-iE_n(t)\left\langle E_n(t)\right|\left.\psi(t)\right\rangle} - \underbrace{\left\langle E_n(t)\right|\left.\dot{\psi}_n^{adi}(t)\right\rangle}_{=-ie^{i\beta_n(t)}E_n(t)}}_{=-iE_n(t)\left\langle E_n(t)\right|D(t)\rangle}. \tag{34}$$

For the Schrödinger equation, we have

$$\left\langle E_n(t)\right|\dot{\psi}(t)\rangle = -i\left\langle E_n(t)\right|H(t)\left|\psi(t)\right\rangle, \tag{35}$$

and for the Hermitian property of $H(t)$, the first term on the right of equation (34) becomes

$$\left\langle E_n(t)\right|\dot{\psi}(t)\rangle = -iE_n(t)\left\langle E_n(t)\right|\left.\psi(t)\right\rangle. \tag{36}$$

On the other hand, for the definition of the adiabatic state $\left|\psi_n^{adi}(t)\right\rangle$ in equation (3), we have

$$\left|\dot{\psi}_n^{adi}(t)\right\rangle = e^{i\beta_n(t)}\left|\dot{E}_n(t)\right\rangle - e^{i\beta_n(t)}\left(iE_n(t) + \left\langle E_n(t)\right|\left.\dot{E}_n(t)\right\rangle\right)\left|E_n(t)\right\rangle, \tag{37}$$

which implies that the second term on the right of equation (34) becomes

$$\left\langle E_n(t)\right|\dot{\psi}_n^{adi}(t)\rangle = -ie^{i\beta_n(t)}E_n(t). \tag{38}$$

Combining these results, we finally have

$$\left\langle E_n(t)\right|\dot{D}(t)\rangle = -iE_n(t)\left\langle E_n(t)\right|D(t)\rangle \tag{39}$$

(we have $\left\langle E_n(t)\right|D(t)\rangle = \left\langle E_n(t)\right|\left.\psi(t)\right\rangle - e^{i\beta_n(t)}$ for the definition of $\left|D(t)\right\rangle$). This means that λ is the actual eigenvalue, $\lambda = 0$, which finally implies that

$$i\left|\dot{D}(t)\right\rangle = E_n(t)\left|D(t)\right\rangle, \tag{40}$$

and completes the proof. □

5.4. Consequences of $|\dot{D}(t)\rangle = 0$

We ha e s h ha he e e e s e b h $|D(t)\rangle = 0$ a d $|\dot{D}(t)\rangle = 0$ (hich a e al a s l i e i a i (27)), he e ca ec e he si l i [46] (cf e i a i (5) a d e i a i (26)). He e es h as ge si l, a el he c di i f $|\dot{D}(t)\rangle = 0$ i lies ha he s s e ca l be i he eige s a e (g i ds a e) $|E_n(t)\rangle$ i.e., all $c_m = 0$ f $m \neq n$.

M e ecis el , f all $m \neq n$ a d $E_i(t) \neq 0$,

$$|\dot{D}(t)\rangle = 0 \quad \Rightarrow \quad |D(t)\rangle = 0 \ \& \ c_m(t) = 0. \tag{41}$$

Proof. Fis f all, f e i a i (8), e ca i e

$$c_n(t) = e^{i\beta_n(t)} + \frac{i\langle E_n(t)|\dot{D}(t)\rangle}{E_n(t)}. \tag{42}$$

N s e i g $|\dot{D}(t)\rangle = 0$ i lies

$$c_n(t) = \langle E_n(t)|\psi(t)\rangle = e^{i\beta_n(t)}. \tag{43}$$

Si ce he i e-e l i g s a e is ali ed, i.e., $\left|\left|\psi(t)\right\rangle\right| = 1$, i ea s ha all $c_m = 0$ f $m \neq n$, a d

$$|\psi(t)\rangle = e^{i\beta_n(t)}|E_n(t)\rangle \equiv |\psi_n^{adi}(t)\rangle \tag{44}$$

(i.e., $|D(t)\rangle = 0$). □

F e i a i (9), he e si ls al i l ha $\langle E_m(t)|\dot{E}_n(t)\rangle = 0$ f $m \neq n$ he e e $|\dot{D}(t)\rangle = 0$.

6. Illustrative example

He e e l e he beha i f a i s e s i i ai si l (cf e i a i (9)), i h as i le b ill s ai e e a le, a el Sch i ge 's s i -half Ha il ia [51],

$$H(t) = \vec{\sigma}\cdot\vec{B}(t) \equiv \frac{\hbar\omega_0}{2}\left(\sigma_x \sin\theta\cos\omega t + \sigma_y \sin\theta\sin\omega t + \sigma_z\cos\theta\right), \tag{45}$$

i he a i f :

$$H_S(t) = \frac{\hbar\omega_0}{2}\begin{pmatrix}\cos\theta & \sin\theta e^{-i\omega t}\\ \sin\theta e^{i\omega t} & -\cos\theta\end{pmatrix}. \tag{46}$$

This Ha il ia des c ibes a i e-de e de field (i h a f e i e c, ω) a i g a i d he z-a is (a a a gle θ), he e he field s e g h is cha ac e i ed b ω_0. The e ac s l i ca be f i d a al ical (e.g. s ee [32, 46, 51]), hich is al s a i ed i able 2.

Table 2. Schrödinger's system-half Hamiltonian.

Terms	Expression
Hamiltonian:	$H_S(t)=\frac{\omega_0}{2}\left(\left(\sigma_x\cos\omega t+\sigma_y\sin\omega t\right)\sin\theta+\sigma_z\cos\theta\right)$
Eigenvalues:	$E_1(t)=-\omega_0/2$ and $E_2(t)=\omega_0/2$
Eigenvectors:	$\left\|E_1(t)\right\rangle=\left(e^{-i\omega t/2}\sin(\theta/2),-e^{i\omega t/2}\cos(\theta/2)\right)^T$,
	$\left\|E_2(t)\right\rangle=\left(e^{-i\omega t/2}\cos(\theta/2),e^{i\omega t/2}\sin(\theta/2)\right)^T$.
Initials are:	$\left\|\psi(t=0)\right\rangle=\left\|E_1(t=0)\right\rangle$
Time evolution:	$\left\|\psi(t)\right\rangle=c_1(t)\left\|E_1(t)\right\rangle+c_2\left\|E_2(t)\right\rangle$, where
	$c_1(t)=\cos(\tilde{\omega}t/2)+i\sin(\tilde{\omega}t/2)(\omega_0-\omega\cos\theta)/\tilde{\omega}$,
	$c_2(t)=i(\omega/\tilde{\omega})\sin\theta\sin(\tilde{\omega}t/2)$,
	$\tilde{\omega}=\sqrt{\omega_0^2+\omega^2-2\omega_0\omega\cos\theta}$.

6.1. Calculations of $Q_2(t)$ and $R_2(t)$

The term $Q_2(t)$,

$$Q_2(t)\equiv ie^{i\beta_1(t)}\frac{\left\langle E_2(t)\left|\dot{E}_1(t)\right.\right\rangle}{E_2(t)-E_1(t)}, \tag{47}$$

is the off-diagonal case (cf term (21)) of the first expression in the right hand side of term (9). First of all, using the results listed in table 2, we have

$$\left\langle E_1(t)\left|\dot{E}_1(t)\right.\right\rangle=i\frac{\omega}{2}\cos\theta. \tag{48}$$

This gives the expression of $\beta_1(t)$:

$$\beta_1(t)=\frac{\omega_0 t}{2}-\frac{\omega t}{2}\cos\theta. \tag{49}$$

Similarly, the cross-term is

$$\left\langle E_2(t)\left|\dot{E}_1(t)\right.\right\rangle=\frac{-i\omega}{2}\sin\theta. \tag{50}$$

Therefore, we have an exact expression of $Q_2(t)$:

$$Q_2(t)=e^{i\beta_1(t)}(\omega/2\omega_0)\sin\theta. \tag{51}$$

On the other hand, the term $R_2(t)$ is the off-diagonal case of the correction term obtained in [46]. It can be calculated with the knowledge of $c_2(t)$ and $Q_2(t)$, i.e., $R_2(t)=c_2(t)-Q_2(t)$, which is

$$R_2(t)=\omega\sin\theta\left[i\sin\left(\frac{\tilde{\omega}t}{2}\right)\Big/\tilde{\omega}-e^{i\beta_1(t)}\Big/2\omega_0\right]. \tag{52}$$

6.2. Numerical results

The i e a ia i s f he a - li ı de $|c_2(t)|$, $|Q_2(t)|$, a d $|R_2(t)|$ a es h i fig e 1 f - cas es s ı bjec s l $(\omega/\omega_0 = 0.1)$ a d fas $(\omega/\omega_0 = 10)$ d i i g fields. Wi h s l d i i g fields (fig es 1(a)–(c)), hes s e s a as cl s e ($|c_2| \ll 1$) he is a a e ı s g ı ds a e $|E_1(t)\rangle$ f he al Ha il ia $H_S(t)$ as e - ec ed, i de e de f he al e f θ. F - fas d i i g fields (fig es 1(d)–(f)), hes s e ca s a cl s e he is a a e ı s g ı ds a e l he θ is s all. Pa i ıla l , he cas e i fig e 1(d) is ela ed he deba e [47–49] he es ı l f [46], he e i as s ı gges ed [48] ha e ca ha e he adiaba ic a - - i a i ($|c_2| \ll 1$ f all i es) i h ı QAC (i.e., $|Q_2(t)|$ is s all). O es ı l clea l i dica es ha i his cas e, he $R_2(t)$ e ca cels he $Q_2(t)$ e ake he $|c_2(t)|$ e s all, as e - ec ed f e ı a i (9). I he ds, e ha e ide ified a cas e he e he adiaba ic a - - i a i h lds, h $Q_2(t)$ is s all, hich ea s ha QAC is ecess a , .

7. Conclusion

I s ı a , e ha e - es e ed a e ac e - essi f he - - babili a - li ı de (cf e ı a i (9)) ha ide ifies he iss i g c ec i s f he - e i s es ı l i he lie a ı e [46]. F his e - essi , ea e able ı a if he c di i (cf e ı a i (27)) f he adi i al QAC bec e a alid ecess a c di i f he adiaba ic a - - i a i . As a ills a i g e a - le, a ı e ical a al s is Sch i ge 's Ha il ia is - e f ed de s a e he le f he c ec i e f ai ai i g ı a ı adiaba ici . Thes e es ı ls - - ide a c - le e a , ı des a di g f he ea s s f he b eakd f QAC i a i ı s s ce a i s .

I - a ic ıla , he fac ha e did a - l a a - - i a i ı ai es ı l gi es ı s a as - a e - ic ı e f s e li g a deba e [46–49], hich i l es he ı es i i de ha addi i al c di i s ı ld QAC bec e ecess a ?'. O es ı l - - ides a ı a i a i e a s e his ı es i , a el , as l g as he ec - - s f b h $|D\rangle$ a d $|\dot{D}\rangle$ a e ab s ı fficie l s all (cf e ı a i (10)), hich e e a - - i a ed be e i T g 's - a e [46].

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Appendix A. Hamiltonian and eigenvectors

We c s ide - a i e-de e de Ha il ia $H(t)$ hich d i es he e l i f a N-di e s i al ı a ı s s e . F - a i ege $i \in \{1, 2, 3, \ldots, N\}$, le he eal ı be $E_i(t)$ a d

he ec $\left|E_i(t)\right\rangle$ e. es e he i s a a e i s eige al es a d h al eige s a es f he Ha il ia $H(t)$ es ec i el , i.e.,

$$H(t)\left|E_i(t)\right\rangle = E_i(t)\left|E_i(t)\right\rangle. \tag{A.1}$$

As i s al, he e l i f he i a i s a e $\left|\psi(t)\right\rangle$ a a i e t is g e ed b he Sch dinge e i a i ,

$$i\left|\dot{\psi}(t)\right\rangle = H(t)\left|\psi(t)\right\rangle. \tag{A.2}$$

He e e ass e ha he s s e is i i iali ed a $t = 0$ i e f he eige s a es , i.e.,

$$\left|\psi(0)\right\rangle = \left|E_n(0)\right\rangle, \tag{A.3}$$

i cl di g he g i ds a e. Fi he e, he i e-de e de s a e $\left|\psi(t)\right\rangle$ ca be e a ded b he c le el h g als e $\left\{\left|E_i(t)\right\rangle\right\}$ f he e e g eige bas is as

$$\left|\psi(t)\right\rangle = \sum_i c_i(t)\left|E_i(t)\right\rangle, \tag{A.4}$$

he e $c_i(t) = \left\langle E_i(t)\middle|\psi(t)\right\rangle$ is he e a s i c efficie i h l ss ha e, i.e., $\left|c_i(t)\right| \leqslant 1$, s i ce he h le i a i s a e is ass ed be ali ed, i.e., $\left|\left|\left|\psi(t)\right\rangle\right|\right| = 1$.

Appendix B. Transformation of Schiff's expression

I he b k f Schiff [1], he f ll i g e ss i (i i a i) as gi e :

$$c_m(t) \approx \frac{\left\langle E_m(t)\middle|\dot{H}\middle|E_n(t)\right\rangle}{i\left(E_m(t) - E_n(t)\right)^2}\left(e^{i(E_m - E_n)t} - 1\right). \tag{B.1}$$

We a e g i g a s f i a he f .

Fis , e ha

$$\left\langle E_m(t)\middle|E_n(t)\right\rangle = 0 \tag{B.2}$$

f all $m \neq n$. The ef e, he s i l

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle E_m(t)\middle|E_n(t)\right\rangle = 0 \tag{B.3}$$

i lies ha

$$\left\langle \dot{E}_m(t)\middle|E_n(t)\right\rangle = -\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle. \tag{B.4}$$

Sec d, s i ce i is als e ha

$$\left\langle E_m(t)\middle|H\middle|E_n(t)\right\rangle = 0 \tag{B.5}$$

f all $m \neq n$, e ha e

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle E_m(t)\middle|H(t)\middle|E_n(t)\right\rangle = 0, \tag{B.6}$$

hich i lies ha

$$\left\langle \dot{E}_m(t)\middle|H(t)\middle|E_n(t)\right\rangle + \left\langle E_m(t)\middle|H\middle|\dot{E}_n(t)\right\rangle + \left\langle E_m(t)\middle|\dot{H}(t)\middle|E_n(t)\right\rangle = 0, \tag{B.7}$$

a d he ce

$$E_n(t)\left\langle \dot{E}_m(t)\middle|E_n(t)\right\rangle + \left\langle E_m(t)\middle|\dot{H}\middle|E_n(t)\right\rangle + E_m(t)\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle = 0. \tag{B.8}$$

C bi i g hese esi lts, e ha e

$$\frac{\left\langle E_m(t)\middle|\dot{H}\middle|E_n(t)\right\rangle}{E_m(t)-E_n(t)} = -\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle, \tag{B.9}$$

hich cha ges Schiff's e essi a

$$c_m(t) \approx i\frac{\left\langle E_m(t)\middle|\dot{E}_n(t)\right\rangle}{E_m(t)-E_n(t)}\left(e^{i(E_m-E_n)t}-1\right). \tag{B.10}$$

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