Supplemental note for "Two-fermion emission from spin-singlet and triplet resonances in one dimension"

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Time-dependent calculation has been a suitable method to investigate the quantum dynamical processes. In Ref. [1] = [T. Oishi et al., J. of Phys. G **45**, 105101 (2018)], we applied this method to the one-dimensional two-fermion tunneling in the nuclear-physics scale. Beside the specific results presented therein, some basic formalism and methods, which can be helpful for further discussions and developments to investigate time-dependent quantum systems, have been awaiting our description. This note is devoted to describe those supplemental contents. We do not limit the story to the nuclear physics, but keep it applicable to other scales and/or targets.

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I. INTRODUCTION

Quantum-mechanical dynamics is an essential concept to understand various aspects of the nuclear and subatomic physics. Thanks to the modern development of computers, it is getting possible to simulate the quantum-dynamical processes with high accuracy. These processes are generally described by the time-development equation,

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{\mathcal{H}}\left|\psi(t)\right\rangle, \tag{1}$$

where $\hat{\mathcal{H}}$ is the Schrödinger (Dirac) Hamiltonian for the non-relativistic (relativistic) system of interest.

In Refs. [1–5], we employed the time-dependent computation to investigate the nuclear meta-stable phenomena, e.g. two-nucleon emission. Besides the specific results therein, we have utilized the formalism and methods, which can be commonly useful for the theoretical and computational approach throughout the different scales or domains. In this note, we describe these contents for the time-dependent framework.

In the following sections, except in Appendix, we assume that the time-development operator (Hamiltonian), $\hat{\mathcal{H}}$, is (i) static, (ii) not self-consistently dependent on the state of interest, and (iii) deterministic without random numbers. This assumption, however, cannot be suitable to several applications in the nuclear and atomic physics. For that purpose, in Appendix, we also describe some ideas for the case with non-static Hamiltonian. Also, we do not determine the specific form of $\hat{\mathcal{H}}$, in order to keep our story linkable to various interests.

II. CONTINUUM EXPANSION

We start with the eigenstates of the Hamiltonian $\hat{\mathcal{H}}$. Those can also contain the unbound, continuum-energy states. Considering the degeneration, they can be formulated as

$$\begin{aligned}&\hat{\mathcal{H}}\left|E, i(E)\right\rangle = E\left|E, i(E)\right\rangle, \\ &\left\langle E', j(E')\,\middle|\,E, i(E)\right\rangle = \delta(E'-E)\delta_{ji}.\end{aligned} \tag{2}$$

Here the eigenenergy E is real, and thus, we consider the pure Hermite space [1]. The $i(E)$ identifies one of the degenerating states with the same energy E. However, in the following, we omit these labels for simplicity. We recount these labels only when it needs.

The quantum-dynamical phenomena, containing some particle-emitting radioactive decays of atomic nuclei [2], can be treated as the time-development of the meta-stable state. Employing the eigenstates for the basis, an arbitrary meta-stable state, $|\psi_0\rangle$, can be expanded as

$$\left|\psi_0\right\rangle = \int \mu(E)\left|E\right\rangle dE, \tag{3}$$

where $\{\mu(E)\} \in \mathbb{C}$ are the expanding coefficients. Thus, $|\mu(E)|^2$ gives the energy spectrum. In Refs. [1–5], these coefficients were determined by "confining potential" procedure [6–9], where a meta-stable state is fixed to have the similar, compact distribution of density to the bound state. The normalization is represented as

$$1 = \left\langle\psi_0\,\middle|\,\psi_0\right\rangle = \int dE\left|\mu(E)\right|^2. \tag{4}$$

Several physical properties of $|\psi_0\rangle$ are characterized by the expanding coefficients, as we discuss in the following.

A. time evolution

Assuming $|\psi_0\rangle$ as the initial state, now we consider the time evolution via $\hat{\mathcal{H}}$. Because $\hat{\mathcal{H}}$ is static, the time-

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[1] This assumption is in contrast to several theoretical methods, in which one employs the model space with complex eigenenergies [10–12], e.g. Berggren space [13–16].

[2] Those include, e.g. alpha decay, proton emission, and two-proton emission.

developed state can be trivially given as

$$|\psi(t)\rangle = e^{-it\hat{\mathcal{H}}/\hbar}|\psi_0\rangle = \int \mu(E)e^{-itE/\hbar}|E\rangle\, dE. \quad (5)$$

The expectation value of $\hat{\mathcal{H}}$, indicated as E_0, obviously conserves during the time evolution. That is,

$$E_0 \equiv \left\langle \psi_0 \middle| \hat{\mathcal{H}} \middle| \psi_0 \right\rangle = \left\langle \psi(t) \middle| \hat{\mathcal{H}} \middle| \psi(t) \right\rangle = \int E\,|\mu(E)|^2\, dE. \quad (6)$$

This conservation, of course, originates from that the energy spectrum should be timely invariant in the Hermite space [3]. Note that, for radioactive decays of nuclei, E_0 corresponds to the mean Q value (resonance energy) carried out by the emitted particle(s).

The survival coefficient, $\beta(t)$, is defined as the overlap between the initial and the present states. That is,

$$\beta(t) \equiv \langle \psi_0 | \psi(t)\rangle \quad (7)$$
$$= \int dE'\mu(E') \int dE\mu(E) \left\langle E' \middle| e^{-itE/\hbar} \middle| E \right\rangle$$
$$= \int dE\,|\mu(E)|^2\, e^{-itE/\hbar}. \quad (8)$$

Notice that $\beta(0) = 1$, consistently to the initial normalization. From Eq.(8), one can read that the survival coefficient is given by the Fourier transformation of the invariant-energy spectrum. This is nothing but the "Krylov-Fock theorem" [17, 18]. As one of the important quantities, the survival probability is also given as

$$P_{\rm surv}(t) = |\beta(t)|^2, \quad (9)$$

which physically corresponds to the decay rule of this meta-stable state. One important application, especially in the nuclear physics, is so-called "exponential-decay rule" and its coincidence to the Breit-Wigner (BW) spectrum.

B. exponential-decay rule

Exponential-decay rule is a typical aspect of nuclear radioactive processes. That is,

$$P(t) = e^{-t/\tau}P(0), \quad (10)$$

where $P(t)$ means the probability for one radioactive nucleus to survive with its characteristic lifetime, τ. Indeed, one can show that the exponential-decay rule is equivalent to the BW distribution of the energy spectrum. Namely, $|\mu(E)|^2$ is assumed to have the Cauchy-Lorentz form, whose center and full width at the half maximum (FWHM) are E_0 and Γ_0, respectively:

$$|\mu(E)|^2 = \frac{1}{\pi}\frac{(\Gamma_0/2)}{(E-E_0)^2 + (\Gamma_0/2)^2} \quad (11)$$

with $-\infty \le E \le \infty$ [4]. Or equivalently,

$$|\psi_0\rangle = \int_{-\infty}^{\infty} dE \sqrt{\frac{\Gamma_0}{2\pi}} \frac{e^{ia(E)}}{(E_0 - i\Gamma_0/2) - E}|E\rangle, \quad (12)$$

where $\left\{e^{ia(E)}\right\}$ with $a(E) \in \mathbb{R}$ are arbitrary phase-factors. If we consider the degeneration, Eq.(11) is modified as

$$|\mu(E)|^2 = \sum_{i(E)} |\mu(E, i(E))|^2 = \frac{1}{\pi}\frac{(\Gamma_0/2)}{(E-E_0)^2 + (\Gamma_0/2)^2}. \quad (13)$$

It is worthwhile to note the following points.

- The normalization is trivially guaranteed:

$$\langle \psi(t) | \psi(t)\rangle = \int_{-\infty}^{+\infty} dE \frac{1}{\pi}\frac{(\Gamma_0/2)}{(E-E_0)^2 + (\Gamma_0/2)^2} = 1. \quad (14)$$

- Next considering the Q value, however, how to define the first-moment value for the BW distribution is not obvious: one should be careful for the range of the integration. At this moment, we assume the isotropic infinite range with the central value of E_0. That is,

$$\int_I dE \equiv \lim_{R\to\infty} \int_{E_0-R}^{E_0+R} dE. \quad (15)$$

Thus, the first moment of the energy is identical to the Cauchy's principal value:

$$\left\langle \psi_0 \middle| \hat{\mathcal{H}} \middle| \psi_0 \right\rangle = \left\langle \psi(t) \middle| \hat{\mathcal{H}} \middle| \psi(t) \right\rangle$$
$$= \int_I dE'\mu(E') \int_I dE\mu(E) \left\langle E' \middle| \hat{\mathcal{H}} \middle| E \right\rangle$$
$$= \int_I dE'\mu(E') \int_I dE\mu(E)\delta(E'-E)E$$
$$= \int_I dE\,|\mu(E)|^2\, E = E_0, \quad (16)$$

In the following, we omit the subscript I.

[3] In the non-Hermite space, on the other hand, there is usually a leak or gain of energy.

[4] In practical applications, however, there should be the lower limit of the energy, as we mention in the next section.

By substituting Eq.(11) into Eq.(8), the survival coefficient is obtained from the residue at the pole, $E = E_0 - i\Gamma_0/2$. That is,

$$\beta(t) = \frac{1}{\pi}\int dE \frac{(\Gamma_0/2)}{(E-E_0)^2+(\Gamma_0/2)^2} e^{-itE/\hbar} = \cdots = e^{-it(E_0 - i\Gamma_0/2)/\hbar}. \quad (17)$$

Then, the survival probability yields the well-known exponential-decay rule:

$$P_{\rm surv}(t) = |\beta(t)|^2 = e^{-t/\tau}, \quad (18)$$

where $\tau = \hbar/\Gamma_0$ is the lifetime of this meta-stable state. This conclusion is indeed a natural product of Krylov-Fock theorem applied to the BW spectrum [5].

C. multi-resonance case

It is worthwhile to mention the case, where there exist two modes of finite-lifetime processes. In this case, the survival probability should read

$$P_{\rm surv}(t) = P^{(1)}_{\rm surv}(t)\cdot P^{(2)}_{\rm surv}(t) = e^{-t/\tau_1}\cdot e^{-t/\tau_2}, \quad (19)$$

where $\tau_i = \hbar/\Gamma_i$ is the lifetime due to the ith mode. The consistent energy spectrum can be given as the convolution of two Cauchy-Lorentz functions. That is,

$$|\mu(E)|^2 = \int dE' L^{(1)}(E-E')L^{(2)}(E'),$$
$$L^{(i)}(x) = \frac{1}{\pi}\frac{(\Gamma_i/2)}{(x-E_i)^2+(\Gamma_i/2)^2}, \quad (20)$$

where E_i and Γ_i indicate the position and width, respectively, of the ith resonance. One can naturally extend this conclusion to the general N-resonance case, where the spectrum should be $(N-1)$-fold convolution.

III. PRACTICAL PROBLEMS

In practical applications, however, one often encounters the situation, which looks more complicated than above discussions. Here we mention some points worthwhile to remember.

- There should be the lower limit for the expansion in the continuum energy space, consistently to the threshold of the emission. Fixing it as $E = 0$, we should modify Eq.(12) as

$$\int_{-\infty}^{\infty} dE \longrightarrow \int_0^{\infty} dE. \quad (21)$$

- The actual energy spectra are not limited to the simple BW distribution, but can show more complicated forms. Even in the nuclear radioactivity, especially when the spectrum has the broad width, the BW distribution may not be suitable for practical analysis.

Because of these two affairs, indeed, the nuclear radioactivity can have the deviation from the exponential-decay rule [19–22]. In such a case, the exponential-decay rule is a good approximation, but only for $t \simeq \tau$.

In numerical calculations, some additional affairs should be concerned.

- The model space needs a truncation by the energy cutoff, $E_{\rm cut}$. Of course, this cutoff should be sufficiently large to ensure the convergence of results.

- It is often necessary to discretize the continuum-energy space. Thus, Eq.(5) should be modified as

$$|\psi(t)\rangle = \sum_N \mu_N e^{-itE_N/\hbar}|E_N\rangle, \quad (22)$$

where $E_N \le E_{\rm cut}$. In Refs. [1–5], we employed the radial box, $R_{\rm box}$, for discretization. There, we had to employ a large box to obtain the convergence in the time-development calculation: if that box was not sufficiently large, there should be a contamination by the reflected component at $R_{\rm box}$.

- Even with the energy cutoff and continuum discretization, the numerical solution of the eigenstates, $\{|E\rangle\}$, may need efforts, especially for three-body or more-body systems. Before going to the meta-stable problem, it is better to check the accuracy of that solution method by some benchmark calculations for the well-known, bound systems.

- Number of basic states, $N_{\rm max}$, should be sufficiently large to ensue the convergence. In Ref. [1], typically $N_{\rm max} = 100$-1000.

- The way to fix the initial state, as well as its correspondence with the experimental situation, should be considered carefully. The initial state, especially of the (multi-)particle emission, is usually characterized as the state, where the emitted particles are confined in the narrow region, and/or the state, which obeys the outgoing condition. Even with these constraints, however, there may remain an ambiguity. Furthermore, obtained results after the time evolution may significantly depend on the selected initial state. In Refs. [1–5], we employed the phenomenological procedure with the confining potential. This procedure has provided a good approximation for the nuclear radioactive processes [6–9]. On the other hand, we also expect that a more smart way to determine the initial state will be available in future.

[5] In another example, when one starts with the Gaussian spectrum, $|\mu(E)|^2 \propto e^{-aE^2}$, it naturally concludes the Gaussian-decay rule, $P_{\rm surv}(t) \propto e^{-At^2}$

Notice also that some of the above issues were not seen in the static, bound-state problems. However, they turn out to be present, when one starts to consider the unbound, meta-stable states.

A. quantum recurrence theorem

For the original statement of this theorem, see Refs. [23, 24].

It is worthwhile to point out the link between the time-dependent calculation and the quantum-mechanics version of the recurrence theorem. In the following, we assume the continuum-discretized space: $\int dE \longrightarrow \sum_{E_N}$.

First we consider the two-component mixture state. Namely, at $t = 0$,

$$|\psi(0)\rangle = \mu_1 |E_1\rangle + \mu_2 |E_2\rangle , \tag{23}$$

where the normalization is also assumed: $\langle\psi(0)\,|\,\psi(0)\rangle = |\mu_1|^2 + |\mu_2|^2 = 1$. The time-development then gives,

$$\begin{aligned} P_{\rm surv}(t) &\equiv |\langle\psi(0)\,|\,\psi(t)\rangle|^2 \\ &= |\mu_1|^4 + |\mu_2|^4 + 2\,|\mu_1|^2\,|\mu_2|^2 \cos\Delta_{12}t, \end{aligned} \tag{24}$$

where $\Delta_{12} = (E_1 - E_2)/\hbar$. Because of the normalization, the survival probability can be reformulated as

$$P_{\rm surv}(t) = 1 - 2\,|\mu_1|^2\,|\mu_2|^2\,(1 - \cos\Delta_{12}t). \tag{25}$$

Thus, when $t = 2N\pi/\Delta_{12}$, the time-developed state can be equivalent to the initial state.

We next start the same story but for the three-component mixture state. That is,

$$|\psi(0)\rangle = \mu_1 |E_1\rangle + \mu_2 |E_2\rangle + \mu_3 |E_3\rangle , \tag{26}$$

where $\langle\psi(0)\,|\,\psi(0)\rangle = \sum_{i=1-3} |\mu_i|^2 = 1$ (normalization). In this case, the time development concludes that

$$P_{\rm surv}(t) = 1 - 2\sum_{(ij)} |\mu_i|^2\,|\mu_j|^2\,(1 - \cos\Delta_{ij}t), \tag{27}$$

where $\Delta_{ij} = (E_i - E_j)/\hbar$, and (ij) indicates the combination of two labels $(i < j)$.

Indeed, Eq.(27) is valid in a more general case, where the initial state is given by the arbitrary-number superposition. Namely,

$$|\psi(0)\rangle = \sum_{i=1}^{N_{\rm max}>2} \mu_i |E_i\rangle . \tag{28}$$

In this case, of course, the summation $\sum_{(ij)}$ contains $N_{\rm max}(N_{\rm max} - 1)/2$ terms. Notice also the time-reversal symmetry, $P_{\rm surv}(-t) = P_{\rm surv}(t)$, as long as in the Hermite model space.

From Eq.(27), the situation looks different from the two-component case: there is not the simple, periodic solution for $P_{\rm surv}(t \neq 0) = 1$. However, there can be still the solution of recurrence. To see this, we consider the gap probability,

$$\begin{aligned} g(t) &= 1 - P_{\rm surv}(t) \\ &= 2\sum_{(ij)=(12)}^{J_{\rm max}} \left|a_{(ij)}\right|^2 (1 - \cos\Delta_{ij}t), \end{aligned} \tag{29}$$

where $\left|a_{(ij)}\right|^2 \equiv |\mu_i|^2\,|\mu_j|^2$ and $J_{\rm max} \equiv N_{\rm max}(N_{\rm max} - 1)/2$. Because $g(t)$ is an almost-periodic function, there can be the time T to satisfy $g(T) < \delta^2$, where δ is the arbitrary positive number [6]. Indeed, one can obtain the same conclusion more easily by evaluating the norm of $|\psi(t)\rangle - |\psi(0)\rangle$ [23, 24].

IV. SUMMARY

In this supplemental note following Ref. [1], the basic ideas and formalism of the time-dependent quantum-mechanical calculation have been presented. Several, typical aspects of the nuclear radioactive processes have been also discussed. However, we expect that some contents in this note can be helpful for other applications, and enable us to proceed the wholistic study on quantum dynamical processes.

Appendix: NON-STATIC OPERATOR

In the main text, the time-development operator (Hamiltonian) is limited to be static and independent of the present state. However, in several applications of quantum many-body problems, Hamiltonian may contain, e.g. a time-dependent external field, and/or the many-body interaction, which should be determined self-consistently to the corresponding state, $\psi(t)$. In such a case, it is necessary to deal with the non-static Hamiltonian,

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}(t, \psi(t)). \tag{A.1}$$

In this section, we summarize the basic ideas for those applications.

The general time-dependent equation is now given as

$$i\frac{\partial}{\partial t}\,|\psi(t)\rangle = \hat{\mathcal{O}}(t, \psi(t))\,|\psi(t)\rangle , \tag{A.2}$$

where $\hat{\mathcal{O}} \equiv \hat{\mathcal{H}}/\hbar$. In addition, it is worthwhile to introduce the other two equations, which can be equivalent to Eq.(A.2). Namely,

$$|\psi(t+\epsilon)\rangle = e^{-i\epsilon\hat{\mathcal{O}}(t,\psi(t))}\,|\psi(t)\rangle , \tag{A.3}$$

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[6] Note that, if one employs the non-Hermite space, this recurrence is not guaranteed.

and also,

$$\hat{\mathcal{O}}(t,\psi(t)) = i\frac{\partial}{\partial\epsilon}\ln\left[|\psi(t+\epsilon)\rangle\right]. \tag{A.4}$$

Here ϵ means the infinitesimal time evolution. Equivalence between these equations is shown as follows.

- Equivalence of Eq.(A.2) and Eq.(A.3). First we expand the left-hand side (LHS) of Eq.(A.3) with respect to ϵ:

$$|\psi(t+\epsilon)\rangle = |\psi(t)\rangle + \epsilon\left(\frac{\partial}{\partial t}\right)|\psi(t)\rangle + \cdots$$

We next expand the exponential operator in the right-hand side (RHS) of Eq.(A.3):

$$\begin{aligned} &e^{-i\epsilon\hat{\mathcal{O}}(t,\psi(t))}|\psi(t)\rangle \\ &= \left[1 + (-i\epsilon)\hat{\mathcal{O}}(t,\psi(t)) + \cdots\right]|\psi(t)\rangle. \end{aligned}$$

By comparing the first-order terms, we can conclude Eq.(A.2).

- Equivalence of Eq.(A.3) and Eq.(A.4). From the derivative of Eq.(A.3), one obtains that

$$i\frac{\partial}{\partial\epsilon}|\psi(t+\epsilon)\rangle = \hat{\mathcal{O}}(t,\psi(t))\,|\psi(t+\epsilon)\rangle.$$

This is equivalent to Eq.(A.4).

Remember that we have not assumed the specific form of $\hat{\mathcal{O}}(t)$, in order to keep generality. In some applications, one often needs to employ a kind of iterative methods, in order to compute the time development. For implementation of that method, the most convenient form is probably Eq.(A.3), which guarantees that $\psi(t+N\epsilon)$ can be obtained from $\hat{\mathcal{O}}(t+(N-1)\epsilon)$ and $\psi(t+(N-1)\epsilon)$. That is,

$$\begin{aligned} i=0: &\quad \psi(t) \implies \hat{\mathcal{O}}(t) \\ &\qquad\qquad \swarrow \\ i=1: &\quad \psi(t+\epsilon) \implies \hat{\mathcal{O}}(t+\epsilon) \\ &\qquad\qquad \swarrow \\ i=2: &\quad \psi(t+2\epsilon) \implies \hat{\mathcal{O}}(t+2\epsilon) \\ &\qquad\qquad \swarrow \\ &\qquad\quad \vdots \end{aligned}$$

Of course, ϵ should be sufficiently small compared with the typical timescale of the process of interest. On the other hand, Eq.(A.4) can be helpful when the time-development operator is unknown, but only the time-dependent wave function is given. In such a case, one can infer $\hat{\mathcal{O}}(t)$ by evaluating the logarithmic derivative of $\psi(t+\epsilon)$.

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