Formation spectra of pionic atoms in the Green’s function method

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We study the formation spectra of deeply bound pionic atoms in the \((d,^{3}\text{He})\) reactions using the Green’s function method, stimulated by recent developments in experimental techniques. The Green’s function method is considered to be a better theoretical formalism than the effective number approach to evaluate the formation rate of unstable systems. We compare the calculated results by the Green’s function method with those by the effective number approach in various cases. We find that the differences between the results obtained by both methods are reasonably small and we can reaffirm that the effective number approach is a good theoretical method for the analyses of the previous experimental data with typical binding-energy errors of \(\Delta B.E. \gtrsim 20\) keV for the deeply bound pionic atoms. On the other hand, we think that theoretical results using the Green’s function method will be necessary in the near future to deduce precise information on the pion properties in nuclei from analyses of the pionic atom data with better accuracy than before.

Subject Index D15, D22, D25, D33

1. Introduction

It is important to know the pion properties in a nucleus since they are believed to provide valuable information on aspects of quantum chromodynamics (QCD) symmetry at finite density. The deeply bound pionic atom is one of the best system to perform accurate spectroscopic studies of pionic states in nuclei. In the previous experiments at GSI \cite{1}, experimental \((d,^{3}\text{He})\) spectra of pionic 1\(s\) states in \(^{115,119,123}\text{Sn}\) isotopes were observed with an experimental resolution of \(\Delta E = 400\) keV FWHM (full width half maximum) based on the theoretical prediction \cite{2}. From these observed spectra, Suzuki et al. \cite{1} precisely determined the binding energies (B.E.) and the widths (\(\Gamma\)) of the pionic 1\(s\) states with total errors of \(\Delta B.E. \simeq 20\) keV and \(\Delta \Gamma \simeq 80\) keV. From the observed B.E. and \(\Gamma\), they extracted the value of a parameter \(b_1\) in the pion–nucleus potential, which can be connected to the value of the chiral condensate, and concluded that there is partial restoration of chiral symmetry \cite{1,3}. Therefore, for obtaining the value of the chiral condensate from the observables in pionic atoms, it is quite important to determine the pion–nucleus interaction parameters reliably from the data.

Recently, experimental studies on pionic atoms have been started in the RIBF/RIKEN facility. In RIBF/RIKEN, the spectral energy resolution can be improved to \(\Delta E \simeq 150–200\) keV with...
much higher statistics (K. Itahashi, private communication). We can also expect the possibility of determining the precise binding energies of pionic states with smaller errors $\Delta B.E. < 20\text{ keV}$ than previous experiments. New experimental data, though still preliminary, have been reported in Ref. [4]. From these data, we can expect the future possibility of precise spectroscopy of pionic atoms in the $(d,^3\text{He})$ reactions at forward and finite angles.

These developments on the experimental side indicate the necessity of further developments in the theoretical calculations to obtain more systematic results of the $(d,^3\text{He})$ spectra for various targets and to deduce more accurate information on pion properties in nuclei. In this article, we study theoretically the $(d,^3\text{He})$ spectra for pionic atom formation using the Green’s function method. So far, our theoretical results obtained by the effective number approach have predicted and reproduced the experimental data reasonably well, and provided a reliable interpretation of the observed $(d,^3\text{He})$ spectra, as we have discussed in Refs. [5–8]. It is known that the effective number approach is a good method to calculate the formation spectra of meson–nucleus systems with relatively small imaginary potentials, such as pionic atoms. However, stimulated by the recent developments in experimental techniques and the possibility of obtaining data with significantly better accuracy, we think that it is important to consider the improvements in the theoretical calculation for the $(d,^3\text{He})$ reactions for pionic atom formation. In this context, we study the Green’s function method in this article as a better theoretical formalism than the effective number approach to obtain more realistic formation spectra of deeply bound pionic atoms. We think that the advantages of the Green’s function method can be summarized in the following three points.

(i) We can calculate the contributions from both bound and quasi-free pion production in the final state in a unified manner with the Green’s function method. In the effective number approach, we have to calculate them separately and add all contributions to get the total spectrum.

(ii) In principle, we can sum up all the contributions from an infinite number of bound pionic states coherently to obtain the formation spectrum in the Green’s function method. In the effective number approach, this is impossible practically.

(iii) We can obtain the formation spectrum without assuming the existence of the discrete bound states or the shape of the peak structure in the Green’s function method. In the effective number approach, we assume a Lorentz distribution function as the shape of the peak structure, and thus the calculated subcomponent of the spectrum has a symmetric peak located exactly at the resonance energy. In general, this is not always true. The shapes of the peak structure in the spectrum could affect the determination of background in the experimental analyses, and thus it is important to identify realistic peak-structure shapes in the spectrum.

Therefore, to obtain valuable information on pion properties, it seems interesting to calculate the formation spectra of the pionic atoms in the Green’s function method and compare the results with those obtained by the effective number approach.

In Sect. 2, we describe the formulation of the Green’s function method to calculate the formation spectra of pionic atoms. In Sect. 3, we show the numerical results and compare the results obtained by both methods. Section 4 is devoted to the conclusion. Part of this article has been reported in the doctoral thesis written by one of the authors [9].

## 2. Formulation

We calculate the formation cross sections of the pionic atoms in the $(d,^3\text{He})$ reaction using the Green’s function method. The Green’s function method is known to be suited for evaluations of the...
formation rates of both stable and unstable systems, which decay rapidly because of the large imaginary potential due to the strong absorptive interaction [10–12]. Because of their short lifetimes, unstable states have large widths in the energy spectrum and have some overlap with neighbor states in general, while stable states are well isolated from other states. By the Green’s function method, we can consider both states simultaneously [13]. In addition, we can also include the contributions from quasi-free pion production in the final states in a unified manner in this formalism. For these reasons, it is known that the Green’s function method is good for obtaining more realistic reaction spectra theoretically.

On the other hand, it is also known that we need a significantly longer computational time to obtain numerical results in the Green’s function method than in the effective number approach because of the multidimensional integrations. Thus, we have mainly adopted the effective number approach to get numerical results for pionic atoms so far, since they are known to have isolated energy levels with relatively small widths. This formulation of the Green’s function method should be used in our future work whenever it is necessary to obtain better calculated results, which could be required for analyses of future experimental data with better accuracy than the previous data. The details of the application of the Green’s function method to the reactions of the meson–nuclear system formation are found in Refs. [13–16].

In the Green’s function method, the formation cross sections of the pionic atoms in the \((d, ^3\text{He})\) reaction are written as

\[
\left( \frac{d^2\sigma}{dE_{\text{He}}d\Omega_{\text{He}}} \right)_A = \left( \frac{d\sigma}{d\Omega_{\text{He}}} \right)_{\text{ele}} \times S(E) \tag{1}
\]

in the laboratory system. Here, \(\left( \frac{d\sigma}{d\Omega_{\text{He}}} \right)_{\text{ele}}\) indicates the elementary differential cross section for the \(d + n \rightarrow ^3\text{He} + \pi^-\) reaction in the laboratory system as in the case of the effective number approach. We use the same value for the elementary cross section as in Ref. [7]. The nuclear response function \(S(E)\) is given by the Green’s function \(G(E)\) as

\[
S(E) = -\frac{1}{\pi} \text{Im} \sum_f K \int dr dr' \tau_f^\dagger(r) G(E; r, r') \tau_f(r'),
\]

where the summation is taken over all possible final states. The kinematical correction factor \(K\) is defined as

\[
K = \left[ \frac{p_{\text{He}}^A E_n E_\pi}{|p_{\text{He}}^A E_n E_\pi| \left( 1 + \frac{E_{\text{He}}}{E_\pi} \frac{|p_{\text{He}}| - |p_d| \cos \theta_{d\text{He}}}{|p_{\text{He}}|} \right) \right]_{\text{lab}}^{1/3},
\]

where the superscript “A” indicates that the momentum and energies are evaluated in the kinematics of the nuclear target case [7]. The superscript “lab” indicates that all kinematical variables are evaluated in the laboratory frame. This correction factor is the same for the effective number approach in Refs. [7,8]. We introduce this correction factor again into the Green’s function method to take into account the differences of the kinematics between the elementary process and meson bound-state production. The calculation of the nuclear response function with complex potential was formulated by Morimatsu and Yazaki [10–12] in a generic form. The amplitude \(\tau_f\) denotes the transition of the incident particle \((d)\) to the neutron-hole and the outgoing particle \((^3\text{He})\) and is written as

\[
\tau_f(r) = \chi_{\text{He}}^*(r) \xi_j^\dagger \left[ Y_{\ell\pi}^*(\hat{r}) \otimes \psi_{jn}(r) \right]_{JM} \chi_d(r),
\]
where $\psi_{j_h}$ is the neutron-hole wave function, $\chi_d$ and $\chi_{He}^*$ the distorted waves of the projectile and ejectile, $Y_{\ell\pi}(\hat{r})$ the angular wave function of the meson, and $\xi_{^{1/2}m_z}^{*}$ the spin wave function of the ejectile.

The distorted waves $\chi_d$ and $\chi_{He}^*$ are written in the eikonal approximation with the distortion factor $F(r)$ as

$$\chi_{He}^*(r)\chi_d(r) = \exp(iq \cdot r) F(r),$$

(5)

where $q$ is the momentum transfer between projectile and ejectile. Here, we introduce the correction factor $(m_C/(m_C + m_\pi))$ to take into account the recoil effect in this formalism, and replace $r$ in Eq. (5) with $r'$ as

$$r \to r' = r\frac{m_C}{m_C + m_\pi},$$

(6)

where $m_C$ and $m_\pi$ are the masses of the daughter nucleus and pion. In this article, we consider pionic atom formation in the $(d,^3He)$ reaction on $^{122}$Sn and $^{206}$Pb targets; thus, the daughter nuclear mass $m_C$ means the mass of the $^{121}$Sn and/or $^{205}$Pb nucleus. This factor is very close to 1 for the formation of deeply bound pionic atoms since the mass of the daughter nucleus $m_C$ is much larger than the pion mass $m_\pi$, and this effect is usually neglected for systems with pions and heavy nuclei. Here, we include explicitly this factor in the formulation of the Green’s function method. A similar consideration was also given in Refs. [17,18] for lighter nuclear systems. The distortion factor $F(r)$ is defined as

$$F(r) = F(z, b) = \exp\left[ -\frac{1}{2} \sigma_{dN} \int_z^\infty dz' \rho_A(z', b) - \frac{1}{2} \sigma_{hN} \int_z^\infty dz' \rho_{A-1}(z', b) \right].$$

(7)

Here, the deuteron–nucleon and $^3$He–nucleon total cross sections are denoted as $\sigma_{dN}$ and $\sigma_{hN}$. The functions $\rho_A(z, b)$ and $\rho_{A-1}(z, b)$ are the density distributions of the target and daughter nuclei at beam-direction coordinate $z$ with impact parameter $b$. As for the evaluation of the $(d, ^3He)$ reaction rate at finite angles, we assume the same expression for the distortion factor as Eq. (7), in which straight trajectories are assumed for the projectile and ejectile, since the scattering angles considered in this article are smaller than three degrees in the laboratory frame. The most important effect at finite angles is the change in the momentum transfer $q$ of the reaction in this energy region.

We should mention here that the $(d, ^3He)$ reactions considered in this article are used to obtain the shape of the energy spectrum of the emitted $^3$He in a very narrow energy region ($\Delta E \approx 10$ MeV) with an intermediate-energy deuteron and $^3$He, and, in our analysis, the absolute strengths of the total spectra are less important. In this narrow energy region, the energy dependences of the spectra are expected to be dominated by pionic processes and the energy dependence of the interaction between the projectile/ejectile and nucleus is considered to be safely neglected unless it has quite a strong energy dependence in the narrow energy region. Thus, improvements in the distorted waves will cause a change in the absolute strength of the cross section in this narrow energy region while keeping the shape of the spectra almost the same. Hence, we think that the eikonal approximation is considered to be reasonably good in the present cases for projectiles and ejectiles with intermediate energies. In order to evaluate the absolute strength in addition to the shape of the energy spectrum, we think that we need to incorporate a more realistic distorted wave in the formula.

The Green’s function $G(E)$ contains the pion–nucleus optical potential $V_{opt}$ in the Hamiltonian $H_\pi$ as

$$G(E, r, r') = \left\langle n^{-1} \phi_\pi(r) \frac{1}{E - H_\pi + i\epsilon} \phi_\pi^*(r') n^{-1} \right\rangle,$$

(8)
where $\phi^\dagger_\pi$ is the pion creation operator and $|n^{-1}\rangle$ the neutron-hole state. The relativistic pion energy $E$ is defined as

$$E = T_d - T_{He} - S_n(j_n) + (M_n + M_d - M_{He}),$$

where $M$ and $T$ are the masses and kinetic energies of the particles participating in the reaction, as indicated by the subscripts, and $M_n + M_d - M_{He} = 6.787$ MeV. The neutron separation energy from the $j_n$ single-particle level is indicated as $S_n(j_n)$. By these kinematical variables, the reaction Q-value of the $(d,^3\text{He})$ reaction can be expressed as $Q = T_{He} - T_d = -E - S_n(j_n) + (M_n + M_d - M_{He})$, as described in the effective number approach in Refs. [7,8].

Obtaining the Green’s function with the optical potential is essentially the same as solving the associated equation of motion, and is explained in detail in Refs. [10–13]. We can then calculate the nuclear response function $S(E)$ from $\tau_f^\dagger(r)G(E; \tau, \tau')\tau_f(r')$ by performing the appropriate numerical integrations for the variables $r$ and $r'$. In the Green’s function formalism, we can calculate the response function $S(E)$ for both the bound and quasi-free pion production energy regions in a unified manner, and we can also perform the summation of the pion final states without assuming the existence of discrete pion bound states.

To take into account the realistic ground-state configurations for the target nucleus, the nuclear excitation energies, and the relative excitation strengths leading to the excited states of the daughter nucleus, we can write the nuclear response function $S(E)$ as

$$S(E) \rightarrow -\frac{1}{\pi} \text{Im} \sum_{f,N} K \int dr \, dr' \tau_f^\dagger(r)G(E; r, r')\tau_f(r')F_O(j_n)F_R((j_n^{-1})_N).$$

Here, the index $N$ indicates the number of states of the daughter nucleus with $j_n^{-1}$ quantum number. $F_O$ is the normalization factor due to the occupation probabilities of the neutron states $j_n$ in the target nucleus, and $F_R$ the relative strength factor of the $N$th excited state of the daughter nucleus with the quantum number $j_n^{-1}$. The values of $F_O$, $F_R$, and $S_n$, which are deduced from data, are compiled in tables in Refs. [6,19].

3. Numerical results

We show the numerical results obtained by the Green’s function method, and compare them with those by the effective number approach. In this article, we consider the $\pi^-$ production processes only and neglect the contributions from the quasi-free $\pi^0$ production since the contribution of the quasi-free $\pi^0$ production is much smaller than that of the quasi-free $\pi^-$ production, as shown in Fig. 1 in Ref. [8].

In both numerical methods, we have used the harmonic oscillator (HO) wave function as the neutron wave function and assumed the instrumental energy resolution to be 300 keV FWHM. The theoretical spectra are obtained by folding the calculated spectra with the Gaussian distribution with the width of the instrumental energy resolution. In the results of the Green’s function method, we include the recoil and the vacuum polarization corrections, as described in Sect. 2 and the Appendix.

In Fig. 1, we show the calculated $^{122}\text{Sn}(d,^3\text{He})$ spectra at forward angle by the Green’s function method and by the effective number approach. The results for the pion bound-state formation of the effective number approach (Fig. 1, right) are the same as those shown in Fig. 3 (upper) in Ref. [7]. The dominant subcomponents are indicated in the figure with their quantum numbers. In the result of the effective number approach, the line with the symbol $[(1s)_{\pi} \otimes (3s_{1/2})_{n}^{-1}], [(2s)_{\pi} \otimes (3s_{1/2})_{n}^{-1}], \text{and } [(3s)_{\pi} \otimes (3s_{1/2})_{n}^{-1}]$. In
Fig. 1. Calculated spectra in the $^{122}$Sn($d$,\(^3\)He) reaction for the formation of pionic atoms at forward angle by the Green's function method (left) and by the effective number approach (right), plotted as functions of the reaction $Q$-value. The dominant subcomponents are also shown in the figures by dotted and dashed lines. The incident deuteron kinetic energy is fixed at $T_d = 500$ MeV. The instrumental energy resolution is assumed to be 300 keV FWHM. The vertical lines indicate the pion production threshold $Q = -141.6$ MeV. The effect of the vacuum polarization of the electromagnetic interaction is included in the results of the Green's function method, but not in the result of the effective number approach.

In order to see the differences in the numerical results obtained by both methods in detail, we show in Fig. 2 an overlay of the total spectra of both methods shown in Fig. 1. From Fig. 2, we think that we can summarize the features of the discrepancies between the spectra in the following three points. Firstly, there is a clear difference in the behaviors of the two spectra near the threshold. The spectrum by the effective number approach clearly shows a smaller cross section at $Q \simeq -141.6$ MeV than that by the Green's function method. This is because we could not include a sufficient number of pion bound-state contributions near the threshold in the spectrum with the effective number approach. Secondly, the heights and positions of the peaks are slightly different in the calculated spectra in both methods. This fact indicates that we will need theoretical results using the Green's function method to analyze the data with high accuracy in the near future. Finally, the shapes of the peak structures are not the same in the two spectra. For example, at the highest peaks of the spectra at $Q \simeq -138$ MeV, we see clearly that the peaks have different shapes, and the tails of the peaks at $Q \simeq -136$ MeV show different behavior. This is important since knowledge of the precise behavior of the tail in the spectrum is essential for determining the background of the experimental data correctly (K. Itahashi, private communication).

In Fig. 3, we show the dominant subcomponents of the ($d$,\(^3\)He) spectra in the region of $Q = -140.5$ to $-136.5$ MeV to see precisely the difference in the peak structure obtained by the two theoretical formulas and the effects of the vacuum polarization. We can see from the figure that the contributions from the $[(1s)\pi \otimes (3s_{1/2})_n^{-1}]$, $[(2s)\pi \otimes (3s_{1/2})_n^{-1}]$ (effective number approach), and $[(s)\pi \otimes (3s_{1/2})_n^{-1}]$ (Green's function method) components in each formalism have different peak shapes, namely, different energy dependences in the spectra around the peak energy. Also, it is quite
Fig. 2. Calculated total spectra for the formation of pionic atoms in the $^{122}\text{Sn}(d,^3\text{He})$ reactions at forward angle, plotted as functions of the reaction $Q$-value. Contributions of quasi-free $\pi^0$ production are not included. The solid line indicates the result of the Green’s function method and the dashed line that of the effective number approach. The incident deuteron kinetic energy is fixed at $T_d = 500$ MeV. The instrumental energy resolution is assumed to be 300 keV FWHM. The vertical lines indicate the pion production threshold $Q = -141.6$ MeV.

obvious that the discrepancy is larger for the stronger imaginary potential, as expected. Similar results were obtained in the case of kaon bound states in Ref. [13]. In the result of the effective number approach, the structure of the isolated peak is symmetric, as we mentioned above, since we assume a symmetric Lorentz distribution function as the shape of the peak structure. On the other hand, in the result of the Green’s function method, the dominant subcomponent $[s_\pi \otimes (3s_{1/2})_n^{-1}]$ has an asymmetric peak, even for the isolated case, for the results of the calculation without assuming the shape of the peak structure. We can also see the effect of the vacuum polarization in the figure by comparing the dashed and dotted lines. The vacuum polarization effects are not large but are visible in the figure.

We summarize in Table 1 the $Q$-values corresponding to the peak of the $(1s)_\pi$ formation for all cases shown in Fig. 3 as an important parameter to evaluate the difference between the effective number approach ($N_{\text{eff}}$) and the Green’s function method, and the vacuum polarization effects. We can see from Table 1 that the effects of the vacuum polarization are around 20 keV for $0.5–2 \text{Im}V_{\text{opt}}$ and consistent with the results shown in the Appendix. The discrepancy between the effective number approach and the Green’s function method can be large and serious for the larger imaginary potential. In the case of the pionic atom with the original imaginary potential $\text{Im}V_{\text{opt}}$, the discrepancy is around 10 keV. Thus, these effects should be considered carefully, even though they are not large, if the experimental accuracy of the peak energy is comparable to this value.

In Fig. 4, we also show the calculated spectra of the $^{122}\text{Sn}(d,^3\text{He})$ reaction at finite angles for the formation of pionic atoms by the effective number approach and the Green’s function method. We find that both methods provide qualitatively the same spectra, even at larger angles. Thus, we can conclude again at finite angles that the effective number approach provides reasonably good theoretical results for the analysis of the previous data; however, the Green’s function method will be necessary for further studies of pionic atom formation by the $(d,^3\text{He})$ reactions.

For completeness, we consider another case to compare the results by both methods. We study the spectra of the $^{206}\text{Pb}$ target case at $T_d = 600$ MeV, for which the theoretical calculations using the effective number approach are reported in Refs. [2,19], and the experimental result in Ref. [20]. Since the binding energies and widths of the pionic state in the Pb nucleus are larger than those in the
Fig. 3. The dominant subcomponents of the $^{122}$Sn($d$, $^{3}$He) reaction spectra for pionic atom formation are plotted as functions of the reaction $Q$-value. The solid line shows the calculated results of the contribution from the $[s_{\pi} \otimes (3s_{1/2})^{-1}]$ components by the Green’s function method. The dashed and dotted lines show the calculated results of the contribution from the $[(1s)_{\pi} \otimes (3s_{1/2})^{-1}]$ and $[(2s)_{\pi} \otimes (3s_{1/2})^{-1}]$ components by the effective number approach. The effects of the vacuum polarization of the electromagnetic interaction are included in the solid and dashed lines. The strength of the imaginary part of the optical potential is varied from its original value, as indicated in the figure. The same real optical potential is included in all calculations. The instrumental energy resolution is not taken into account in this figure.
Table 1. The $Q$-values of the peak position of the $|(1s)_\pi \otimes (3s_{1/2})_n^{-1}|$ subcomponent for the formation of pionic atoms in the $^{122}$Sn$(d,^3$He) reactions for all cases shown in Fig. 3 in units of MeV. The same real optical potential is included in all calculations. The effects of the vacuum polarization (VP) of the electromagnetic interaction are included in the results of Green’s function method and $N_{\text{eff}}(V_{\text{FS+VP}})$. FS: finite size.

| Imaginary potential | Green’s function method | $N_{\text{eff}}(V_{\text{FS+VP}})$ | $N_{\text{eff}}(V_{\text{FS}})$ |
|---------------------|-------------------------|-----------------------------------|--------------------------------|
| 0.5 Im$V_{\text{opt}}$ | $-137.780$               | $-137.783$                        | $-137.804$                     |
| Im$V_{\text{opt}}$   | $-137.793$               | $-137.803$                        | $-137.824$                     |
| 2 Im$V_{\text{opt}}$ | $-137.834$               | $-137.871$                        | $-137.891$                     |
| 10 Im$V_{\text{opt}}$| $-138.200$               | $-138.473$                        | $-138.488$                     |

![Fig. 4](image-url)  

Calculated spectra in the $^{206}$Pb$(d,^3$He) reaction for the formation of pionic atoms at $\omega_{\text{lab}} = 0^\circ$ (solid lines), $1^\circ$ (dashed lines), $2^\circ$ (dash-dotted lines), and $3^\circ$ (dotted lines) by the Green’s function method (left) and by the effective number approach (right), plotted as functions of the reaction $Q$-value. Contributions of quasi-free $\pi^0$ production are not included. The incident deuteron kinetic energy is fixed at $T_d = 500$ MeV. The instrumental energy resolution is assumed to be 300 keV FWHM. The effect of the vacuum polarization is included in the results of the Green’s function method, but not in the result of the effective number approach.

Sn nucleus, we can expect that the formation spectrum of pionic atoms in the $^{206}$Pb$(d,^3$He) reaction spreads over a wider energy range than that in the $^{122}$Sn$(d,^3$He) reaction and, thus, could be more suited to study the energy dependence of the differences between both methods.

In Fig. 5, we show the calculated $^{206}$Pb$(d,^3$He) spectra together with the main subcomponents by the effective number approach and the Green’s function method. In the result of the effective number approach (right), the line with the symbol $[(2p,3p,4p)_\pi \otimes (3p)_n^{-1}]$ indicates the sum of the three subcomponents $[(2p)_\pi \otimes (3p)_n^{-1}], [(3p)_\pi \otimes (3p)_n^{-1}], $ and $[(4p)_\pi \otimes (3p)_n^{-1}]$. In the $^{206}$Pb target reaction at $T_d = 600$ MeV, the contributions from the pionic $p$ states become considerably large and the largest peak structure at $Q \simeq -136$ MeV is mainly composed of the $[(2p)_\pi \otimes (3p)_n^{-1}]$ subcomponent. The contributions from the pionic $1s$ state coupled to the neutron $(3p)_n^{-1}$ hole state are seen at $Q \simeq -134$ MeV in the $^{206}$Pb$(d,^3$He) spectrum. We also show, in Fig. 6, the overlay of the total spectra of both methods shown in Fig. 5. As in the $^{122}$Sn target case, both methods provide very similar formation spectra in the $^{206}$Pb target case. We also find that the discrepancies of the two calculated spectra have exactly the same features, as discussed in Fig. 2 for the Sn target case. In addition, we find that differences between the effective number approach and the Green’s function method are even enhanced for the Pb target case. An interesting feature of the spectra for the Pb target case is the height of the peak at $Q \simeq -134$ MeV, which is composed of the $|(1s)_\pi \otimes (3p)_n^{-1}|$ subcomponent. We find that the calculated peak in the Green’s function method is larger than that by the effective number approach, mainly because of the tail of the $|(2p)_\pi \otimes (3p)_n^{-1}|$ subcomponent.
Fig. 5. Calculated spectra in the $^{206}$Pb($d$, $^3$He) reaction for the formation of pionic atoms at forward angle by the Green’s function method (left) and by the effective number approach (right), plotted as functions of the reaction $Q$-value. Contributions of quasi-free $\pi^0$ production are not included. The dominant subcomponents are also shown in the figures. The incident deuteron kinetic energy is fixed at $T_d = 600$ MeV. The instrumental energy resolution is assumed to be 300 keV FWHM. The vertical lines indicate the pion production threshold $Q = -140.9$ MeV. The effect of the vacuum polarization is included in the results of the Green’s function method, but not in the result of the effective number approach.

Fig. 6. Calculated total spectra for the formation of pionic atoms in the $^{206}$Pb($d$, $^3$He) reactions at forward angle, plotted as functions of the reaction $Q$-value. Contributions of quasi-free $\pi^0$ production are not included. The solid line indicates the result of the Green’s function method and the dashed line that of the effective number approach. The incident deuteron kinetic energy is fixed at $T_d = 600$ MeV. The instrumental energy resolution is assumed to be 300 keV FWHM. The vertical lines indicate the pion production threshold $Q = -140.9$ MeV.

This observation again indicates that we definitely need careful analyses of highly precise data to obtain precise information on in-medium pion properties for the ($d$, $^3$He) spectra.

4. Conclusion

We have calculated the ($d$, $^3$He) spectra in the effective number approach and the Green’s function method. The Green’s function method is known to be a better theoretical formalism than the effective number approach to obtain more realistic formation spectra of unstable bound states with large widths. The effective number approach is known to be a good method to evaluate the formation rate of quasi-stable bound states with small widths, such as pionic atoms, and is known to require much fewer numerical calculations than the Green’s function method.

We found that both methods provide similar spectra for whole energy regions of bound and quasi-free pion production, as we expected. From the overlay plots of the total spectra obtained by both
methods, we found that small discrepancies between the two spectra appeared at the following three points: (i) the behaviors of the spectra near the threshold, (ii) the heights and positions of peaks, and (iii) the shapes of the peak structures. The origin of these discrepancies can be attributed to the following differences in the two formalisms. In the effective number approach, we cannot include all contributions of the pion bound states in the spectrum near the threshold and we need to assume a symmetric Lorentz distribution function as the shape of the peak structure. On the other hand, in the Green’s function method, we can, in principle, sum up all the contributions from an infinite number of the bound pionic states, and we do not need to assume the shape of the peak structure.

In Sect. 3, we investigated numerically the size of the discrepancies and showed the quantitative results. As one of the most important observables in our analysis, we compiled the dependence of the position of the largest peak in the \((d, ^3\text{He})\) reaction on the formalism for calculating the reaction spectra in addition to the vacuum polarization effects. For relatively small imaginary potential cases, such as pionic atoms, we think that we can conclude that the Green’s function method should be used for cases where an accuracy better than 10 keV is required for the peak position of the deepest 1s atomic states.

Since the discrepancies are reasonably small compared to the accuracy of the data for previous analyses of pionic atoms, we have reaffirmed that the effective number approach is a good theoretical method for getting the spectra for the analyses of the previous experimental data obtained so far. However, in the near future, we think that theoretical results using the Green’s function method will be necessary to deduce precise information on the pion properties from analyses of the data with better accuracy, as described above.

We would also like to mention here that the absolute sizes of the observed \((d, ^3\text{He})\) cross section reactions are different from the theoretical results. Though the absolute size of the spectra is less important in our analysis than the shapes of the spectra and the peak position, this discrepancy should be revisited and studied by using realistic distorted waves for the projectile and ejectile.

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Appendix A. Vacuum polarization correction

In this appendix, we describe how to include the vacuum polarization effects of the pion–nucleus electromagnetic interaction in our theoretical calculation. We follow the same method adopted in Ref. [21].

The energy spectra and wave functions of the pionic atoms can be obtained theoretically by solving the Klein–Gordon equation:

\[
-\nabla^2 + \mu^2 + 2\mu V_{\text{opt}}(r) \phi(r) = \left[ E - V_{\text{em}}(r) \right] \phi(r),
\]

where \(\mu\) is the pion–nucleus reduced mass, and \(E\) is the eigenenergy written as \(E = \mu - \text{B.E.} - \frac{i}{2} \Gamma\) with the binding energy B.E. and the width \(\Gamma\) of the atomic states. The two terms, \(V_{\text{opt}}\) and \(V_{\text{em}}\), indicate the pion–nucleus interactions. The first term \(V_{\text{opt}}\) is the pion–nucleus optical potential and the second term \(V_{\text{em}}\) is the electromagnetic interaction.
The simplest electromagnetic interaction between two charged particles with a distance of $r$ is the well known point Coulomb (PC) interaction $V_{PC} = -\frac{\alpha}{r}$ with the fine structure constant $\alpha \approx \frac{1}{137}$.

To obtain precise theoretical results for the structure of pionic atoms, we need to modify the PC interaction by introducing corrections due to the finite size (FS) charge distribution of the nucleus and the vacuum polarization (VP) of the photon propagator. The correction due to the VP effects to the point Coulomb potential is described in detail in, e.g., Ref. [22] and the PC potential should be modified as

$$V_{PC} \rightarrow V_{PC+VP} = -\frac{\alpha}{r} Q(r),$$  

(A2)

where $Q(r)$ is given in Eq. (7.24) in Ref. [22] and defined as

$$Q(r) = 1 + \frac{2\alpha}{3\pi} \int_1^\infty du e^{-mru} \left(1 + \frac{1}{2u^2}\right) \frac{(u^2 - 1)^{1/2}}{u^2},$$  

(A3)

where $m$ indicates the electron mass. To further include the FS effects on this potential non-perturbatively, we consider the folding form of $V_{PC+VP}$ by the nuclear charge distribution $\rho(r)$ as

$$V_{FS+VP}(r) = -\alpha \int \frac{\rho(r') Q(|r - r'|)}{|r - r'|} dr'.$$  

(A4)

The $V_{FS+VP}$ potential is used in the Klein–Gordon equation to obtain the results with the vacuum polarization effects.

We calculate the pion binding energies and widths by solving the Klein–Gordon equation with the pion–nucleus electromagnetic interaction Eq. (A4). We show in Table A1 the calculated pion binding energies and widths in units of keV.

**Table A1.** Calculated binding energies B.E. and widths $\Gamma$ of $\pi^- -^{121}\text{Sn}$ atoms in units of keV. The results calculated without the vacuum polarization effects (right) are the same as those shown in Table VII in Ref. [6] and are listed again for the comparison with those with the vacuum polarization effects (left). The same optical potential is included in both calculations and $V_{FS}$ is defined as in Eq. (A4), replacing $Q(r)$ with unity.

| state | $V_{FS+VP}$ | $V_{FS}$ |
|-------|-------------|-----------|
|       | B.E. [keV] | $\Gamma$ [keV] | B.E. [keV] | $\Gamma$ [keV] |
| $1s$  | 3850.0     | 323.6     | 3829.2     | 320.6     |
| $2s$  | 1421.5     | 77.5      | 1415.6     | 76.8      |
| $3s$  | 734.8      | 29.5      | 732.5      | 29.3      |
| $4s$  | 447.8      | 14.2      | 446.6      | 14.1      |
| $5s$  | 301.1      | 7.9       | 300.5      | 7.8       |
| $6s$  | 216.2      | 4.8       | 215.8      | 4.8       |
| $2p$  | 2275.9     | 118.6     | 2262.7     | 116.7     |
| $3p$  | 1017.9     | 40.1      | 1013.6     | 39.6      |
| $4p$  | 574.7      | 17.7      | 572.9      | 17.5      |
| $5p$  | 368.6      | 9.3       | 367.7      | 9.2       |
| $6p$  | 256.3      | 5.4       | 255.8      | 5.4       |
| $3d$  | 1044.8     | 2.6       | 1040.5     | 2.5       |
| $4d$  | 587.5      | 1.6       | 585.6      | 1.5       |
| $5d$  | 375.5      | $9.2 \times 10^{-1}$ | 374.6 | $9.0 \times 10^{-1}$ |
| $6d$  | 260.4      | $5.7 \times 10^{-1}$ | 259.9 | $5.6 \times 10^{-1}$ |
| $4f$  | 583.3      | $5.7 \times 10^{-3}$ | 581.8 | $5.6 \times 10^{-3}$ |
| $5f$  | 373.2      | $5.0 \times 10^{-3}$ | 372.5 | $4.8 \times 10^{-3}$ |
| $6f$  | 259.1      | $3.6 \times 10^{-3}$ | 258.7 | $3.5 \times 10^{-3}$ |
energies and widths for $\pi^{-}\!^{121}\text{Sn}$ with and without the vacuum polarization effects. The differences between the binding energies in the two cases are found to be around 1\% or less.

In the latest experiments at GSI, reported in Ref. [1], the experimental energy resolution is about 400 keV and the evaluated error of the pion binding energy is about 20 keV. This error is almost the same as the vacuum polarization effects for the pionic $1s$ state, as we can see in Table A1.

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