Low energy valence photoemission in the Anderson impurity model for Ce compounds

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The valence level photoemission spectra in the Anderson impurity model for Ce compounds at zero temperature are studied as a function of the photon energy \( \omega \). Most of former studies on Ce compounds are based on the sudden approximation, which is valid in high energy region. For the photoemission in the adiabatic limit of low energy region, one should consider the dipole matrix elements and the hole-induced photoelectron scattering potential. We can manage it by combining the time-evolution formalism and the 1/\( N_f \) scheme in a large \( f \)-level degeneracy \( N_f \). This gives the exact results as \( N_f \to \infty \). In view of experiments on the valence photoemission, two contributions of 4f- and band emissions are mixed. We study the separate 4f and band contributions (from Ce 5d) and total emission including the interference between two on an equal footing with varying the photon energy. In the 4f-emission case, we also explore the effects of hole-induced scattering potential of the photoelectron with respect to \( \omega \). Its effects are found very similar to the core level photoemission in shake down case with a localized charge transfer excitation. Additionally, we examine the adiabatic-sudden transition in valence level photoemission for the present localized system through the simplified two-level model.

I. INTRODUCTION

The Anderson impurity model (AIM) was originally proposed to discuss the property of magnetic impurities in nonmagnetic metals. After that, AIM has been widely applied to the analysis of spectroscopic data for \( f \) and \( d \) electron systems, i.e. rare earth compounds or transition metal compounds, where electron states are treated to be an impurity and they are hybridized with the valence or conduction electron states. Also, AIM has been often used to describe the Ce mixed-valence compounds, where one considers the \( f \) level on one atom and its interaction with the conduction bands. In investigations of Ce and its compounds, the basic question concerns the nature of a 4f electron and other electronic states and how they mix with the 4f state. Much of the interests are therefore imposed on the properties of the 4f states, i.e. the occupation, position, width, coupling to the metallic band, intra-atomic Coulomb interaction and so on. There were numerous studies of thermodynamic and transport properties for them, which has been followed by the electron-spectroscopy studies.

The photoemission spectroscopy (PES) is a very useful tool for studying the electronic structure of matters and could have provided a lot of insights also for Ce studies. But it’s worth noting PES cannot always give a simple answer about the underlying electronic structure because the photoelectron may perturb the system left behind. Actual description of theoretical PES is quite complicated and therefore the sudden approximation is frequently used, where the photoelectron is assumed decoupled from the remaining solid. The sudden approximation becomes exact when the kinetic energy of the emitted electron gets large infinitely.

Gunnarsson and Schönhammer have extensively studied the electron spectroscopies for Ce compounds, i.e. core level photoemission, x-ray absorption, and bremsstrahlung isochromat spectroscopy as well as the valence photoemission. For the information of the position and width of \( f \)-level in the compounds, the valence photoemission has often been used. Through their studies of valence photoemission in \( f \)-emission channel, they reproduced two-peak structure in Ce compound using AIM consistent with the experiments. In the earlier evolution stage for Ce materials, it was found that the valence PES shows just a single \( f \)-related structure 2-3 eV below the Fermi level. Later PES experiments have demonstrated the 4f spectrum has the additional structure interestingly near the Fermi level. Subsequently, it was shown that the particular structure is due to the Kondo resonance singlet characterized by the small energy \( T_K \). In the actual experiments on valence photoemission, two contributions of 4f-emission and band emission (from Ce 5d or other bands) are mixed. The identification of 4f-emission from the experiments is a highly nontrivial work. Wieliczka et al. have done the comparison of spectra taken at the different photon energies showing the resonance of 4f-emission and reported the additional peak near the Fermi level. Another possibility is to assume the behaviors of 4f- and band emissions with respect to the photon energies, especially in 20 – 80 eV. Nevertheless, they could have said nothing about the interference between two. These works can motivate to explore a more explicit analysis for the interference effects of two emission channels with the photon energy varied. Gunnarsson and Schönhammer have also studied the band emission contribution as well as 4f-emission and discussed the interference effects of two. However, all their works were within the sudden approximation.

We consider both the contributions of 4f- and 5d-emission on an equal footing by introducing two dipole matrix elements, \( \Delta_f(E) \) and \( \Delta_d(\epsilon, E) \), where \( E \) is the...
kinetic energy of photoelectrons. In the sudden approximation, the dipole matrix elements are normally treated constant with $E$. But in the low energy PES, it can be crucial. Combining the time-dependent formalism and $1/N_f$ idea, we can calculate the PES exactly up to $\mathcal{O}(1/N_f^0)$ as the photon energy varies. $N_f = \infty$ can be a good approximation to $N_f = 14$ in Ce compounds. Then we study the separate contributions of $4f$- and $5d$-emission and more interestingly the nontrivial interference effects between two. The relative sign or strength of $\Delta_f(E)$ and $\Delta_d(\epsilon, E)$ are important. Difference in the energy scale of $\Delta_f(E)$ and $\Delta_d(\epsilon, E)$ makes the spectra from each channel separate with respect to $\omega$ in the low energy PES. It is also found that, because the interference contribution has a peak near the Fermi level, the $4f$-derived peak near the Fermi level may be enhanced or suppressed in a total spectra.

It is recently reported that the adiabatic-sudden transition due to the photoelectron scattering potential will be governed by the characteristic of relevant excitations to which the emitted electron couples in the system. When the photoelectron couples to the extended excitation like plasmon, the sudden transition occurs in very large kinetic energies ($\sim$ keV), while to the localized excitations, the sudden approximation occurs much quicker.

In our study, the extrinsic effects beyond the sudden approximation will be considered only through the hole-induced scattering potential. Effects like surface or several damping mechanisms will not be taken into account. The system of Ce compounds has also included the localized excitations represented by $f^0$, $f^1$, $f^2$ created from the hole potential. We can consider the scattering potential in the valence PES due to $f$-hole in the impurity model within the formalism. The scattering effects will not be important for band emission channel. The crossover from adiabatic to sudden limit can be also re-examined in this localized system, for which we simplify the model to have only two relevant levels. The same criterion for the transition is found as in the previous work\cite{landau}, the energy scale of $E = 1/(2R^2)$, where $R$ is a scattering potential range.

We organize the paper as follows. Our model and the formalism for calculation are given in Sec. II. The simple sudden approximation results for separate and both channels are described in Sec. III. In Sec. IV, we present the model for necessary dipole matrix elements and calculate the spectra for the separate contributions for $4f$- and $5d$-emission and for both with respect to the photon energies. We also discuss the interference contribution between two. In Sec. V, for $4f$-emission, we include the photoelectron scattering potential within the same formalism. In Sec. VI, we try to reexamine the adiabatic-sudden crossover in the system by way of the simplified two-level model. In Sec. VII, we give the discussion and conclusion.

II. MODEL AND FORMALISM

As mentioned in the introduction, we consider the AIM Hamiltonian in the energy basis used in Gunnarsson and Schönhammer’s discussion for Ce compounds\cite{gunnarsson2002}.

$$\mathcal{H} = \mathcal{H}_0 + \Delta,$$

$$\mathcal{H}_0 = \sum_{\nu} \int E \psi_{\nu E}^\dagger \psi_{\nu E} dE + \sum_{\nu} \epsilon \psi_{\nu E}^\dagger \psi_{\nu E} d\epsilon + \epsilon \sum_{\nu} n_{\nu} + \sum_{\nu} V(\epsilon)(\psi_{\nu E}^\dagger \psi_{\nu E} + \psi_{\nu E}^\dagger \psi_{\nu E}) d\epsilon + \frac{U}{2} \sum_{\nu \neq \nu'} n_{\nu} n_{\nu'}, \quad (1)$$

where $\psi_{\nu E}^\dagger(\psi_{\nu E})$ is a photoelectron operator, $\epsilon$ denotes the 5d conduction states, $\epsilon$ describes the impurity 4f level, and $V(\epsilon)$ is a hybridization matrix element between the conduction states and localized $f$ level. $|V(\epsilon)|^2$ can be modeled to have a semilcutical form symmetric with respect to $\epsilon = 0$, $|V(\epsilon)|^2 = 2V^2/(B^2 - \epsilon^2)^{1/2} / B^2$, where $2B$ is the bandwidth. $\Delta$ in the Hamiltonian is the dipole descriptor describing the photon-matter interaction. The one particle basis used in Eq. (1) is introduced by assuming\cite{landau}

$$\sum_{k} V_{km} V_{km'} = |V(\epsilon)|^2 \delta_{mm'},$$

and so $\nu$ is the orbital and spin magnetic quantum number and from $\nu = 1$ to $\nu = N_f$ if we assume the magnetic degeneracy $N_f$ of $f$-level. In Ce, $N_f$ is normally taken as 14. To apply $1/N_f$ idea, we need one subsidiary condition that $N_f^{1/2}|V(\epsilon)|$ should be independent of $N_f$.

In $\Delta$, we will generally have two interaction terms due to $4f$ level and $5d$ conduction bands, so

$$\Delta = \sum_{\nu} \int dE \left[ \Delta_f(E) \psi_{\nu E}^\dagger \psi_{\nu E} + \Delta_d(E) \psi_{\nu E}^\dagger \psi_{\nu E} \right]$$

$$+ \frac{1}{N_f^{1/2}} \sum_{\nu} \sum_{E} d\epsilon \left[ \Delta_d(\epsilon, E) \psi_{\nu E}^\dagger \psi_{\nu E} + \Delta_d^*(\epsilon, E) \psi_{\nu E}^\dagger \psi_{\nu E} \right].$$

By giving the explicit time-dependency $f(\tau)$ in $\Delta$ and re-defining the dipole matrix elements, $\Delta_f(E)$ and $\Delta_d(E, \epsilon)$, we use a time-dependent formulation and solve the Schrödinger equation for the total Hamiltonian $\mathcal{H}$.

We first introduce a state $|0\rangle$,

$$|0\rangle = \prod_{\nu \epsilon < \epsilon_F} \psi_{\nu E}^\dagger |\text{vac}\rangle,$$
where all the conduction electron states below Fermi energy are occupied and the $f$ level is empty. For the simplicity, we keep only the lowest order terms of $1/N$ before and after the photoemission, which means the results will be exact as $N_f \to \infty$.

$$|\epsilon\rangle = \frac{1}{N_f^{1/2}} \sum_{\nu} \psi_{\nu}^{f} \psi_{\nu}^{c}|0\rangle,$$

$$|\epsilon, \epsilon'\rangle = \frac{1}{N_f^{1/2}(N_f - 1)^{1/2}} \sum_{\nu \neq \nu'} \psi_{\nu}^{f} \psi_{\nu'}^{f} \psi_{\nu}^{c} \psi_{\nu'}^{c}|0\rangle,$$

$$|E, \epsilon\rangle = \frac{1}{N_f^{1/2}} \sum_{\nu} \psi_{\nu}^{E} \psi_{\nu}^{f} |0\rangle,$$

$$|E, \epsilon, \epsilon'\rangle = \frac{1}{N_f^{1/2}(N_f - 1)^{1/2}} \sum_{\nu \neq \nu'} \psi_{\nu}^{E} \psi_{\nu'}^{f} \psi_{\nu}^{f} \psi_{\nu'}^{c} |0\rangle,$$

$$|E, \epsilon, \epsilon', \epsilon''\rangle = \frac{1}{N_f^{1/2}(N_f - 1)^{1/2}(N_f - 2)^{1/2}} \times \sum_{\nu \neq \nu' \neq \nu''} \psi_{\nu}^{E} \psi_{\nu'}^{f} \psi_{\nu''}^{f} \psi_{\nu'}^{f} \psi_{\nu''}^{c} \psi_{\nu'}^{c} |0\rangle.$$

Within the above basis set, after time $\tau$, the wave function $|\Psi(\tau)\rangle$ of the system is given by

$$|\Psi(\tau)\rangle = a(\tau)|0\rangle + \int b(\epsilon; \tau)\epsilon|\epsilon\rangle d\epsilon + \int c(\epsilon, \epsilon'; \tau)|\epsilon, \epsilon'\rangle d\epsilon d\epsilon'$$

$$+ \int d(E, \epsilon; \tau)|E, \epsilon\rangle dE d\epsilon$$

$$+ \int e(E, \epsilon, \epsilon'; \tau)|E, \epsilon, \epsilon'\rangle dE d\epsilon d\epsilon'$$

$$+ \int f(E, \epsilon, \epsilon', \epsilon''; \tau)|E, \epsilon, \epsilon', \epsilon''\rangle dE d\epsilon d\epsilon' d\epsilon''.$$

The coefficients of $|\Psi(\tau)\rangle$ can be determined by the time dependent Schrödinger equation,

$$i \frac{\partial}{\partial \tau} |\Psi(\tau)\rangle = \mathcal{H}|\Psi(\tau)\rangle,$$

where the initial condition of the state should be corresponding to the ground state before the photoemission, $|\Psi(\tau = 0)\rangle = |\Psi_0\rangle$,

$$|\Psi(0)\rangle = a(0)|0\rangle + \int b(\epsilon; 0)\epsilon|\epsilon\rangle d\epsilon + \int c(\epsilon, \epsilon'; 0)|\epsilon, \epsilon'\rangle d\epsilon d\epsilon'$$

and the equations for $a(0)$, $b(\epsilon; 0)$, and $c(\epsilon, \epsilon'; 0)$ are found in Ref.15. The coefficients $M_f$ and $M_d$ represent the external field strength. In the present formalism, we solve the equation in the limit of $M_f \to 0$ and $M_d \to 0$ and let the system evolve for a time of the order $1/\eta$. Then we can show the solution identical to the more conventional photoemissionubo. $\eta$ is a small positive number and gives a life-time broadening in the spectra. In the actual calculation, $\eta$ is taken as 0.3 eV (0.01 au). The photoemission spectra will now be proportional to

$$I(E) = \int |d(E, \epsilon; \tau)|^2 d\epsilon + \int |e(E, \epsilon, \epsilon'; \tau)|^2 d\epsilon d\epsilon'$$

$$+ \int |f(E, \epsilon, \epsilon', \epsilon''; \tau)|^2 d\epsilon d\epsilon' d\epsilon'',$$

and we see, due to $M_f \to 0$ and $M_d \to 0$,

$$I(E) = \alpha(\epsilon)M_f^2 + \beta(\epsilon)M_d^2 + \gamma(\epsilon)M_f M_d,$$

where $\alpha(\epsilon)$, $\beta(\epsilon)$, and $\gamma(\epsilon)$ correspond to 4$f$-, 5$d$-emission, and interference between those, respectively.

### III. SUDDEN APPROXIMATION

In the sudden approximation, we normally neglect $E$-dependency of the dipole matrix elements, i.e. $\Delta_f(E) = M_f$ and $\Delta_d(\epsilon, E) = M_d\Delta_f(\epsilon)$, where $E$ is a kinetic energy of photoelectron. Gunnarsson and Schönhammer\[12\] assumed $\Delta_f(\epsilon)$ have the same shape as $V(\epsilon)$ for the conduction band emission, which we’ll simply follow.

The AIM has often been studied in the limit of $U = \infty$, where it becomes so simple as to allow the analytic solutions. In our formalism, to neglect $|\epsilon, \epsilon'\rangle$ and $|E, \epsilon, \epsilon', \epsilon''\rangle$ corresponds to the limit. However the assumption $U = \infty$ is not really justified because $U$ is just about 5 ~ 6 eV\[13\] and thus $f^0$ and $f^2$ configurations are energetically comparable, i.e. $\epsilon_f$ is about $-2 \sim -3$ eV\[13\] and $2\epsilon_f + U \approx 0$. In the calculations, we have always taken $U = 5.0$ eV and $\epsilon_f = -2.5$ eV to be $2\epsilon_f + U = 0$. In Fig.4, we give the simple valence PES results for 4$f$- and 5$d$-emission, respectively.
FIG. 1. In the upper panel, the f-derived valence PES is provided \((M_d = 0)\) and in the lower panel, the conduction band emission is given \((M_f = 0)\) for \(U = 5.0\) eV, \(\epsilon_f = -2.5\) eV, \(V = 0.5\) eV, and \(B = 6\) eV. Both calculations are based on the sudden approximation. Spectral curves are normalized to have the same area.

It is seen in Fig.[1] that we nicely reproduce the well-known sudden 4f-PES results\(^5\) having the double-peak structure in the upper panel and also get 5d-PES simulating the broad structureless conduction band. The 4f-PES is especially interesting because of its ample physics. The peak well below the Fermi level corresponds to 4f ionization peak, \(4f^1 \to 4f^0\), and the peak near the Fermi level (also called Kondo resonance peak) arise from a 4f hole screened by a 4f electron (making a 5d hole near the Fermi level), \(4f^1 \to 4f^1\).

In the separate calculations of emission channels, the absolute values or signs of \(M_f\) and \(M_d\) are surely irrelevant to the results. There can be however some subtleties when we consider both emission channels. The PES curves drastically change with respect to the relative sign or relative ratio of \(M_f\) and \(M_d\). For the relative strength, we parametrize the ratio of \(|M_d\Delta'(0)/M_f|\) (note \(|M_d\Delta'(0)/M_f| > 1\) does not always mean the band emission is dominant over the \(f\)-emission). The relative sign is related to whether the interference will be constructive or destructive.

As shown in Fig.[2] the relative ratio and signs of two dipole components are crucial in valence PES. Interestingly, the interference contributions show a peak near the Fermi level, which may enhance the Kondo resonance peak from 4f-emission in the constructive case or suppress in the destructive case. In Fig.[2](b), even if we can see a clear ionization peak near \(\epsilon_f\), we see only the shoulder structure not a peak near the Fermi level due to a strong destructive interference. These destructive interferences may be one of the reasons that several groups in the former stage have failed to see a double-peak structure and reported only an ionization peak near \(\epsilon_f\).

IV. LOW ENERGY VALENCE PHOTOEMISSION: EFFECTS OF DIPOLE MATRIX

In the last section, we have illustrated the sudden approximation results valid in the high energy PES. To see how the PES behaves in the low energy regime, first off we should account for the \(E\)-dependent dipole matrix elements. Using the Slater-type orbital\(^6\) for the corresponding atomic orbital, we calculate \(E\)-dependent dipole matrix elements. The Slater orbital for \(R_{nl}(r)\) is given by

\[ R_{nl}(r) = (2\zeta)^{n+1/2}[(2n)!]^{-1/2}r^{n-1}e^{-\zeta r}, \]

where the orbital exponent is determined by a suitable rule. But in \(4f^55d^6\) configuration of Ce, the Slater orbital for 5d gives actually the poor representation compared to a more accurate LSD calculation\(^2\) for the atomic wavefunction of Ce. We adopt therefore the same functional form of Eq.(16), but determine the exponent \(\zeta\) suitably by comparing with the accurate result, i.e. we take \(\zeta_{4f} = 5.0\) and \(\zeta_{5d} = 2.0\) (by a Slater-rule, \(\zeta_{5d}\) will be 0.75). In principle, the atomic orbital and photoelectron basis function having an explicit angular momentum channel \(l\) should be obtained by solving the Schrödinger equation under the same Ce atomic potential. But in our discussion the basis function is simply assumed to be a spherical Bessel function of \(l\),

\[ \varphi_E^l(r) = \frac{\sqrt{2}}{\sqrt{\pi}}(2E)^{1/4}j_0(\sqrt{2Er}), \]

and its normalization follows

\[ \int r^2 dr \varphi_E^*(r) \varphi_E^l(r) = \delta(E - E'). \]

So the dipole matrix elements for 4f-emission is given by

\[ \Delta_f(E) = M_f \int r^2 dr R_{4f}(r) r \varphi_E^{l=4}(r), \]

and for the 5d-conduction band emission, we assume \(\Delta_d(\epsilon, E)\) has the simple separable form like

\[ \Delta_d(\epsilon, E) = M_d \Delta_d'(\epsilon) \Delta_d(E). \]

\[\text{FIG. 2. The valence PES including both contributions of 4f- and 5d-emission is shown. The solid line is the total spectra corresponding to constructive or destructive interference, where interference effects (labeled "intf") is added or subtracted. In (a), we use } |M_d\Delta'(0)/M_f| = 2 \text{ and in (b), } |M_d\Delta'(0)/M_f| = 6. \text{ The used parameters are same in Fig.1.}\]
$\Delta_f'(\epsilon)$ is still assumed to have the shape of $V(\epsilon)$ as in the last section and $\Delta_d(E)$ can be expected to have much 5d atomic orbital character if we think of the tight binding idea for the corresponding energy band. Thus we assume the behavior of $\Delta_d(E)$ as

$$\Delta_d(E) \propto \int r^2 \, dr \, R_{5d}(r) \, r \varphi_{l=3}^l(r).$$

\hfill (21)

Here it should be noted that the possible $l$-channel of photoelectrons are $l = 2, 4$ for 4f-emission and $l = 1, 3$ for 5d-emission due to the angular momentum selection rule, but the major channel will be $l = 4$ and $l = 3$, respectively.

In Fig.3, we give the dipole matrix behaviors of $\Delta_f(E)$ and $\Delta_d(E)$. This is obtained from very crude calculations, but qualitatively quite consistent with Yeh and Lindau's calculation of photoionization cross sections for Ce. We can simply expect from the behaviors of dipole elements the general trend is that in the low energy, d-emission will be dominant over f-emission, while in the high energy, f-emission dominant over d-emission. We first show the calculation result for separate 4f and 5d contributions with respect to various photon energies $\omega$.

Figure 4 shows $\omega$-dependent 4f- and 5d-emission, the changes of spectral height and shape with $\omega$ varied. The spectral height will be proportional to the square of dipole matrix elements at the corresponding energies and the shape related to the behaviors of dipole element. If the 5d radial wave function does not vary significantly for La and Ce, the bottom panel of the figure can be compared with the PES for La[4] and found to be consistent with the experiment. We can also find as $\omega$ increases the spectral shape approaches the sudden approximation results (see the insets).

Now we investigate the total valence PES to which both 4f- and 5d-emission contribute with respect to various photon energies $\omega$. To parameterize the relative strength of two dipole matrix effects, we define $\tilde{\Delta}_f$ and $\tilde{\Delta}_d$ as $\tilde{\Delta}_f = \Delta_f(E)|_{E=4.0}$, $\tilde{\Delta}_d = \max\{\Delta_d(\epsilon, E)\}$. That is, $\tilde{\Delta}_f$ is defined as the value of $\Delta_f(E)$ at $E = 4.0$ and $\tilde{\Delta}_d$ as the value of $\Delta_d(\epsilon, E)$ at $\epsilon = 0.0$ and $E \approx 0.6$ (see Fig.3). We give the behaviors of valence PES as $\omega$ varied for $|\Delta_d/\Delta_f| = 2.0$ and $|\Delta_d/\Delta_f| = 6.0$, respectively.
In tensility (arb. unit), experiments, using He resonance lines, to subtract $|\tilde{\Delta}f|$ to approximately a 4 decay. We used to separate the 4d electrons because $\Delta$ is the total emission spectra involving the interference (of 4d and 5d) as a dominant contribution is from 5d band emission because $\Delta$ at $\omega = 0$ au, most of the spectra in Ce arises from the 4f electrons. Gunnarsson and Schönhammer have obtained the total emission spectra involving the interference (of 4f and 5d) based on the sudden approximation, but could not have discussed these behaviors with respect to $\omega$. In the experiments, on the other hand, the increasing 4f and decreasing band features with varying $\omega$ has been used to separate the 4f structure. That is, in the experiments, using He resonance lines, to subtract $\omega = 0.78$ (21.2 eV) result from $\omega = 1.5$ (40.8 eV) result leads to approximately a 4f-emission for a moderate value of $|\tilde{\Delta}d/\tilde{\Delta}f|$ (i.e., say for $|\tilde{\Delta}d/\tilde{\Delta}f| \sim 2$).

In Figs. 5 and 6, we see that at $\omega = 0.5$ au, the dominant contributions are from 5d-band emission because $\tilde{\Delta}f(E)$ increases slowly compared to $\tilde{\Delta}d(\epsilon, E)$, however at $\omega = 4.0$ au, most of the spectra in Ce arises from the 4f electrons because $\Delta_d(\epsilon, E)$ rapidly falls off over $E \sim 0.6$ au. Gunnarsson and Schönhammer have obtained the total emission spectra involving the interference (of 4f and 5d) based on the sudden approximation, but could not have discussed these behaviors with respect to $\omega$. In the experiments, on the other hand, the increasing 4f and decreasing band features with varying $\omega$ has been used to separate the 4f structure. That is, in the experiments, using He resonance lines, to subtract $\omega = 0.78$ (21.2 eV) result from $\omega = 1.5$ (40.8 eV) result leads to approximately a 4f-emission for a moderate value of $|\tilde{\Delta}d/\tilde{\Delta}f|$ (i.e., say for $|\tilde{\Delta}d/\tilde{\Delta}f| \sim 2$).

Below, in Fig. 5, we can see the behaviors of interference as $\omega$ varies. As $\omega$ increases, the interference become stronger at first and then weaker again. And about $\omega = 1.0$ or 2.0 au, we see the strong interference, where the spectra cannot be understood from two separate emission spectra. Particularly in the case of strong destructive interference, although the 4f-emission always comprises two peaks (see the inset of upper panel in Fig. 6), the peak near the Fermi level may be smeared until $\omega$ becomes a bit larger.

FIG. 5. The valence PES with respect to photon energies are provided. The relative strength of two channels is taken as $|\tilde{\Delta}d/\tilde{\Delta}f| = 2.0$. Here the solid line is the total spectra corresponding to constructive or destructive interference. The dashed line represents $4f$-emission, the dotted line $5d$-emission, and the dot-dashed line the interference contribution.

FIG. 6. The valence PES with respect to photon energies. The relative strength of two channels is taken as $|\tilde{\Delta}d/\tilde{\Delta}f| = 6.0$. Notations are same as in Fig. 5.

FIG. 7. The contribution of interferences are given with respect to the photon energies. In the intermediate energies, the interferences are very strong.

V. LOW ENERGY VALENCE PHOTOEMISSION: EFFECTS OF PHOTOELECTRON SCATTERING

In the low photon energy region, we should consider the effects of photoelectron scattering potential induced by the hole left by the electron emission as well as the dipole matrix behavior. The band emission can also raise the shake-up effects like plasmon satellites due to the fluctuation potential. Nevertheless, in the present model, within $1/N_f$ expansion, the relevant bases of Eqs. (5)–(10) in the limit of $N_f \to \infty$ do not allow any conduction electron-hole excitation. Any shake-up behaviors from dielectric responses by band emissions then cannot be seen in the taken limit, but in the next higher order of $1/N_f$. For a hole in a localized $f$-level, however, a small number of electrons may undergo measurable shifts in response to the potential induced by a hole. For the photoelectron scattering potential, we should go back to Eq. (1) and see the interaction of a $f$-level impurity electron. In this section, we’ll confine our discussion only to the $f$-level valence photoemission, i.e., here we do not consider the interference with band contributions. In $\mathcal{H} (= \mathcal{H}_0 + \Delta)$, it needs noting that the $f$-electron correlation is actually a quantity renormalized by the conduction electrons, that is,

$$U_{ff}n_ff + U_{fd}n_f \sum_{n} \int d\epsilon \psi^\dagger_{\epsilon f} \psi^{\nu}_{\epsilon f} = (U_{ff} - U_{fd}) n_fn_f = U_{ff} n_f,$$

where we have used $n _f + \sum_{\nu} \int d\epsilon \psi^\dagger_{\epsilon f} \psi^{\nu}_{\epsilon f}$ is a conserved quantity. In the similar way, we can compose the scattering potential $V_{SC}$ which must be added to $\mathcal{H}_0$

$$V_{SC} = V_{4f}(r)n_f + V_{5d}(r) \sum_{\nu} \int d\epsilon \psi^\dagger_{\epsilon f} \psi^{\nu}_{\epsilon f} - V_{4f}(r),$$

where it should be noted that the initial neutral (ground) state is $4f^1$. Then we have
We know $V_{sd}(r)$ is much broader and weaker than $V_{4f}(r)$ and better to be neglected. So we take $V_{SC}$ as

$$V_{SC} = (V_{4f}(r) - V_{5d}(r))n_f - V_{4f}(r) = (V_{4f}(r) - V_{5d}(r))(n_f - 1) - V_{5d}(r).$$

(24)

If we assume the $f$-level charge density $\rho_f(r)$ and $f$-level is quite localized like the core level. Thus $V(r)$ should be redefined by $\frac{1}{\varepsilon}V(r)$, where $\varepsilon$ is a dielectric constant chosen to make sure of Eq. (25), being due to screening by the surrounding, so $\varepsilon$ is $V(0)/U \approx 5.24$. The behavior of $V(r)$ is given in Fig. 8(a).

Then we express the scattering potential in terms of the photoelectron basis function,

$$V_{SC} = \sum_{\nu} \int dE dE' V(E, E') \psi_{E\nu}^\dagger \psi_{E'\nu} \left[ \sum_{\nu'} \psi_{E\nu'}^\dagger \psi_{E'\nu} - 1 \right],$$

(27)

where the potential matrix element $V(E, E')$ are

$$V(E, E') = \int d\mathbf{r} \varphi_{E\nu}(r) V(r) \varphi_{E'\nu}(r).$$

(28)

As in calculating the dipole matrix, the photoelectron basis function $\varphi_{E\nu}(r)$ must be obtained by solving the Schrödinger equation under the atomic potential. But here we use simple spherical Bessel function of $l = 4$ as in the last section. We hopefully expect the essential feature will not be spoiled by neglecting the phase shift $\delta(k)$. So the desirable $\varphi_{E\nu}(r)$ is

$$\varphi_{E\nu}(r) = \frac{\sqrt{2}}{\sqrt{\pi}} (2E)^{1/4} j_4(\sqrt{2Er}) Y_{4m}(\hat{r}),$$

(29)

and the matrix element $V(E, E')$ is

$$V(E, E') = \frac{2}{\pi} (4E')^{1/4} \int d\mathbf{r} r^2 j_4(\sqrt{2Er}) V(r) j_4(\sqrt{2E'r}),$$

(30)

whose explicit behaviors are shown in Fig. 8(b).

As $V_{SC}$ added, the total Hamiltonian $\mathcal{H}$ becomes $\mathcal{H}_0 + \Delta + V_{SC}$. Under $\mathcal{H}$, the valence PES via $f$-channel can be calculated. The comparison of the results with $V_{SC}$ to those without $V_{SC}$ (still including the dipole elements) is provided in Fig. 9. The effects of scattering potential are quite small as shown in Fig. 9, which must be due to a weak scattering potential in a typical Ce compounds. Nevertheless, it’s very meaningful to pursue a general consensus in the valence PES about the photoelectron scattering effects. In order to be more instructive, we also investigate the resulting behaviors for a slightly different potential whose range is a bit larger by 50% (see Fig. 9).
In both Figs. 9 and 10, it’s notable that there are no appreciable changes in the peak near the Fermi level, while an increase in the ionization peak. This will be under-

FIG. 10. Notations are same as in Fig. 1. Here the scattering potential range has been made a bit larger than in a Ce case, \( r_{mt} = 5.24 \) au.

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VI. ADIABATIC-SUDDEN TRANSITION FOR 2-ELECTRON AND \( N_f = 2 \)

The AIM can be reduced into the two-level model, i.e. the whole continuum band is replaced by one level. The Hamiltonian \( \mathcal{H}_0 \) we should now consider is

\[
\mathcal{H}_0 = \epsilon_d \sum_{\sigma} \psi_{d\sigma}^+ \psi_{d\sigma} + \epsilon_f \sum_{\sigma} \psi_{f\sigma}^+ \psi_{f\sigma} \\
+ V \sum_{\sigma} (\psi_{f\sigma}^+ \psi_{d\sigma} + \psi_{d\sigma}^+ \psi_{f\sigma}) + U n_{f\uparrow} n_{f\downarrow},
\]

(31)

where \( n_{f\sigma} = \psi_{f\sigma}^+ \psi_{f\sigma} \). Then the analogy of the present problem with the core level PES for the shake down case (having "level crossing" as the hole is created) is more evident. The change of relevant electronic levels is given schematically before and after the photoemission in the following Fig. 11.

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\[
\mathcal{H}_0 = \epsilon_d \sum_{\sigma} \psi_{d\sigma}^+ \psi_{d\sigma} + \epsilon_f \sum_{\sigma} \psi_{f\sigma}^+ \psi_{f\sigma} \\
+ V \sum_{\sigma} (\psi_{f\sigma}^+ \psi_{d\sigma} + \psi_{d\sigma}^+ \psi_{f\sigma}) + U n_{f\uparrow} n_{f\downarrow},
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where \( n_{f\sigma} = \psi_{f\sigma}^+ \psi_{f\sigma} \). Then the analogy of the present problem with the core level PES for the shake down case (having "level crossing" as the hole is created) is more evident. The change of relevant electronic levels is given schematically before and after the photoemission in the following Fig. 11.

We can introduce three states \( |f^0\rangle, |f^1\rangle, \) and \( |f^2\rangle \) as follows,

\[
|f^0\rangle = \psi_{d\uparrow}^+ \psi_{d\downarrow} |0\rangle,
\]

\[
|f^1\rangle = \frac{1}{\sqrt{2}} (\psi_{d\uparrow}^+ \psi_{f\downarrow} |0\rangle - \psi_{d\downarrow}^+ \psi_{f\uparrow} |0\rangle),
\]

\[
|f^2\rangle = \psi_{f\uparrow}^+ \psi_{f\downarrow} |0\rangle,
\]

then we can express \( \mathcal{H}_0 \) in these bases,

\[
\mathcal{H}_0 = \begin{pmatrix}
0 & \hat{V} \\
\hat{V} & \Delta \epsilon
\end{pmatrix} + 2\epsilon_d, \quad (32)
\]

where \( \Delta \epsilon = \epsilon_f - \epsilon_d \). For simplicity, we will put \( 2\Delta \epsilon + U = 0 \). The ground state corresponding to the initial state of photoemission, \( |\Psi_0\rangle \) is

\[
|\Psi_0\rangle = \frac{\hat{V}}{\sqrt{\Delta_0^2 + 2V^2}} \left[ |f^0\rangle + \frac{\Delta_0}{V} |f^1\rangle + |f^2\rangle \right], \quad (33)
\]

where \( \Delta_0 = \frac{1}{2} \Delta \epsilon - \frac{1}{2} \sqrt{\Delta_\epsilon^2 + 8V^2} \) and its energy \( E_0 \) is

\[
E_0 = \Delta_0 + 2\epsilon_d. \quad (34)
\]
The final states of the target are given by the following another set of bases,

\[
|\vec{f}^0; \sigma\rangle = \psi_{d\sigma}^\dagger |0\rangle,
\]
\[
|\vec{f}^1; \sigma\rangle = \psi_{f\sigma}^\dagger |0\rangle,
\]
then the Hamiltonian \( \hat{H}_0 \) with one \( f \)-electron emitted is

\[
\hat{H}_0 = \left( \begin{array}{c}
0 \\
\hat{V}/\sqrt{2} \\
\Delta \epsilon
\end{array} \right) + \epsilon_d. \tag{35}
\]

Note \( \psi_{f\sigma}|f^0\rangle = 0 \), \( \psi_{f\sigma}|f^1\rangle = \frac{1}{\sqrt{2}} \sigma|\vec{f}^0; -\sigma\rangle \), and \( \psi_{f\sigma}|f^2\rangle = \sigma|\vec{f}^1; -\sigma\rangle \) and \( \sigma \) is \( \pm 1 \). Here \( \sigma \) is actually a redundant parameter. The possible final target states will be given by the eigenstates of \( \hat{H}_0 \) in Eq. (35),

\[
|\Psi_1; \sigma\rangle = \cos \varphi|\vec{f}^0; \sigma\rangle - \sin \varphi|\vec{f}^1; \sigma\rangle,
\]
\[
|\Psi_2; \sigma\rangle = \sin \varphi|\vec{f}^0; \sigma\rangle + \cos \varphi|\vec{f}^1; \sigma\rangle,
\]
where \( E_2 = \frac{1}{2} \Delta \epsilon + \frac{1}{2} \sqrt{\Delta \epsilon^2 + 2 \epsilon_d^2} \) and \( \Delta \epsilon = \sqrt{\Delta \epsilon^2 + 2 \epsilon_d^2} \), and the parameter \( \varphi \) (\( \frac{\pi}{4} < \varphi < \frac{\pi}{2} \)) is determined by

\[
\tan \varphi = \frac{1}{\sqrt{2}}(w^2 + 2 - w), \quad w = \frac{\Delta \epsilon}{\sqrt{V}}. \tag{38}
\]

Also noticeable is

\[
\psi_{f\sigma}|\Psi_0\rangle = \frac{1}{\sqrt{2}} \left[ -\sin \theta|\vec{f}^0; -\sigma\rangle + \cos \theta|\vec{f}^1; -\sigma\rangle \right], \tag{39}
\]
where the parametric angle \( \theta \) (\( \frac{\pi}{4} < \theta < \frac{\pi}{2} \)) is

\[
\cot \theta = \frac{1}{2\sqrt{2}}(w^2 + 8 + w). \tag{40}
\]

Now we consider the optical activation Hamiltonian \( \Delta \),

\[
\Delta = \sum_{k\sigma} M_k \psi_{k\sigma}^\dagger \psi_{f\sigma}, \quad \text{(or } \Delta = \int dE \Delta(E) \psi_{E\sigma}^\dagger \psi_{f\sigma}) \tag{41}.
\]

Within the first order perturbation theory, the photoemission matrix element \( M(i, k\sigma) \) (\( i = 1, 2 \)) will be

\[
M(i, k\sigma)
= \langle \Psi_i; -\sigma| \psi_{k\sigma} \left[ 1 + \frac{1}{E - \hat{H}_0 - T + i\eta} \right] \Delta|\Psi_0\rangle
= m_i M_k + \sum_j c_{ij} m_j \sum_{k'} \frac{V_{kk'} M_{k'}}{\omega + E_0 - E_j - \frac{1}{2} k'^2 + i\eta}, \tag{42}
\]
where the scattering potential \( V_{SC} \) is taken as

\[
V_{SC} = V(r)(n_f - 1), \quad V_{kk'} = \int d\varphi \varphi_{k\sigma}^*(r) V(r) \varphi_{k'\sigma}(r)
\]
and thus

\[
m_1 = \langle \Psi_i; -\sigma| \psi_{f\sigma}|\Psi_0\rangle, \quad c_{ij} = \langle \Psi_i; -\sigma|n_f|\Psi_j; -\sigma\rangle - \delta_{ij}.
\]

That is, the coefficients are

\[
c_{11} = -\cos^2 \varphi, \quad c_{22} = -\sin^2 \varphi, \quad c_{12} = c_{21} = -\sin \varphi \cos \varphi.
\]

If we consider a ratio between the main and the satellite absorption intensity divided by a noninteracting case \( r(\omega)/r_0(\omega) \), \( r(\omega)/r_0(\omega) \) is

\[
\left. \frac{r(\omega)}{r_0(\omega)} \right| = \left( \frac{1 + \frac{1}{2} \sin^2 \theta}{1 + \frac{1}{2} \cos^2 \theta} \right)^2 \tag{44}
\]

\[
\left. \left( 1 + \frac{1}{2} \cos^2 \theta \right) \right| = \sin \left( \frac{\theta}{2} \right) V_{E\sigma} F_{k2} \left( \frac{\omega}{E} \right) - \sin \left( \frac{\theta}{2} \right) V_{E\sigma} F_{k1} \left( \frac{\omega}{E} \right) V_{E\sigma} F_{k2} \left( \frac{\omega}{E} \right) - \sin \left( \frac{\theta}{2} \right) V_{E\sigma} F_{k1} \left( \frac{\omega}{E} \right),
\]

where \( k_2 = \sqrt{2(\omega + E_k - E_2)} \), \( \omega = E_2 - E_0 \) (threshold energy for the satellite), and we have extended the model matrix elements \( M_k \) and \( V_{kk'} \) used in the previous core level case,

\[
\sum_{k'} \frac{V_{kk'} M_{k'}}{\epsilon - \epsilon_{k'} + i\eta} = -\bar{V} E M_k F_k(\epsilon/\bar{E}), \tag{45}
\]

\[
F_k(\epsilon) = \frac{1}{\pi} \int_0^\infty \frac{x^{10} dx}{[1 + x^5]^2 [1 + (\bar{R}k - x)^2] [x^2 - \epsilon - i\eta]}, \tag{46}
\]

\[
M_k = \frac{(\bar{R}k)^5}{1 + (\bar{R}k)^5}, \tag{47}
\]

\[
V_{kk'} = \frac{\bar{R} \bar{R}}{\bar{R} [1 + (\bar{R}k)^5][1 + (\bar{R}k')^5][1 + \bar{R}^2(k - k')^2]}, \tag{48}
\]

where \( \bar{R} \) is the characteristic length scale of the system directly related to the potential range and \( \bar{E} = 1/2 \bar{R}^2 \). Here it is found that from Eq. (44), \( r(\omega)/r_0(\omega) \) can be written essentially in the same mathematics as in the core level case. In the following Fig. we give the behaviors of \( F(\epsilon) \).
Similarly to the core case, we always have an overshoot behavior in \( r(\omega)/r_0(\omega) \) in the low energy limit, when \( \delta E = 0 \),

\[
\frac{r(\omega_{th})}{r_0(\omega_{th})} = \left[ \frac{1 - F(0) \frac{\tilde{V}}{\tilde{E}} \sin \varphi \sin \theta}{1 + F(0) \frac{\tilde{V}}{\tilde{E}} \cos \varphi \cos \theta} \right]^2 > 1, \tag{49}
\]

where \( F(0) = 0.052286 \) and \( \frac{\pi}{4} < \varphi < \frac{3\pi}{4}, \frac{\pi}{2} < \theta < \frac{3\pi}{2} \), and \( \frac{\pi}{2} < \varphi + \theta < \pi \) should be noted. In Fig. 13, we show \( r(\omega)/r_0(\omega) \) as a function of \( \tilde{\omega}/\tilde{E} \) for a few values of \( \tilde{V}/\tilde{E} \) (\( \tilde{\omega} \equiv \omega - \omega_{th} \)).

\[ \begin{align*}
\tilde{V} = 0.2 \\
\tilde{E} = 0.2 \left( \frac{\tilde{V}}{\tilde{E}} - 1.0 \right) \\
\tilde{E} = 0.3 \left( \frac{\tilde{V}}{\tilde{E}} - 0.7 \right) \\
\tilde{E} = 0.4 \left( \frac{\tilde{V}}{\tilde{E}} - 0.5 \right) \\
\tilde{E} = 0.5 \left( \frac{\tilde{V}}{\tilde{E}} - 0.4 \right)
\end{align*} \]

FIG. 13. The ratio \( r(\omega)/r_0(\omega) \) as a function of \( \tilde{\omega}/\tilde{E} \) for several values of \( \tilde{V}/\tilde{E} \). \( \Delta \epsilon/\tilde{V} = -2.0 \) is taken.

Fig. 13 shows as \( \omega \) increases the ratio also increases and reaches a maximum. From the arguments in our previous work, we see roughly \( \tilde{R} \sim R_0/3 \) and \( \tilde{V} \sim 3V(0)/2 \) and for Ce, \( \tilde{R} \sim 1 \) and \( \tilde{V} \sim 0.3 \), which leads to \( \tilde{V}/\tilde{E} \sim 0.6 \). Most notable is that the curves have the universal feature independent of \( \tilde{V}/\tilde{E} \), i.e. the overshoots disappear at about \( \tilde{\omega}/\tilde{E} \sim 10 \) in all relevant parameter region. This means the adiabatic-sudden transition depends only on \( \tilde{E} \), that is, \( \tilde{R} \), even if the amplitude of overshoot is from \( \tilde{V}/\tilde{E} \). Beyond the first order perturbation, the overshoot range will be reduced due to the multiple scattering, but the universal behavior not changed. This conclusion is exactly identical to that in the core level case and implies the same criteria can be applied also to the valence PES case.

VII. CONCLUSION

We have studied the valence photoemission spectra in the Anderson impurity model aiming at Ce compounds. Using the time-dependent formulation and \( 1/N_f \) expansion, we can treat the problem exactly up to \( O(1/N_f)^0 \). For Ce compounds, \( N_f = \infty \) can be a good approximation for \( N_f = 14 \). Within the formalism, to evaluate the photoemission spectra is corresponding to solving the time-dependent Schrödinger equation.

To investigate the low energy photoemission spectra, we should consider the dipole matrix and photoelectron scattering matrix additionally compared to the sudden approximation valid in high energy limit. In view of experiment, the valence PES always consist of \( f \)-emission and band emission. So we considered both dipole matrix elements having explicit \( E \)-dependencies and obtained the total spectra as well as two separate spectra with respect to the photon energies. The relative strength and sign of two dipole elements are crucial in the total spectra. Due to differences in the energy scales of \( 4f \) and \( 5d \) dipole elements, the general trends are that, in a very low energy (\( \omega \lesssim 1.0 \) au), the \( 5d \) emission is dominant, while the \( 4f \) emission increases and dominates over the \( 5d \) emission in a high energy (\( \omega \gtrsim 2.0 \) au). It is also found that the interference effects of \( f \)-emission and band emission (from \( d \)) are highly nontrivial especially in the intermediate energy region. In the intermediate region (\( \omega \sim 1.0 \) or 2.0 au depending on the relative strength), due to a strong peak of the interferences near the Fermi level, the Kondo resonance peak of \( 4f \) emission may be smeared in the case of destructive interference. The constructive or destructive interference will be determined by the relative sign.

We also studied the effects of scattering potential for the \( f \)-electron emission. Scattering effects on the band emission is neglected in the infinite \( N_f \) limit. The potential matrix also includes the kinetic energy dependencies. It’s a general result that, in the case where the photoelectron couples to the localized excitation, the arrival at the sudden transition is much faster compared to the extended excitation. Effects of scattering potential gives the similar spectral changes to the core level PES in shake down case if we assign the Kondo resonance and ionization peak to the main and satellite peak, respectively. Behaviors of two-peak ratio is reminiscent of the previous analysis of core level PES. Therefore, this can be a motivation to do a further analysis for the adiabatic-sudden behavior. We can then cast a question, "The criteria found in core level case can be also valid in the valence case?" To explore it, first we simplify the model into just a two-level one, where the whole conduction band is replaced by one level. Then it is found the intensity ratio
of two peaks can be written actually in the same way as in the core case. Through the same analysis, we can find that also in the valence PES, the sudden transition happens on the energy scale of $E = 1/(2 \tilde{R}^2)$, where $\tilde{R}$ is a typical length scale of the scattering potential.

Finally, we would like to make it clear the limit or shortcomings of our present model. Within the model, we cannot yet arrive at the realistic photoemission in a true solid. The AIM includes the continuum band describing a crystal, which has a surface. Then the position of a surface with respect to the created hole will enter as an important parameter. In a true solid, we never reach a vanishing extrinsic scattering because the corresponding cross section goes to zero, while the photoelectron is emitted from an infinite depth. And to correctly predict the amount of photocurrent, we also should use the damped wavefunctions, not undamped partial wave. These additional extrinsic effects may be as important as the hole-induced scattering potential treated here. Therefore, it should be understood that the scope of this paper is to explore the effects of hole-induced scattering potential in the valence PES in AIM describing the Ce compounds apart from additional ingredients.

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