Variational ground state for the periodic Anderson model with an indirect hybridization

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As the direct on-site hybridization is forbidden by inversion symmetry in most of the mixed-valence compounds, an indirect on-site hybridization mediated by phonons has been introduced into the periodic Anderson model to constitute our model system. Then we try to construct a variational ground state for the model Hamiltonian by the following steps. First, we develop a new procedure to transform the model Hamiltonian by a unitary transformation of the displacement-operator type. Second, a two-phonon coherent state is taken as the trial-state vector for the ground state of the phonon subsystem and the parameters of the two-phonon coherent state, which are regarded as the adjustable parameters of the variational treatment, remain to be determined. Third, a Bogoliubov transformation is introduced to deal with the electron subsystem; the ground state and low-lying excited states are constructed directly. Finally, the parameters of the two-phonon coherent state are adjusted to ensure that the energy functional of our variational ground state is a stable minimum. Numerical calculations have been done and a nonzero energy gap and fluctuating valence have been obtained in various cases. Our results could be used to explain the small energy gap and valence-fluctuation phenomena observed in some Sm-based compounds.

I. INTRODUCTION

The problem of valence fluctuation, which occurs in certain rare-earth metals and compounds, has aroused considerable interest among solid-state physicists.[1-12] Many essential aspects of valence-fluctuation phenomena can be described by the nondegenerate periodic Anderson model (PAM),[1-9] which describes hybridization between a wide d band and a strongly correlated dispersionless f band,

$$\hat{H}_{\rm PAM}=\sum_{\mathbf{k},\sigma}E_{\mathbf{k}}d^{\dagger}_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}+\sum_{l,\sigma}E_f f^{\dagger}_{l\sigma}f_{l\sigma}+\sum_{l}Uf_{l\uparrow}f^{\dagger}_{l\uparrow}f_{l\downarrow}f^{\dagger}_{l\downarrow}+\sum_{\mathbf{k},\sigma}\sum_{l}(V_{\mathbf{k}}d^{\dagger}_{\mathbf{k}\sigma}f_{l\sigma}e^{i\mathbf{k}\cdot l}+V^{*}_{\mathbf{k}}f^{\dagger}_{l\sigma}d_{\mathbf{k}\sigma}e^{-i\mathbf{k}\cdot l}) , \quad (1)$$

where l is a lattice-site vector, $E_{\mathbf{k}}$ is the bare d-band function, E_f is the bare f level, U represents the Coulomb repulsion between f holes, and $V_{\mathbf{k}}$ and $V^{*}_{\mathbf{k}}$ are hybridization functions. It is well known that when the function $V_{\mathbf{k}}$ satisfies some conditions, a hybridization gap is opened in the density of states of the electrons.[4-10] Some authors have explained the nature of the gap in Sm-based compounds, such as SmB_6 and SmS, observed in experiments as such a d-f-hybridization gap.[4-9]

But in this paper, we shall discuss another possible mechanism of inducing a gap in the density of states: a gap might be induced by electron-phonon interaction alone. The influence of electron-phonon interaction in the valence-fluctuation phenomena described by $\hat{H}_{\rm PAM}$ has been discussed by a number of authors,[13-18] and the renormalization of the electron-energy levels and the hybridization function $V_{\mathbf{k}}$ has been obtained.[13,15-17] However, because of the approximations used by them, their results could be questioned. In the following we review briefly their methods and approximations in treating electron-phonon interaction.

It was pointed out that because most of mixed-valence compounds (MVC's), such as SmB_6 and SmS, are of the highest symmetry of the O_h point group, the on-site hybridization between d and f states are forbidden by inversion symmetry.[9,11,12] However, the indirect on-site hybridization mediated by phonons may still be permitted because the participation of phonons in the d-f-hybridization processes may cause the Hamiltonian to remain parity conservative.[13] In Refs. 4 and 13-18, an indirect hybridization of the following form,

$$\hat{H}_{df\text{-ph}}=\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}\sum_{l,\sigma}g(\mathbf{q})e^{-i\mathbf{q}\cdot l}(f^{\dagger}_{l\sigma}d_{l\sigma}+d^{\dagger}_{l\sigma}f_{l\sigma})\times(b^{\dagger}_{\mathbf{q}}+b_{-\mathbf{q}}) , \quad (2)$$

has been added into $\hat{H}_{\rm PAM}$, where $b_{\mathbf{q}}$ and $b^{\dagger}_{\mathbf{q}}$ are the phonon annihilation and creation operators, respectively. Khomskii[4] used the mean-field approximation

$$\langle b^{\dagger}_{l}+b_{l}\rangle=\text{const}\neq 0 \quad (3)$$

in $\hat{H}_{df\text{-ph}}$, that is, assumed that strains near every site are the same nonzero quantity. Alascio *et al.*[14] proposed that a local lattice distortion breaking the symmetry of the electron states may produce a direct on-site hybridization. This idea is identical in practice with Khomskii's, as we can obtain a direct on-site hybridization after substituting the mean-field approximation (3) into (2).

Brouers and de Menezes[15] introduced a unitary trans-

formation to cancel the first-order term of $g(\mathbf{q})$ from the total Hamiltonian and ignored terms of $g(\mathbf{q})$ of higher than second order after the unitary transformation was performed. Giner and Brouers[16] utilized the transformed Hamiltonian of Brouers and de Menezes[15] to reconsider the results of Entel *et al.*,[17] whose conclusions have led to some debate. They obtained within the Hartree-Fock approximation a renormalized d-f hybridization and then investigated the effects of phonons on valence transitions in MVC's. Although some interesting results have been obtained by Brouers and de Menezes and by Giner and Brouers, the reliability of their conclusions might be suspect, because in their treatment the higher-order terms of $g(\mathbf{q})$ were all omitted. It is worthwhile to discuss the effects of the higher-order terms of $g(\mathbf{q})$ on the valence-fluctuation phenomena.

Karnaukhov[18] introduced a different unitary transformation than Brouers and de Menezes[15] to remove the first-order term of $g(\mathbf{q})$, and derived a Kondo-lattice Hamiltonian. But in Karnaukhov's transformation, terms of $g(\mathbf{q})$ higher than second order were also omitted, so his procedure could not be used for the valence-fluctuation case.

Recently, Nunez-Regueiro and Avignon[13] have again studied the renormalization of the hybridization by the d-f Coulomb repulsion, by using the electron-phonon interaction within the same approximation as Giner and Brouers.[16] They have pointed out that the local $d \leftrightarrow f$ electron-phonon processes may exist even in the absence of direct on-site hybridization, and such processes may be the origin of the d-f hybridization in some mixed-valence systems.

These remarks and insufficiencies have led us to reconsider carefully the effects of the phonon-mediated d-f hybridization on the valence-fluctuation phenomena within the framework of the PAM. In this paper, a new unitary-transformation procedure will be developed and our model Hamiltonian $\hat{H}$ (which will be detailed in Sec. II) will be transformed into a unitary-transformed form $\hat{\tilde{H}}$ without any higher-order terms being omitted. Then, we will construct a variational ground state for $\hat{\tilde{H}}$ and discuss its physical properties, especially the energy gap and the fluctuating valence. Finally, in Sec. V, the approximations involved in our variational treatment will be discussed and a comparison between our treatment and those of Refs. 13–18 will be made.

II. MODEL HAMILTONIAN AND UNITARY TRANSFORMATIONS

In this paper, the model Hamiltonian we consider is as follows,

$$\hat{H} = -T_0 \sum_{\langle l,l' \rangle} \sum_{\sigma} d^{\dagger}_{l\sigma} d_{l'\sigma} + \sum_{l,\sigma} E_f f^{\dagger}_{l\sigma} f_{l\sigma} + \sum_{l} U f_{l\uparrow} f^{\dagger}_{l\uparrow} f_{l\downarrow} f^{\dagger}_{l\downarrow} + \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \sum_{l,\sigma} g(\mathbf{q}) e^{-i\mathbf{q}\cdot l} (f^{\dagger}_{l\sigma} d_{l\sigma} + d^{\dagger}_{l\sigma} f_{l\sigma})(b^{\dagger}_{\mathbf{q}} + b_{-\mathbf{q}}) + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} b^{\dagger}_{\mathbf{q}} b_{\mathbf{q}} , \tag{4}$$

where the direct d-f hybridization has not been included because we are interested in the phonon-mediated indirect d-f hybridization alone. The last term in (4) is the harmonic Hamiltonian of phonons. We have taken the tight-binding approximation for the d-electron band function $E_{\mathbf{k}}$, and $\sum_{\langle l,l' \rangle}$ represents a summation over nearest-neighbor ion pairs. Without loss of generality, we have chosen the center of the d band as the zero point of the energy scale.

In $\hat{H}$, we have not included the f-electron–phonon coupling,

$$\hat{H}_{f\text{-ph}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \sum_{l,\sigma} g_f(\mathbf{q}) e^{-i\mathbf{q}\cdot l} f^{\dagger}_{l\sigma} f_{l\sigma} (b^{\dagger}_{\mathbf{q}} + b_{-\mathbf{q}}) , \tag{5}$$

and the d-electron–phonon coupling,

$$\hat{H}_{d\text{-ph}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \sum_{l,\sigma} g_d(\mathbf{q}) e^{-i\mathbf{q}\cdot l} d^{\dagger}_{l\sigma} d_{l\sigma} (b^{\dagger}_{\mathbf{q}} + b_{-\mathbf{q}}) , \tag{6}$$

while the former was included in Refs. 4, 13, and 15–17, and the latter was included in Ref. 15. The reason for this exclusion is as follows. If the interaction functions $g(\mathbf{q})$ in (2), $g_f(\mathbf{q})$ in (5), and $g_d(\mathbf{q})$ in (6) are taken to be $\mathbf{q}$ independent, as is the case in Refs. 4, 13, and 15–17, the interaction Hamiltonian $\hat{H}_{df\text{-ph}}$, $\hat{H}_{f\text{-ph}}$, and $\hat{H}_{d\text{-ph}}$ would take the following forms,

$$\hat{H}_{df\text{-ph}} = \sum_{l,\sigma} g (f^{\dagger}_{l\sigma} d_{l\sigma} + d^{\dagger}_{l\sigma} f_{l\sigma})(b^{\dagger}_{l} + b_{l}) , \tag{2'}$$

$$\hat{H}_{f\text{-ph}} = \sum_{l,\sigma} g_f f^{\dagger}_{l\sigma} f_{l\sigma} (b^{\dagger}_{l} + b_{l}) , \tag{5'}$$

and

$$\hat{H}_{d\text{-ph}} = \sum_{l,\sigma} g_d d^{\dagger}_{l\sigma} d_{l\sigma} (b^{\dagger}_{l} + b_{l}) . \tag{6'}$$

Because the electron number operators $f^{\dagger}_{l\sigma} f_{l\sigma}$ and $d^{\dagger}_{l\sigma} d_{l\sigma}$ are parity conservative, being different from the hybridization operator $f^{\dagger}_{l\sigma} d_{l\sigma} + d^{\dagger}_{l\sigma} f_{l\sigma}$, the local-phonon operators in $\hat{H}_{df\text{-ph}}$ and those in $\hat{H}_{f\text{-ph}}$ and $\hat{H}_{d\text{-ph}}$ must belong to different branches, so one can deal with the electron-phonon interaction in (2′) and that in (5′) and (6′) separately. In this paper only $\hat{H}_{df\text{-ph}}$ is considered as we are interested in the energy gap induced by the phonon-mediated d-f hybridization. The method presented in this paper can also be used to deal with $\hat{H}_{f\text{-ph}}$ and $\hat{H}_{d\text{-ph}}$ without difficulty.

As we have said above, the goal of this paper is to construct a variational ground state $|\Phi_g\rangle$ of the model Hamiltonian $\hat{H}$ and to obtain the energy spectrum and

the density of states of electrons in this variational ground state. In order to arrive at this goal, in this section we first introduce a unitary transformation. In general, if we make a unitary transformation $|\Phi\rangle = U^{-1}|\bar{\Psi}\rangle$ in the Schrödinger equation $\hat{H}|\Phi\rangle = E|\Phi\rangle$, it follows that $U\hat{H}U^{-1}|\bar{\Psi}\rangle = E|\bar{\Psi}\rangle$. Thus, the Hamiltonian is transformed as $\hat{H} \rightarrow \hat{\bar{H}} = U\hat{H}U^{-1}$. The $\hat{\bar{H}}$ describes the same physical system as $\hat{H}$ does.

Our unitary transformation is

$$\hat{\bar{H}} = e^{\hat{R}}\hat{H}e^{-\hat{R}} , \tag{7}$$

$$\hat{R} = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \sum_{l,\sigma} \frac{g(\mathbf{q})}{\hbar\omega_{\mathbf{q}}} e^{-i\mathbf{q}\cdot l}(f^{\dagger}_{l\sigma}d_{l\sigma} + d^{\dagger}_{l\sigma}f_{l\sigma})(b^{\dagger}_{\mathbf{q}} - b_{-\mathbf{q}}) , \tag{8}$$

where $g(-\mathbf{q}) = g^{*}(\mathbf{q})$ because of the unitarity of the operator $e^{\hat{R}}$.

We develop a new procedure for the transformation (7), which is different from that used in Refs. 15 and 18. The practical processes of this transformation are quite cumbersome and therefore are given in Appendix A, where the terms in $\hat{H}$ are transformed one after another. The transformed Hamiltonian $\hat{\bar{H}}$ reads as follows:

$$\begin{aligned}
\hat{\bar{H}} = {} & \tfrac{1}{2}E_f \sum_{l,\sigma}(d^{\dagger}_{l\sigma}d_{l\sigma} + f^{\dagger}_{l\sigma}f_{l\sigma}) - \tfrac{1}{2}E_f \sum_{l,\sigma}(d^{\dagger}_{l\sigma}d_{l\sigma} - f^{\dagger}_{l\sigma}f_{l\sigma})\cosh\hat{B}(l+l) \\
& - \tfrac{1}{2}E_f \sum_{l,\sigma}(d^{\dagger}_{l\sigma}f_{l\sigma} - f^{\dagger}_{l\sigma}d_{l\sigma})\sinh\hat{B}(l+l) + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} b^{\dagger}_{\mathbf{q}} b_{\mathbf{q}} \\
& - \tfrac{1}{2}T_0 \sum_{\langle l,l'\rangle} \sum_{\sigma} \{(d^{\dagger}_{l\sigma}f_{l'\sigma} - f^{\dagger}_{l'\sigma}d_{l\sigma})[\sinh\hat{B}(l'-l) + \sinh\hat{B}(l'+l)] \\
& \qquad + d^{\dagger}_{l\sigma}d_{l'\sigma}[\cosh\hat{B}(l-l) + \cosh\hat{B}(l'+l)] + f^{\dagger}_{l\sigma}f_{l'\sigma}[\cosh\hat{B}(l'-l) - \cosh\hat{B}(l'+l)]\} \\
& - \frac{1}{N} \sum_{\mathbf{q}} \sum_{\mathbf{m},\sigma} \sum_{\mathbf{n},\sigma'} [\,|g(\mathbf{q})|^2/\hbar\omega_{\mathbf{q}}] e^{i\mathbf{q}\cdot(\mathbf{m}-\mathbf{n})}(f^{\dagger}_{\mathbf{m}\sigma}d_{\mathbf{m}\sigma} + d^{\dagger}_{\mathbf{m}\sigma}f_{\mathbf{m}\sigma})(f^{\dagger}_{\mathbf{n}\sigma'}d_{\mathbf{n}\sigma'} + d^{\dagger}_{\mathbf{n}\sigma'}f_{\mathbf{n}\sigma'}) \\
& + \frac{U}{4} \sum_{l} \{d_{l\uparrow}d^{\dagger}_{l\uparrow}[1 - \cosh\hat{B}(l+l)] + f_{l\uparrow}f^{\dagger}_{l\uparrow}[1 + \cosh\hat{B}(l+l)] + (d^{\dagger}_{l\uparrow}f_{l\uparrow} - f^{\dagger}_{l\uparrow}d_{l\uparrow})\sinh\hat{B}(l+l)\} \\
& \qquad \times \{d_{l\downarrow}d^{\dagger}_{l\downarrow}[1 - \cosh\hat{B}(l+l)] + f_{l\downarrow}f^{\dagger}_{l\downarrow}[1 + \cosh\hat{B}(l+l)] + (d^{\dagger}_{l\downarrow}f_{l\downarrow} - f^{\dagger}_{l\downarrow}d_{l\downarrow})\sinh\hat{B}(l+l)\} ,
\end{aligned} \tag{9}$$

where

$$\hat{B}(\mathbf{n}\pm\mathbf{m}) = -\frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \frac{g(\mathbf{q})}{\hbar\omega_{\mathbf{q}}}(e^{-i\mathbf{q}\cdot\mathbf{n}} \pm e^{-i\mathbf{q}\cdot\mathbf{m}})(b^{\dagger}_{\mathbf{q}} - b_{-\mathbf{q}}) . \tag{10}$$

We should emphasize again that the difference between our transformation method and that used in Refs. 15 and 18 is embodied by the different manners of treating the higher-order terms of $g(\mathbf{q})$. Our unitary transformation (7) has been performed exactly and no higher-order terms are omitted. The higher-order terms of $g(\mathbf{q})$ in $\hat{\bar{H}}$ are all contained within the hyperbolic functions $\sinh(\hat{B})$ and $\cosh(\hat{B})$.

The variational evaluation of the ground-state energy E_g of $\hat{\bar{H}}$ will follow the general procedure of the variational method. Firstly, we construct a trial state vector $|\bar{\Psi}\rangle$ for the ground state of $\hat{\bar{H}}$, which contains some adjustable parameters. Then these parameters are adjusted so as to minimize the expectation value $\langle\bar{\Psi}|\hat{\bar{H}}|\bar{\Psi}\rangle$. This minimum value, which will be denoted E_g, will be taken as an approximation to the true ground-state energy. Moreover, the corresponding-state vector $|\bar{\Psi}_g\rangle$, which is obtained by making the adjustable parameters in $|\bar{\Psi}\rangle$ equal to the values that minimize the expectation value $\langle\bar{\Psi}|\hat{\bar{H}}|\bar{\Psi}\rangle$, will be taken as an approximation to the true ground-state vector.

We suppose that in the ground state of $\hat{\bar{H}}$ the phonon variables and electron variables could be separated approximately. In other words, we assume that the trial state vector $|\bar{\Psi}\rangle$ for the ground state of $\hat{\bar{H}}$ could be written as a product of two state vectors,

$$|\bar{\Psi}\rangle = |\bar{\Psi}_{\mathrm{ph}}\rangle|\bar{\Psi}_e\rangle , \tag{11}$$

where $|\bar{\Psi}_{\mathrm{ph}}\rangle$ contains only phonon variables and $|\bar{\Psi}_e\rangle$ contains only electron variables. Because of such an approximate separation, we can consider the phonon subsystem and electron subsystem separately. The following part of this section serves for the discussion of $|\bar{\Psi}_{\mathrm{ph}}\rangle$ and that of $|\Psi_e\rangle$ will be presented in Sec. III.

If there is no electron-phonon interaction, that is, if $g(\mathbf{q})$ in $\hat{H}$ is equal to zero, the ground state of the phonon subsystem should be the multiplied zero-phonon eigenstate of the phonon number operators of each mode,

$$|\bar{\Psi}_{\mathrm{ph}}\rangle_0 = \prod_{\mathbf{q}} |n_{\mathbf{q}} = 0\rangle , \tag{12}$$

where the subscript 0 denotes the case in which $g(\mathbf{q}) = 0$ and $|n_{\mathbf{q}} = 0\rangle$ is the zero-phonon eigenstate of mode $\mathbf{q}$. As in reality, $g(\mathbf{q}) \neq 0$, and the zero-phonon state $|\bar{\Psi}_{\mathrm{ph}}\rangle_0$ cannot be the ground state of the phonon subsystem be-

cause we must minimize the total expectation value of $\hat{\bar{H}}$ in the state $|\bar{\Psi}_g\rangle = |\bar{\Psi}_{\rm phg}\rangle |\bar{\Psi}_{eg}\rangle$,

$$E_g = \langle \bar{\Psi}_{eg} | \langle \bar{\Psi}_{\rm phg} | \hat{\bar{H}} | \bar{\Psi}_{\rm phg}\rangle | \bar{\Psi}_{eg}\rangle \ . \tag{13}$$

It is evident that any eigenstate of phonon number operators can not also be the ground state of the phonon subsystem because of the same reason mentioned above. Therefore we should search for other state vectors to meet our aim. As a trial state vector for the ground state of the phonon subsystem, we propose the following form,

$$|\bar{\Psi}_{\rm ph}\rangle = e^{-\hat{S}} \prod_{\mathbf{q}} |n_{\mathbf{q}}=0\rangle \ , \tag{14}$$

where

$$\hat{S} = \sum_{\mathbf{q}} \alpha_{\mathbf{q}} (b_{\mathbf{q}} b_{-\mathbf{q}} - b_{\mathbf{q}}^{\dagger} b_{-\mathbf{q}}^{\dagger}) \tag{15}$$

and $\alpha_{\mathbf{q}}$'s are real numbers because of the unitarity of $e^{\hat{S}}$. The adjustable parameters $\alpha_{\mathbf{q}}$ will be adjusted to minimize the energy functional of our variational ground state. When $\alpha_{\mathbf{q}}=0$ for every $\mathbf{q}$ mode $|\bar{\Psi}_{\rm ph}\rangle$ becomes the zero-phonon state $|\bar{\Psi}_{\rm ph}\rangle_0$. As long as $\alpha_{\mathbf{q}}\neq 0$ for some or all $\mathbf{q}$ modes, our trail state vector $|\bar{\Psi}_{\rm ph}\rangle$ should be a new and special state of the phonon subsystem, other than any eigenstate of phonon number operators. Because the unitary operator $e^{-\hat{S}}$ is similar to that of the two-photon coherent state in quantum optics proposed firstly by Yuen,[19] we call $|\bar{\Psi}_{\rm ph}\rangle$ in Eq. (14) the two-phonon coherent state in which the average values of phonon creation and annihilation operators are zero but the average values of phonon number operators are nonzero.[19] We shall show in Sec. IV that the minimized value of the variational ground-state energy is indeed obtained when the adjustable parameters $\alpha_{\mathbf{q}}$'s are equal to some nonzero value.

According to the variational method we should derive the energy functional E from the following formula,

$$E = \langle \bar{\Psi} | \hat{\bar{H}} | \bar{\Psi}\rangle = \langle \bar{\Psi}_e | \langle \bar{\Psi}_{\rm ph} | \hat{\bar{H}} | \bar{\Psi}_{\rm ph}\rangle | \bar{\Psi}_e\rangle \ . \tag{16}$$

E is a functional of all adjustable parameters. In order to treat the problem clearly we designate $\langle \bar{\Psi}_{\rm ph} | \hat{\bar{H}} | \bar{\Psi}_{\rm ph}\rangle$ as an effective Hamiltonian $\hat{H}_{\rm eff}$ for the electron subsystem,

$$\hat{H}_{\rm eff} = \langle \bar{\Psi}_{\rm ph} | \hat{\bar{H}} | \bar{\Psi}_{\rm ph}\rangle = \left[\prod_{\mathbf{q}} \langle n_{\mathbf{q}}=0| \right] e^{+\hat{S}} \hat{\bar{H}} e^{-\hat{S}} \left[\prod_{\mathbf{q}} |n_{\mathbf{q}}=0\rangle\right] \ , \tag{17}$$

into which Eq. (14) has been substituted. The unitary transformation

$$\hat{\bar{H}} = e^{+\hat{S}} \hat{\bar{H}} e^{-\hat{S}} \tag{18}$$

is performed in Appendix A and the result is

$$\begin{aligned}
\hat{\bar{H}} = {} & \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} (b_{\mathbf{q}}^{\dagger} \cosh 2\alpha_{\mathbf{q}} + b_{-\mathbf{q}} \sinh 2\alpha_{\mathbf{q}})(b_{-\mathbf{q}}^{\dagger} \sinh 2\alpha_{\mathbf{q}} + b_{\mathbf{q}} \cosh 2\alpha_{\mathbf{q}}) \\
& - \tfrac{1}{2} E_f \sum_{l,\sigma} (d_{l\sigma}^{\dagger} d_{l\sigma} - f_{l\sigma}^{\dagger} f_{l\sigma}) \cosh \hat{A}(l+l) - \tfrac{1}{2} E_f \sum_{l,\sigma} (d_{l\sigma}^{\dagger} f_{l\sigma} - f_{l\sigma}^{\dagger} d_{l\sigma}) \sinh \hat{A}(l+l) \\
& + \tfrac{1}{2} E_f \sum_{l,\sigma} (d_{l\sigma}^{\dagger} d_{l\sigma} + f_{l\sigma}^{\dagger} f_{l\sigma}) - \tfrac{1}{2} T_0 \sum_{\langle l,l'\rangle} \sum_{\sigma} \{ (d_{l\sigma}^{\dagger} f_{l'\sigma} - f_{l'\sigma}^{\dagger} d_{l\sigma}) [\sinh \hat{A}(l'-l) + \sinh \hat{A}(l'+l)] \\
& \qquad + d_{l\sigma}^{\dagger} d_{l'\sigma} [\cosh \hat{A}(l'-l) + \cosh \hat{A}(l'+l)] \\
& \qquad + f_{l\sigma}^{\dagger} f_{l'\sigma} [\cosh \hat{A}(l'-l) - \cosh \hat{A}(l'+l)] \} \\
& - \frac{1}{N} \sum_{\mathbf{q}} \sum_{\mathbf{m},\sigma} \sum_{\mathbf{n},\sigma'} [\, |g(\mathbf{q})|^2 / \hbar\omega_{\mathbf{q}}] e^{i\mathbf{q}\cdot(\mathbf{m}-\mathbf{n})} (f_{\mathbf{m}\sigma}^{\dagger} d_{\mathbf{m}\sigma} + d_{\mathbf{m}\sigma}^{\dagger} f_{\mathbf{m}\sigma}) (f_{\mathbf{n}\sigma'}^{\dagger} d_{\mathbf{n}\sigma'} + d_{\mathbf{n}\sigma'}^{\dagger} f_{\mathbf{n}\sigma'}) \\
& + \frac{U}{4} \sum_{l} \{ d_{l\uparrow} d_{l\uparrow}^{\dagger} [1 - \cosh \hat{A}(l+l)] + f_{l\uparrow} f_{l\uparrow}^{\dagger} [1 + \cosh \hat{A}(l+l)] + (d_{l\uparrow}^{\dagger} f_{l\uparrow} - f_{l\uparrow}^{\dagger} d_{l\uparrow}) \sinh \hat{A}(l+l) \} \\
& \times \{ d_{l\downarrow} d_{l\downarrow}^{\dagger} [1 - \cosh \hat{A}(l+l)] + f_{l\downarrow} f_{l\downarrow}^{\dagger} [1 + \cosh \hat{A}(l+l)] + (d_{l\downarrow}^{\dagger} f_{l\downarrow} - f_{l\downarrow}^{\dagger} d_{l\downarrow}) \sinh \hat{A}(l+l) \} \ ,
\end{aligned} \tag{19}$$

where

$$\hat{A}(\mathbf{n} \pm \mathbf{m}) = -\frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \frac{g(\mathbf{q})}{\hbar\omega_{\mathbf{q}}} e^{-2\alpha_{\mathbf{q}}} (e^{-i\mathbf{q}\cdot\mathbf{n}} \pm e^{-i\mathbf{q}\cdot\mathbf{m}}) (b_{\mathbf{q}}^{\dagger} - b_{-\mathbf{q}}) \ . \tag{20}$$

After substituting $\hat{\tilde{H}}$ into (17) we obtain the effective Hamiltonian:

$$\hat{H}_{\rm eff}=\sum_{\mathbf{q}}\hbar\omega_{\mathbf{q}}(\sinh 2\alpha_{\mathbf{q}})^2+E_d'\sum_{l,\sigma}d_{l\sigma}^{\dagger}d_{l\sigma}-T_d\sum_{\langle l,l'\rangle}\sum_{\sigma}d_{l\sigma}^{\dagger}d_{l'\sigma}+E_f'\sum_{l,\sigma}f_{l\sigma}^{\dagger}f_{l\sigma}$$
$$-T_f\sum_{\langle l,l'\rangle}\sum_{\sigma}f_{l\sigma}^{\dagger}f_{l'\sigma}-\sum_{\mathbf{m},\sigma}\sum_{\mathbf{n},\sigma'}J_{\mathbf{mn}}(f_{\mathbf{m}\sigma}^{\dagger}d_{\mathbf{m}\sigma}+d_{\mathbf{m}\sigma}^{\dagger}f_{\mathbf{m}\sigma})(f_{\mathbf{n}\sigma'}^{\dagger}d_{\mathbf{n}\sigma'}+d_{\mathbf{n}\sigma'}^{\dagger}f_{\mathbf{n}\sigma'})+U_f\sum_{l}f_{l\uparrow}f_{l\uparrow}^{\dagger}f_{l\downarrow}f_{l\downarrow}^{\dagger}$$
$$+U_d\sum_{l}d_{l\uparrow}d_{l\uparrow}^{\dagger}d_{l\downarrow}d_{l\downarrow}^{\dagger}+U_{fd}\sum_{l,\sigma}d_{l\sigma}d_{l\sigma}^{\dagger}f_{l\bar{\sigma}}f_{l\bar{\sigma}}^{\dagger}-U_{fd}\sum_{l}(f_{l\uparrow}^{\dagger}d_{l\uparrow}-d_{l\uparrow}^{\dagger}f_{l\uparrow})(f_{l\downarrow}^{\dagger}d_{l\downarrow}-d_{l\downarrow}^{\dagger}f_{l\downarrow})\ . \tag{21}$$

The various quantities are given by

$$\left.\begin{matrix}E_d'\\E_f'\end{matrix}\right\}=\tfrac{1}{2}E_f(1\mp e^{-2\rho}),\quad \rho=\frac{1}{N}\sum_{\mathbf{q}}\frac{|g(\mathbf{q})|^2}{(\hbar\omega_{\mathbf{q}})^2}e^{-4\alpha_{\mathbf{q}}}\ ,$$

$$U_{fd}=\frac{U}{8}(1-e^{-8\rho}),\quad \left.\begin{matrix}U_f\\U_d\end{matrix}\right\}=\frac{U}{4}(\tfrac{3}{2}\pm 2e^{-2\rho}+\tfrac{1}{2}e^{-8\rho})\ ,$$

$$\left.\begin{matrix}T_d\\T_f\end{matrix}\right\}=\tfrac{1}{2}T_0\left[\exp\left[-\frac{2}{N}\sum_{\mathbf{q}}[\,|g(\mathbf{q})|/\hbar\omega_{\mathbf{q}}]^2e^{-4\alpha_{\mathbf{q}}}C_1(\mathbf{q})\right]\pm\exp\left[-\frac{2}{N}\sum_{\mathbf{q}}[\,|g(\mathbf{q})|/\hbar\omega_{\mathbf{q}}]^2e^{-4\alpha_{\mathbf{q}}}C_2(\mathbf{q})\right]\right]\ , \tag{22}$$

$$C_1(\mathbf{q})=\frac{1}{z}\sum_{\delta}\sin^2\left[\frac{\mathbf{q}\cdot\delta}{2}\right],\quad C_2(\mathbf{q})=\frac{1}{z}\sum_{\delta}\cos^2\left[\frac{\mathbf{q}\cdot\delta}{2}\right],$$

$$J_{\mathbf{mn}}=\frac{1}{N}\sum_{\mathbf{q}}\frac{|g(\mathbf{q})|^2}{\hbar\omega_{\mathbf{q}}}e^{i\mathbf{q}\cdot(\mathbf{m}-\mathbf{n})}\ ,$$

where z is the nearest-neighbor number and δ is a nearest-neighbor vector.

We can see that the form of $\hat{H}_{\rm eff}$ is something like the transformed Hamiltonians in Refs. 13, 15, 16, and 18, which were obtained after respective unitary transformations had been performed and the higher-order terms of $g(\mathbf{q})$ had been omitted. But it should be pointed out that, in fact, there are differences between $\hat{H}_{\rm eff}$ and the transformed Hamiltonian in Refs. 13, 15, 16, and 18. In $\hat{H}_{\rm eff}$, the renormalized quantities E_d', E_f', T_d, T_f, U_d, U_f, and U_{fd} are all functionals of the adjustable parameters $\alpha_{\mathbf{q}}$'s. In addition, besides the f-f Hubbard term, in $\hat{H}_{\rm eff}$ there are d-d and d-f Hubbard terms which did not appear in the transformed Hamiltonian in Refs. 13, 15, 16, and 18. de Menezes and Troper[20] had derived a phonon-mediated attraction between d and f electrons, but their physical background is different from ours.

III. BOGOLIUBOV TRANSFORMATION AND THE ENERGY FUNCTIONAL E

In this section we will obtain the energy functional E [see Eq. (16)]. In order to achieve this, we should write out the explicit form of our trial state vector $|\bar{\Psi}_e\rangle$ of the electron subsystem, which may contain some adjustable parameters, and derive the expectation value of $\hat{H}_{\rm eff}$ in $|\bar{\Psi}_e\rangle$; that is, $E=\langle\bar{\Psi}_e|H_{\rm eff}|\bar{\Psi}_e\rangle$, as is indicated by Eqs. (16) and (17).

In analogy with Brandow's variational ground state for the PAM,[8] we propose the following form of the trial state vector $|\bar{\Psi}_e\rangle$,

$$|\bar{\Psi}_e\rangle=\left[\prod_{\mathbf{k},\sigma}(u_{\mathbf{k}}+v_{\mathbf{k}}f_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}^{\dagger})\right]\left[\prod_{l}f_{l\uparrow}^{\dagger}f_{l\downarrow}^{\dagger}\right]|\,\text{vacuum}\rangle\ , \tag{23}$$

where $u_{\mathbf{k}}$'s and $v_{\mathbf{k}}$'s are adjustable parameters. $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are real numbers and must satisfy the normalizing condition

$$u_{\mathbf{k}}^2+v_{\mathbf{k}}^2=1\ . \tag{24}$$

This trial state vector $|\bar{\Psi}_e\rangle$ is an exact eigenstate of the total electron number operator $\hat{N}_e$ and the eigenvalue of it is $2N$,

$$\begin{aligned}\hat{N}_e|\bar{\Psi}_e\rangle&=\sum_{l,\sigma}(f_{l\sigma}^{\dagger}f_{l\sigma}+d_{l\sigma}^{\dagger}d_{l\sigma})|\bar{\Psi}_e\rangle\\&=\sum_{\mathbf{k},\sigma}(f_{\mathbf{k}\sigma}^{\dagger}f_{\mathbf{k}\sigma}+d_{\mathbf{k}\sigma}^{\dagger}d_{\mathbf{k}\sigma})|\bar{\Psi}_e\rangle\\&=\sum_{\mathbf{k},\sigma}(f_{\mathbf{k}\sigma}^{\dagger}f_{\mathbf{k}\sigma}+d_{\mathbf{k}\sigma}^{\dagger}d_{\mathbf{k}\sigma})(u_{\mathbf{k}}+v_{\mathbf{k}}f_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}^{\dagger})(u_{\mathbf{k}}+v_{\mathbf{k}}f_{\mathbf{k}\bar{\sigma}}d_{\mathbf{k}\bar{\sigma}}^{\dagger})\prod_{\substack{\mathbf{k}'\\\mathbf{k}'\neq\mathbf{k}}}\prod_{\sigma'}(u_{\mathbf{k}'}+v_{\mathbf{k}'}f_{\mathbf{k}'\sigma'}d_{\mathbf{k}'\sigma'}^{\dagger})\left[\prod_{l}f_{l\uparrow}^{\dagger}f_{l\downarrow}^{\dagger}\right]|\,\text{vacuum}\rangle\\&=\sum_{\mathbf{k},\sigma}[u_{\mathbf{k}}(f_{\mathbf{k}\sigma}^{\dagger}f_{\mathbf{k}\sigma}+d_{\mathbf{k}\sigma}^{\dagger}d_{\mathbf{k}\sigma})+v_{\mathbf{k}}f_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}^{\dagger}](u_{\mathbf{k}}+v_{\mathbf{k}}f_{\mathbf{k}\bar{\sigma}}d_{\mathbf{k}\bar{\sigma}}^{\dagger})\\&\quad\times\prod_{\substack{\mathbf{k}'\\\mathbf{k}'\neq\mathbf{k}}}\prod_{\sigma'}(u_{\mathbf{k}'}+v_{\mathbf{k}'}f_{\mathbf{k}'\sigma'}d_{\mathbf{k}'\sigma'}^{\dagger})\left[\prod_{l}f_{l\uparrow}^{\dagger}f_{l\downarrow}^{\dagger}\right]|\,\text{vacuum}\rangle=2N|\bar{\Psi}_e\rangle\ ,\end{aligned} \tag{25}$$

where N is the total number of the unit cells. Equation (25) indicates that our trial state vector $|\bar{\Psi}_e\rangle$ can serve only for those systems in which the average number of electrons per unit cell is two. This is just the case for a model system being suitable to SmB_6 or SmS.[1,4–6,8]

The problem now is to derive the expectation value of $\hat{H}_{\text{eff}}$ in the state vector (23) and adjust the parameters $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ under the condition (24) to make this expectation value a minimum. This problem has a similar form as that discussed by Bardeen, Cooper, and Schrieffer (BCS) in their famous paper[21] concerning the superconducting state of metals. It had been proved by Valatin[22] and Bogoliubov[23] that the BCS variational method is equivalent, in essence, to the method of introducing new collective fermion operators by a Bogoliubov transformation and constructing the ground state and low-lying excited states by these collective fermion operators. In this section we use the method of Valatin and Bogoliubov to deal with our variational problem stated above because by this method the excitation spectrum of the electron subsystem can be discussed in a more straightforward manner.

We introduce the new collective fermion operators $\xi_{\mathbf{k}\sigma}$, $\xi^{\dagger}_{\mathbf{k}\sigma}$, $\eta_{\mathbf{k}\sigma}$, and $\eta^{\dagger}_{\mathbf{k}\sigma}$ in the Bloch representation by means of the Bogoliubov transformation

$$d_{\mathbf{k}\sigma}=u_{\mathbf{k}}\xi_{\mathbf{k}\sigma}+v_{\mathbf{k}}\eta^{\dagger}_{-\mathbf{k}\sigma},\quad f_{\mathbf{k}\sigma}=v_{\mathbf{k}}\xi_{\mathbf{k}\sigma}-u_{\mathbf{k}}\eta^{\dagger}_{-\mathbf{k}\sigma},\quad u_{\mathbf{k}}^2+v_{\mathbf{k}}^2=1\ . \tag{26}$$

$\xi_{\mathbf{k}\sigma}$, $\xi^{\dagger}_{\mathbf{k}\sigma}$, $\eta_{-\mathbf{k}\sigma}$, and $\eta^{\dagger}_{-\mathbf{k}\sigma}$ satisfy the anticommutation relations in a standard fashion. The practical process of this transformation is given in Appendix B because the algebraic operations of it are quite cumbersome. In Appendix B the parameters $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are determined by the condition (24) and that the second-order nondiagonal terms of the collective fermion operators in the Bogoliubov-transformed Hamiltonian must be eliminated. They are

$$u_{\mathbf{k}}=\left[\frac{1}{2}+\frac{1}{2}\frac{F(\mathbf{k})}{[F^2(\mathbf{k})+4G^2(\mathbf{k})]^{1/2}}\right]^{1/2},\qquad v_{\mathbf{k}}=\left[\frac{1}{2}-\frac{1}{2}\frac{F(\mathbf{k})}{[F^2(\mathbf{k})+4G^2(\mathbf{k})]^{1/2}}\right]^{1/2}. \tag{27}$$

The definitions of $F(\mathbf{k})$ and $G(\mathbf{k})$ are given in Appendix B. Our effective Hamiltonian $\hat{H}_{\text{eff}}$ after the transformation (26) and (27) has been made is

$$\hat{H}_{\text{eff}}=E+\sum_{\mathbf{k},\sigma}E_{\xi}(\mathbf{k})\xi^{\dagger}_{\mathbf{k}\sigma}\xi_{\mathbf{k}\sigma}+\sum_{\mathbf{k},\sigma}E_{\eta}(\mathbf{k})\eta^{\dagger}_{\mathbf{k}\sigma}\eta_{\mathbf{k}\sigma}+\hat{H}^{(4)}_{\text{eff}}\ , \tag{28}$$

where

$$E_{\xi}(\mathbf{k})=\tfrac{1}{2}[F^2(\mathbf{k})+4G^2(\mathbf{k})]^{1/2}+\tfrac{1}{2}S(\mathbf{k})\ ,\quad E_{\eta}(\mathbf{k})=\tfrac{1}{2}[F^2(\mathbf{k})+4G^2(\mathbf{k})]^{1/2}-\tfrac{1}{2}S(\mathbf{k})\ , \tag{29}$$

$$\begin{aligned}E=&\sum_{\mathbf{q}}\hbar\omega_{\mathbf{q}}[\sinh(2\alpha_{\mathbf{q}})]^2+\sum_{\mathbf{k}}\left[E'_d+E'_f+\frac{T_d+T_f}{T_0}E_{\mathbf{k}}-J_0+\tfrac{1}{2}U_f n_d+\tfrac{1}{2}U_d n_f+\tfrac{1}{2}U_{fd}\right]\\&+\sum_{\mathbf{k}}\frac{F(\mathbf{k})}{[F^2(\mathbf{k})+4G^2(\mathbf{k})]^{1/2}}\frac{1}{N}\sum_{\mathbf{q}}J(\mathbf{q})\frac{F(\mathbf{k}+\mathbf{q})}{[F^2(\mathbf{k}+\mathbf{q})+4G^2(\mathbf{k}+\mathbf{q})]^{1/2}}-\sum_{\mathbf{q}}[F^2(\mathbf{k})+4G^2(\mathbf{k})]^{1/2}\\&+2\sum_{\mathbf{k}}\frac{G^2(\mathbf{k})}{[F^2(\mathbf{k})+4G^2(\mathbf{k})]^{1/2}}+\frac{N}{2}(U_f n_d-U_d n_f-U_{fd}n_d+U_{fd}n_f)(n_f-n_d)\ .\end{aligned} \tag{30}$$

$S(\mathbf{k})$, n_d, and n_f are also defined in Appendix B.

The collective fermion operators $\xi^{\dagger}_{\mathbf{k}\sigma}$ and $\eta^{\dagger}_{\mathbf{k}\sigma}$ are considered to create the excited states of the electrons subsystem, so that the ground state $|\bar{\Psi}_{eg}\rangle$ of this subsystem should therefore satisfy

$$\xi_{\mathbf{k}\sigma}|\bar{\Psi}_{eg}\rangle=0,\quad \eta_{\mathbf{k}\sigma}|\bar{\Psi}_{eg}\rangle=0\ . \tag{31}$$

Thus $|\bar{\Psi}_{eg}\rangle$ is an eigenstate of the collective fermion number operators and the eigenvalues are zero:

$$\xi^{\dagger}_{\mathbf{k}\sigma}\xi_{\mathbf{k}\sigma}|\bar{\Psi}_{eg}\rangle=0,\quad \eta^{\dagger}_{\mathbf{k}\sigma}\eta_{\mathbf{k}\sigma}|\bar{\Psi}_{eg}\rangle=0\ . \tag{32}$$

It follows from the properties of the fermion operators that $\xi_{\mathbf{k}\sigma}\xi_{\mathbf{k}\sigma}=0$, $\eta_{\mathbf{k}\sigma}\eta_{\mathbf{k}\sigma}=0$; according to this fact the ground state $|\bar{\Psi}_{eg}\rangle$ satisfying (31) may now be constructed as

$$\begin{aligned}|\bar{\Psi}_{eg}\rangle&=\left[\prod_{\mathbf{k},\sigma}\frac{1}{v_{\mathbf{k}}}\xi_{\mathbf{k}\sigma}\eta_{\mathbf{k}\sigma}\right]\left[\prod_{l}f^{\dagger}_{l\uparrow}f^{\dagger}_{l\downarrow}\right]|\text{vacuum}\rangle\\&=\left[\prod_{\mathbf{k},\sigma}(u_{\mathbf{k}}+v_{\mathbf{k}}f_{\mathbf{k}\sigma}d^{\dagger}_{\mathbf{k}\sigma})\right]\left[\prod_{l}f^{\dagger}_{l\uparrow}f^{\dagger}_{l\downarrow}\right]|\text{vacuum}\rangle\ ,\end{aligned} \tag{33}$$

which has been normalized already. This state vector has the same form as that in Eq. (23). The expectation value of $\hat{H}_{\text{eff}}$ in $|\bar{\Psi}_{eg}\rangle$ is

$$\langle\bar{\Psi}_{eg}|E+\sum_{\mathbf{k},\sigma}E_{\xi}(\mathbf{k})\xi^{\dagger}_{\mathbf{k}\sigma}\xi_{\mathbf{k}\sigma}+\sum_{\mathbf{k},\sigma}E_{\eta}(\mathbf{k})\eta^{\dagger}_{\mathbf{k}\sigma}n_{\mathbf{k}\sigma}+\hat{H}^{(4)}_{\text{eff}}|\bar{\Psi}_{eg}\rangle=E\ . \tag{34}$$

In Eq. (34) we have made use of Eq. (32) and the fact that the collective fermion operators are of normal order in $\hat{H}^{(4)}_{\rm eff}$. E is just the energy functional we are going to obtain in this section and its explicit form is in Eq. (30). We should emphasize again that E is still a functional of the parameters $\alpha_{\rm q}$. By adjusting the $\alpha_{\rm q}$'s in Sec. IV we shall show that E may arrive at a minimum.

As has been proved in Eq. (25), the ground state $|\overline{\Psi}_{eg}\rangle$ is an eigenstate of the total electron number operator $\hat{N}_e$ and the eigenvalue is $2N$. However, $|\overline{\Psi}_{eg}\rangle$ is neither an eigenstate of the total d-electron number operator $\hat{N}_d=\sum_{l,\sigma}d^{\dagger}_{l\sigma}d_{l\sigma}$ nor an eigenstate of the total f-electron number operator $N_f=\sum_{l,\sigma}f^{\dagger}_{l\sigma}f_{l\sigma}$; the average values of these two number operators in $|\overline{\Psi}_{eg}\rangle$ are

$$N_d=\langle\overline{\Psi}_{eg}|\hat{N}_d|\overline{\Psi}_{eg}\rangle=2\sum_{\rm k}v_k^2$$

and (35)

$$N_f=\langle\overline{\Psi}_{eg}|\hat{N}_f|\overline{\Psi}_{eg}\rangle=2\sum_{\rm k}u_k^2\ .$$

Thus we may consider that the average d-electron number and f-electron number per site per spin direction is

$$n_d=N_d/2N=(1/N)\sum_{\rm k}v_{\rm k}^2$$

and (36)

$$n_f=N_f/2N=(1/N)\sum_{\rm k}u_{\rm k}^2\ ,$$

respectively. This is Eq. (B9). It follows from condition (24) that $n_d+n_f=1$, which is consistent with the fact that the total electron number in our system is $2N$ since in our discussion we do not consider any magnetic ordering.

The low-lying excited states of our model system may be obtained more conveniently by means of the collective fermion operators. With the aid of (24) the transformation (26) can be easily inverted:

$$\begin{aligned}\xi^{\dagger}_{\mathbf{k}\sigma}&=u_{\mathbf{k}}d^{\dagger}_{\mathbf{k}\sigma}+v_{\mathbf{k}}f^{\dagger}_{\mathbf{k}\sigma}\ ,\\ \eta^{\dagger}_{\mathbf{k}\sigma}&=v_{\mathbf{k}}d_{-\mathbf{k}\sigma}-u_{\mathbf{k}}f_{-\mathbf{k}\sigma}\ .\end{aligned}\tag{37}$$

It follows from Eq. (32) that the states $\xi^{\dagger}_{\mathbf{k}\sigma}|\overline{\Psi}_{eg}\rangle$ and $\eta^{\dagger}_{\mathbf{k}\sigma}|\overline{\Psi}_{eg}\rangle$ are excited states of the system. It is apparent from Eq. (37) that $\xi^{\dagger}_{\mathbf{k}\sigma}|\overline{\Psi}_{eg}\rangle$ is a state of wave vector $\mathbf{k}$ involving a superposition of a d electron and an f electron, both of wave vector $\mathbf{k}$, and $\eta^{\dagger}_{\mathbf{k}\sigma}|\overline{\Psi}_{eg}\rangle$ is a state of wave vector $\mathbf{k}$ involving a superposition of a d hole and an f hole; both of them are of wave vector $-\mathbf{k}$. These states are quasiparticle states and their excitation energy may be determined by $\hat{H}_{\rm eff}$ in Eq. (28). To this end $\hat{H}^{(4)}_{\rm eff}$ in $\hat{H}_{\rm eff}$ may be ignored because the terms in $\hat{H}^{(4)}_{\rm eff}$ represents the interactions between quasiparticles. After ignoring this it is evident that the excitation energy of $\xi^{\dagger}_{\mathbf{k}\sigma}|\overline{\Psi}_{eg}\rangle$ is $E_{\xi}(\mathbf{k})$ and that of $\eta^{\dagger}_{\mathbf{k}\sigma}|\overline{\Psi}_{eg}\rangle$ is $E_{\eta}(\mathbf{k})$. The explicit forms of $E_{\xi}(\mathbf{k})$ and $E_{\eta}(\mathbf{k})$ are in Eq. (29).

It should be pointed out that external fields do not create these quasiparticles singly. Since $\xi^{\dagger}_{\mathbf{k}\sigma}$ is a linear combination of single-electron operators and $\eta^{\dagger}_{\mathbf{k}\sigma}$ is a linear combination of single-hole operators, the $\xi^{\dagger}_{\mathbf{k}\sigma}$'s and $\eta^{\dagger}_{\mathbf{k}\sigma}$'s always occur in pairs in an interaction Hamiltonian which describes the interaction between our model system and external fields and must conserve the electron number. As a result, the quasiparticles are created in pairs and the energy gap observed experimentally should be

$$\begin{aligned}\Delta&=E_{\xi}(\mathbf{k})|_{\rm min}+E_{\eta}(\mathbf{k})|_{\rm min}\\ &=\{\tfrac{1}{2}[F^2(\mathbf{k})+4G^2(\mathbf{k})]^{1/2}+\tfrac{1}{2}S(\mathbf{k})\}|_{\rm min}\\ &\quad+\{\tfrac{1}{2}[F^2(\mathbf{k})+4G^2(\mathbf{k})]^{1/2}-\tfrac{1}{2}S(\mathbf{k})\}|_{\rm min}\ ,\end{aligned}\tag{38}$$

where min denotes "minimum." The model system will appear as a small-gap semiconductor so long as Δ is a small positive quantity.

IV. THE RESULTS OF NUMERICAL CALCULATIONS

In this section we are going to minimize the energy functional E to get the variational ground-state energy E_g and calculate the energy gap Δ and the fluctuating valence of ions in the variational ground state. As can be seen from Eqs. (30), (36), and (38), for these goals we must solve the simultaneous equations (B6), (B7), and (B9) first to obtain the quantities $G(\mathbf{k})$, $F(\mathbf{k})$, and n_d ($n_f=1-n_d$) in explicit form since in these equations $G(\mathbf{k})$, $F(\mathbf{k})$, and n_d are defined in the forms of implicit functions. For clarity, we rewrite Eqs. (B6), (B7), and (B9) as follows:

$$G(\mathbf{k})=\frac{8}{N}\sum_{\mathbf{k}'}J(0)G(\mathbf{k}')/[F^2(\mathbf{k}')+4G^2(\mathbf{k}')]^{1/2}-\frac{2}{N}\sum_{\rm q}J(\mathbf{q})G(\mathbf{k}+\mathbf{q})/[F^2(\mathbf{k}+\mathbf{q})+4G^2(\mathbf{k}+\mathbf{q})]^{1/2}\ ,\tag{39}$$

$$F(\mathbf{k})=E'_d-E'_f+\frac{T_d-T_f}{T_0}E_{\mathbf{k}}+U_fn_d-U_dn_f-U_{fd}n_d+U_{fd}n_f+\frac{2}{N}\sum_{\rm q}J(\mathbf{q})F(\mathbf{k}+\mathbf{q})/[F^2(\mathbf{k}+\mathbf{q})+4G^2(\mathbf{k}+\mathbf{q})]^{1/2}\ ,\tag{40}$$

$$n_d=\frac{1}{2}-\frac{1}{2N}\sum_{\rm k}F(\mathbf{k})/[F^2(\mathbf{k})+4G^2(\mathbf{k})]^{1/2}\ .\tag{41}$$

These simultaneous equations could be solved by self-consistent methods.

A simple assumption concerning the functions $g(\mathbf{q})$ and $\omega_{\mathbf{q}}$ should be introduced to facilitate solutions of Eqs. (39)–(41). We suppose that $g(\mathbf{q})$ and $\omega_{\mathbf{q}}$ are constants that are $\mathbf{q}$ independent,

$$g(\mathbf{q})=g \quad \text{and} \quad \omega_{\mathbf{q}}=\omega_0 \; ; \tag{42}$$

that is, we use the local-phonon-mediated d-f hybridization (2′) instead of (2) and let the local-phonon frequency to be equal to a constant ω_0. This assumption is consistent with the model parameters used in Refs. 13 and 15–17 and it can largely simplify the calculations without loss of physical contents. According to this assumption,

$$J(\mathbf{q})=|g(\mathbf{q})|^2/\hbar\omega_{\mathbf{q}}=g^2/\hbar\omega_0=J_0 \tag{43}$$

is also $\mathbf{q}$ independent and the adjustable parameters $\alpha_{\mathbf{q}}$ may be taken to be $\mathbf{q}$ independent too, $\alpha_{\mathbf{q}}=\alpha$ for every $\mathbf{q}$ mode. Thus the various quantities in Eq. (22) are rewritten as

$$\rho=\frac{J_0}{\hbar\omega_0}\frac{1}{N}\sum_{\mathbf{q}} e^{-4\alpha}=\frac{J_0}{\hbar\omega_0}\tau^2, \text{ i.e., } \tau=e^{-2\alpha} \; , \tag{44}$$

$$J_{\mathbf{mn}}=J_0\delta_{\mathbf{mn}} \; , \tag{45}$$

$$\begin{aligned}&(1/N)\sum_{\mathbf{q}} C_1(\mathbf{q})=(1/N)\sum_{\mathbf{q}} C_2(\mathbf{q})=\tfrac{1}{2} \; ,\\ &T_d=T_0e^{-\rho}, \quad T_f=0 \; .\end{aligned} \tag{46}$$

Equation (40) becomes

$$\begin{aligned}F(k)=&E_d'-E_f'+(T_d/T_0)E_k+U_fn_d-U_dn_f\\ &-U_{fd}n_d+U_{fd}n_f-2J_0(n_d-n_f) \; ,\end{aligned} \tag{40′}$$

so $G(\mathbf{k})$ in Eq. (39) may be taken to be $\mathbf{k}$ independent,

$$G=\frac{6}{N}J_0\sum_{\mathbf{k}} G/[F^2(\mathbf{k})+4G^2]^{1/2} \; . \tag{39′}$$

Equation (39′) can be solved more easily than Eq. (39) can. It may be seen that for Eq. (39′) $G=0$ is a trivial solution, but our interest is in a nontrivial solution $G\neq 0$. In the following we shall show that when $G\neq 0$ a nonzero energy gap Δ is opened in the density of states of electrons and the variational ground-state energy E_g of this case is lower than that of the case of $G=0$ in which $\Delta=0$ also. Divided by G on both sides of Eq. (39′) it becomes

$$1=\frac{6}{N}\sum_{\mathbf{k}}\frac{J_0}{[F^2(\mathbf{k})+4G^2]^{1/2}} \; . \tag{39″}$$

We should solve Eqs. (39″) and (41); the function $F(\mathbf{k})$ is defined as (40′).

In order to make the $\mathbf{k}$ summation ($\mathbf{k}$ integration) in various expressions in the paper be summed (integrated) analytically, we take the band function $E_{\mathbf{k}}$ to be of a constant density of states $1/2D$;[24] that is, the density of states is

$$\rho(\varepsilon)=\frac{1}{N}\sum_{\mathbf{k}}\delta(\varepsilon-E_{\mathbf{k}})=\begin{cases}0, & \varepsilon>D \text{ or } \varepsilon<-D\\ 1/2D, & -D<\varepsilon<D \; .\end{cases} \tag{47}$$

Adopting this $\rho(\varepsilon)$, Eqs. (39″) and (41) are changed into

$$1=\frac{1}{2D}\int_{-D}^{D} d\varepsilon\, bJ_0/[F^2(\varepsilon)+4G^2]^{1/2}$$

and

$$\tfrac{1}{2}-n_d=\frac{1}{4D}\int_{-D}^{D} d\varepsilon\, F(\varepsilon)/[F^2(\varepsilon)+4G^2]^{1/2} \; ,$$

where $F(\varepsilon)$ is the same function as $F(\mathbf{k})$ in Eq. (40′), but replacing $E_{\mathbf{k}}$ by ε. The results of integrations in the two equations are

$$\begin{aligned}&1=\frac{3J_0}{De^{-\rho}}\ln\left[\frac{F(D)+[F^2(D)+4G^2]^{1/2}}{F(-D)+[F^2(-D)+4G^2]^{1/2}}\right] \; ,\\ &\tfrac{1}{2}-n_d=\{[F^2(D)+4G^2]^{1/2}-[F^2(-D)+4G^2]^{1/2}\}/4De^{-\rho} \; .\end{aligned}$$

G and n_d can be solved from these equations,

$$\begin{aligned}G=&\left[\frac{2n_dDe^{-\rho}}{\exp(De^{-\rho}/3J_0)-1}\right]^{1/2}\left[De^{-\rho}+X+Yn_d+\frac{2n_dDe^{-\rho}}{\exp(De^{-\rho}/3J_0)-1}\right]^{1/2} \; ,\\ n_d=&\frac{De^{-\rho}[\exp(De^{-\rho}/3J_0)+1]/[\exp(De^{-\rho}/3J_0)-1]-X}{Y+2De^{-\rho}[\exp(De^{-\rho}/3J_0)+1]/[\exp(De^{-\rho}/3J_0)-1]} \; ,\end{aligned} \tag{48}$$

where

$$\begin{aligned}X=&-E_fe^{-2\rho}-\frac{U}{4}+\frac{U}{2}e^{-2\rho}-\frac{U}{4}e^{-8\rho}+2J_0 \; ,\\ Y=&\frac{U}{2}+\frac{U}{2}e^{-8\rho}-4J_0 \; .\end{aligned} \tag{49}$$

It should be pointed out that, as indicated in Eq. (48), G and n_d are still related to the parameter ρ, the actual value of which is undetermined now. Because of the functional relation between ρ and τ and the adjustable parameter α as

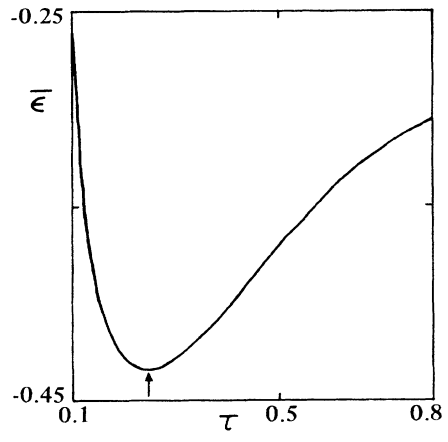

FIG. 1. $\bar{\varepsilon}$ vs τ relation in the case of $\bar{J}_0=0.045$, $\bar{\varepsilon}_f=-0.4$, $\hbar\bar{\omega}_0=0.02$, and $\bar{U}=0$. See text for details.

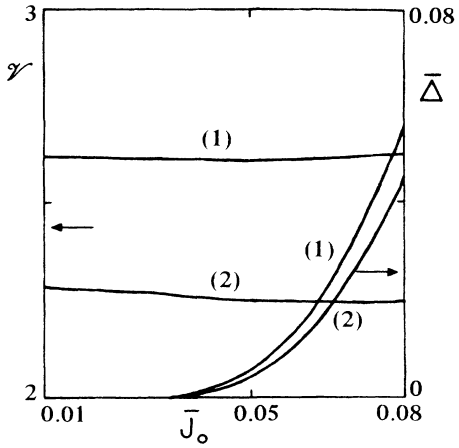

FIG. 2. v and $\bar{\Delta}$ vs $\bar{J}_0$ relations in the case of $\bar{\varepsilon}_f=-0.4$, $\hbar\bar{\omega}_0=0.02$, and $\bar{U}=0$ (1) or $\bar{U}=2$ (2). See text for details.

shown in Eq. (44), we could consider ρ or τ as our adjustable parameter and determine both by the variational method as mentioned in Sec. II. Using the assumptions (42) and (47) and doing some complicated algebraic operations and integrations, an analytical formula of the energy functional E can be derived from Eq. (30),

$$\frac{E}{2N}=\frac{1}{8}\hbar\omega_0(\tau-1/\tau)^2+G^2/6J_0+\tfrac{1}{2}E_f+\frac{U}{16}(1-e^{8\rho})+\left[\frac{U}{4}(1+e^{-8\rho})-2J_0\right](n_d-n_d^2)$$
$$-\frac{G^2}{2De^{-\rho}}\ln\left[\frac{F(D)+[F^2(D)+4G^2]^{1/2}}{F(-D)+[F^2(-D)+4G^2]^{1/2}}\right]$$
$$-\frac{1}{8De^{-\rho}}F(D)[F^2(D)+4G^2]^{1/2}+\frac{1}{8De^{-\rho}}F(-D)[F^2(-D)+4G^2]^{1/2}\ , \tag{50}$$

in which the variational parameter τ should be determined by the condition that when τ is equal to a special value τ_0, $E/2W$ must arrive at its minimum $E_g/2N$. After τ_0 is determined, the various quantities in Eqs. (22) and (46) that are related to parameter ρ may be fixed by making ρ in these quantities equal to ρ_0 corresponding to $\tau=\tau_0$. That is, $\rho_0=(J_0/\hbar\omega_0)\tau_0^2$ and

$$\begin{aligned}&E_d'=(E_f/2)(1-e^{-2\rho_0}),\quad E_f'=(E_f/2)(1+e^{-2\rho_0})\ ,\\ &T_d=T_0e^{-\rho_0},\quad T_f=0,\quad U_{fd}=(U/8)(1-e^{-8\rho_0})\ ,\\ &U_d=(U/8)(3-4e^{-2\rho_0}+e^{-8\rho_0})\ ,\\ &U_f=(U/8)(3+4e^{-2\rho_0}+e^{-8\rho_0})\ .\end{aligned} \tag{51}$$

Then these fixed quantities are substituted into Eqs. (B8), (40′), and (48) to obtain the actual values of $S(\mathbf{k})$, $F(\mathbf{k})$, G, and n_d. Substituting $S(\mathbf{k})$, $F(\mathbf{k})$, and G thus obtained into Eq. (38), the energy gap Δ becomes

$$\Delta=\tfrac{1}{2}[F^2(-D)+4G^2]^{1/2}+\tfrac{1}{2}[F^2(D)+4G^2]^{1/2}-De^{-\rho_0}\ . \tag{52}$$

In our model the ions have two valence states—one is the state having two f electrons localized at one site and the other having one f electron. We will regard the former as the divalent state and the latter as the trivalent state for the sake of comparing our results with the experimental data for some Sm-based compounds.[1,2,8] Thus the number of trivalent ions is equal to $2N-2n_fN=2n_dN$, so $v=2+2n_d$ may be used to represent the fluctuating valence of the ions (the origin of the constant 2 in $v=2+2n_d$ is that the valence of the ions is fluctuating between 2 and 3).

Equations (48), (50), and (52), in which ρ is replaced by ρ_0, comprise the starting point of the following numerical calculations. In the calculations, all quantities—being of the energy dimension—are expressed in units of half the bandwidth D of the bare d electrons: $\bar{E}_f=E_f/D$, $\bar{J}_0=J_0/D$, $\bar{U}=U/D$, $\hbar\bar{\omega}_0=\hbar\omega_0/D$, $\bar{G}=G/D$, $\bar{\Delta}=\Delta/D$, $\bar{E}=E/D$, $\bar{E}_g=E_g/D$, etc. The employed values of these parameters in the calculations are given in the following figures and table separately, which are reasonable as D is of the order of 1 eV.[1-5,9]

The $\bar{\varepsilon}=\bar{E}/2N$ versus the two-phonon coherent state parameter τ [see Eq. (44), $\tau=e^{-2\alpha}$] relation is illustrated in Fig. 1 for a special case offered as an example. From the figure we see that when $\tau=\tau_0=0.25$, $\bar{\varepsilon}$ decreases to its stable minimum value $\bar{\varepsilon}_g$. So in this case the ground state of the phonon subsystem is the two-phonon coherent state with the parameter α equal to $\alpha_0=-\frac{1}{2}\ln\tau_0=0.7$. We have made the calculations in some other cases with the employed values of the param-

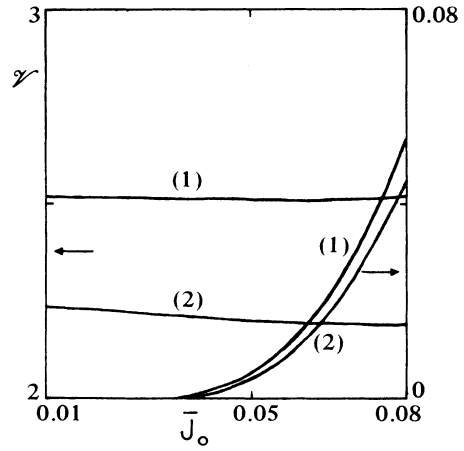

FIG. 3. v and $\bar{\Delta}$ vs $\bar{J}_0$ relations in the case of $\bar{\varepsilon}_f=-0.5$, $\hbar\bar{\omega}_0=0.03$, and $\bar{U}=0$ (1) or $\bar{U}=2$ (2). See text for details.

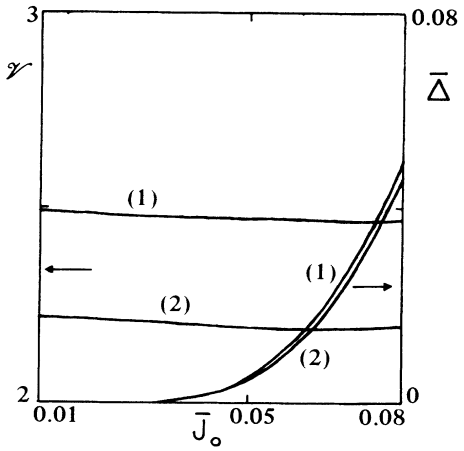

FIG. 4. v and $\bar{\Delta}$ vs $\bar{J}_0$ relations in the case of $\bar{\varepsilon}_f=0$, $\hbar\bar{\omega}_0=0.02$, and $\bar{U}=2(1)$ or $\bar{\varepsilon}_f=-0.8$, $\hbar\bar{\omega}_0=0.02$, and $\bar{U}=0$ (2). See text for details.

eters $\bar{J}_0$, $\bar{E}_f$, $\hbar\omega_0$, and $\bar{U}$ being different from those of Fig. 1, and found that a stable minimum value $\bar{\varepsilon}_g$ always exists in every case as the variational parameter τ arrives at some particular point.

Figures 2–4 are the fluctuation valence v and the energy gap $\bar{\Delta}$ versus $\bar{J}_0$ relations in various cases. The variation of $\bar{J}_0$ may result from the external pressure or from the changed chemical composition, because the electron-phonon interaction is sensitive to them.[1,2,4,17] In the figures we see that as $\bar{J}_0$ increases $\bar{\Delta}$ also increases, but v keeps a constant value, approximately. The values of v are sensitive to the adopted values of $\bar{E}_f$ and $\bar{U}$, as we can see in these three figures.

For the sake of clarity, in Table I the calculated values of v and $\bar{\Delta}$ are listed. From the table we see that when $\bar{J}_0$ is in the reasonable range of 0.02–0.07, the calculated values of v and $\bar{\Delta}$ are consistent with the experimental data for SmB_6 and SmS [SmB_6, $v\sim2.67$ and $\Delta\sim3$ meV (Ref. 5); SmS, $v\sim2.6$ and $\Delta\sim1$ meV (Ref. 5)], at least being of the same order of the magnitude (the unit of energy is $D\sim1$ eV).

TABLE I. Values of v and $\bar{\Delta}$ in some cases.

$\bar{J}_0$	v and $\bar{\Delta}$	$\bar{\varepsilon}_f=-0.4$ $\hbar\bar{\omega}_0=0.02$ $\bar{U}=0$	$\bar{\varepsilon}_f=-0.4$ $\hbar\bar{\omega}_0=0.02$ $\bar{U}=2$	$\bar{\varepsilon}_f=-0.5$ $\hbar\bar{\omega}_0=0.03$ $\bar{U}=0$	$\bar{\varepsilon}_f=-0.5$ $\hbar\bar{\omega}_0=0.03$ $\bar{U}=2$	$\bar{\varepsilon}_f=0$ $\hbar\bar{\omega}_0=0.02$ $\bar{U}=0$	$\bar{\varepsilon}_f=0$ $\hbar\bar{\omega}_0=0.02$ $\bar{U}=2$	$\bar{\varepsilon}_f=-0.8$ $\hbar\bar{\omega}=0.02$ $\bar{U}=0$	$\bar{\varepsilon}_f=-0.8$ $\hbar\bar{\omega}_0=0.03$ $\bar{U}=0$
0.01	v	2.615	2.283	2.517	2.232	3	2.491	2.217	2.217
	$\bar{\Delta}$	0	0	0	0	0	0	0	0
0.02	v	2.617	2.274	2.518	2.222	3	2.482	2.215	2.215
	$\bar{\Delta}$	4.17×10^{-7}	2.38×10^{-7}	3.58×10^{-7}	2.98×10^{-7}	5.96×10^{-7}	2.98×10^{-7}	2.38×10^{-7}	2.38×10^{-7}
0.03	v	2.615	2.266	2.515	2.213	3	2.477	2.208	2.208
	$\bar{\Delta}$	8.40×10^{-5}	6.09×10^{-5}	7.78×10^{-5}	5.92×10^{-5}	1.02×10^{-4}	7.07×10^{-5}	6.32×10^{-5}	6.29×10^{-5}
0.04	v	2.613	2.258	2.512	2.205	3	2.472	2.199	2.200
	$\bar{\Delta}$	1.15×10^{-3}	8.66×10^{-4}	1.08×10^{-3}	8.47×10^{-4}	1.35×10^{-3}	9.81×10^{-4}	9.0×10^{-4}	9.01×10^{-4}
0.05	v	2.611	2.252	2.509	2.197	3	2.469	2.192	2.192
	$\bar{\Delta}$	5.44×10^{-3}	4.23×10^{-3}	5.14×10^{-3}	4.13×10^{-3}	6.27×10^{-3}	4.71×10^{-3}	4.40×10^{-3}	4.39×10^{-3}
0.06	v	2.612	2.250	2.509	2.192	3	2.467	2.188	2.187
	$\bar{\Delta}$	0.015	0.012	0.014	0.012	0.017	0.013	0.013	0.013
0.07	v	2.617	2.246	2.513	2.190	3	2.468	2.189	2.189
	$\bar{\Delta}$	0.032	0.026	0.030	0.025	0.036	0.028	0.027	0.027

V. DISCUSSIONS AND CONCLUSIONS

Since the method used in this paper is a variational one, there are no small parameters involved explicitly in our treatment. In the above presentations we have not mentioned what approximations are used and why they should be introduced. But it goes without saying that some approximations must be involved.

Although we have said in Sec. II that in the two unitary transformations we have not omitted any higher-order terms, in the variational treatment in Secs. II and III some approximations have been introduced implicitly. The first is that of Eq. (11), by which we could deal with the phonon subsystem and the electron subsystem separately. We consider this approximation to be satisfactory because the effects of the electron-phonon interaction have been included in our theory by means of the first unitary transformation (7).

When we eliminate the electron-phonon operators in $\hat{\tilde{H}}$ by taking the expectation value of $\hat{\tilde{H}}$ over the two-phonon coherent state $|\bar{\Psi}_{\rm ph}\rangle$ with nonzero variational parameters $\alpha_{\rm q}$ to obtain the effective Hamiltonian $\hat{H}_{\rm eff}$, as indicated in Eq. (17), another approximation has been introduced. It is obvious that the odd functions of the operators $\hat{B}$ in $\hat{\tilde{H}}$ contribute nothing to the effective Hamiltonian $\hat{H}_{\rm eff}$ and the contribution of the even functions of $\hat{B}$ results from taking their expectation values over the two-phonon coherent state. This approximation is something like that used in dealing with the small-polaron problem.[25]

The small polaron corresponds to an electron in some ionic crystal, which is in a narrow band but interacting with phonons strongly. In the treatment of the small-polaron problem,[25] it was considered that in the lowest-temperature region the diagonal transition of the phonon subsystem, described by even functions of phonon operators, plays a dominant role, and the probability of the nondiagonal transition, described by odd functions of phonon operators, is so small that it could be disregarded. In fact, the approximation adopted in the small-polaron problem is the narrow-band approximation;[25] that is, the terms in the Hamiltonian corresponding to the band energy of the electron may be treated as a perturbation, but the electron-phonon interaction could not be treated by any perturbation method. Therefore, our approximation used in deriving $\hat{H}_{\rm eff}$ from $\hat{\tilde{H}}$ in Sec. II is also a narrow-band one. It was pointed out by many authors[1–8] that for the d band in MVC's the narrow-band approximation is a good one.

Although there are similarities between our model system and the small-polaron one, some differences exist. The first is that in the small-polaron problem the interaction between electrons, in general, is not taken into account, but in our problem the interaction between electrons plays a very important role. The second and more influential difference is that the population of the small polarons in the conduction band is very few, but that of the electrons in the d band of our model is of the same order of magnitude as the number of the total unit cells, N. It was shown[25] that for the small polaron the concept of an energy band is still valid, but the bandwidth is renormalized and narrowed by the action of phonons, even if the phonon system is in the ground state. Since the population of the small polarons is very few, this narrowing of the band has no effect on the total energy of the system. However, in our model system it is not the case. Because the population of electrons in the d band is of the order of magnitude N, narrowing the d band by the action of phonons must make the total energy of the system increase. In order to lower the total energy in our variational treatment, we introduce the adjustable parameters $\alpha_{\rm q}$. The nonzero $\alpha_{\rm q}$'s, which serve as the parameters of the two-phonon coherent state, can offset the narrowing of the d band mentioned above. When the $\alpha_{\rm q}$'s tend to infinity, we can see from Eq. (22) that $\rho=0$ and $E_d'=0$, $E_f'=E_f$, $T_d=T_0$, $T_f=0$, $U_{fd}=U_d=0$, and $U_f=U$; that is, these quantities are not affected by the action of phonons. However, the nonzero $\alpha_{\rm q}$'s may increase the harmonic energy of the phonon subsystem and when $\alpha_{\rm q}$'s tend to infinity this energy tends to infinity also. Therefore, these two effects of $\alpha_{\rm q}$'s compete with each other and our variational treatment consists of selecting the proper values of $\alpha_{\rm q}$'s at which a stable minimum of the total energy of the system can be obtained.

Some comparisons between our effective Hamiltonian $\hat{H}_{\rm eff}$ and the transformed Hamiltonian in Refs. 13, 15, 16, and 18 were made at the end of Sec. II. At present, we will emphasize a further point. In Refs. 13, 15, 16, and 18, after the unitary transformation and omission of the higher-order terms of $g(\mathbf{q})$, the interplay between the phonon subsystem and the electron subsystem is cut off completely. But in our treatment the interplay between the two subsystems is considered in the following way. The renormalized quantities in $\hat{H}_{\rm eff}$, E_d', E_f', T_d, T_f, U_d, U_f, and U_{fd} are all functionals of the adjustable parameters $\alpha_{\rm q}$'s, and the $\alpha_{\rm q}$'s should be determined by minimizing the total ground-state energy of the two subsystems. This is the reaction of the electron subsystem on the phonon subsystem since the selected values of the $\alpha_{\rm q}$'s fix the state of the phonon subsystem.

Finally, we arrive at the following conclusions.

(1) We have obtained a variational ground state of the periodic Anderson model with an indirect hybridization, which is composed of the two-phonon coherent state of the phonon subsystem and the pairing state of the electron subsystem. In such a ground state a nonzero energy gap and a fluctuating valence exist, the calculated values of which are consistent semiquantitatively with the experimental data for SmB_6 and SmS.

(2) In this paper a new concept—the two-phonon coherent state—has been introduced to make the energy of the ground state arrive at a stable minimum value.

(3) By means of a Bogoliubov transformation we have constructed the pairing state as the ground state of the electron subsystem. This procedure could be used only when the total electron number is equal to $2N$, because the pairing state is also the eigenstate of the total electron number operator $\hat{N}_e$ and the eigenvalue of it is $2N$. So it is obvious that only when the total electron number is $2N$ can a nonzero energy gap be observed experimentally.

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APPENDIX A: THE TWO UNITARY TRANSFORMATIONS

In this appendix we give the practical processes of the two transformations (7) and (18). For the first one, it can easily be verified that

$$e^{\hat{R}}b_{-\mathbf{q}}e^{-\hat{R}}=b_{-\mathbf{q}}-\frac{1}{\sqrt{N}}\sum_{l,\sigma}[g^*(\mathbf{q})/\hbar\omega_{\mathbf{q}}]e^{i\mathbf{q}\cdot l}(f^\dagger_{l\sigma}d_{l\sigma}+d^\dagger_{l\sigma}f_{l\sigma}) ,$$
$$e^{\hat{R}}b^\dagger_{\mathbf{q}}e^{-\hat{R}}=b^\dagger_{\mathbf{q}}-\frac{1}{\sqrt{N}}\sum_{l,\sigma}[g^*(\mathbf{q})/\hbar\omega_{\mathbf{q}}]e^{i\mathbf{q}\cdot l}(f^\dagger_{l\sigma}d_{l\sigma}+d^\dagger_{l\sigma}f_{l\sigma}) . \tag{A1}$$

In order to transform several electron operators in $\hat{H}$, we define two operator functions,

$$D^\sigma_{\mathbf{mn}}(\lambda)=e^{\lambda\hat{R}}d^\dagger_{\mathbf{m}\sigma}d_{\mathbf{n}\sigma}e^{-\lambda\hat{R}} ,$$
$$F^\sigma_{\mathbf{mn}}(\lambda)=e^{\lambda\hat{R}}f^\dagger_{\mathbf{m}\sigma}f_{\mathbf{n}\sigma}e^{-\lambda\hat{R}} , \tag{A2}$$

and perform differential operations on these operator functions as follows:

$$\frac{d}{d\lambda}D^\sigma_{\mathbf{mn}}(\lambda)=\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}[g(\mathbf{q})/\hbar\omega_{\mathbf{q}}]e^{\lambda\hat{R}}(f^\dagger_{\mathbf{m}\sigma}d_{\mathbf{n}\sigma}e^{-i\mathbf{q}\cdot\mathbf{m}}-d^\dagger_{\mathbf{m}\sigma}f_{\mathbf{n}\sigma}e^{-i\mathbf{q}\cdot\mathbf{n}})e^{-\lambda\hat{R}}(b^\dagger_{\mathbf{q}}-b_{-\mathbf{q}}) , \tag{A3}$$

$$\frac{d}{d\lambda}F^\sigma_{\mathbf{mn}}(\lambda)=\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}[g(\mathbf{q})/\hbar\omega_{\mathbf{q}}]e^{\lambda\hat{R}}(d^\dagger_{\mathbf{m}\sigma}f_{\mathbf{n}\sigma}e^{-i\mathbf{q}\cdot\mathbf{m}}-f^\dagger_{\mathbf{m}\sigma}d_{\mathbf{n}\sigma}e^{-i\mathbf{q}\cdot\mathbf{n}})e^{-\lambda\hat{R}}(b^\dagger_{\mathbf{q}}-b_{-\mathbf{q}}) , \tag{A4}$$

$$\frac{d^2}{d\lambda^2}D^\sigma_{\mathbf{mn}}(\lambda)=\frac{1}{N}\sum_{\mathbf{q},\mathbf{q}'}[g(\mathbf{q})g(\mathbf{q}')/\hbar\omega_{\mathbf{q}}\hbar\omega_{\mathbf{q}'}][D^\sigma_{\mathbf{mn}}(\lambda)(e^{-i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{m}}+e^{-i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{n}})$$
$$-F^\sigma_{\mathbf{mn}}(\lambda)(e^{-i\mathbf{q}\cdot\mathbf{m}-i\mathbf{q}'\cdot\mathbf{n}}+e^{-i\mathbf{q}\cdot\mathbf{n}-i\mathbf{q}'\cdot\mathbf{m}})](b^\dagger_{\mathbf{q}}-b_{-\mathbf{q}})(b^\dagger_{\mathbf{q}'}-b_{-\mathbf{q}'}) , \tag{A5}$$

$$\frac{d^2}{d\lambda^2}F^\sigma_{\mathbf{mn}}(\lambda)=\frac{1}{N}\sum_{\mathbf{q},\mathbf{q}'}[g(\mathbf{q})g(\mathbf{q}')/\hbar\omega_{\mathbf{q}}\hbar\omega_{\mathbf{q}'}][F^\sigma_{\mathbf{mn}}(\lambda)(e^{-i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{n}}+e^{-i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{m}})$$
$$-D^\sigma_{\mathbf{mn}}(\lambda)(e^{-i\mathbf{q}\cdot\mathbf{n}-i\mathbf{q}'\cdot\mathbf{m}}+e^{-i\mathbf{q}\cdot\mathbf{m}-i\mathbf{q}'\cdot\mathbf{n}})](b^\dagger_{\mathbf{q}}-b_{-\mathbf{q}})(b^\dagger_{\mathbf{q}'}-b_{-\mathbf{q}'}) . \tag{A6}$$

Equations (A5) and (A6) are simultaneous differential equations and in order to solve them conveniently they may be changed into the following forms,

$$\frac{d^2}{d\lambda^2}[D^\sigma_{\mathbf{mn}}(\lambda)+F^\sigma_{\mathbf{mn}}(\lambda)]=[D^\sigma_{\mathbf{mn}}(\lambda)+F^\sigma_{\mathbf{mn}}(\lambda)]\left[\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}[g(\mathbf{q})/\hbar\omega_{\mathbf{q}}](e^{-i\mathbf{q}\cdot\mathbf{m}}-e^{-i\mathbf{q}\cdot\mathbf{n}})(b^\dagger_{\mathbf{q}}-b_{-\mathbf{q}})\right]^2 , \tag{A7}$$

$$\frac{d^2}{d\lambda^2}[D^\sigma_{\mathbf{mn}}(\lambda)-F^\sigma_{\mathbf{mn}}(\lambda)]=[D^\sigma_{\mathbf{mn}}(\lambda)-F^\sigma_{\mathbf{mn}}(\lambda)]\left[\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}[g(\mathbf{q})/\hbar\omega_{\mathbf{q}}](e^{-i\mathbf{q}\cdot\mathbf{m}}+e^{-i\mathbf{q}\cdot\mathbf{n}})(b^\dagger_{\mathbf{q}}-b_{-\mathbf{q}})\right]^2 . \tag{A8}$$

The initial ($\lambda=0$) conditions for solving the differential equations (A7) and (A8) can be derived from Eqs. (A2)–(A4); they are

$$[D^\sigma_{\mathbf{mn}}(\lambda)\pm F^\sigma_{\mathbf{mn}}(\lambda)]\,|_{\lambda=0}=d^\dagger_{\mathbf{m}\sigma}d_{\mathbf{n}\sigma}\pm f^\dagger_{\mathbf{m}\sigma}f_{\mathbf{n}\sigma} \tag{A9}$$

and

$$\frac{d}{d\lambda}[D^\sigma_{\mathbf{mn}}(\lambda)\pm F^\sigma_{\mathbf{mn}}(\lambda)]\Big|_{\lambda=0}=(f^\dagger_{\mathbf{m}\sigma}d_{\mathbf{n}\sigma}\pm d^\dagger_{\mathbf{m}\sigma}f_{\mathbf{n}\sigma})\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}[g(\mathbf{q})/\hbar\omega_q](e^{-i\mathbf{q}\cdot\mathbf{m}}\mp e^{-i\mathbf{q}\cdot\mathbf{n}})(b^\dagger_{\mathbf{q}}-b_{-\mathbf{q}}) . \tag{A10}$$

Equations (A7) and (A8) are second-order ordinary differential equations, the solutions of which under the initial conditions (A9) and (A10) can be obtained without difficulty,

$$D^\sigma_{\mathbf{mn}}(\lambda)+F^\sigma_{\mathbf{mn}}(\lambda)=(d^\dagger_{\mathbf{m}\sigma}f_{\mathbf{n}\sigma}+f^\dagger_{\mathbf{m}\sigma}d_{\mathbf{n}\sigma})\sinh[\lambda\hat{B}(\mathbf{n}-\mathbf{m})]+(d^\dagger_{\mathbf{m}\sigma}d_{\mathbf{n}\sigma}+f^\dagger_{\mathbf{m}\sigma}f_{\mathbf{n}\sigma})\cosh[\lambda\hat{B}(\mathbf{n}-\mathbf{m})] , \tag{A11}$$

$$D^\sigma_{\mathbf{mn}}(\lambda)-F^\sigma_{\mathbf{mn}}(\lambda)=(d^\dagger_{\mathbf{m}\sigma}f_{\mathbf{n}\sigma}-f^\dagger_{\mathbf{m}\sigma}d_{\mathbf{n}\sigma})\sinh[\lambda\hat{B}(\mathbf{n}+\mathbf{m})]+(d^\dagger_{\mathbf{m}\sigma}d_{\mathbf{n}\sigma}-f^\dagger_{\mathbf{m}\sigma}f_{\mathbf{n}\sigma})\cosh[\lambda\hat{B}(\mathbf{n}+\mathbf{m})] , \tag{A12}$$

where

$$\hat{B}(\mathbf{n}\pm\mathbf{m})=-\frac{1}{\sqrt{N}}\sum_{\mathbf{q}}[g(\mathbf{q})/\hbar\omega_{\mathbf{q}}](e^{-i\mathbf{q}\cdot\mathbf{n}}\pm e^{-i\mathbf{q}\cdot\mathbf{m}})(b_{\mathbf{q}}^{\dagger}-b_{-\mathbf{q}}) , \tag{A13}$$

and sinh and cosh represent the hyperbolic sine and cosine functions. From Eqs. (A11) and (A12) we can write out $D_{\mathrm{mn}}^{\sigma}(\lambda)$ and $F_{\mathrm{mn}}^{\sigma}(\lambda)$, respectively, as

$$\begin{aligned}e^{\hat{R}}d_{\mathrm{m}\sigma}^{\dagger}d_{\mathrm{n}\sigma}e^{-\hat{R}}=D_{\mathrm{mn}}^{\sigma}(1)=&\tfrac{1}{2}\{\cosh[\hat{B}(\mathbf{n}-\mathbf{m})]+\cosh[\hat{B}(\mathbf{n}+\mathbf{m})]\}d_{\mathrm{m}\sigma}^{\dagger}d_{\mathrm{n}\sigma}\\&+\tfrac{1}{2}\{\cosh[\hat{B}(\mathbf{n}-\mathbf{m})]-\cosh[\hat{B}(\mathbf{n}+\mathbf{m})]\}f_{\mathrm{m}\sigma}^{\dagger}f_{\mathrm{n}\sigma}\\&+\tfrac{1}{2}\{\sinh[\hat{B}(\mathbf{n}-\mathbf{m})]+\sinh[\hat{B}(\mathbf{n}+\mathbf{m})]\}d_{\mathrm{m}\sigma}^{\dagger}f_{\mathrm{n}\sigma}\\&+\tfrac{1}{2}\{\sinh[\hat{B}(\mathbf{n}-\mathbf{m})]-\sinh[\hat{B}(\mathbf{n}+\mathbf{m})]\}f_{\mathrm{m}\sigma}^{\dagger}d_{\mathrm{n}\sigma} ,\end{aligned} \tag{A14}$$

$$\begin{aligned}e^{\hat{R}}f_{\mathrm{m}\sigma}^{\dagger}f_{\mathrm{n}\sigma}e^{-\hat{R}}=F_{\mathrm{mn}}^{\sigma}(1)=&\tfrac{1}{2}\{\cosh[\hat{B}(\mathbf{n}-\mathbf{m})]-\cosh[\hat{B}(\mathbf{n}+\mathbf{m})]\}d_{\mathrm{m}\sigma}^{\dagger}d_{\mathrm{n}\sigma}\\&+\tfrac{1}{2}\{\cosh[\hat{B}(\mathbf{n}-\mathbf{m})]+\cosh[\hat{B}(\mathbf{n}+\mathbf{m})]\}f_{\mathrm{m}\sigma}^{\dagger}f_{\mathrm{n}\sigma}\\&+\tfrac{1}{2}\{\sinh[\hat{B}(\mathbf{n}-\mathbf{m})]-\sinh[\hat{B}(\mathbf{n}+\mathbf{m})]\}d_{\mathrm{m}\sigma}^{\dagger}f_{\mathrm{n}\sigma}\\&+\tfrac{1}{2}\{\sinh[\hat{B}(\mathbf{n}-\mathbf{m})]+\sinh[\hat{B}(\mathbf{n}+\mathbf{m})]\}f_{\mathrm{m}\sigma}^{\dagger}d_{\mathrm{n}\sigma} ,\end{aligned} \tag{A15}$$

where we have made the parameter λ equal to 1. Substituting Eqs. (A1), (A14), and (A15) into the unitary transformation $\hat{\tilde{H}}=e^{\hat{R}}\hat{H}e^{-\hat{R}}$, the transformed Hamiltonian $\hat{\tilde{H}}$ can be obtained and its explicit form is given in Eq. (9). It should be pointed out that in our treatment we have collected all higher-order terms of $g(\mathbf{q})$, so that the transformation making above is exact and no approximation has been involved.

For making the second unitary transformation (18), we need to define an operator function

$$f_{\mathbf{q}}(\lambda)=e^{\lambda\hat{S}}b_{\mathbf{q}}^{\dagger}e^{-\lambda\hat{S}} . \tag{A16}$$

Performing the differential operation on $f_{\mathbf{q}}(\lambda)$ and making use of the commutation relation $[\hat{S},b_{\mathbf{q}}^{\dagger}]=2\alpha_{\mathbf{q}}b_{-\mathbf{q}}$, we can obtain

$$\frac{d}{d\lambda}f_{\mathbf{q}}(\lambda)=e^{\lambda\hat{S}}2\alpha_{\mathbf{q}}b_{\mathbf{q}}e^{-\lambda\hat{S}}=2\alpha_{\mathbf{q}}e^{\lambda\hat{S}}b_{-\mathbf{q}}e^{-\lambda\hat{S}} . \tag{A17}$$

Performing the differential operation again we can obtain the following second-order ordinary differential equation:

$$\frac{d^2}{d\lambda^2}f_{\mathbf{q}}(\lambda)=2\alpha_{\mathbf{q}}e^{\lambda\hat{S}}[\hat{S},b_{-\mathbf{q}}]e^{-\lambda\hat{S}}=(2\alpha_{\mathbf{q}})^2e^{\lambda\hat{S}}b_{\mathbf{q}}^{\dagger}e^{-\lambda\hat{S}}=(2\alpha_{\mathbf{q}})^2f_{\mathbf{q}}(\lambda) . \tag{A18}$$

The solution of this equation under the initial conditions

$$f_{\mathbf{q}}(0)=b_{\mathbf{q}}^{\dagger} \tag{A19}$$

and

$$\left.\frac{d}{d\lambda}f_{\mathbf{q}}(\lambda)\right|_{\lambda=0}=2\alpha_{\mathbf{q}}b_{-\mathbf{q}} \tag{A20}$$

are

$$f_{\mathbf{q}}(\lambda)=b_{\mathbf{q}}^{\dagger}\cosh(2\alpha_{\mathbf{q}}\lambda)+b_{-\mathbf{q}}\sinh(2\alpha_{\mathbf{q}}\lambda) . \tag{A21}$$

It may be derived from Eqs. (A16) and (A21) that

$$e^{\lambda\hat{S}}b_{-\mathbf{q}}e^{-\lambda\hat{S}}=b_{\mathbf{q}}^{\dagger}\sinh(2\alpha_{\mathbf{q}}\lambda)+b_{-\mathbf{q}}\cosh(2\alpha_{\mathbf{q}}\lambda) . \tag{A22}$$

After making the parameter λ equal to 1 in Eqs. (A21) and (A22), they take the form of

$$e^{\hat{S}}b_{\mathbf{q}}^{\dagger}e^{-\hat{S}}=b_{\mathbf{q}}^{\dagger}\cosh(2\alpha_{\mathbf{q}})+b_{-\mathbf{q}}\sinh(2\alpha_{\mathbf{q}}) \tag{A23}$$

and

$$e^{\hat{S}}b_{-\mathbf{q}}e^{-\hat{S}}=b_{\mathbf{q}}^{\dagger}\sinh(2\alpha_{\mathbf{q}})+b_{-\mathbf{q}}\cosh(2\alpha_{\mathbf{q}}) . \tag{A24}$$

The following two equations can be derived from Eqs. (A23) and (A24) very easily,

$$e^{\hat{S}}(b_{\mathbf{q}}^{\dagger}\pm b_{-\mathbf{q}})e^{-\hat{S}}=(b_{\mathbf{q}}^{\dagger}\pm b_{-\mathbf{q}})e^{\pm 2\alpha_{\mathbf{q}}}\ , \tag{A25}$$

$$e^{\hat{S}}b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}e^{-\hat{S}}=(b_{\mathbf{q}}^{\dagger}\cosh 2\alpha_{\mathbf{q}}+b_{-\mathbf{q}}\sinh 2\alpha_{\mathbf{q}})(b_{-\mathbf{q}}^{\dagger}\sinh 2\alpha_{\mathbf{q}}+b_{\mathbf{q}}\cosh 2\alpha_{\mathbf{q}})\ . \tag{A26}$$

Substituting these two equations into the second unitary transformation (18), the transformed Hamiltonian $\hat{\tilde{H}}$ has been written out in Eq. (19). The second unitary transformation is also performed exactly and there are no omitted higher-order terms of this transformation.

APPENDIX B: BOGOLIUBOV TRANSFORMATION

In this appendix we give the practical procedure of the Bogoliubov transformation (26). In the Bloch representation, $\hat{H}_{\text{eff}}$ may be written as

$$\begin{aligned}\hat{H}_{\text{eff}}=&\sum_{\mathbf{q}}\hbar\omega_{\mathbf{q}}(\sinh 2\alpha_{\mathbf{q}})^2+\sum_{\mathbf{k},\sigma}\left[E_d'+\frac{T_d}{T_0}E_{\mathbf{k}}\right]d_{\mathbf{k}\sigma}^{\dagger}d_{\mathbf{k}\sigma}\\&+\sum_{\mathbf{k},\sigma}\left[E_f'+\frac{T_f}{T_0}E_{\mathbf{k}}\right]f_{\mathbf{k}\sigma}^{\dagger}f_{\mathbf{k}\sigma}+\frac{1}{N}U_{fd}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\sum_{\sigma}d_{\mathbf{k}\sigma}d_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}f_{\mathbf{k}'\bar{\sigma}}f_{\mathbf{k}'-\mathbf{q}\bar{\sigma}}^{\dagger}+\frac{1}{N}U_f\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}f_{\mathbf{k}\uparrow}f_{\mathbf{k}+\mathbf{q}\uparrow}^{\dagger}f_{\mathbf{k}'\downarrow}f_{\mathbf{k}'-\mathbf{q}\downarrow}^{\dagger}\\&+\frac{1}{N}U_d\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}d_{\mathbf{k}\uparrow}d_{\mathbf{k}+\mathbf{q}\uparrow}^{\dagger}d_{\mathbf{k}'\downarrow}d_{\mathbf{k}'-\mathbf{q}\downarrow}^{\dagger}-\frac{1}{N}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\sum_{\sigma,\sigma'}J(\mathbf{q})(f_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}d_{\mathbf{k}\sigma}+d_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}f_{\mathbf{k}\sigma})(f_{\mathbf{k}'-\mathbf{q}\sigma'}^{\dagger}d_{\mathbf{k}'\sigma'}+d_{\mathbf{k}'-\mathbf{q}\sigma'}^{\dagger}f_{\mathbf{k}'\sigma'})\\&-\frac{1}{N}U_{fd}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}(f_{\mathbf{k}+\mathbf{q}\uparrow}^{\dagger}d_{\mathbf{k}\uparrow}-d_{\mathbf{k}+\mathbf{q}\uparrow}^{\dagger}f_{\mathbf{k}\uparrow})(f_{\mathbf{k}'-\mathbf{q}\downarrow}^{\dagger}d_{\mathbf{k}'\downarrow}-d_{\mathbf{k}'-\mathbf{q}\downarrow}^{\dagger}f_{\mathbf{k}'\downarrow})\ ,\end{aligned} \tag{B1}$$

where $J(\mathbf{q})=|g(\mathbf{q})|^2/\hbar\omega_{\mathbf{q}}$ and $E_{\mathbf{k}}$ is the d-band function. Substituting the transformation (26) into (B1), $\hat{H}_{\text{eff}}$ is changed into the following form:

$$\begin{aligned}\hat{H}_{\text{eff}}=&\sum_{\mathbf{q}}\hbar\omega_{\mathbf{q}}(\sinh 2\alpha_{\mathbf{q}})^2+\sum_{\mathbf{k},\sigma}\left[u_{\mathbf{k}}^2\left[E_d'+\frac{T_d}{T_0}E_{\mathbf{k}}\right]+v_{\mathbf{k}}^2\left[E_f'+\frac{T_f}{T_0}E_{\mathbf{k}}\right]\right]\xi_{\mathbf{k}\sigma}^{\dagger}\xi_{\mathbf{k}\sigma}\\&+\sum_{\mathbf{k},\sigma}\left[v_{\mathbf{k}}^2\left[E_d'+\frac{T_d}{T_0}E_{\mathbf{k}}\right]+u_{\mathbf{k}}^2\left[E_f'+\frac{T_f}{T_0}E_{\mathbf{k}}\right]\right]\eta_{\mathbf{k}\sigma}\eta_{\mathbf{k}\sigma}^{\dagger}+\sum_{\mathbf{k},\sigma}u_{\mathbf{k}}v_{\mathbf{k}}\left[E_d'-E_f'+\frac{T_d-T_f}{T_0}E_{\mathbf{k}}\right](\xi_{\mathbf{k}\sigma}^{\dagger}\eta_{-\mathbf{k}\sigma}^{\dagger}+\eta_{-\mathbf{k}\sigma}\xi_{\mathbf{k}\sigma})\\&-\frac{1}{N}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\sum_{\sigma,\sigma'}J(\mathbf{q})[(v_{\mathbf{k}+\mathbf{q}}v_{\mathbf{k}}-u_{\mathbf{k}+\mathbf{q}}u_{\mathbf{k}})(\xi_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}\eta_{-\mathbf{k}\sigma}^{\dagger}+\eta_{-\mathbf{k}-\mathbf{q}\sigma}\xi_{\mathbf{k}\sigma})-2u_{\mathbf{k}}v_{\mathbf{k}}\delta_{\mathbf{q}0}\\&\qquad+(v_{\mathbf{k}+\mathbf{q}}u_{\mathbf{k}}+u_{\mathbf{k}+\mathbf{q}}v_{\mathbf{k}})\xi_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}\xi_{\mathbf{k}\sigma}+(u_{\mathbf{k}+\mathbf{q}}v_{\mathbf{k}}+v_{\mathbf{k}+\mathbf{q}}u_{\mathbf{k}})\eta_{-\mathbf{k}\sigma}^{\dagger}\eta_{-\mathbf{k}-\mathbf{q}\sigma}]\\&\qquad\times[(u_{\mathbf{k}'-\mathbf{q}}v_{\mathbf{k}'}-u_{\mathbf{k}'-\mathbf{q}}u_{\mathbf{k}'})(\xi_{\mathbf{k}'-\mathbf{q}\sigma'}^{\dagger}\eta_{-\mathbf{k}'\sigma'}^{\dagger}+\eta_{-\mathbf{k}'+\mathbf{q}\sigma'}\xi_{\mathbf{k}'\sigma'})-2u_{\mathbf{k}'}v_{\mathbf{k}'}\delta_{\mathbf{q}0}\\&\qquad\quad+(v_{\mathbf{k}'-\mathbf{q}}u_{\mathbf{k}'}+u_{\mathbf{k}'-\mathbf{q}}v_{\mathbf{k}'})\xi_{\mathbf{k}'-\mathbf{q}\sigma'}^{\dagger}\xi_{\mathbf{k}'\sigma'}+(u_{\mathbf{k}'-\mathbf{q}}v_{\mathbf{k}'}+v_{\mathbf{k}'-\mathbf{q}}u_{\mathbf{k}'})\eta_{-\mathbf{k}'\sigma'}^{\dagger}\eta_{-\mathbf{k}'+\mathbf{q}\sigma'}]\\&+\frac{1}{N}U_f\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}(v_{\mathbf{k}}^2\delta_{\mathbf{q}0}-v_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}}\xi_{\mathbf{k}+\mathbf{q}\uparrow}^{\dagger}\xi_{\mathbf{k}\uparrow}+u_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}}\eta_{-\mathbf{k}\uparrow}^{\dagger}\eta_{-\mathbf{k}-\mathbf{q}\uparrow}-u_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}}\eta_{-\mathbf{k}\uparrow}^{\dagger}\xi_{\mathbf{k}+\mathbf{q}\uparrow}^{\dagger}-v_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}}\xi_{\mathbf{k}\uparrow}\eta_{-\mathbf{k}-\mathbf{q}\uparrow})\\&\qquad\times(v_{\mathbf{k}'}^2\delta_{\mathbf{q}0}-v_{\mathbf{k}'}v_{\mathbf{k}'-\mathbf{q}}\xi_{\mathbf{k}'-\mathbf{q}\downarrow}^{\dagger}\xi_{\mathbf{k}'\downarrow}+u_{\mathbf{k}'}u_{\mathbf{k}'-\mathbf{q}}\eta_{-\mathbf{k}'\downarrow}^{\dagger}\eta_{-\mathbf{k}'+\mathbf{q}\downarrow}-u_{\mathbf{k}'}v_{\mathbf{k}'-\mathbf{q}}\eta_{-\mathbf{k}'\downarrow}^{\dagger}\xi_{\mathbf{k}'-\mathbf{q}\downarrow}^{\dagger}-v_{\mathbf{k}'}u_{\mathbf{k}'-\mathbf{q}}\xi_{\mathbf{k}'\downarrow}\eta_{-\mathbf{k}'+\mathbf{q}\downarrow})\\&+\frac{1}{N}U_d\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}(u_{\mathbf{k}}^2\delta_{\mathbf{q}0}-u_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}}\xi_{\mathbf{k}+\mathbf{q}\uparrow}^{\dagger}\xi_{\mathbf{k}\uparrow}+v_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}}\eta_{-\mathbf{k}\uparrow}^{\dagger}\eta_{-\mathbf{k}-\mathbf{q}\uparrow}+v_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}}\eta_{-\mathbf{k}\uparrow}^{\dagger}\xi_{\mathbf{k}+\mathbf{q}\uparrow}^{\dagger}+u_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}}\xi_{\mathbf{k}\uparrow}\eta_{-\mathbf{k}-\mathbf{q}\uparrow})\\&\qquad\times(u_{\mathbf{k}'}^2\delta_{\mathbf{q}0}-u_{\mathbf{k}'}u_{\mathbf{k}'-\mathbf{q}}\xi_{\mathbf{k}'-\mathbf{q}\downarrow}^{\dagger}\xi_{\mathbf{k}'\downarrow}+v_{\mathbf{k}'}v_{\mathbf{k}'-\mathbf{q}}\eta_{-\mathbf{k}'\downarrow}^{\dagger}\eta_{-\mathbf{k}'+\mathbf{q}\downarrow}+v_{\mathbf{k}'}u_{\mathbf{k}'-\mathbf{q}}\eta_{-\mathbf{k}'\downarrow}^{\dagger}\xi_{\mathbf{k}'-\mathbf{q}\downarrow}^{\dagger}+u_{\mathbf{k}'}v_{\mathbf{k}'-\mathbf{q}}\xi_{\mathbf{k}'\downarrow}\eta_{-\mathbf{k}'+\mathbf{q}\downarrow})\\&+\frac{1}{N}U_{fd}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\sum_{\sigma}(u_{\mathbf{k}}^2\delta_{\mathbf{q}0}-u_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}}\xi_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}\xi_{\mathbf{k}\sigma}+v_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}}\eta_{-\mathbf{k}\sigma}^{\dagger}\eta_{-\mathbf{k}-\mathbf{q}\sigma}+v_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}}\eta_{-\mathbf{k}\sigma}^{\dagger}\xi_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger}+u_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}}\xi_{\mathbf{k}\sigma}\eta_{-\mathbf{k}-\mathbf{q}\sigma})\\&\qquad\times(v_{\mathbf{k}'}^2\delta_{\mathbf{q}0}-v_{\mathbf{k}'}v_{\mathbf{k}'-\mathbf{q}}\xi_{\mathbf{k}'-\mathbf{q}\bar{\sigma}}^{\dagger}\xi_{\mathbf{k}'\bar{\sigma}}+u_{\mathbf{k}'}u_{\mathbf{k}'-\mathbf{q}}\eta_{-\mathbf{k}'\mathbf{q}}^{\dagger}\eta_{-\mathbf{k}'+\mathbf{q}\bar{\sigma}}-u_{\mathbf{k}'}v_{\mathbf{k}'-\mathbf{q}}\eta_{-\mathbf{k}'\bar{\sigma}}^{\dagger}\xi_{\mathbf{k}'-\mathbf{q}\bar{\sigma}}^{\dagger}-v_{\mathbf{k}'}u_{\mathbf{k}'-\mathbf{q}}\xi_{\mathbf{k}'\bar{\sigma}}\eta_{-\mathbf{k}'+\mathbf{q}\bar{\sigma}})\\&-\frac{1}{N}U_{fd}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}[(v_{\mathbf{k}+\mathbf{q}}\xi_{\mathbf{k}+\mathbf{q}\uparrow}^{\dagger}-u_{\mathbf{k}+\mathbf{q}}\eta_{-\mathbf{k}-\mathbf{q}\uparrow})(u_{\mathbf{k}}\xi_{\mathbf{k}\uparrow}+v_{\mathbf{k}}\eta_{-\mathbf{k}\uparrow}^{\dagger})-(u_{\mathbf{k}+\mathbf{q}}\xi_{\mathbf{k}+\mathbf{q}\uparrow}^{\dagger}+v_{\mathbf{k}+\mathbf{q}}\eta_{-\mathbf{k}-\mathbf{q}\uparrow})(v_{\mathbf{k}}\xi_{\mathbf{k}\uparrow}-u_{\mathbf{k}}\eta_{-\mathbf{k}\uparrow}^{\dagger})]\\&\qquad\times[(v_{\mathbf{k}'-\mathbf{q}}\xi_{\mathbf{k}'-\mathbf{q}\downarrow}^{\dagger}-u_{\mathbf{k}'-\mathbf{q}}\eta_{-\mathbf{k}'+\mathbf{q}\downarrow})(u_{\mathbf{k}'}\xi_{\mathbf{k}'\downarrow}+v_{\mathbf{k}'}\eta_{-\mathbf{k}'\downarrow}^{\dagger})\\&\qquad\quad-(u_{\mathbf{k}'-\mathbf{q}}\xi_{\mathbf{k}'-\mathbf{q}\downarrow}^{\dagger}+v_{\mathbf{k}'-\mathbf{q}}\eta_{-\mathbf{k}'+\mathbf{q}\downarrow})(v_{\mathbf{k}'}\xi_{\mathbf{k}'\downarrow}-u_{\mathbf{k}'}\eta_{-\mathbf{k}'\downarrow}^{\dagger})]\ .\end{aligned} \tag{B2}$$

This form is more complicated and it contains c-number terms, second-order diagonal terms, second-order nondiagonal terms, and fourth-order terms which should be normal ordered. The c-number terms are

$$E=\sum_{\mathbf{q}}\hbar\omega_{\mathbf{q}}[\sinh 2\alpha_{\mathbf{q}}]^2+\sum_{\mathbf{k},\sigma}\left[v_{\mathbf{k}}^2\left[E_d'+\frac{T_d}{T_0}E_{\mathbf{k}}\right]+u_{\mathbf{k}}^2\left[E_f'+\frac{T_f}{T_0}E_{\mathbf{k}}\right]\right]$$
$$-\frac{16}{N}J(0)\sum_{\mathbf{k},\mathbf{k}'}u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{k}'}v_{\mathbf{k}'}+\frac{4}{N}\sum_{\mathbf{k},\mathbf{q}}J(\mathbf{q})u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}}v_{\mathbf{k}+\mathbf{q}}$$
$$-\frac{2}{N}\sum_{\mathbf{k},\mathbf{q}}J(\mathbf{q})(v_{\mathbf{k}+\mathbf{q}}^2v_{\mathbf{k}}^2+u_{\mathbf{k}}^2u_{\mathbf{k}+\mathbf{q}}^2)+\frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'}(u_fv_{\mathbf{k}}^2v_{\mathbf{k}'}^2+u_du_{\mathbf{k}}^2u_{\mathbf{k}'}^2+2u_{fd}u_{\mathbf{k}}^2v_{\mathbf{k}'}^2)\ , \tag{B3}$$

where we have designated the sum of the c-number terms as E because we shall show below that this sum is just the quantity $E=\langle\bar{\Psi}_e\,|\,\hat{H}_{\rm eff}\,|\,\bar{\Psi}_e\rangle$ we want to obtain. The second-order diagonal terms are

$$\sum_{\mathbf{k},\sigma}\xi_{\mathbf{k}\sigma}^{\dagger}\xi_{\mathbf{k}\sigma}\left[u_{\mathbf{k}}^2\left[E_d'+\frac{T_d}{T_0}E_{\mathbf{k}}\right]+v_{\mathbf{k}}^2\left[E_f'+\frac{T_f}{T_0}E_{\mathbf{k}}\right]+16J(0)u_{\mathbf{k}}v_{\mathbf{k}}\left[\frac{1}{N}\sum_{\mathbf{k}'}u_{\mathbf{k}'}v_{\mathbf{k}'}\right]\right.$$
$$-\frac{1}{N}\sum_{\mathbf{q}}J(\mathbf{q})[(v_{\mathbf{k}}u_{\mathbf{k}-\mathbf{q}}+u_{\mathbf{k}}v_{\mathbf{k}-\mathbf{q}})^2-(v_{\mathbf{k}+\mathbf{q}}v_{\mathbf{k}}-u_{\mathbf{k}+\mathbf{q}}u_{\mathbf{k}})^2]$$
$$\left.-U_fv_{\mathbf{k}^2}\left[\frac{1}{N}\sum_{\mathbf{k}}v_{\mathbf{k}'}^2\right]-U_du_{\mathbf{k}}^2\left[\frac{1}{N}\sum_{\mathbf{k}'}u_{\mathbf{k}'}^2\right]-U_{fd}u_{\mathbf{k}}^2\left[\frac{1}{N}\sum_{\mathbf{k}'}v_{\mathbf{k}'}^2\right]-U_{fd}v_{\mathbf{k}}^2\left[\frac{1}{N}\sum_{\mathbf{k}'}u_{\mathbf{k}'}^2\right]\right]$$
$$+\sum_{\mathbf{k},\sigma}\eta_{\mathbf{k}\sigma}^{\dagger}\eta_{\mathbf{k}\sigma}\left[-v_{\mathbf{k}}^2\left[E_d'+\frac{T_d}{T_0}E_{\mathbf{k}}\right]-u_{\mathbf{k}}^2\left[E_f'+\frac{T_f}{T_0}E_{\mathbf{k}}\right]+16J(0)u_{\mathbf{k}}v_{\mathbf{k}}\left[\frac{1}{N}\sum_{\mathbf{k}'}u_{\mathbf{k}'}v_{\mathbf{k}'}\right]\right.$$
$$-\frac{1}{N}\sum_{\mathbf{q}}J(\mathbf{q})[(u_{\mathbf{k}+\mathbf{q}}v_{\mathbf{k}}+v_{\mathbf{k}+\mathbf{q}}u_{\mathbf{k}})^2-(v_{\mathbf{k}-\mathbf{q}}v_{\mathbf{k}}-u_{\mathbf{k}-\mathbf{q}}u_{\mathbf{k}})^2]$$
$$\left.+U_fu_{\mathbf{k}}^2\left[\frac{1}{N}\sum_{\mathbf{k}'}v_{\mathbf{k}'}^2\right]+U_dv_{\mathbf{k}}^2\left[\frac{1}{N}\sum_{\mathbf{k}'}u_{\mathbf{k}'}^2\right]+U_{fd}u_{\mathbf{k}}^2\left[\frac{1}{N}\sum_{\mathbf{k}'}u_{\mathbf{k}'}^2\right]+U_{fd}v_{\mathbf{k}}^2\left[\frac{1}{N}\sum_{\mathbf{k}'}v_{\mathbf{k}'}^2\right]\right]$$
$$=\sum_{\mathbf{k},\sigma}[\tfrac{1}{2}(u_{\mathbf{k}}^2-v_{\mathbf{k}}^2)F(\mathbf{k})+2G(\mathbf{k})u_{\mathbf{k}}v_{\mathbf{k}}+\tfrac{1}{2}S(\mathbf{k})]\xi_{\mathbf{k}\sigma}^{\dagger}\xi_{\mathbf{k}\sigma}+\sum_{\mathbf{k},\sigma}[\tfrac{1}{2}(u_{\mathbf{k}}^2-v_{\mathbf{k}}^2)F(\mathbf{k})+2G(\mathbf{k})u_{\mathbf{k}}v_{\mathbf{k}}-\tfrac{1}{2}S(\mathbf{k})]\eta_{\mathbf{k}\sigma}^{\dagger}\eta_{\mathbf{k}\sigma}\ . \tag{B4}$$

The second-order nondiagonal terms are

$$\sum_{\mathbf{k},\sigma}(\xi_{\mathbf{k}\sigma}^{\dagger}\eta_{-\mathbf{k}\sigma}^{\dagger}+\eta_{-\mathbf{k}\sigma}\xi_{\mathbf{k}\sigma})\left[u_{\mathbf{k}}v_{\mathbf{k}}\left[E_d'-E_f'+\frac{T_d-T_f}{T_0}E_{\mathbf{k}}\right]+8J(0)(v_{\mathbf{k}}^2-u_{\mathbf{k}}^2)\left[\frac{1}{N}\sum_{\mathbf{k}'}u_{\mathbf{k}'}v_{\mathbf{k}'}\right]\right.$$
$$-\frac{2}{N}\sum_{\mathbf{q}}J(\mathbf{q})(u_{\mathbf{k}+\mathbf{q}}v_{\mathbf{k}}+v_{\mathbf{k}+\mathbf{q}}u_{\mathbf{k}})(v_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}}-u_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}})$$
$$\left.+u_{\mathbf{k}}v_{\mathbf{k}}\left[\frac{U_f}{N}\sum_{\mathbf{k}'}v_{\mathbf{k}'}^2-\frac{U_d}{N}\sum_{\mathbf{k}'}u_{\mathbf{k}'}^2-\frac{U_{fd}}{N}\sum_{\mathbf{k}'}(v_{\mathbf{k}'}^2-u_{\mathbf{k}'}^2)\right]\right]$$
$$=\sum_{\mathbf{k},\sigma}[F(\mathbf{k})u_{\mathbf{k}}v_{\mathbf{k}}+G(\mathbf{k})(v_{\mathbf{k}}^2-u_{\mathbf{k}}^2)](\xi_{\mathbf{k}\sigma}^{\dagger}\eta_{-\mathbf{k}\sigma}^{\dagger}+\eta_{-\mathbf{k}\sigma}\xi_{\mathbf{k}\sigma})\ . \tag{B5}$$

In Eqs. (B4) and (B5) we have used the following functions:

$$G(\mathbf{k})=\frac{8}{N}J(0)\sum_{\mathbf{k}'}u_{\mathbf{k}'}v_{\mathbf{k}'}-\frac{2}{N}\sum_{\mathbf{q}}J(\mathbf{q})u_{\mathbf{k}+\mathbf{q}}v_{\mathbf{k}+\mathbf{q}}\ , \tag{B6}$$

$$F(\mathbf{k})=E_d'-E_f'+\frac{T_d-T_f}{T_0}E_{\mathbf{k}}-\frac{2}{N}\sum_{\mathbf{q}}J(\mathbf{q})(v_{\mathbf{k}+\mathbf{q}}^2-u_{\mathbf{k}+\mathbf{q}}^2)+U_fn_d-U_dn_f-U_{fd}n_d+U_{fd}n_f\ , \tag{B7}$$

$$S(\mathbf{k})=E_d'+E_f'+\frac{T_d-T_f}{T_0}E_{\mathbf{k}}-U_dn_f-U_fn_d-U_{fd}\ , \tag{B8}$$

$$n_f=\frac{1}{N}\sum_{\mathbf{k}}u_{\mathbf{k}}^2,\quad n_d=\frac{1}{N}\sum_{\mathbf{k}}v_{\mathbf{k}}^2\ . \tag{B9}$$

The sum of fourth-order terms, in which the collective fermion operators are of normal order already, is designated as

$\hat{H}_{\text{eff}}^{(4)}$ and the explicit form of $\hat{H}_{\text{eff}}^{(4)}$ is not given here because in this paper we are concerned only about the properties of the variational ground state.

According to the method of Valatin[22] and Bogoliubov,[23] we should eliminate the second-order nondiagonal terms in Eq. (B5) by proper choice of $u_{\mathbf{k}}$'s and $v_{\mathbf{k}}$'s. This aim can be easily arrived at under the condition that

$$F(\mathbf{k})u_{\mathbf{k}}v_{\mathbf{k}}+G(\mathbf{k})(v_{\mathbf{k}}^2-u_{\mathbf{k}}^2)=0\ . \tag{B10}$$

Equation (B10) and $u_{\mathbf{k}}^2+v_{\mathbf{k}}^2=1$ must be solved simultaneously to determine $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. The solutions are

$$u_{\mathbf{k}}=\left[\frac{1}{2}+\frac{1}{2}\frac{F(\mathbf{k})}{[F^2(\mathbf{k})+4G^2(\mathbf{k})]^{1/2}}\right]^{1/2},\quad v_{\mathbf{k}}=\left[\frac{1}{2}-\frac{1}{2}\frac{F(\mathbf{k})}{[F^2(\mathbf{k})+4G^2(\mathbf{k})]^{1/2}}\right]^{1/2}. \tag{B11}$$

After substituting (B11) into (B3) and (B4), we obtain the Bogoliubov-transformed form of $\hat{H}_{\text{eff}}$ and it is written out in Eq. (28).

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