Correlated squeezed-state approach for the ground state of a system with strong electron-phonon interaction

C. F. Lo
Department of Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong

E. Manousakis
Department of Physics, Florida State University, Tallahassee, Florida 32306

R. Sollie
Department of Physics, University of Trondheim, N-7034 Trondheim-NTH, Norway and IKU, Sintef, N-7034 Trondheim, Norway

Y. L. Wang
Department of Physics, Florida State University, Tallahassee, Florida 32306
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We have investigated the ground state of an electron-phonon system with strong electron-phonon interaction and a weak on-site Coulomb repulsion using the correlated squeezed-state approach. We have introduced a variational ground state in which the phonon subsystem is in a correlated squeezed state and the electron subsystem is in a superconducting pairing state. In addition to the anharmonicity of each phonon mode induced by the linear coupling with the electrons, the correlated squeezed state is able to take into account the nonlinearity of the induced interaction between different phonon modes beyond the Hartree approximation. Also, with optimal values of the variational parameters this trial state will by construction yield an energy lower than those obtained in previous studies, and thus our variational ansatz is a more stable ground state for this system. Furthermore, in this approximate ground state the reduction effect of phonons is much more alleviated, and thus the mass enhancement inherent to the polaron effect is considerably weakened. This weakening of the reduction effect should, in turn, affect other physical properties of the system; for instance, it does suggest the possibility of higher critical temperatures for superconductivity in the strong-coupling limit where the superfluidlike bipolaronic superconductivity is supposed to occur.

I. INTRODUCTION

The study of the behavior of coupled electron-phonon systems has long been an active research area in condensed matter physics because of its significance in determining the resultant electronic properties such as superconductivity or electron-driven instabilities. Recently the interest in the interplay of electron-electron and electron-phonon interactions in strongly correlated fermion systems has been further intensified by the discovery of high-temperature superconducting materials. The role of electron-phonon coupling is of special interest in view of the close proximity of these materials, e.g., $La_{2-x}Ba_xCuO_4$, to structural, insulating antiferromagnetic, and superconducting instabilities. A simple model that could account for such a complex phase diagram is an extension of the Hubbard model where one couples the electrons to phonons linearly. In this paper we shall study a model which involves optical Holstein-phonon modes coupled strongly to electrons which interact via an effective on-site Coulomb repulsion. Such a model could be general enough to also capture some aspects of the physics of the C_{60}-based superconductors where it is possible that the electrons coupled to the on-fullerene phonons may give rise to the observed superconductivity in these materials.

The physics of narrow-band electrons coupled to Holstein phonons is governed by three competing effects: the itinerancy of the electrons, the Coulomb repulsion, and the local electron-phonon coupling. With strong electron-phonon interaction each electron carries with itself a lattice deformation in a coherent way, forming what is called a small polaron, severely localized in its own potential well.[1] Provided that the interaction is strong enough for the on-site electron-electron correlation to be attractive after renormalization, the small polarons form spatially overlapping Cooper pairs with superconducting properties similar to ordinary BCS superconductivity, except for a few differences in the gap equations as well as in the expressions for the critical temperature T_c.[2–4] Furthermore, if the polaron-polaron attractive interaction is strong enough, a superfluidlike superconductivity, so-called bipolaronic superconductivity, will occur.[5–9] The polaron effect can increase the electron mass by a factor 10^2–10^4, and much more for a bipolaron. Thus, starting from the BCS limit the pairing first increases with the coupling, but for too large coupling the local pairs become essentially localized and the critical temperatures

extremely small. The intermediate region is very difficult to treat due to the failure of perturbation theories. Nevertheless, this region is of the greatest interest for it is expected to yield the highest critical temperatures for superconductivity.

Recently Zheng proposed a squeezed-state approach for dealing with the superconducting properties of systems of strong electron-phonon interaction which are described by the Hubbard model with a local Holstein-type electron-phonon interaction.[10] He showed that a better variational ground state of such a system is obtained by assuming a squeezed state for the phonon subsystem instead of the conventional coherent state. The squeezed state has the virtue that the anharmonicity of each phonon mode induced by coupling with the electrons is being taken into account.[11–14] It is shown that the "squeezing" effect noticeably weakens the mass enhancement inherent to the polaron effect. Therefore, despite that Zheng's investigation is based on a weak-coupling mean-field theory treatment, it is sugguested that by means of the squeezed polaronic state higher critical temperatures for superconductivity can be attained in the strong-coupling limit where the superfluidlike bipolaronic superconductivity is supposed to occur.

Nevertheless, both the squeezed-state and conventional coherent-state trial wave functions for the ground state of the phonon subsystem are within the Hartree approximation and thus uncorrelated. In order to account for the strong phonon correlation and anharmonicity of the interaction between different phonon modes induced by the linear coupling with the electrons, one needs to go beyond the Hartree approximation. In this paper we shall introduce the correlated squeezed-state ansatz as a candidate for the ground state of the phonon subsystem. The variational treatment consists of the following steps: First, a unitary displacement transformation and a squeezing transformation are applied to our model Hamiltonian. Next, a variational wave function for the phonon subsystem is used to take into account the intersite phonon correlation effects and we integrate out the phonon degrees of freedom to obtain an effective electronic Hamiltonian which can yield an attractive on-site interaction for strong enough electron-phonon coupling. A weak-coupling mean-field theory treatment of the resulting effective Hamiltonian is used to obtain the ground state of our model system.[7] Our results are in general agreement with those obtained by Zheng but somewhat more accurate.[10] We generally find that the usual Holstein factor is much larger in our correlated approach compared to Holstein's result and thus the polaron hopping suppression effect is much more alleviated in our calculation.

In Sec. II we shall apply the correlated squeezed-state approach to the ground state of a system of strong electron-phonon interaction described by the Hubbard model with a local Holstein-type electron-phonon coupling. Numerical results for some special cases as well as our conclusions will be discussed in Sec. III.

II. FORMULATION

Our model Hamiltonian is a generalization of the standard Hamiltonian first introduced by Holstein[1] to describe electrons locally coupled to molecularlike oscillators; it includes an additional Hubbard correlation term

$$H=\sum_{i,\sigma}(E-\mu)d_{i\sigma}^{\dagger}d_{i\sigma}+\sum_{(i,j)}\sum_{\sigma}Td_{i\sigma}^{\dagger}d_{j\sigma}+\sum_{i}\hbar\omega b_i^{\dagger}b_i+\sum_{i}Ud_{i\uparrow}^{\dagger}d_{i\uparrow}d_{i\downarrow}^{\dagger}d_{i\downarrow}+\sum_{i,\sigma}gd_{i\sigma}^{\dagger}d_{i\sigma}(b_i^{\dagger}+b_i), \tag{1}$$

where μ is the chemical potential, $d_{i\sigma}^{\dagger}$ and $d_{i\sigma}$ are the creation and annihilation operators of electrons, $b_i^{\dagger}$ and b_i are the creation and annihilation operators of phonons, and $\sum_{(i,j)}$ denotes the sum over nearest neighbor sites. This model is an example of a more general class of coupled electron-phonon models. It is characterized by a dispersionless branch of phonons, and by a linear and local coupling between the electron density and the lattice deformation. We shall hereafter limit ourselves to this simple model which contains essentially all the important physics of the problem. Generalization to phonons with dispersion or nonlocal coupling is straightforward and will be presented elsewhere.

Applying the Lang-Firsov unitary displacement transformation[15]

$$D=\exp\left\{-\frac{g}{\hbar\omega}\sum_{i,\sigma}d_{i\sigma}^{\dagger}d_{i\sigma}(b_i^{\dagger}-b_i)\right\} \tag{2}$$

to the Hamiltonian in Eq. (1), we obtain

$$\bar{H}=D^{\dagger}HD=\sum_{i,\sigma}(E-\mu)d_{i\sigma}^{\dagger}d_{i\sigma}+\sum_{(i,j)}\sum_{\sigma}Td_{i\sigma}^{\dagger}d_{j\sigma}\exp\left\{\frac{g}{\hbar\omega}[(b_i^{\dagger}-b_i)-(b_j^{\dagger}-b_j)]\right\}+\sum_{i}\hbar\omega b_i^{\dagger}b_i+\sum_{i}Ud_{i\uparrow}^{\dagger}d_{i\uparrow}d_{i\downarrow}^{\dagger}d_{i\downarrow}-\sum_{i}\sum_{\sigma,\sigma'}\frac{g^2}{\hbar\omega}d_{i\sigma}^{\dagger}d_{i\sigma}d_{i\sigma'}^{\dagger}d_{i\sigma'}\ . \tag{3}$$

This shows that the linear coupling with the electrons induces nonlinear interactions between phonons not only in the same mode, but also in different modes. At this point one could suppose that the electron and the phonon subsystems might be decoupled by making an average of $\bar{H}$ over the vacuum state of the phonon subsystem and a Holstein reduction factor $\exp[-g^2/(\hbar\omega)^2]$ is obtained. This is the usual way of dealing with the electron-phonon interaction in discussing the small polaron problem.[1,16,17] However, as pointed out in Sec. I, for a strong electron-phonon interaction the reduction effect would be fairly strong and make the ground-state energy of the inter-

acting system increase. In order to lower the ground-state energy, we shall develop here a variational treatment based on the correlated squeezed states.

First, to account for the anharmonicity of each phonon mode, we shall perform the unitary squeezing transformation[11–14]

$$S = \exp\left\{\alpha \sum_i (b_i^{\dagger 2} - b_i^2)\right\} \tag{4}$$

to the Hamiltonian $\bar{H}$ such that

$$\begin{aligned}\tilde{H} &= S^\dagger \bar{H} S \\ &= \sum_{i,\sigma}(E-\mu) d_{i\sigma}^\dagger d_{i\sigma} + \sum_{(i,j)}\sum_\sigma T d_{i\sigma}^\dagger d_{j\sigma} \exp\left\{\frac{g}{\hbar\omega}\exp(-2\alpha)[(b_i^\dagger - b_i) - (b_j^\dagger - b_j)]\right\} \\ &\quad + \frac{1}{4}\sum_i \hbar\omega \exp(4\alpha)(b_i^\dagger + b_i)^2 - \frac{1}{4}\sum_i \hbar\omega \exp(-4\alpha)(b_i^\dagger - b_i)^2 \\ &\quad - \frac{1}{2}\sum_i \hbar\omega + \sum_i U d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow} - \sum_i \sum_{\sigma,\sigma'} \frac{g^2}{\hbar\omega} d_{i\sigma}^\dagger d_{i\sigma} d_{i\sigma'}^\dagger d_{i\sigma'} \ .\end{aligned} \tag{5}$$

It is quite obvious that the Hamiltonian $\tilde{H}$ cannot be solved exactly, and so we shall tackle it approximately by the variational approach. Taking into account the correlation between different phonon modes, we next propose a generalized multimode squeezed vacuum state as the trial wave function for the ground state of the phonon subsystem:[18]

$$\begin{aligned}|\Psi_p\rangle &= \exp\left\{\frac{1}{2}\sum_{i\neq j}\beta_{ij}(b_i^\dagger b_j^\dagger - b_i b_j)\right\}|\text{vac}\rangle \\ &\equiv \tilde{S}(\{\beta_{ij}\})|\text{vac}\rangle \ ,\end{aligned} \tag{6}$$

where $\beta_{ij} = \beta_{ji}$. The generalized multimode squeeze operator $\tilde{S}(\{\beta_{ij}\})$ transforms the annihilation and creation operators as follows:

$$\tilde{S}^\dagger \mathbf{a}\, \tilde{S} = \cosh(|\boldsymbol{\beta}|)\,\mathbf{a} + \sinh(|\boldsymbol{\beta}|)\,|\boldsymbol{\beta}|^{-1}\boldsymbol{\beta}\,\mathbf{a}^\dagger \ , \tag{7}$$

$$\tilde{S}^\dagger \mathbf{a}^\dagger \tilde{S} = \cosh(|\boldsymbol{\beta}|^T)\,\mathbf{a}^\dagger + \sinh(|\boldsymbol{\beta}|^T)\,(|\boldsymbol{\beta}|^T)^{-1}\boldsymbol{\beta}^*\,\mathbf{a} \ , \tag{8}$$

where $|\boldsymbol{\beta}|^T$ is the transpose of $|\boldsymbol{\beta}|$, i.e., $(|\boldsymbol{\beta}|^T)_{ij} = |\boldsymbol{\beta}|_{ji}$, $\mathbf{a}$ is the column vector consisting of annihilation operators a_i $(i = 1, 2, ..., N)$, and $\mathbf{a}^\dagger$ is the vector of creation operators. Here the matrices $|\boldsymbol{\beta}|$ and $|\boldsymbol{\beta}|^{-1}$ are defined in the following way:

$$(|\boldsymbol{\beta}|^2)_{ij} = \sum_{k=1}^N (|\boldsymbol{\beta}|)_{ik}(|\boldsymbol{\beta}|)_{kj} = \sum_{k=1}^N \beta_{ik}\beta_{kj}^* \ , \tag{9}$$

$$\delta_{ij} = \sum_{k=1}^N (|\boldsymbol{\beta}|^{-1})_{ik}(|\boldsymbol{\beta}|)_{kj} \ , \tag{10}$$

so that

$$[\cosh(|\boldsymbol{\beta}|)]_{ij} = \delta_{ij} + \frac{1}{2!}\sum_{k=1}^N \beta_{ik}\beta_{kj}^* + \frac{1}{4!}\sum_{k,l,m=1}^N \beta_{ik}\beta_{kl}^*\beta_{lm}\beta_{mj}^* + \cdots \ , \tag{11}$$

$$\begin{aligned}[\sinh(|\boldsymbol{\beta}|)\,|\boldsymbol{\beta}|^{-1}\boldsymbol{\beta}]_{ij} &= \sum_{k,l=1}^N [\sinh(|\boldsymbol{\beta}|)]_{ik}(|\boldsymbol{\beta}|^{-1})_{kl}(\boldsymbol{\beta})_{lj} \\ &= \frac{1}{1!}\beta_{ij} + \frac{1}{3!}\sum_{k,l=1}^N \beta_{ik}\beta_{kl}^*\beta_{lj} \\ &\quad + \frac{1}{5!}\sum_{k,l,m,n=1}^N \beta_{ik}\beta_{kl}^*\beta_{lm}\beta_{mn}^*\beta_{nj} \\ &\quad + \cdots .\end{aligned} \tag{12}$$

[Note that we have set $\beta_{ii} = 0$ $(i = 1, 2, ..., N)$ so that the restriction on the double sum in Eq. (6) can be lifted.] Furthermore, provided $\boldsymbol{\beta}$ is real, the generalized multimode squeezed state is a multimode minimum-uncertainty state, which exhibits generalized multimode squeezing in the fluctuations of the phonon field modes.

This correlated squeezed-state approach has been applied earlier to the linear E-e Jahn-Teller effect, a tunneling particle coupled to phonons and some coupled electron-phonon systems.[19–22] Taking the average of $\tilde{H}$ over the state $|\Psi_p\rangle$, we obtain an effective Hamiltonian for the electron subsystem as follows:

$$\begin{aligned}H_{\text{eff}} &= \langle\Psi_p|\tilde{H}|\Psi_p\rangle \\ &= \sum_{i,\sigma}(E_e-\mu) d_{i\sigma}^\dagger d_{i\sigma} + \sum_{(i,j)}\sum_\sigma T_e d_{i\sigma}^\dagger d_{j\sigma} + \frac{1}{4}\sum_i \hbar\omega\exp(4\alpha)[\exp(2\boldsymbol{\beta})]_{00} \\ &\quad + \frac{1}{4}\sum_i \hbar\omega\exp(-4\alpha)[\exp(-2\boldsymbol{\beta})]_{00} - \frac{1}{2}\sum_i \hbar\omega + \sum_i U_e d_{i\uparrow}^\dagger d_{i\uparrow} d_{i\downarrow}^\dagger d_{i\downarrow},\end{aligned} \tag{13}$$

where $E_e = E - J$, $U_e = U - 2J$ and $J = g^2/\hbar\omega$. The renormalized hopping integral T_e has the form

$$T_e = \eta T = T\exp\left\{-\frac{J}{\hbar\omega}\exp(-4\alpha)\{[\exp(-2\beta)]_{00} - [\exp(-2\beta)]_{0\delta}\}\right\}. \quad (14)$$

Here 0 denotes the origin and δ its nearest neighbor site. It is clear that the renormalized correlation U_e could be negative, and in what follows we would concentrate on the case that $U_e < 0$. Also, it should be noted that a new factor $\exp(-4\alpha)\{[\exp(-2\beta)]_{00} - [\exp(-2\beta)]_{0\delta}\}$ has appeared in the exponent of the usual reduction factor. As long as $\alpha \neq 0$ and $\beta_{ij} \neq 0$, the band-narrowing effect of phonons would be modified and the ground-state energy of the interacting system lowered. If $\alpha = \beta_{ij} = 0$, $|\Psi_p\rangle$ will return to the vacuum state $|\text{vac}\rangle$, whereas if only β_{ij} vanishes, $|\Psi_p\rangle$ will reduce to Zheng's squeezed-state ansatz. Therefore, our variational wave function by construction gives a better representation of the ground state of the phonon subsystem.

Thus after integrating out the phonon degrees of freedom our effective Hamiltonian is the negative-U Hubbard model. Here we shall consider the weak-coupling limit of the model (since we expect that U_e to be smaller than the electron bandwidth) where a mean-field approach[7] to obtain the ground state of our model system may be applicable. Taking advantage of the results of Ref. 7, we can write directly the expressions for the ground-state energy (Ω_0) and the gap (Δ_0) equation of the superconducting state of the effective Hamiltonian H_{eff} as follows:

$$\frac{\Omega_0}{N} = \frac{1}{4}\hbar\omega\{\exp(4\alpha)[\exp(2\beta)]_{00} + \exp(-4\alpha)[\exp(-2\beta)]_{00}\} - \frac{1}{2}\hbar\omega + E_e - \mu_0 - \frac{|U_e|n}{2} + \frac{|U_e|n^2}{4} + \frac{\Delta_0^2}{|U_e|} - \frac{1}{N}\sum_{\vec{k}}\sqrt{E(\vec{k})^2 + \Delta_0^2}, \quad (15)$$

$$n = 1 - \frac{1}{N}\sum_{\vec{k}}\frac{E(\vec{k})}{\sqrt{E(\vec{k})^2 + \Delta_0^2}}, \quad (16)$$

$$\Delta_0 = \frac{1}{2N}\sum_{\vec{k}}\frac{|U_e|\Delta_0}{\sqrt{E(\vec{k})^2 + \Delta_0^2}}, \quad (17)$$

where

$$E(\vec{k}) = E_e - \mu_0 - \frac{|U_e|n}{2} + \eta E_{\vec{k}}, \quad (18)$$

$$E_{\vec{k}} = T\sum_{j(0)}\exp(i\vec{k}\cdot\vec{r}_j), \quad (19)$$

with $\sum_{j(0)}$ denoting the sum over the nearest neighbor sites around the origin. Clearly, $\Delta_0 = 0$ is a trivial solution of Eq. (17). Assuming a square density of states of the electrons,

$$\rho(\epsilon) = \begin{cases} \frac{1}{2D} & \text{for } |\epsilon| \leq D, \\ 0 & \text{otherwise,} \end{cases} \quad (20)$$

analytical results can be obtained, and it can be easily verified that the solutions of Eqs. (15)–(17) are given by (i) $\Delta_0 \neq 0$:

$$E_e - \mu_0 - \frac{|U_e|n}{2} = (1-n)\eta D\coth\left(\frac{2\eta D}{|U_e|}\right), \quad (21)$$

$$\Delta_0 = \frac{\sqrt{n(2-n)}\,\eta D}{\sinh(2\eta D/|U_e|)}, \quad (22)$$

$$\frac{\Omega_0}{N} = \frac{1}{4}\hbar\omega\{\exp(4\alpha)[\exp(2\beta)]_{00} + \exp(-4\alpha)[\exp(-2\beta)]_{00}\} - \frac{1}{2}\hbar\omega + \frac{|U_e|n^2}{4} - \frac{n^2\eta D}{2}\coth\left(\frac{2\eta D}{|U_e|}\right); \quad (23)$$

(ii) $\Delta_0 = 0$:

$$E_e - \mu_0 - \frac{|U_e|n}{2} = (1-n)\eta D, \quad (24)$$

$$\frac{\Omega_0}{N} = \frac{1}{4}\hbar\omega\{\exp(4\alpha)[\exp(2\beta)]_{00} + \exp(-4\alpha)[\exp(-2\beta)]_{00}\} - \frac{1}{2}\hbar\omega + \frac{|U_e|n^2}{4} - \frac{n^2\eta D}{2}. \quad (25)$$

For the sake of simplicity, we shall assume here $\beta_{ij} = \beta\sum_{k(i)}\delta_{jk}$ where the sum is over the nearest neighbor sites around the site i. In other words, β_{ij} is nonzero only if i and j are nearest neighbors. With this choice of β_{ij}, we are left with only two variational parameters $\tau \equiv \exp(-2\alpha)$ and β. The optimal values of τ and β are determined by the variational approach, that is, when the energy Ω_0 arrives at its stable minimum. Numerical results in some special cases will be given in the next section.

III. RESULTS AND DISCUSSION

The best estimates for the energies are obtained by adjusting the variational parameters α and β so as to minimize Eqs. (23) and (25). Since the minimized values of the energies would be achieved at nonzero α and β, numerical calculations are needed to determine the optimal values of the variational parameters. For convenience, we shall set the energy unit such that $D = 1$ in the following.

In Fig. 1 we show the energy vs β for the same set of parameters as those in Fig. 1 of Ref. 10. For each value of β we let τ vary to minimize the energy; the values at $\beta = 0$ correspond to the result of Ref. 10. The variational calculations have been performed for both a square lattice and a simple cubic lattice. It is clear that keeping a finite β lowers the energies in both cases:

(i) square lattice:

$$\frac{\Omega_0(\Delta_0=0)_m}{N} = -0.04767 \text{ at } (\tau_m = 0.4332\ ,\ \beta_m = -0.06855)\ , \tag{26}$$

$$\frac{\Omega_0(\Delta_0\neq 0)_m}{N} = -0.04795 \text{ at } (\tau_m = 0.4337\ ,\ \beta_m = -0.06850)\ ; \tag{27}$$

(ii) simple cubic lattice:

$$\frac{\Omega_0(\Delta_0=0)_m}{N} = -0.04500 \text{ at } (\tau_m = 0.4278\ ,\ \beta_m = -0.04380)\ , \tag{28}$$

$$\frac{\Omega_0(\Delta_0\neq 0)_m}{N} = -0.04531 \text{ at } (\tau_m = 0.4295\ ,\ \beta_m = -0.04375)\ ; \tag{29}$$

and that the reduction is as much as 12% for simple cubic lattice and 18% for square lattice. Thus, the phonon correlations are important and have to be accounted for to obtain a good estimate of the ground-state energy. The nonzero gap function Δ_0 takes the value of 0.030 20 for the square lattice and 0.031 23 for the simple cubic lattice, whereas Zheng's estimate gives $\Delta_0 = 0.033\,14$. From the minimized energies given above, the superconducting condensation energy can be determined as follows:

$$\delta \equiv \frac{\Omega_0(\Delta_0\neq 0)_m}{N} - \frac{\Omega_0(\Delta_0=0)_m}{N} = \begin{cases} -0.000\,28 & \text{for square lattice,} \\ -0.000\,31 & \text{for simple cubic lattice.} \end{cases} \tag{30}$$

Again, this shows a considerable correction to Zheng's result ($\delta = -0.000\,35$) even though both are of the same order of magnitude. Furthermore, if only the conventional small polaron approximation is used, i.e., $\alpha = \beta = 0$, we would have $\delta = -0.04$, which is a hundred times larger than the value in Eq. (30) and is too large to be a correct condensation energy.

In Fig. 2 the optimal narrowing factor $\eta(\Delta_0 \neq 0)$ is plotted as a function of J and n. Figure 2(a) indicates that when the electron-phonon interaction becomes stronger, η decreases but its rate of decrease is much slower than the usual Holstein factor, which is represented by a dotted curve in the inset. In Fig. 2(b) it is shown that unlike the usual Holstein factor which is independent of n (dotted curve in the inset), η increases with the population of electrons. These results are consistent with Zheng's (dot-dashed curve). Also, in both cases our estimates of η is much larger than the usual Holstein factor; in other words, the suppression effect is much more alleviated in our correlated squeezed-state ansatz approach and in Zheng's approach as compared to the Holstein's result. This weakening mechanism of the narrowing effect suggests a much smaller effective mass of polarons. Furthermore, in both cases our results show considerable improvement with respect to Zheng's.

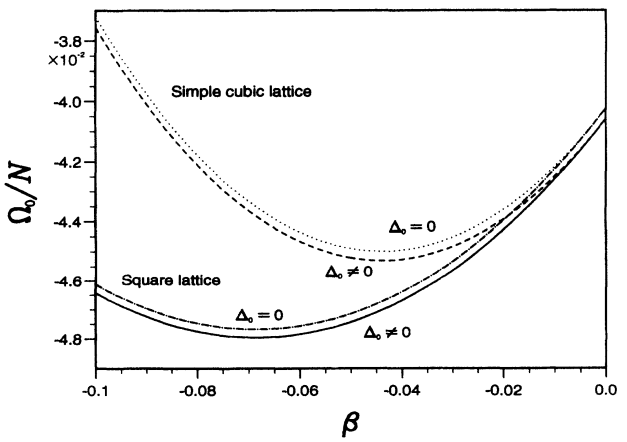

FIG. 1. Minimum energy vs β in the case of $\hbar\omega = 0.08$, $J = 0.3$, $U = 0.3$, and $n = 0.8$. (a) Simple cubic lattice: the dotted curve is the result for $\Delta_0 = 0$, and the dashed curve for nonzero Δ_0. (b) Square lattice: the dot-dashed curve is the result for $\Delta_0 = 0$, and the solid curve for nonzero Δ_0.

In Fig. 3 the nonzero gap function $\Delta_0/\hbar\omega$ is plotted against J and n. Figure 3(a) indicates that $\Delta_0/\hbar\omega$ increases with the strength of the electron-phonon interaction, just as we might expect. On the other hand, as shown in Fig. 3(b), $\Delta_0/\hbar\omega$ decreases on increase in the population of electrons. This type of behavior for Δ_0 arises because $\eta(\Delta_0 \neq 0)$ increases when the population of electrons increases, as can be seen from Eq. (22). In both cases Zheng's results are also plotted for comparison. It is clear that our results are not only consistent with his, but also show considerable improvement.

Now we shall try to estimate the critical temperature T_c based upon the above results. In the finite-temperature region the method of Robaszkiewicz *et al.*,[7] can be applied to derive the gap equation from the effective Hamiltonian H_{eff} in Eq. (13):

$$\Delta = \frac{\Delta}{2N}\sum_{\vec{k}} \frac{|U_e|}{\sqrt{E(\vec{k})^2+\Delta^2}} \tanh\left(\frac{\beta\sqrt{E(\vec{k})^2+\Delta^2}}{2}\right), \tag{31}$$

with

$$E(\vec{k}) = E_e - \mu(T) - \frac{|U_e|n}{2} + \eta_m E_{\vec{k}}, \tag{32}$$

$$n = 1 - \frac{1}{N}\sum_{\vec{k}} \frac{E(\vec{k})}{\sqrt{E(\vec{k})^2+\Delta^2}} \tanh\left(\frac{\beta\sqrt{E(\vec{k})^2+\Delta^2}}{2}\right), \tag{33}$$

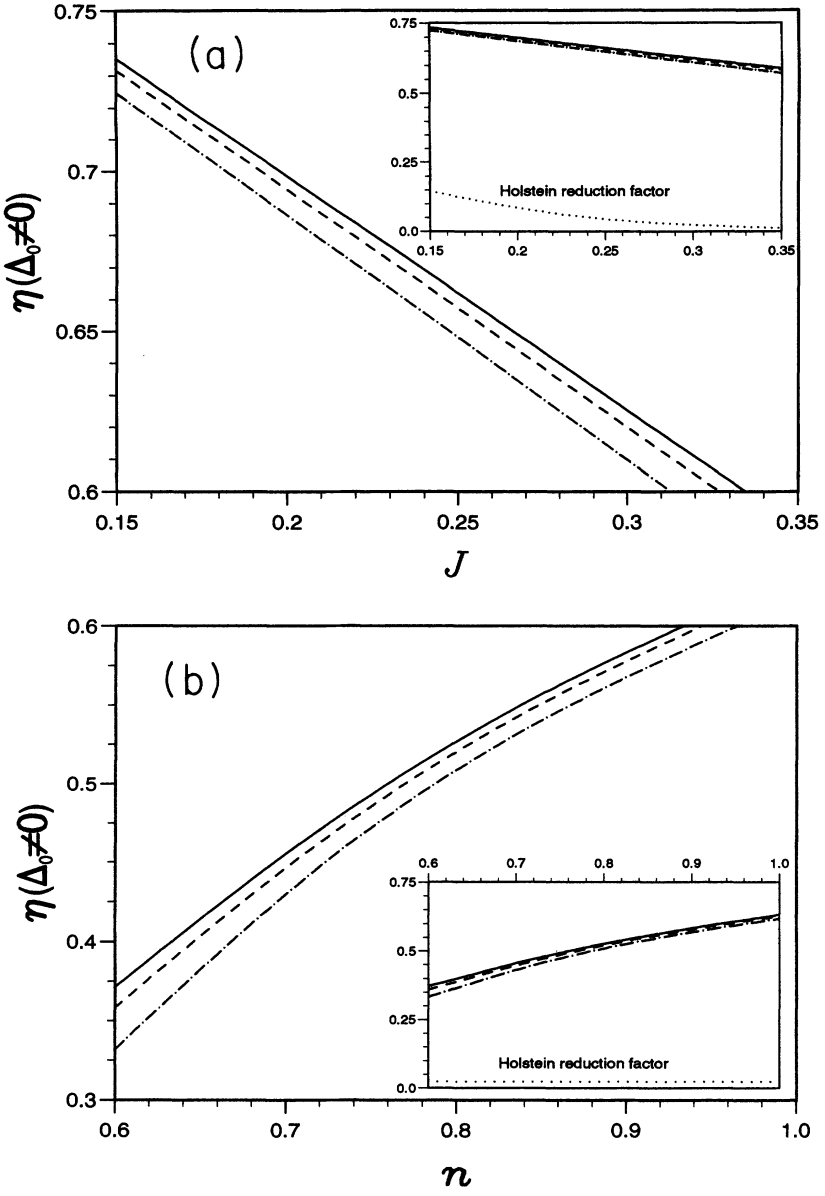

FIG. 2. (a) $\eta(\Delta_0 \neq 0)$ plotted against J for $\hbar\omega = 0.08$, $U = 0.3$, and $n = 1$. (b) $\eta(\Delta_0 \neq 0)$ plotted against n for $\hbar\omega = 0.08$, $U = 0.3$, and $J = 0.3$. The solid curve is our result for the square lattice, and the dashed curve for the simple cubic. Zheng's result is represented by the dot-dashed curve. The dotted curve in the inset denotes the usual Holstein reduction factor.

where $\mu(T)$ is the chemical potential, $\beta^{-1} = k_B T$, and η_m is abbreviated from $\eta_m(\Delta_0 \neq 0)$. Obviously, finding solutions to these equations is a formidable task. However, if we are interested in the critical temperature T_c only, we can solve these equations without much difficulty because $\Delta \to 0$ when $T \to T_c$. When $\beta^{-1} = \beta_c^{-1} = k_B T_c$, Eqs. (31)–(33) become

$$1 = \frac{1}{2N} \sum_{\vec{k}} \frac{|U_e|}{E(\vec{k})} \tanh\left(\frac{\beta_c E(\vec{k})}{2}\right), \tag{34}$$

where

$$E(\vec{k}) = E_e - \mu(T_c) - \frac{|U_e| n}{2} + \eta_m E_{\vec{k}} \tag{35}$$

and

$$n = 1 - \frac{1}{N} \sum_{\vec{k}} \tanh\left(\frac{\beta_c E(\vec{k})}{2}\right). \tag{36}$$

Using the simplified density of states in Eq. (20), it can easily be verified that Eq. (34) can be rewritten as

$$\frac{4D}{|U_e|} = \int_{-D}^{D} \frac{d\epsilon}{F_c + \eta_m \epsilon} \tanh\left(\frac{\beta_c [F_c + \eta_m \epsilon]}{2}\right), \tag{37}$$

where

$$\begin{aligned} F_c &= E_e - \mu(T_c) - \frac{|U_e| n}{2}, \\ &= (1-n)\eta_m D \\ &\quad - \frac{1}{\beta_c} \log_e \left\{ \frac{1 - \exp(-n\beta_c \eta_m D)}{1 - \exp[-(2-n)\beta_c \eta_m D]} \right\}. \end{aligned} \tag{38}$$

It is clear that this equation cannot be solved analytically, and we have to resort to numerical calculations.

Numerical results for the critical temperature T_c vs J and n are shown in Fig. 4. As shown in Fig. 4(a), T_c is getting higher when J increases; in other words, the stronger the electron-phonon interaction is, the higher

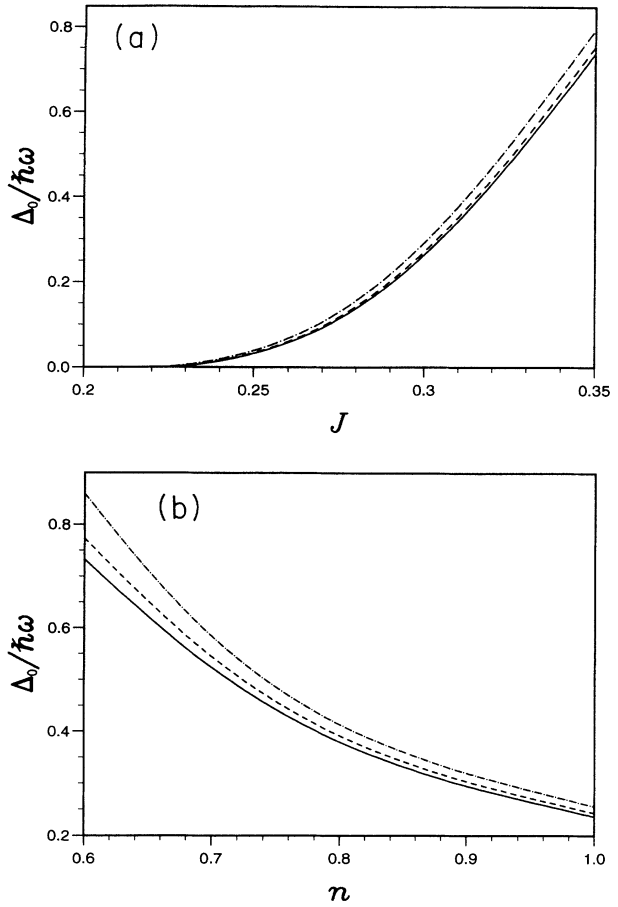

FIG. 3. (a) $\Delta_0/\hbar\omega$ plotted against J for $\hbar\omega = 0.08$, $U = 0.3$, and $n = 1$. (b) $\Delta_0/\hbar\omega$ plotted against n for $\hbar\omega = 0.08$, $U = 0.3$, and $J = 0.3$. The solid curve is our result for the square lattice, and the dashed curve for the simple cubic. Zheng's result is represented by the dot-dashed curve.

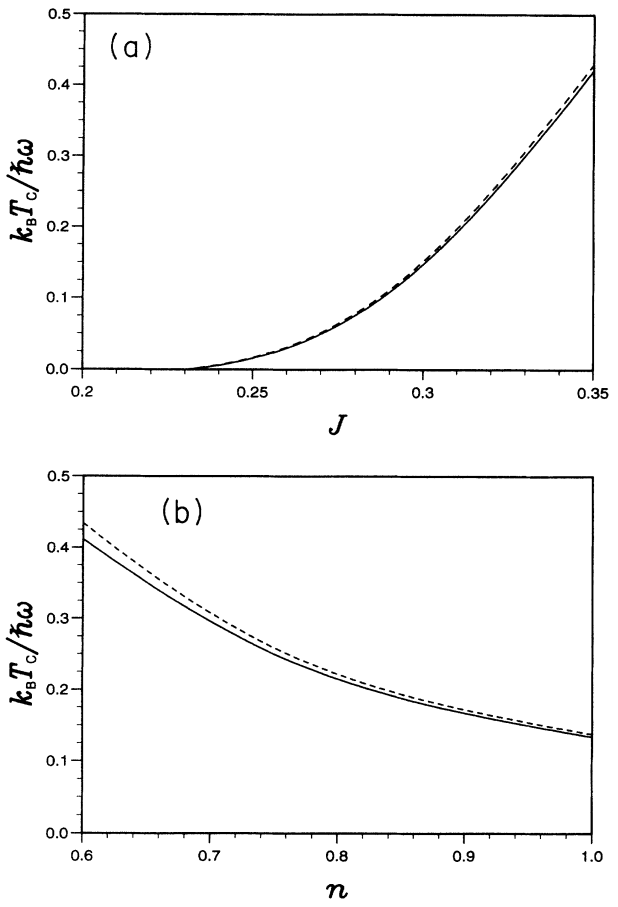

FIG. 4. (a) $k_BT_c/\hbar\omega$ plotted against J for $\hbar\omega = 0.08$, $U = 0.3$, and $n = 1$. (b) $k_BT_c/\hbar\omega$ plotted against n for $\hbar\omega = 0.08$, $U = 0.3$, and $J = 0.3$. The solid curve is our result for the square lattice, and the dashed curve for the simple cubic.

the critical temperature. This is consistent with what we might expect. On the other hand, Fig. 4(b) shows that T_c decreases when n increases from 0.6 to 1.0, which is qualitatively different from the results of Robaszkiewicz *et al.*[7] According to their work, T_c should increase when n increases from 0.6 to 1.0. The reason for the decrease in T_c in our work when n increases is the increase in η_m in the same n range.

In summary, using the correlated squeezed-state approach we have investigated the ground state of an electron-phonon system with strong electron-phonon interaction and a weak on-site Coulomb repulsion. The crux of our treatment is to decouple the electron and the phonon subsystems approximately by introducing a variational correlated squeezed-state ansatz for the phonons. This correlated squeezed state has the virtue that the nonlinearity of the interaction between different phonon modes induced by the linear coupling with the electrons are being taken into account beyond the Hartree approximation. Then assuming the renormalized on-site electron correlation of the effective electronic Hamiltonian to be attractive, we have applied the weak-coupling mean-field theory treatment to obtain the ground state of the system, which is a superconducting pairing state. With optimal values of the variational parameters the correlated squeezed state will by construction yield a ground-state energy lower than those obtained in previous studies. This means that our variational ansatz is more stable as the ground state of the system. Furthermore, our variational study shows that in the correlated squeezed state the polaronic reduction effect of phonons is much more alleviated, and thus the mass enhancement inherent to the polaron effect is noticeably weakened. This weakening of the reduction effect should, in turn, affect other physical properties of the system; for instance, it does suggest that in the strong-coupling limit, where the superfluidlike bipolaronic superconductivity is supposed to occur, higher critical temperatures for superconductivity can be attained by means of the correlated squeezed polaronic state.

Besides, in our theoretical treatment of this system, although an approximate decoupling of the electron-phonon interaction is assumed, the interplay between the two subsystems is still being considered within the mean-

field approximation through the adjustable squeezing parameters α and β. The optimal values of α and β, which describe the state of phonons, are dependent upon the state of the electrons and the strength of the electron-phonon interaction. This situation is completely different from the small polaron case, where the phonon subsystem is in the vacuum state. Hence, we believe that our correlated squeezed-state approach is necessary for dealing with strong electron-phonon interacting systems from first principles.

As a final remark, we would like to mention a recent numerical analysis of the excitation spectrum for the two-site polaron problem: electrons hopping between two diatomic molecular units.[23] In this study it has been shown that in general the eigenspectrum of the single-polaron problem cannot be obtained by simply renormalizing the electron hopping integral, $T \rightarrow T_e \equiv \eta T$ [see Eq. (14)], as in the conventional small-polaron approach; in other words, polarons are no longer describable in terms of quasiparticles having a well-defined dispersion like that in Eq. (18). Also, for sufficiently strong electron-phonon coupling, the conventional small-polaron theory can no longer adequately describe the system. Of course, these results are from the study of a small cluster of two diatomic molecules only; nevertheless, they do shed doubt on the conventional assumption of the existence of single-polaron band states for the case of sufficiently large electron-phonon coupling. As a result, one might need a new approach to treat the system more adequately.

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