Variational treatment of the strong electron-phonon interaction

1989 J. Phys.: Condens. Matter 1 1641

(http://iopscience.iop.org/0953-8984/1/9/009)

J. Phys.: Condens. Matter 1 (1989) 1641–1651. Printed in the UK

Variational treatment of the strong electron–phonon interaction

Zheng Hang
Centre of Theoretical Physics, CCAST (World Laboratory), Beijing, and Department of Applied Physics, Shanghai Jiao Tong University, Shanghai, People's Republic of China

Received 2 November 1987, in final form 6 April 1988

Abstract. In this paper, via discussions of the simple model of a strong electron–phonon interacting system, we develop a new variational treatment for dealing with the superconducting properties of such a system. The key idea of our treatment is to introduce a two-phonon coherent state for the phonon subsystem so that the ground-state energy of the interacting system can arrive at a stable minimum. We have shown that the superconducting condensation energy in our variational state is of a reasonable magnitude and that the effective mass of the polarons is much smaller than that considered by previous researchers. The gap equation and the expression for critical temperature T_c in our theory are also different from those in ordinary polaronic state as well as from those in Bardeen–Cooper–Schrieffer theory. We have pointed out the possibility of high-T_c superconductivity in such an interacting system.

1. Introduction

In recent years, the properties of strong electron–phonon interacting systems (SEPISs) have aroused considerable interest among solid state physicists because such a system has the potential for displaying high-temperature superconductivity. Theoretical research on the superconducting properties of such systems fall into two general classes. One is represented by the so-called strong-coupling theory (for a review, see Scalapino (1969)) which is an extension of the famous Bardeen–Cooper–Schrieffer (BCS) (1957) weak-coupling theory and is a continuum model theory, in which only those electron states near the Fermi surface are strongly coupled to the phonons. However, some workers (Alexandrov *et al* 1986a, b) have pointed out that in strong-coupling narrow-band systems the well known Migdal theorem on which the strong-coupling theory is based breaks down because in such systems one may be in the so-called anti-adiabatic limit (Alexandrov *et al* 1986a, b, Nash 1987)

$$\omega \gtrsim W \tag{1}$$

where ω is the characteristic phonon frequency and W is the renormalised band half-width.

The other is concerned with the strong-coupling narrow-band systems, represented by the theories of electrons on a lattice strongly coupled to the phonons, in which all electron states in the Fermi sea are involved in the superconducting process. In such

0953-8984/89/091641 + 11 $02.50

systems the strong electron–phonon interaction leads to lattice instabilities and the result of it is the formation of the so-called small polarons (Toyazawa 1962, Anderson 1975, Alexandrov *et al* 1986a, b). In accordance with the magnitude of the effective attraction between polarons, which is denoted by V, research belonging to this class could be divided into two subclasses. If the effective attraction is small ($V \leqslant W$), Alexandrov (1983) and Robaszkiewicz *et al* (1981b, 1982) have shown that the small polarons form spatially overlapping Cooper pairs with superconducting properties similar to ordinary BCS theory. There are nevertheless differences in the gap equations and in the expressions for the critical temperature T_c. In the case of strong polaron–polaron coupling ($V \gg W$), Alexandrov and Ranninger (1981), Alexandrov *et al* 1984 and Robaszkiewicz *et al* (1981a) have shown that a new type of superconductivity, the so-called bipolaronic superconductivity, could result and its properties are different in many ways from the BCS properties but are similar to those of the superfluidity of liquid helium.

From the above reviews, we see that the magnitude of W plays an important role in discussing the SEPIS. As is well known, in the low-temperature region, W is connected to the bare band half-width D via a polaronic narrowing factor (Holstein 1959, Toyazawa 1962)

$$W = D \exp(-g^2/\hbar^2\omega^2) \tag{2}$$

where g represents the strength of the electron–phonon interaction. However, as this narrowing factor is obtained in dealing with the so-called small-polaron problem which corresponds to an electron in a narrow band but interacts with phonons strongly (Toyazawa 1962), we should ask a new question: in many-electron and phonon interacting systems, what is the situation?

We can see from equation (2) that, if the ratio $g/\hbar\omega$ is larger than unity, which is exactly the case for the SEPIS (Alexandrov *et al* 1986a, b, Nash 1987), the band-narrowing effect should be fairly strong even if the temperature is zero. However, when such a strong narrowing effect is taken into account the ground-state energy of the SEPIS would increase as the mass centre of the band is not influenced by the electron–phonon interaction (without including the polaronic binding energy). If the average number n ($=N_e/N$) of electrons per unit cell is a negligibly small quantity, the increase in the ground-state energy is also negligible. However, the situation is the completely different case when n is a finite quantity. In this paper, via the discussion of a simple model for the SEPIS, we want to illustrate the increase in the ground-state energy in the $n \neq 0$ case and develop a variational treatment to lower it. We shall point out that in practice the narrowing effect could be much weaker than equation (2) indicates provided that n is some finite quantity and this weakening mechanism of our variational treatment has some interesting influences on other physical propeties of the interacting system.

The variational treatment in this paper consists of the following steps. Firstly, a unitary transformation of displaced-operator type is used to transform our model Hamiltonian H into $\bar{H}$; as is well known, $\bar{H}$ describes the same physical system as H does. Secondly, for the state vector $|\Psi\rangle$ of $\bar{H}$, we assume that the phonon and the electron subsystems could be decoupled approximately, i.e.

$$|\Psi\rangle = |\Psi_p\rangle|\Psi_e\rangle \tag{3}$$

where $|\Psi_p\rangle$ contains only phonon variables and $|\Psi_e\rangle$ only electron variables. Thirdly, a variational state $|\Psi_p\rangle$, which is new and called the two-phonon coherent state (Zheng 1987), is introduced for phonon subsystem, in which some variational parameter is included for the ground-state energy to arrive at a stable minimum. Fourthly, the method

of Robaszkiewicz *et al* (1981b, 1982) is used to obtain the ground-state energy of our model system. Finally, the variational parameter is adjusted to arrive at a stable minimum of the ground-state energy of the system.

2. Theoretical analysis

Our model Hamiltonian is the Hubbard model of the electron subsystem plus an electron–phonon interaction with the phonon subsystem,

$$H = \sum_{i,\sigma} (E - \mu) d_{i\sigma}^{+} d_{i\sigma} + \sum_{i,j(i\neq j)} \sum_{\sigma} T_{ij}^{0} d_{i\sigma}^{+} d_{j\sigma} + \sum_{i} \hbar\omega b_i^{+} b_i + \sum_{i} U d_{i\uparrow}^{+} d_{i\uparrow} d_{i\downarrow}^{+} d_{i\downarrow} + \sum_{i,\sigma} g d_{i\sigma}^{+} d_{i\sigma} (b_i^{+} + b_i) \tag{4}$$

where μ is the chemical potential, $d_{i\sigma}^{+}$ and $d_{i\sigma}$ are the creation and annihilation operators of electrons, and b_i^{+} and b_i are the creation and annihilation operators of phonons. The third term of equation (4) represents the harmonic energy of phonons and the other notation in equation (4) is as usual. For simplicity, the strength g of the electron–phonon interaction and the phonon frequency ω are assumed to be dispersionless. Applying a unitary transformation of the displaced-operator type to H, we obtain

$$\bar{H} = \exp(R)\, H \exp(-R) \tag{5}$$

$$R = \sum_{i,\sigma} \frac{g}{\hbar\omega} d_{i\sigma}^{+} d_{i\sigma} (b_i^{+} - b_i) \tag{6}$$

and, using the transformation relations

$$\exp(R)\, b_i \exp(-R) = b_i - \sum_{\sigma} \frac{g}{\hbar\omega} d_{i\sigma}^{+} d_{i\sigma} \tag{7}$$

$$\exp(R)\, d_{i\sigma}^{+} d_{j\sigma} \exp(-R) = d_{i\sigma}^{+} d_{j\sigma} \exp\{(g/\hbar\omega)\,[(b_i^{+} - b_i) - (b_j^{+} - b_j)]\} \tag{8}$$

we have

$$\bar{H} = \sum_{i} \hbar\omega b_i^{+} b_i + \sum_{i,\sigma} (E - \mu) d_{i\sigma}^{+} d_{i\sigma} + \sum_{i} U d_{i\uparrow}^{+} d_{i\uparrow} d_{i\downarrow}^{+} d_{i\downarrow} + \sum_{i,j(i\neq j)} \sum_{\sigma} T_{ij}^{0} d_{i\sigma}^{+} d_{j\sigma} \exp\left(\frac{g}{\hbar\omega}[(b_i^{+} - b_i) - (b_j^{+} - b_j)]\right) - \sum_{i} \sum_{\sigma,\sigma'} \frac{g^2}{\hbar\omega} d_{i\sigma}^{+} d_{i\sigma} d_{i\sigma'}^{+} d_{i\sigma'}\,. \tag{9}$$

At this point, one could suppose that, when the temperature is low enough, the state of the phonon subsystem does not change as electrons move, so that the electron and the phonon subsystems could be decoupled by averaging H over the vacuum state of the phonon subsystem and the band-narrowing factor $\exp(-g^2/\hbar^2\omega^2)$ thus obtained. This is the usual way of dealing with the electron–phonon interaction in discussing the small-polaron problem (Holstein 1959, Toyozawa 1962, Mahan 1981). However, in our many-electron and phonon interacting system, such a narrowing effect would bring about an increase in the ground-state energy of the system, as pointed out in § 1. In order to lower

this energy, we introduce a new variational state $|\Psi_p\rangle$ for the phonon subsystem,

$$|\psi_p\rangle = \exp(-S)\,|\text{vac}\rangle \tag{10}$$

$$S = \sum_i \alpha(b_i b_i - b_i^+ b_i^+) \tag{11}$$

where α is a variational parameter for the ground-state energy to be a stable minimum. If $\alpha = 0$, $|\Psi_p\rangle$ returns to the vacuum state $|\text{vac}\rangle$; as long as $\alpha \neq 0$, $|\Psi_p\rangle$ is a new and special state of the phonon subsystem other than any eigenstate of phonon number operators. Because the unitary operator $\exp(-S)$ is similar to that of the two-photon coherent state in quantum optics proposed firstly by Yuen (1976), we call $|\Psi_p\rangle$ the two-phonon coherent state (Zheng 1987).

Using the relations

$$\exp(S)\,(b_i^+ \pm b_i)\exp(-S) = (b_i^+ \pm b_i)\exp(\pm 2\alpha) \tag{12}$$

and

$$\exp(S)\,b_i^+ b_i \exp(-S)$$
$$= [b_i^+ \cosh(2\alpha) + b_i \sinh(2\alpha)][b_i^+ \sinh(2\alpha) + b_i \cosh(2\alpha)] \tag{13}$$

we can average $\bar{H}$ over the variational state $|\Psi_p\rangle$ of the phonon subsystem and thus decouple the electron and the phonon subsystems approximately. In so doing, an effective Hamiltonian of the electron subsystem is obtained:

$$H_{\text{eff}} = N\hbar\omega[\sinh(2\alpha)]^2 + \sum_{i,\sigma}(E_e - \mu)d_{i\sigma}^+ d_{i\sigma}$$
$$+ \sum_{i,j(i\neq j)}\sum_{\sigma} T_{ij} d_{i\sigma}^+ d_{j\sigma} - \sum_i |U_e| d_{i\uparrow}^+ d_{i\uparrow} d_{i\downarrow}^+ d_{i\downarrow} \tag{14}$$

where

$$E_e = E - J \qquad U_e = U - 2J \qquad J = g^2/\hbar\omega \tag{15}$$

and $U_e < 0$ has been assumed. The renormalised hopping integral T_{ij} has the form

$$T_{ij} = \rho T_{ij}^0 = T_{ij}^0 \exp[-(J/\hbar\omega)\exp(-4\alpha)] = T_{ij}^0 \exp[-(J/\hbar\omega)\tau^2] \tag{16}$$

i.e. in the exponent of the band-narrowing factor there appears a new factor $\tau^2 = \exp(-4\alpha)$ which is connected with the variational parameter α. So long as $\alpha > 0$ the band-narrowing effect of phonons would be weakened and it could lower the ground-state energy of the interacting system. However, the first term in equation (14) represents the harmonic energy of the phonon subsystem and it would increase when α increases. These two effects of the variational parameter α compete with each other and the result is that a stable minimum of the ground-state energy could be obtained at some non-zero α. The procedure of how to determine the practical value of α will be given out in § 3.

3. Ground state

In this section, we consider the $T = 0$ case. For simplicity, we can take advantage of the results of Robaszkiewicz *et al* (1981b, 1982) to write directly expressions for the ground-state energy and the gap equation of the superconducting state of the interacting system

from the effective Hamiltonian H_{eff}:

$$\frac{\Omega_0}{N} = \hbar\omega[\sinh(2\alpha)]^2 + E_e - \mu_0 - \frac{|U_e|n}{2} + \frac{|U_e|n^2}{4} + \frac{\Delta_0^2}{|U_e|} - \frac{1}{N}\sum_k \sqrt{E^2(k) + \Delta_0^2} \tag{17}$$

$$n = 1 - \frac{1}{N}\sum_k \frac{E(k)}{\sqrt{E^2(k) + \Delta_0^2}} \tag{18}$$

$$\Delta_0 = \frac{1}{2N}\sum_k \frac{|U_e|\Delta_0}{\sqrt{E^2(k) + \Delta_0^2}} \tag{19}$$

where

$$E(k) = E_e - \mu_0 - |U_e|n/2 + \rho E_k \tag{20}$$

and

$$T_{ij}^0 = \frac{1}{N}\sum_k E_k \exp[ik \cdot (i - j)]. \tag{21}$$

In equations (17)–(20) all the subscripts 0 denote that the corresponding quantities are evaluated in the $T = 0$ case. Obviously, $\Delta_0 = 0$ is a trivial solution of equation (19).

In what follows, a square density of states

$$\rho(\varepsilon) = \begin{cases} 1/2D & \text{for } |\varepsilon| \leqslant D \\ 0 & \text{otherwise} \end{cases} \tag{22}$$

of the electrons will be assumed, so that analytical results can be obtained. Using such a simplified density of states, it could be easily verified that the solutions of the above equations are

$$E_e - \mu_0 - |U_e|n/2 = (1 - n)\rho D \coth(\rho D/|U_e|) \tag{23}$$

$$\Delta_0 = \sqrt{n(2 - n)}\rho D/\sinh(2\rho D/|U_e|) \tag{24}$$

$$\Omega_0(\Delta_0 \neq 0)/N = \hbar\omega[\sinh(2\alpha)]^2 + |U_e|n^2/4 - (n^2/2)\rho D \coth(2\rho D/|U_e|). \tag{25}$$

If we take the trivial solution $\Delta_0 = 0$ of equation (19), we have

$$E_e - \mu_0 - |U_e|n/2 = (1 - n)\rho D \tag{26}$$

$$\Omega_0(\Delta_0 = 0)/N = \hbar\omega[\sinh(2\alpha)]^2 + |U_e|n^2/4 - n^2\rho D/2. \tag{27}$$

Differentiating $\Omega_0(\Delta_0 \neq 0)$ and $\Omega_0(\Delta_0 = 0)$ with respect to the variational parameter τ, we can obtain two transcendental equations for determining the minimum points $\tau_m(\Delta_0 \neq 0)$ and $\tau_m(\Delta_0 = 0)$:

$$1/\tau_m^2(\Delta_0 \neq 0) = \{1 + [2n^2JD/(\hbar\omega)^2][\coth Y - Y(\sinh Y)^{-2}] \times \exp[-(J/\hbar\omega)\tau_m^2(\Delta_0 \neq 0)]\}^{1/2} \tag{28}$$

where

$$Y = (2D/|U_e|)\exp[-(J/\hbar\omega)\tau_m^2(\Delta_0 \neq 0)]$$

and

$$1/\tau_m^2(\Delta_0 = 0) = \{1 + [2n^2JD/(\hbar\omega)^2]\exp[-(J/\hbar\omega)\tau_m^2(\Delta_0 = 0)]\}^{1/2}. \tag{29}$$

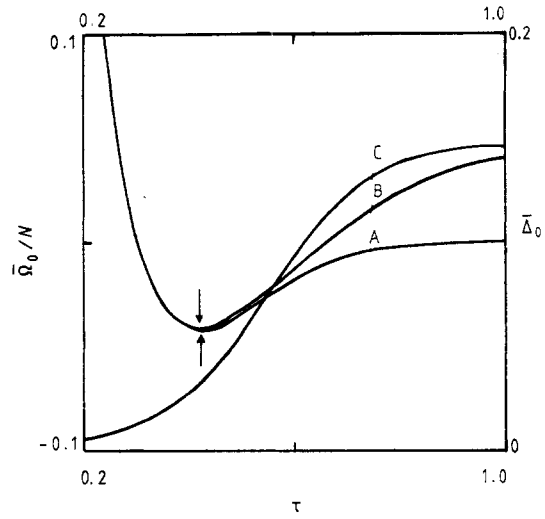

Figure 1. $\bar{\Omega}_0(\Delta_0 \neq 0)$ (curve A), $\bar{\Omega}_0(\Delta_0 = 0)$ (curve B) and $\bar{\Delta}_0$ (curve C) plotted against τ for $\hbar\omega = 0.08$, $\bar{J} = 0.3$, $\bar{U} = 0.3$ and $n = 0.8$. The arrows indicate $\tau_m(\Delta_0 \neq 0) = 0.4228$ $(\bar{\Omega}_0(\Delta_0 \neq 0)_m/N = -0.04059)$ and $\tau_m(\Delta_0 = 0) = 0.4208$ $(\bar{\Omega}_0(\Delta_0 = 0)_m/N = -0.04024)$, respectively.

The corresponding minimised values of ground-state energy can be obtained by replacing τ in $\Omega_0(\Delta_0 \neq 0)$ and $\Omega_0(\Delta_0 = 0)$ by $\tau_m(\Delta_0 \neq 0)$ and $\tau_m(\Delta_0 = 0)$, respectively.

Numerical results in some special cases are given in figures 1, 2 and 3. The values of various parameters employed in the calculations are listed in the figures where the overbar designates that the corresponding parameter is expressed in units of D. In figure 1, we can see that for either $\Delta_0 \neq 0$ or $\Delta_0 = 0$ a stable minimum of Ω_0/N, $\Omega_0(\Delta_0 \neq 0)_m/N$ or $\Omega_0(\Delta_0 = 0)_m/N$ is really achieved at the respective $\tau_m(\Delta_0 \neq 0)$ or $\tau_m(\Delta_0 = 0)$ point, at $\tau_m(\Delta_0 \neq 0)$ the non-zero gap function $\bar{\Delta}_0$ takes a value of 0.033 14. From the minimised energy given in the figure, we derive the superconducting condensation energy as follows:

$$\delta = \bar{\Omega}_0(\Delta_0 \neq 0)_m/N - \bar{\Omega}_0(\Delta_0 = 0)_m/N = -0.00035. \tag{30}$$

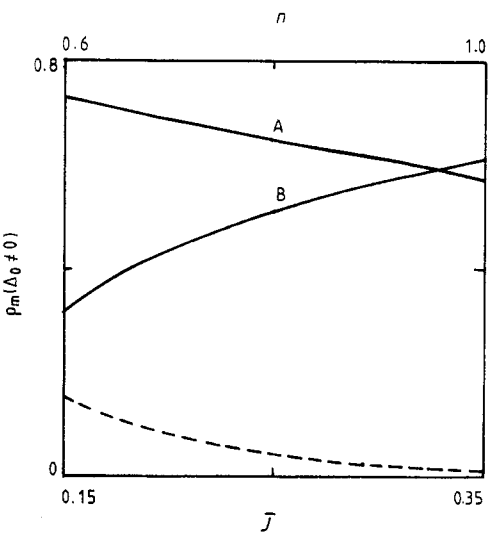

Figure 2. $\rho_m(\Delta_0 \neq 0)$ plotted against $\bar{J}$ for $\hbar\omega = 0.08$, $\bar{U} = 0.3$ and $n = 1$ (curve A) and $\rho_m(\Delta_0 \neq 0)$ plotted against n for $\hbar\omega = 0.08$, $\bar{U} = 0.3$ and $\bar{J} = 0.3$ (curve B): ---, $\exp(-J/\hbar\omega)$.

However, if we do not introduce the two-phonon coherent state ($\alpha = 0$ and $\tau = 1$), we would have $\delta = -0.04$, which is a hundred times larger than the value in equation (30) and is too large to be a correct condensation energy. For comparison, we should note that the energy unit D is of the order of 0.1–1 eV for a narrow-band system and the condensation energy in BCS theory is of the order of 10^{-7} eV.

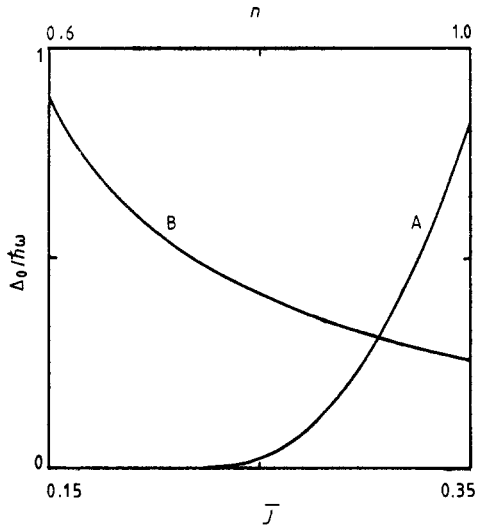

Figure 3. $\Delta_0/\hbar\omega$ plotted against $\bar{J}$ for $\hbar\omega = 0.08$, $\bar{U} = 0.3$ and $n = 1$ (curve A) and $\Delta_0/\hbar\omega$ plotted against n relation for $\hbar\omega = 0.08$, $\bar{U} = 0.3$ and $\bar{J} = 0.3$ (curve B).

In figure 2, the relation between the narrowing factor $\rho_m(\Delta_0 \neq 0)$ (corresponding to that in equation (16) where τ is replaced by $\tau_m(\Delta_0 \neq 0)$) and $\bar{J}$ or n is given. Curve A indicates that, when the electron–phonon interaction $\bar{J}$ becomes stronger, $\rho_m(\Delta_0 \neq 0)$ decreases, but its rate of decrease is much slower than the usual Holstein factor, which is represented by a broken curve in the figure. Curve B indicates that, when the population of electrons increases, $\rho_m(\Delta_0 \neq 0)$ becomes larger. This tendency is consistent with our expectations, as is discussed in § 1. This weakening mechanism of the narrowing effect in our variational treatment should result in a much smaller effective mass of polarons than that considered by previous workers (see, e.g., Toyozawa 1962, Alexandrov *et al* 1986a, b, Nash 1987) because $\rho_m D$ in our theory is the renormalized band half-width of the polaron and thus the effective mass m^* of the polaron should be inversely proportional to $\rho_m D$. As we know, if the effective mass of the charge carriers is too large ($m^* \to \infty$), there would be no superconductivity.

In figure 3, the relation between the non-zero gap function $\Delta_0/\hbar\omega$ (corresponding to that in equation (24) where τ is replaced by $\tau_m(\Delta_0 \neq 0)$) and $\bar{J}$ or n is given. We express Δ_0 in units of $\hbar\omega$ because it is a characteristic energy in the SEPIS. Curve A indicates that, on increase in the strength of the electron–phonon interaction, Δ_0 increases, just as we might expect. Curve B indicates that, on increase in the population of electrons, Δ_0 decreases. This type of behaviour for Δ_0 arises because $\rho_m(\Delta_0 \neq 0)$ increases when the population of electrons increases, as can be seen from equation (24).

4. Critical temperature

In the finite-temperature region the results of Robaszkiewicz *et al* (1981b, 1982) can also be used to write directly the gap equation from the effective Hamiltonian H_{eff}:

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

where

$$E(k) = E_e - \mu(T) - |U_e|n/2 + \rho_m E_k \tag{32}$$

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

$\mu(T)$ is the chemical potential, $\beta = 1/k_B T$ and ρ_m is abbreviated from $\rho_m(\Delta_0 \neq 0)$. The problem of solving equations (31)–(33) is difficult. In this section, only the critical temperature T_c will be discussed because, when $T \to T_c$, $\Delta \to 0$ and we can solve equations (31)–(33) without more difficulty.

When $\beta = \beta_c = 1/k_B T_c$, equations (31)–(33) become

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

where

$$E(k) = E_e - \mu(T_c) - |U_e|n/2 + \rho_m E_k \tag{35}$$

and

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

Using the simplified density of states (22), it can easily be verified that equation (34) can be rewritten as

$$\frac{4D}{|U_e|} = \int_{-D}^{D}\frac{d\varepsilon}{F_c + \rho_m\varepsilon}\tanh\left(\frac{\beta_c(F_c + \rho_m\varepsilon)}{2}\right) \tag{37}$$

where

$$F_c = E_e - \mu(T_c) - |U_e|n/2 = (1-n)\rho_m D - (1/\beta_c) \times \ln\{[1-\exp(-n\beta_c\rho_m D)]/\{1-\exp[-(2-n)\beta_c\rho_m D)]\}\}. \tag{38}$$

Equation (37) can be solved numerically. For the special case of weak coupling, i.e. $2\rho_m D/|U_e| \gg 1$ (in accordance with the parameters employed in figures 2 and 3 the range of this ratio is 2–10), we should have $\beta_c\rho_m D \gg 1$ and the chemical potential $\mu(T_c)$ in equation (38) can be approximated by

$$F_c = E_e - \mu(T_c) - |U_e|n/2 = (1-n)\rho_m D \tag{39}$$

Then the integral in equation (37) can be carried out approximately as follows:

$$\frac{4D}{|U_e|} = \int_0^D\left[\frac{d\varepsilon}{F_c + \rho_m\varepsilon}\tanh\left(\frac{\beta_c(F_c+\rho_m\varepsilon)}{2}\right) + \frac{d\varepsilon}{F_c - \rho_m\varepsilon}\tanh\left(\frac{\beta_c(F_c-\rho_m\varepsilon)}{2}\right)\right]$$

$$= \frac{1}{\rho_m}\left(\int_0^{\beta_c(\rho_m D + F_c)/2} + \int_0^{\beta_c(\rho_m D - F_c)/2}\right)\frac{dz}{z}\tanh z.$$

Integrating by parts, we have

$$4\rho_m D/|U_e| = \tanh z \ln z|_0^{\beta_c(\rho_m D+F_c)/2} + \tanh z \ln z|_0^{\beta_c(\rho_m D-F_c)/2} - \left(\int_0^{\beta_c(\rho_m D+F_c)/2} + \int_0^{\beta_c(\rho_m D-F_c)/2}\right) dz \ln z \,(\operatorname{sech} z)^2.$$

As $\beta_c\rho_m D \gg 1$, this equation may be approximated as

$$2\rho_m D/|U_e| = \ln[(\beta_c/2)\sqrt{(\rho_m D + F_c)(\rho_m D - F_c)}] + \ln(4 \exp \gamma/\pi) \tag{40}$$

where γ is Euler's constant and $(2 \exp \gamma)/\pi = 1.134$. A simple rearrangement yields

$$1/\beta_c = k_B T_c = [(2 \exp \gamma)/\pi]\sqrt{n(2-n)}\rho_m D \exp(-2\rho_m D/|U_e|). \tag{41}$$

We should point out that, according to equation (41),

$$\beta_c\rho_m D = (\pi/2 \exp \gamma)[n(2-n)]^{-1/2} \exp(2\rho_m D/|U_e|) \tag{42}$$

and the condition $\beta_c\rho_m D \gg 1$ is satisfied because, when $2\rho_m D/|U_e|$ is larger than 2, we have $\beta_c\rho_m D > 7.5$.

Using the gap function Δ_0 in the zero-temperature case (equation (24)), we obtain

$$\Delta_0/k_B T_c = 1.764 \tag{43}$$

which is the same relation as in the BCS theory.

In figure 4, the relation between the critical temperature T_c (in units of $\hbar\omega$) and $\bar{J}$ or n is given. T_c increases when $\bar{J}$ increases, as we might expect, since $\bar{J}$ represents the strength of the electron–phonon interaction. However, the relation between $k_B T_c/\hbar\omega$ and n in this figure is different qualitatively from the result of Robaszkiewicz *et al* (1982); according to their work, T_c should increase when n increases from 0.6 to 1. The reason for the decrease in T_c in our work when n increases from 0.6 to 1 is the increase in ρ_m in figure 2 in the same n range.

We can estimate the values of T_c in our model system. It can be seen from figure 4 that in the ranges employed for various parameters the critical temperature T_c is of the

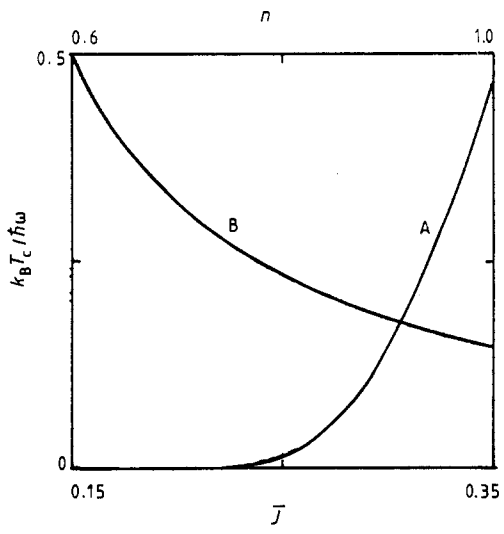

Figure 4. $k_B T_c/\hbar\omega$ plotted against $\bar{J}$ for $\hbar\omega = 0.08$, $\bar{U} = 0.3$ and $n = 1$ (curve A) and $k_B T_c/\hbar\omega$ plotted against n for $\hbar\omega = 0.08$, $\bar{U} = 0.3$ and $\bar{J} = 0.3$ (curve B).

order of (0.1–0.4) $\hbar\omega/k_B$. We can assume that $\hbar\omega/k_B \simeq 300$ K, which corresponds to $\hbar\omega \simeq 26$ meV and is reasonable; thus T_c is of the order of 30–120 K. This range of T_c is the same as that of the high-temperature superconductivity in Ba–La–Cu–O systems (Bednorz and Müller 1986) (for references and a list of compounds see, e.g., Murphy *et al* (1987)).

The results discussed in this paper indicate that the gap equation and the expression for T_c in our theory are different from those of the BCS theory as well as from those of Robaszkiewicz *et al* (1981b, 1982).

5. Concluding remarks

(i) In SEPIS the strong electron–phonon interaction leads to lattice instabilities and it results in the formation of small polarons with an extremely narrow band. However, since the narrowing effect is induced by the random motion of phonons in the phonon cloud around each polaron, when $n \neq 0$ the phonons might form some ordering state of zero momentum to weaken the narrowing effect. The two-phonon coherent state is just such an ordering state in which the phase ordering of the phonon subsystem arises from the interference between phonon clouds around every polaron.

(ii) The role played by the variational parameter α, which may be considered as an ordering parameter, is twofold. It can offset the narrowing effect of phonons, as is indicated by equation (21) (if $\alpha \to \infty$, $\rho = 1$). However, the non-zero α can make the harmonic energy of the phonon subsystem increase; when $\alpha \to \infty$, this energy also tends to infinity. These two effects of α compete with each other and our variational treatment consists in selecting the proper value of it at which a stable minimum of the ground-state energy can be achieved. In such a variational treatment a superconducting condensation energy of reasonable magnitude can be derived and the effective mass of polarons is not as large as considered previously (Holstein 1959, Toyozawa 1962, Alexandrov *et al* 1986a, b, Nash 1987). It is known that, if the effective mass of the charge carriers is too large, the superconductivity would disappear since the thermal conductivity and the permanent current of a superconducting system are inversely proportional to the effective mass of charge carriers.

(iii) Although an approximate decoupling of the electron–phonon interaction is assumed (equation (3)), the interplay between the two subsystems still exists via the action of the variational parameter α. The practical value of α, which describes the state of phonons, is dependent on the state of electrons and the strength of the electron–phonon interaction. This situation is completely different from the small-polaron case (Mahan 1981, Alexandrov *et al* 1986a, b) where the phonon subsystem is in a vacuum state. Moreover, if we take into account the fact that the frequency ω_q and the strength $g(q)$ of the interaction are q dependent, thus α_q is also q dependent and this function of q should be connected by the variational treatment with the spectra of ω_q and $g(q)$. This problem is left for further research.

(iv) We have pointed out in § 4 that in our treatment the ratio $2\rho_m D/|U_e|$ is in the range 2–9, so that our theory is a weak-coupling one although the electron–phonon interaction may be strong. The comparatively high T_c, which is or the order of (0.1–0.4) $\hbar\omega/k_B$, results from the fact that all polarons in the SEPIS are involved in the superconducting process.

(v) We consider that our variational method given in this paper is necessary for dealing with the strong-coupling narrow-band system from first principles. The reason

is as follows. On the one hand, it is a generally accepted viewpoint that the strong electron–phonon interaction can induce an attractive interaction between polarons which may overcompensate for the Coulomb repulsion between them and leads to an effective attraction (Anderson 1975, Alexandrov and Ranninger *et al* 1981, Alexandrov 1986a, b, Robaszkiewicz *et al* 1981a, b). On the other hand, if we consider such a many-polaron system via the usual small-polaron viewpoint, then the band of the small polarons would be extremely narrow and their effective mass would be very large; these will not be consistent with the real cases of some strong-coupling narrow-band systems. Thus we are in a dilemma. The variational treatment in this paper has settled this dilemma.

Acknowledgment

This work was supported in part by the Science Foundation of Shanghai Jiao Tong University (China) under Grant A1173.

References

Alexandrov A S 1983 *Zh. Fiz. Khim.* **57** 273
Alexandrov A and Ranninger J 1981 *Phys. Rev.* B **23** 1796; **24** 1164
Alexandrov A S, Ranninger J and Robaszkiewicz S 1986a *Phys. Rev.* B **33** 4526
—— 1986b *Phys. Rev. Lett.* **56** 949
Anderson P W 1975 *Phys. Rev. Lett.* **34** 953
Bardeen J, Cooper L N and Schrieffer J R 1957 *Phys. Rev.* **108** 1175
Bednorz J G and Müller K A 1987 *Z. Phys.* B **64** 189
Holstein T 1959 *Ann. Phys, NY* **8** 325
Mahan G D 1981 *Many-Particle Physics* (New York: Plenum) ch 6
Murphy D W, Sunshine S, van Dover R B, Cava R J, Batlogg B, Zahurak S M and Schneemeyer L F 1987 *Phys. Rev. Lett.* **58** 1888
Nash K 1987 *Phys. Rev.* B **35** 1748
Robaszkiewicz S, Micnas R and Chao K A 1981a *Phys. Rev.* B **23** 1447; **24** 1579
—— 1981b *Phys. Rev.* B **24** 4018
—— 1982 *Phys. Rev.* B **26** 3915
Scalapino D S 1969 *Superconductivity* vol I, ed. R D Parks (New York: Dekker)
Toyazawa Y 1962 *Polarons and Excitons* ed. G B Kuper and G D Whitfield (Edinburgh: Oliver and Boyd)
Yuen H P 1976 *Phys. Rev.* A **13** 2226
Zheng H 1987 *Phys. Rev.* B **36** 8736