Dynamic Hubbard model: Effect of finite boson frequency

F. Marsiglio,[1] R. Teshima,[1] and J. E. Hirsch[2]
[1]*Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2J1*
[2]*Department of Physics, University of California, San Diego, La Jolla, California 92093-0319, USA*
(Received 16 July 2003; published 11 December 2003)

Dynamic Hubbard models describe coupling of a boson degree of freedom to the on-site electronic double occupancy. In the limit of infinite boson frequency this coupling gives rise to a correlated hopping term in the effective Hamiltonian and to superconductivity when the Fermi level is near the top of the band. Here we study the effect of finite boson frequency through a generalized Lang-Firsov transformation and a high-frequency expansion. It is found that finite frequency enhances the tendency to superconductivity in this model.

DOI: 10.1103/PhysRevB.68.224507 PACS number(s): 74.20.Mn, 71.10.Fd, 71.10.−w

I. INTRODUCTION

An attempt to understand electron-electron interactions in solids over the last few decades has focused on simplified models which single out, for example, on-site or nearest-neighbor Coulombic interactions. While it is usually understood that the parameters that are required in these models are not ''bare'' parameters, it is often tacitly assumed that the omitted physics can be recovered by simply modifying these parameters to effectively incorporate the missing physics. However, the notion that this procedure may in fact leave out much of the interesting physics has been emphasized by one of us recently,[1] and a new class of model Hamiltonians, ''dynamic Hubbard models,'' was introduced to remedy this difficulty.[1–4] These Hamiltonians describe an essential difference between the empty and the doubly occupied Wannier orbital, that the former is representable by a single Slater determinant and the latter one is not. This difference is not described by the conventional models and leads to electron-hole asymmetry and to an unconventional mechanism of superconductivity.[5]

In this paper we focus attention on one particular dynamic Hubbard model, which introduces a modulation of the Hubbard U by coupling the electron double occupancy to a fictitious local boson displacement. The site Hamiltonian that describes this model is given by[1]

$$H_i=\frac{p_i^2}{2M}+\frac{1}{2}Kq_i^2+(U+\alpha q_i)n_{i\uparrow}n_{i\downarrow}, \tag{1}$$

where the boson is characterized by an Einstein oscillator with mass M and spring constant K. The displacement of the local oscillator q_i is coupled to the electron double occupancy with coupling constant α, and as a consequence the on-site repulsion $U+\alpha q_i$ becomes a dynamical variable. The Hamiltonian in electron representation is given by

$$H=\omega_0\sum_i a_i^\dagger a_i-t\sum_{\substack{i\delta\\ \sigma}}(c_{i\sigma}^\dagger c_{i+\delta\sigma}+c_{i+\delta\sigma}^\dagger c_{i\sigma})-\mu\sum_{i\sigma}n_{i\sigma}$$
$$+\sum_i[U+g\omega_0(a_i+a_i^\dagger)]n_{i\uparrow}n_{i\downarrow}, \tag{2}$$

where $c_{i\sigma}^\dagger$ is an electron creation operator for site i and spin σ, $n_{i\sigma}$ is the corresponding number operator and we have introduced the boson creation and annihilation operators, $a_i^\dagger$ and a_i, respectively. The Einstein oscillator frequency is $\omega_0\equiv(K/M)^{1/2}$ and $g\equiv\alpha/(2K\omega_0)^{1/2}$. In addition we have introduced the electron kinetic energy, with nearest-neighbor hopping amplitude t and chemical potential μ. Finally, U describes the static electron-electron repulsion.

Treating the four-fermion term involving the boson in mean field leads to a model with ordinary Holstein-like electron-boson coupling,

$$H_{el-b}=g(n)\omega_0(a_i^\dagger+a_i)(n_{i\uparrow}+n_{i\downarrow}), \tag{3}$$

$$g(n)=\frac{n}{2}g, \tag{4}$$

where the coupling constant $g(n)$ increases with electron occupation and is maximum for the Fermi level at the top of the band. Hence the quasiparticle dressing in this model increases as the Fermi level rises in the band, and conversely it decreases as the system is doped with holes. There are indications in the high T_c cuprates that the quasiparticle dressing decreases with hole doping[6] and this is one of the motivations to study this Hamiltonian. However to fully understand the physics of this model the mean-field decoupling leading to Eqs. (3) and (4) is certainly inappropriate.

We study the Hamiltonian, Eq. (2), in hole rather than electron representation. A particle-hole transformation yields in addition a Holstein-like coupling

$$H=\omega_0\sum_i a_i^\dagger a_i-t\sum_{\substack{i\delta\\ \sigma}}(c_{i\sigma}^\dagger c_{i+\delta\sigma}+c_{i+\delta\sigma}^\dagger c_{i\sigma})-\mu\sum_{i\sigma}n_{i\sigma}$$
$$-g\omega_0\sum_{i\sigma}(a_i+a_i^\dagger)n_{i\sigma}+\sum_i[U+g\omega_0(a_i+a_i^\dagger)]n_{i\uparrow}n_{i\downarrow}, \tag{5}$$

where now $c_{i\sigma}^\dagger$ and $n_{i\sigma}$ are the hole creation operator and the hole number operator, respectively. One of the essential ingredients of this and other similar models is that the system is inherently *not* electron-hole symmetric. This is clear within the Hartree approximation, but the asymmetry is best revealed through a generalized Lang-Firsov transformation.[1,7,8]

In the following section we perform this transformation and derive a Migdal-like expansion valid in the antiadiabatic

limit, which allows us to study corrections due to finite boson frequency. While the antiadiabatic limit is very well understood,[5] the effect of noninfinite boson frequency (retardation) is not. The purpose of this paper is to address this question which is of fundamental importance because derivation of the model from first principles necessarily leads to finite boson frequency.[2] The expansion is performed to first order in inverse boson frequency, and the impact on superconductivity is determined. We find that retardation increases T_c at all hole densities, and increases the range of hole densities over which superconductivity occurs. This is in qualitative agreement with a previous study[3] which determined the effective pairing interaction for two holes within a pseudospin model on small clusters. That study found an increased attractive interaction due to retardation as well.

II. GENERALIZED LANG-FIRSOV TRANSFORMATION

We use the transformation

$$\tilde{H}=e^{G}He^{-G}, \tag{6}$$

where[8]

$$G=\sum_i g(a_i-a_i^\dagger)(n_{i\uparrow}+n_{i\downarrow}-n_{i\uparrow}n_{i\downarrow}). \tag{7}$$

The usual Lang-Firsov transformation serves to diagonalize the nonhopping part of standard electron-phonon Hamiltonians. In contrast, here the ''dressing'' operators $X_{i\sigma}$ [see Eq. (9) below] depend on fermion occupation number: the hole is dressed (undressed) if there is not (is) other hole of opposite spin at the site.

Application of Eq. (6) results in

$$\tilde{H}=\omega_0\sum_i a_i^\dagger a_i-\mu_0\sum_{i\sigma} n_{i\sigma}+U_{\rm eff}\sum_i n_{i\uparrow}n_{i\downarrow}$$

$$-t\sum_{\substack{i\delta\\ \sigma}}(X_{i\sigma}^\dagger X_{i+\delta\sigma}c_{i\sigma}^\dagger c_{i+\delta\sigma}+\text{H.c.}), \tag{8}$$

where $U_{\rm eff}\equiv U-\omega_0 g^2$, $\mu_0\equiv\mu+\omega_0 g^2$, and

$$X_{i\sigma}^\dagger\equiv\exp[g(a_i-a_i^\dagger)(1-n_{i-\sigma})] \tag{9}$$

dresses the hole-hopping amplitudes. These operators are dependent on both the oscillator and hole degrees of freedom.

Equation (8) leads to a low-energy Hamiltonian for the hole degrees of freedom if the ground-state expectation value is taken with respect to the oscillator degrees of freedom. Following Ref. 1, we find

$$\tilde{H}\approx-\tilde{t}_0\sum_{\substack{i\delta\\ \sigma}}(c_{i\sigma}^\dagger c_{i+\delta\sigma}+\text{H.c.})-\mu_0\sum_{i\sigma} n_{i\sigma}+U_{\rm eff}\sum_i n_{i\uparrow}n_{i\downarrow}$$

$$-\Delta t\sum_{\substack{i\delta\\ \sigma}}(c_{i\sigma}^\dagger c_{i+\delta\sigma}+\text{H.c.})(n_{i-\sigma}+n_{i+\delta-\sigma}), \tag{10}$$

where

$$\tilde{t}_0\equiv te^{-g^2} \tag{11}$$

and

$$\Delta t\equiv te^{-g^2}(e^{g^2/2}-1). \tag{12}$$

Equation (10) is the effective quasiparticle Hamiltonian studied in Ref. 5. This model is known to lead to superconductivity at low hole dopings, and to characteristic properties related to ''undressing'' phenomenology.[8] The effective single hole hopping

$$\tilde{t}(n)=\tilde{t}_0+n\Delta t \tag{13}$$

is an increasing function of hole doping, and so is the effective hole bandwidth.

Based on previous studies,[5] superconductivity (and in fact pair binding) occurs in the model in Eq. (8) in the antiadiabatic limit. We wish to answer the question: will superconductivity occur more or less readily with retardation, i.e., away from the antiadiabatic limit? To this end, we use perturbation theory following the generalized Lang-Firsov transformation. That is, we note that the operator $X_{i\sigma}^\dagger$ can be written as

$$\begin{aligned}X_{i\sigma}^\dagger&=n_{i-\sigma}+(1-n_{i-\sigma})\exp[g(a_i-a_i^\dagger)]\\&=n_{i-\sigma}+(1-n_{i-\sigma})e^{-g^2/2}e^{-ga_i^\dagger}e^{ga_i}\\&\approx n_{i-\sigma}+(1-n_{i-\sigma})e^{-g^2/2}[1+g(a_i-a_i^\dagger)],\end{aligned} \tag{14}$$

and similarly for $X_{i\sigma}$. In the last line of Eq. (14) we have expanded the exponential to first order in the oscillator momentum (or, equivalently, the displacement). To put terms involving the linear oscillator operators into ''standard'' form (with the oscillator displacement rather than the momentum), we utilize the canonical transformation

$$\begin{aligned}a_i&\to -ia_i\\ a_i^\dagger&\to ia_i^\dagger.\end{aligned} \tag{15}$$

Finally, Fourier transforming all the operators to momentum space, using a Hartree-Fock approximation and retaining only the reduced part of the Hamiltonian, we obtain

$$\begin{aligned}\tilde{H}=&\omega_0\sum_q a_q^\dagger a_q+\sum_{k\sigma}(\tilde{\epsilon}_k-\tilde{\mu}_0)c_{k\sigma}^\dagger c_{k\sigma}\\&+\frac{1}{N}\sum_{kk'}\left[U_{\rm eff}+2\frac{\Delta t}{\tilde{t}_0+n\Delta t}(\tilde{\epsilon}_k+\tilde{\epsilon}_{k'})\right]\\&\times c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-k'\downarrow}c_{k'\uparrow}\\&+\frac{1}{\sqrt{N}}\sum_{\substack{kk'\\ \sigma}} g_{kk'}(a_{k-k'}+a_{-(k-k')}^\dagger)c_{k\sigma}^\dagger c_{k'\sigma},\end{aligned} \tag{16}$$

where

$$\tilde{\epsilon}_k=-2(\tilde{t}_0+n\Delta t)\sum_\delta\cos(k\delta), \tag{17}$$

$$\tilde{t}_0 = te^{-g^2}, \tag{18}$$

$$\Delta t = \tilde{t}_0(e^{g^2/2}-1), \tag{19}$$

$$U_{\text{eff}} = U - \omega_0 g^2 \tag{20}$$

$$\tilde{\mu}_0 = \mu + \omega_0 g^2 - U_{\text{eff}} n/2, \tag{21}$$

and

$$g_{kk'} \equiv ig \frac{\tilde{t}_0(1-n/2)+n\Delta t/2}{\tilde{t}_0+n\Delta t}(\tilde{\epsilon}_k - \tilde{\epsilon}_{k'}). \tag{22}$$

Note that we have included Hartree corrections already in the hopping and chemical potential terms; these are not to be included again when treating the Hamiltonian (16). The correction to the hole-hopping matrix element in particular leads to a wider bandwidth $\tilde{D}$ for increasing number of holes in the band.

III. ELIASHBERG-LIKE APPROXIMATION FOR HIGH BOSON FREQUENCIES

Equation (16) looks like a standard Hamiltonian with linear electron-phonon coupling. One can determine its properties with the Migdal-Eliashberg approximation. Omitting the detailed steps in the derivation, the final result is

$$\phi(k,i\omega_m) = \frac{1}{N\beta}\sum_{k',m'}\left(\frac{2\omega_0 g_{-k'-k}g_{k'k}}{\omega_0^2+(\omega_m-\omega_{m'})^2} - V_{kk'}\right) \times \frac{\phi(k',i\omega_{m'})}{E(k',i\omega_{m'})}, \tag{23}$$

$$\Sigma(k,i\omega_m) = \frac{1}{N\beta}\sum_{k',m'}\left(\frac{2\omega_0 g_{k'k}g_{kk'}}{\omega_0^2+(\omega_m-\omega_{m'})^2}\right) \times \frac{\tilde{G}_0^{-1}(-k',-i\omega_{m'})}{E(k',i\omega_{m'})}, \tag{24}$$

where $\phi(k,i\omega_m)$ and $\Sigma(k,i\omega_m)$ are the pairing and normal self energies, respectively, and the denominator $E(k,i\omega_m)$ is given by

$$E(k,i\omega_m) \equiv \tilde{G}_0^{-1}(k,i\omega_m)\tilde{G}_0^{-1}(-k,-i\omega_m) + \phi^2(k,i\omega_m) \tag{25}$$

with

$$\tilde{G}_0^{-1}(k,i\omega_m) \equiv i\omega_m - (\tilde{\epsilon}_k - \tilde{\mu}_0) - \Sigma(k,i\omega_m). \tag{26}$$

These equations are standard Eliashberg equations, with $i\omega_m \equiv i\pi T(2m-1)$ a fermion Matsubara frequency, $\beta \equiv 1/(k_B T)$ the inverse temperature, and N the number of lattice sites. The direct electron-electron interaction is given by

$$V_{kk'} = U_{\text{eff}} + \frac{2\Delta t}{\tilde{t}_0+n\Delta t}(\tilde{\epsilon}_k + \tilde{\epsilon}_{k'}). \tag{27}$$

It is also customary to write the normal self-energy in terms of an odd and even (in Matsubara frequency) part

$$\Sigma(k,i\omega_m) \equiv i\omega_m[1-Z(k,i\omega_m)] + \chi(k,i\omega_m), \tag{28}$$

which leads to three coupled equations instead of the two Eqs. (23) and (24). Note that the arguments of the g factors in the kernels of Eqs. (23) and (24) are actually different, and lead, in this case, to kernels with opposite signs in the pairing and normal equations. These equations also require an auxiliary number equation

$$n = 1 + 2\,\text{Re}\frac{1}{N\beta} \times \sum_{k,m} \frac{\tilde{G}_0^{-1}(-k,-i\omega_m)}{\tilde{G}_0^{-1}(k,i\omega_m)\tilde{G}_0^{-1}(-k,-i\omega_m)+\phi^2(k,i\omega_m)}, \tag{29}$$

where n is the hole number density.

These equations are most easily solved by noting that each unknown function can be decomposed into three k-dependent pieces. For example,

$$\phi(k,i\omega_m) \equiv \phi_0(i\omega_m) + \phi_1(i\omega_m)\left(-\frac{\tilde{\epsilon}_k}{\tilde{D}/2}\right) + \phi_2(i\omega_m)\left(\frac{\tilde{\epsilon}_k}{\tilde{D}/2}\right)^2, \tag{30}$$

where $\tilde{D} \equiv \tilde{D}(n) = 8(\tilde{t}_0 + n\Delta t)$ is the n-dependent hole bandwidth. This makes the entire problem only slightly more difficult than the standard Eliashberg equations which require iterative solution in Matsubara frequency space.[9]

Nonetheless, we need not solve these rather complicated equations to determine their properties for large boson frequency ω_0. Equations (23) and (24) contain a kernel of the form

$$\kappa_{kk'}(i\nu_n) = -\frac{\tilde{D}(n)}{\omega_0}\frac{\omega_0^2}{\omega_0^2+\nu_n^2}\frac{g^2}{2}\left(\frac{\tilde{t}_0(1-n/2)+n\Delta t/2}{\tilde{t}_0+n\Delta t}\right)^2 \times \left(\frac{\tilde{\epsilon}_k - \tilde{\epsilon}_{k'}}{\tilde{D}(n)/2}\right)^2, \tag{31}$$

where $i\nu_n \equiv i2\pi Tn$ is a boson Matsubara frequency, and the other variables have been previously defined. We have written Eq. (31) with an explicit prefactor $\tilde{D}(n)/\omega_0$, which shows that for infinite boson frequency ω_0 all of the complications due to the electron-boson coupling can be ignored. This leaves

$$Z(k,i\omega_m) = 1,$$

$$\chi(k,i\omega_m) = 0,$$

$$\phi(k,i\omega_m)\equiv\phi(k)=-\frac{1}{N\beta}\sum_{k',m'}V_{kk'}\frac{\phi(k')}{\tilde{G}_0^{-1}(k',i\omega_{m'})\tilde{G}_0^{-1}(-k',-i\omega_{m'})+\phi^2(k')}, \tag{32}$$

which is a straightforward BCS-like problem which has been solved previously.[5] The result is an extended *s*-wave solution for superconductivity at low hole densities. To understand what happens for large but noninfinite boson frequencies, we adopt a standard approximation for Eliashberg theory, i.e., in the kernel we assume that the boson frequency is much larger than the other energy scales, so that it becomes independent of Matsubara frequency. This allows us to neglect the normal channels, and focus on the gap equation[10]

$$\phi(k)=\frac{1}{N\beta}\tilde{D}(n)\sum_{k',m'}\left[-\kappa(n)\left(\frac{\tilde{\epsilon}_k-\tilde{\epsilon}_{k'}}{\tilde{D}(n)/2}\right)^2-\frac{V_{kk'}}{\tilde{D}(n)}\right]\frac{\phi(k')}{\omega_{m'}^2+(\tilde{\epsilon}_{k'}-\tilde{\mu}_0)^2}, \tag{33}$$

where

$$\kappa(n)\equiv\frac{\tilde{D}(n)}{\omega_0}\frac{g^2}{2}\left(\frac{\tilde{t}_0(1-n/2)+n\Delta t/2}{\tilde{t}_0+n\Delta t}\right)^2. \tag{34}$$

The Matsubara sum in this equation is readily performed:

$$\frac{1}{\beta}\sum_m\frac{\tilde{D}(n)/2}{\omega_m^2+(\tilde{\epsilon}_k-\tilde{\mu}_0)^2}=\frac{\tilde{D}(n)/2}{2(\tilde{\epsilon}_k-\tilde{\mu}_0)}[1-2f(\tilde{\epsilon}_k-\tilde{\mu}_0)]\equiv F_1(\tilde{\epsilon}_k). \tag{35}$$

As noted already in Eq. (30), the k dependence can be decomposed into a constant, a term proportional to $\tilde{\epsilon}_k$, and a third term proportional to $\tilde{\epsilon}_k^2$. The latter term is new, and arises from the fact that a noninfinite boson frequency is used. More explicitly, if we use a constant electron density of states [$g(\tilde{\epsilon})=1/\tilde{D}$, $-\tilde{D}/2<\tilde{\epsilon}<\tilde{D}/2$], then we have

$$\phi(x)=\int_{-1}^{1}dx'\,[-\kappa(n)(x^2+x'^2)+2\kappa(n)xx'-k(x+x')-u_{\rm eff}]\phi(x')F_1(\tilde{\epsilon}'), \tag{36}$$

where $u_{\rm eff}\equiv U_{\rm eff}/\tilde{D}(n)$, $k\equiv 8\Delta t/\tilde{D}(n)$, and $x\equiv\tilde{\epsilon}/(\tilde{D}(n)/2)$, and similarly for the primed quantities. Normally, positive components of the kernels contribute to pairing, and hence to T_c. For example, focusing on the antiadiabatic terms, $u_{\rm eff}$ clearly deters pairing, whereas k will enhance pairing in the energy range where holes dominate (negative $\tilde{\epsilon}$ and negative $\tilde{\epsilon}'$). At the same time k hurts pairing in the electron regime (positive $\tilde{\epsilon}$). Clearly the effect of $\kappa(n)$ is helpful (to pairing) in the central term (and hence adds to the role of k), and is detrimental in the first term. However, a full solution is required to determine the overall impact of a nonzero $\kappa(n)$ [and hence noninfinite ω_0—see Eq. (34)].[11]

IV. BCS-LIKE SOLUTION

A full solution to Eq. (36) is obtained by noting that

$$\phi(x)=a_0-a_1x+a_2x^2. \tag{37}$$

Substitution of Eq. (37) into Eq. (36) leads to three homogeneous equations, so that T_c is given by setting the following 3×3 determinant to zero

$$\det\begin{pmatrix}1+\kappa(n)I_2+uI_0-kI_1 & \kappa(n)I_3+uI_1-kI_2 & \kappa(n)I_4+uI_2-kI_3\\ -kI_0-2\kappa(n)I_1 & 1-kI_1-2\kappa(n)I_2 & -kI_2-2\kappa(n)I_3\\ \kappa(n)I_0 & \kappa(n)I_1 & 1+\kappa(n)I_2\end{pmatrix}=0, \tag{38}$$

where

$$I_\ell\equiv\int_{-\tilde{D}(n)/2}^{\tilde{D}(n)/2}d\tilde{\epsilon}\left(-\frac{\tilde{\epsilon}}{\tilde{D}(n)/2}\right)^\ell\frac{1-2f(\tilde{\epsilon}-\tilde{\mu}_0)}{2(\tilde{\epsilon}-\tilde{\mu}_0)}. \tag{39}$$

For the number equation we assume that all nonpairing interactions are already taken into account in the parameters; thus we obtain, for the chemical potential

$$\frac{\tilde{\mu}_0}{\tilde{D}(n)/2}=-(1-n), \tag{40}$$

where n is the hole density. The evaluation of the determinant, and the determination of $T_c(n)$ is a tedious process; in weak coupling, one can use the relations

$$I_0=\ln\left(\frac{1.13}{k_BT_c}\frac{\tilde{D}(n)}{2}\sqrt{n(2-n)}\right),$$

$$I_1=\rho(I_0-1),$$

$$I_2=\rho^2I_0+\tfrac{1}{2}-\tfrac{3}{2}\rho^2,$$

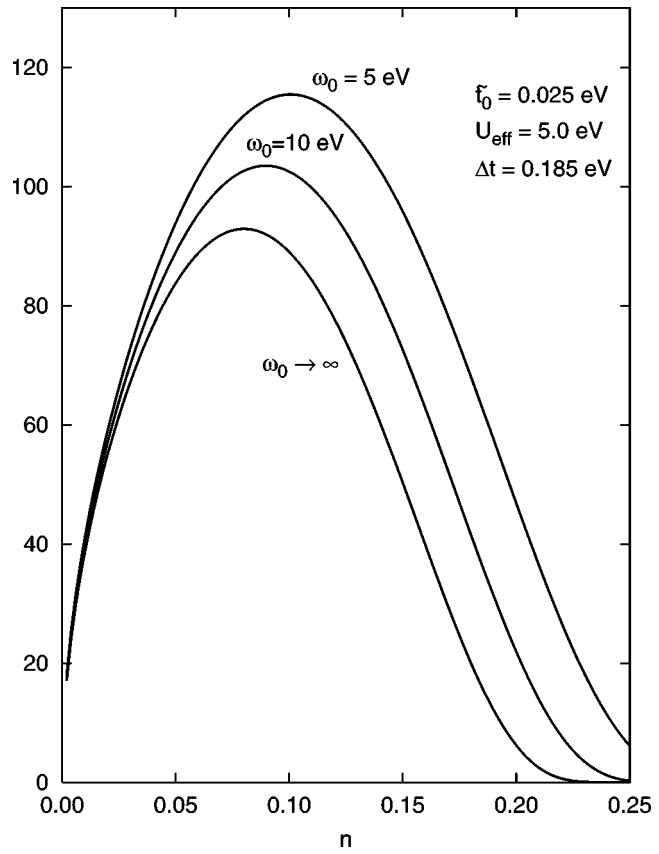

FIG. 1. T_c vs hole doping n. For these parameters $g=2.063$, the hole bandwidth at the top of the band is $\tilde{D}=0.2$ eV, and the electron bandwidth at the bottom of the band is $D=14$ eV. The quasiparticle weight is one at the bottom of the band (electrons) and 0.014 at the top of the band (holes). The boson frequencies are $\omega_0=10$ and 5 eV, which gives $\kappa_0=0.043$ and $\kappa_0=0.085$, respectively.

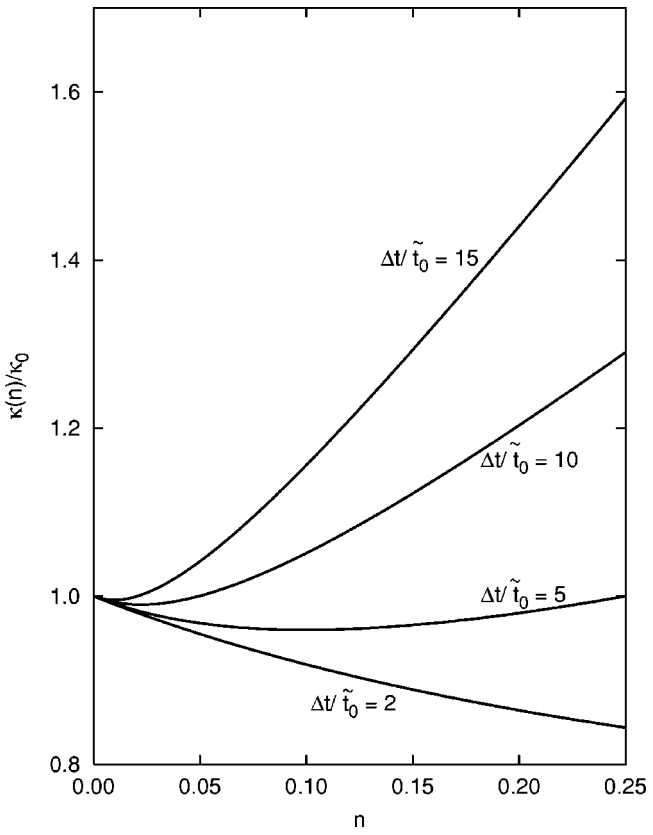

FIG. 2. $\kappa(n)$ vs hole doping n from Eq. (34).

$$I_3=\rho^3 I_0+\tfrac{1}{2}\rho-\tfrac{11}{6}\rho^3,$$

$$I_4=\rho^4 I_0+\tfrac{1}{4}+\tfrac{1}{2}\rho^2-\tfrac{25}{12}\rho^4, \tag{41}$$

where $\rho\equiv 1-n$. Weak coupling is accurate over a wide range of parameters.[12] The end result is

$$k_B T_c=1.13\frac{\tilde{D}(n)}{2}\sqrt{n(2-n)}\exp(-a/b), \tag{42}$$

where

$$a=1+k\rho(2+k\rho)-\kappa\rho(-k-2u\rho+3k\rho^2)+\kappa^2(-9+30\rho^2+7\rho^4)/12-\kappa^3(3-9\rho^2+13\rho^4+\rho^6)/12,$$

$$b=(k^2-2u+4k\rho+k^2\rho^2)/2+\kappa(3u+3u\rho^2-4k\rho^3)/3+\kappa^2(1+6\rho^2+\rho^4)/4-\kappa^3(9-9\rho^2+15\rho^4+\rho^6)/36, \tag{43}$$

with $\kappa\equiv\kappa(n)$. Note that if only the coupling to the boson was present, then, for small hole density, $b/a\approx 2\kappa^2$ for $\kappa \ll 1$. Thus the boson leads to an attractive interaction, independent of the sign of κ, but T_c is unobservably small if $\kappa \ll 1$. However, if T_c already exists (through the presence of the antiadiabatic terms, in this case), then the enhancement due to the coupling to the boson (which, in this case, means a coupling at noninfinite frequency) can be substantial. This nonlinear effect is merely due to the nature of the exponential function.

In Fig. 1 we plot T_c versus hole density n for parameter values $\Delta t=0.185$ eV, $U_{\rm eff}=5.0$ eV, and $\tilde{t}_0=0.025$ eV. The justification for this choice of parameters is the following: the value of U_{eff} is within the generally accepted range; the choice of a large value $\Delta t/\tilde{t}_0=7.4$ (i.e., $g\sim 2$) implies a large dressing of the single hole in the normal state (mass enhancement ~ 70 in the underdoped regime) and a rapid undressing as a function of hole concentration, as seen in the cuprates. The values of Δt and $\tilde{t}$ are then determined by requiring that the maximum T_c be of order of 100 K. As shown in our previous work, Ref. 5, results for this model are not very sensitive to the precise choice of parameters. To explore the effects of retardation, we show results for $\omega_0=\infty$, 10 eV and 5 eV. The explicit n dependence of $\kappa(n)$ is not significant, and is shown in Fig. 2, for a variety of parameter values (note; for Fig. 1, $\Delta t/\tilde{t}_0=7.4$). Figure 1 shows that T_c is enhanced by retardation—as ω_0 decreases, $\kappa_0\equiv\kappa(n=0)$ increases. It is also clear that the range of hole densities increases with increasing amount of retardation.

Finally, we can compute the effective mass and quasiparticle residue as a function of doping. These are obtained in a two-step process. First, in the antiadiabatic limit ($\omega_0\to\infty$), the effective mass ratio is given for low hole densities[8] as

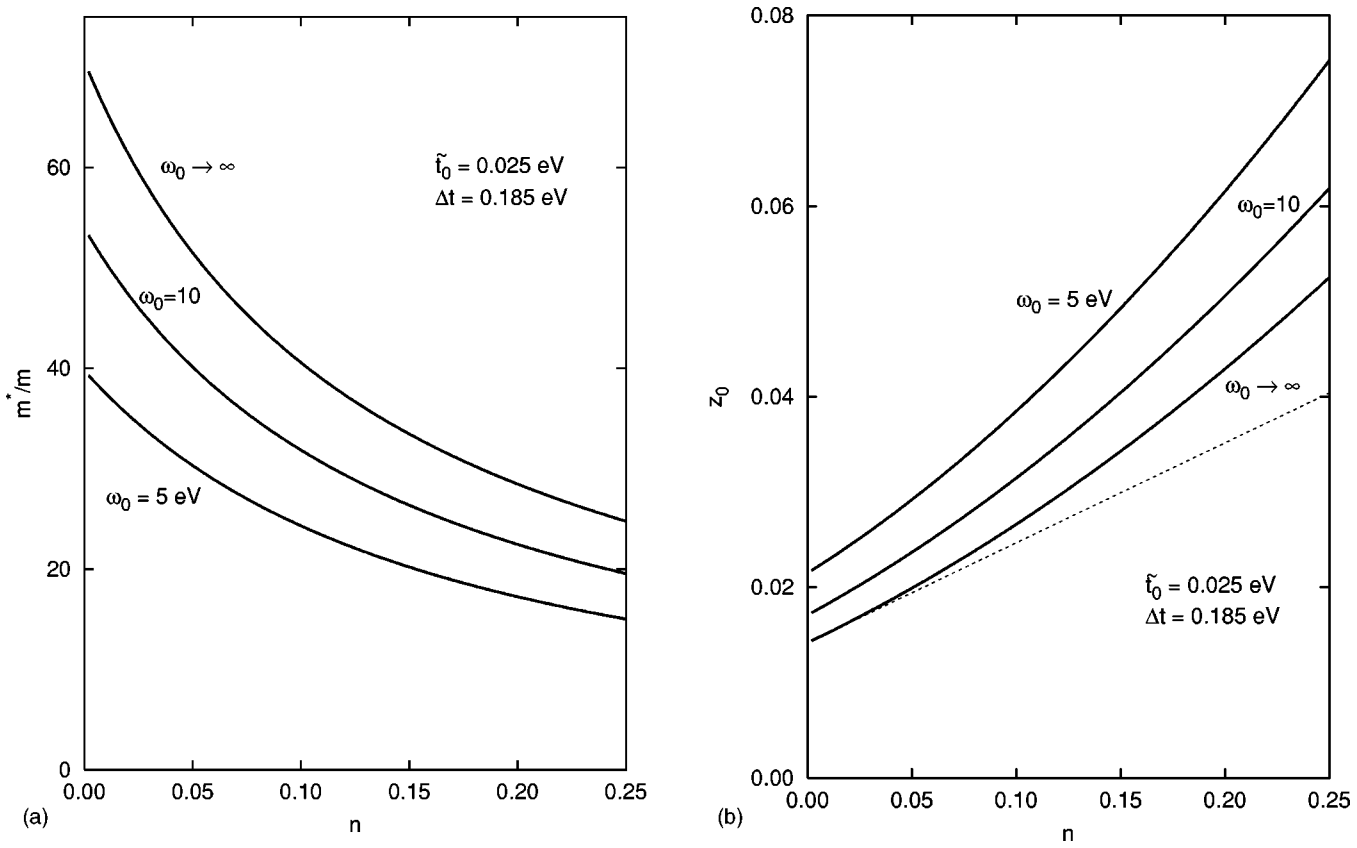

FIG. 3. Effective mass (a) and quasiparticle residue (b) vs hole doping n for several boson frequencies as indicated. As expected, the quasiparticle effective mass decreases as the situation becomes more electronlike; similarly the residue increases towards unity. Note that both quantities have the same tendency, as is made clear by the dashed curve in (b), where the inverse effective mass is plotted for $\omega_0 \to \infty$.

$$m^*_{aa}/m = \frac{(1+\Delta t/\tilde{t}_0)^2}{(1+n\Delta t/\tilde{t}_0)} \tag{44}$$

and the quasiparticle residue is similarly given by[8]

$$z_{aa0} = \frac{\left(1+\frac{n}{2}\Delta t/\tilde{t}_0\right)^2}{(1+\Delta t/\tilde{t}_0)^2}. \tag{45}$$

Here z_{aa0} is the quasiparticle residue on the Fermi surface, and the subscript aa stands for the antiadiabatic limit. To incorporate changes due to retardation effects, we proceed in the usual fashion, and compute the real part of the analytic continuation to the real axis of the self-energy expression, Eq. (24), in the normal state, and without self-consistency (i.e., we omit the self-energy on the right-hand side). Then

$$\frac{m^*}{m} = \frac{m^*_{aa}}{m}\left(\frac{1-a_\omega}{1+a_k}\right) \tag{46}$$

and

$$z_0 = \frac{z_{aa0}}{1-a_\omega}, \tag{47}$$

where

$$a_\omega \equiv \frac{\partial \Sigma_1}{\partial \omega}(\tilde{\epsilon}_k, \omega + i\delta)\big|_{\omega=0,\tilde{\epsilon}_k=\tilde{\mu}_0} \tag{48}$$

and

$$a_k \equiv \frac{\partial \Sigma_1}{\partial \tilde{\epsilon}_k}(\tilde{\epsilon}_k, \omega + i\delta)\big|_{\omega=0,\tilde{\epsilon}_k=\tilde{\mu}_0}, \tag{49}$$

where Σ_1 is the real part of the self-energy. These quantities are given by

$$a_\omega = 2\kappa(n)[1+(1-n)^2] \tag{50}$$

and

$$a_k = \kappa(n)[1+(1-n)^2]. \tag{51}$$

The effective mass and residue are plotted in Fig. 3. It is clear that the effective mass decreases and the quasiparticle residue increases as a function of increasing hole concentration, as expected in this model. Note that retardation actually *decreases* the effective mass and *increases* the quasiparticle residue, because retardation ''undoes'' some of the effects from the generalized Lang-Firsov transformation. Note that retardation has little effect on the doping dependence of these properties. To emphasize the observation made in Ref. 3 we have plotted the inverse effective mass ratio in Fig. 3(b)

(dashed curve) in the antiadiabatic limit to show that the residue and inverse mass behave similarly as a function of doping. This indicates that the frequency dependence of the hole self-energy is most important (as opposed to the momentum dependence).

V. CONCLUSIONS

We have studied the effect of finite boson frequency in a dynamic Hubbard model. The model describes modulation of the Hubbard on-site repulsion by a boson degree of freedom. In the limit of infinite boson frequency the properties of the model are well understood, and here we studied the effect of finite frequencies through a generalized Lang-Firsov transformation and a high-frequency expansion.

One might also ask about the use of cruder approximations. For example, one might first consider the Hamiltonian (5) in the mean-field decoupling given by Eqs. (3) and (4). Doing then the usual Lang-Firsov transformation would yield an effective repulsive Hubbard model, with no superconductivity in the antiadiabatic limit at the BCS-Eliashberg level of approximation. Thus the starting point for such a study would already be in serious error. The dynamics inherent in the coupling of the double occupancy of holes to the boson displacement given in Eq. (5) is crucial for the occurrence of pairing.

The central result of this work is the finding that T_c increases with retardation. That this effect is expected was also indicated by the exact diagonalization study in Ref. 3. In the derivation of this model from first principles[1,2] the boson frequency represents the scale of intra-atomic electronic excitation energies. This scale is expected to be large compared to the scale of interatomic hopping, but is certainly not infinite. Therefore, it is essential to study the effect of finite frequency corrections as done in this paper.

This finding supports the possibility that the model may be relevant to the superconductivity of real materials. It should also be noted that in the microscopic derivation of the model both the coupling constant g increases and the boson frequency decreases as the degree of negative charging of the ion increases. According to the results of this study, both effects enhance superconductivity in this model. Hence our results support the hypothesis that conduction of holes through negative ions is conducive to high-temperature superconductivity. This is in qualitative agreement with the fact that high T_c is found in cuprates (with holes in $O^=$ ions) and in MgB_2 (with holes in B^- ions).

ACKNOWLEDGMENTS

We are grateful to the Natural Sciences and Engineering Research Council of Canada and the Canadian Institute for Advanced Research for support.

[1] J.E. Hirsch, Phys. Rev. Lett. **87**, 206402 (2001).
[2] J.E. Hirsch, Phys. Rev. B **65**, 184502 (2002).
[3] J.E. Hirsch, Phys. Rev. B **65**, 214510 (2002); **66**, 064507 (2002).
[4] J.E. Hirsch, Phys. Rev. B **67**, 035103 (2003).
[5] J.E. Hirsch and F. Marsiglio, Phys. Rev. B **39**, 11 515 (1989); **41**, 6435 (1990).
[6] H. Ding, J.R. Engelbrecht, Z. Wang, J.C. Campuzano, S.C. Wang, H.B. Yang, R. Rogan, T. Takahashi, K. Kadowaki, and D.G. Hinks, Phys. Rev. Lett. **87**, 227001 (2001); Y. Ando, A.N. Lavrov, S. Komiya, K. Segawa, and X.F. Sun, *ibid.* **87**, 017001 (2001); P.D. Johnson, T. Valla, A.V. Fedorov, Z. Yusof, B.O. Wells, Q. Li, A.R. Moodenbaugh, G.D. Gu, N. Koshizuka, C. Kendziora, Sha Jian, and D.G. Hinks, *ibid.* **87**, 177007 (2001).
[7] I.G. Lang and Y.A. Firsov, Zh. Éksp. Teor. Fiz. **43**, 923 (1962) [Sov. Phys. JETP **16**, 1301 (1963)].
[8] J.E. Hirsch, Phys. Rev. B **62**, 14 487 (2000); **62**, 14 498 (2000).
[9] F. Marsiglio and J. P. Carbotte, in *The Physics of Conventional and Unconventional Superconductors*, edited by K.H. Bennemann and J.B. Ketterson (Springer-Verlag, Berlin, 2003), p. 233; cond-mat/0106143.
[10] Strictly speaking, $\chi(k,i\omega_m)$ simply renormalizes the chemical potential, but $Z(k,i\omega_m)$ remains dependent on Matsubara frequency, even if $\kappa_{kk'}(i\nu_n)$ is replaced by a constant independent of Matsubara frequency. These corrections have been neglected, and are expected to cause only minor quantitative changes.
[11] This is apparent by inspection of the kernel as written in Eq. (33), where it *would appear* that the additional electron-boson coupling could only have a detrimental effect on T_c [because of the minus sign in front of the $\kappa(n)$ term]. That this is not the case is clear from the numerical solutions (see Fig. 1).
[12] F. Marsiglio and J.E. Hirsch, Physica C **165**, 71 (1990).