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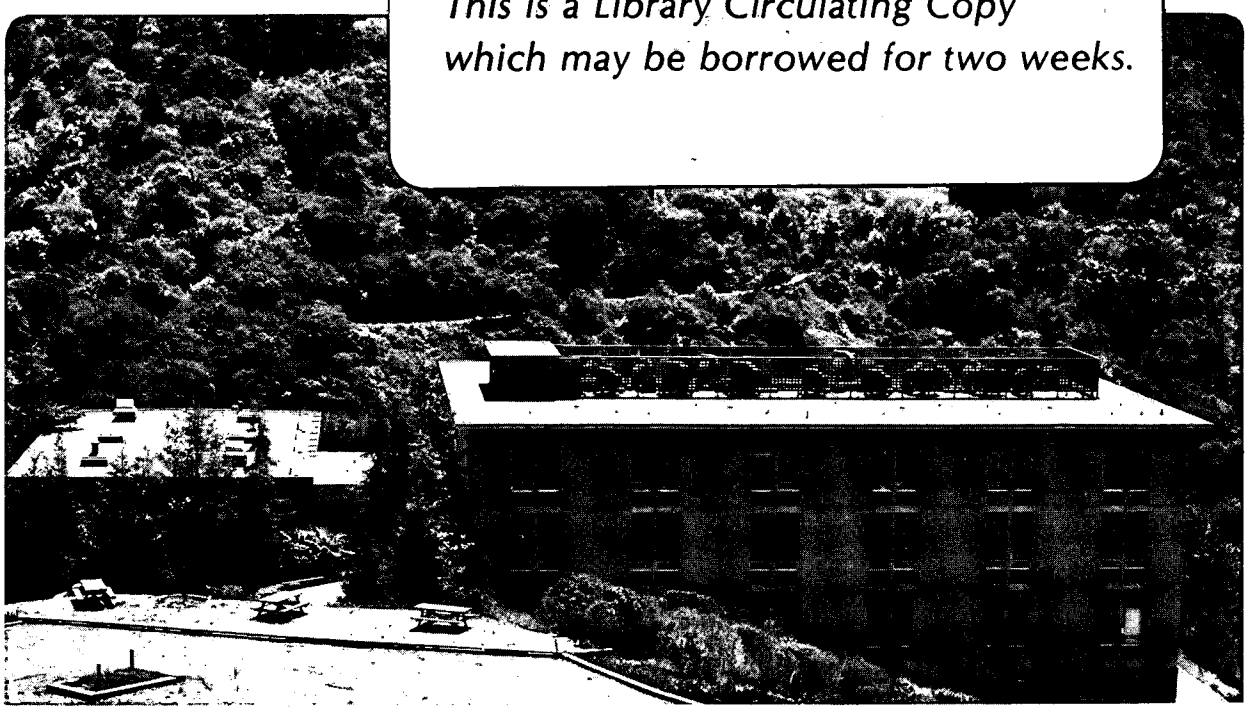

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EXACT SOLUTION OF A PERIODIC-CLUSTER ELECTRON-PHONON SYSTEM*

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ABSTRACT

The ground state of a one-dimensional electron-phonon system is studied by means of a small-crystal approach: an exact solution of a two-site cluster with two electrons and periodic boundary conditions. A single electron band is considered in the tight-binding approximation, together with two-electron interactions between electrons in the same site (Hubbard model); the electrons are coupled to longitudinal acoustic phonons through a bilinear interaction. The problem is isomorphic with that of the homopolar diatomic molecule with a vibronic degree of freedom and coupling between the electronic and vibronic modes. In the adiabatic (large ionic mass, small vibrational frequency) limit there is an analytical solution which indicates that the transition between the non-distorted (weak coupling) and the distorted (strong coupling) phases can be either continuous or discontinuous, depending on whether the value of the electron-electron interaction is larger or smaller than a critical value. In the extremely high-frequency limit (ionic mass $M \rightarrow 0$) it is also possible to find an analytical solution (for $M = 0$) that shows that the system remains undistorted for any value of the electron-phonon coupling and the electron-electron interaction. In the intermediate case (finite, nonvanishing M) numerical solutions exhibit a continuous transition from the non-distorted to the distorted phase.

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I. INTRODUCTION

One-dimensional (1-D) systems[1] are of great intrinsic interest. They are a testing ground for problems in higher dimensions because of the existence, in 1-D, of a variety of exactly soluble problems[1]. Even though several electronic many-body problems have been solved[1–3] exactly in 1-D, the very important problem of a 1-D interacting electron-phonon and electron-electron system has not however produced a model with an exact solution. In dealing with electron-phonon interacting systems several well established approximations exist; the most commonly used one -- the adiabatic or Born-Oppenheimer approximation[4] -- completely neglects quantum fluctuations in the phonon field when solving the interacting electron system.

In this work a study is made of a 1-D Hubbard[1–3,5] Hamiltonian -- with one electron per site, and in the presence of a phonon field and an electron-phonon interaction -- by means of a small-crystal approach[6–17]. This approach samples the Brillouin zone with a finite, small and properly selected set of points which constitute a finite-size space group -- identical, except for the finite number of translations, to the original space group of the infinite system. It should be remembered that this finite sampling approach is exactly equivalent to the study in real space of a cluster of N sites with periodic boundary conditions -- hence the nomenclature of small-crystal approach.

In this contribution the 1-D Brillouin zone is sampled at two points, the zone center and the zone boundary, which results in a cluster of two sites, two electrons and a single vibrational mode. This approach to the problem contains four parameters (three if one of them is taken to be the unit of energy): (i) an electronic bandwidth, (ii) an electron-electron intra-site repulsion, (iii) a lattice vibration frequency, and (iv) an electron-phonon coupling parameter. With the use of a variety of theoretical techniques the problem is reduced, in the various regimes, to situations in which it can be solved *exactly*, albeit sometimes numerically.

The problem here considered is either identical or closely related to other well known problems. The two-point sampling, two-site cluster approximation makes the problem completely isomorphic to the two-electron, two-center homopolar molecule[18] in which a single vibronic degree of freedom plays the role of the zone-boundary phonon mode. The molecular problem is moreover closely related to the dissipative two-state system [19], also known as the spin-boson problem [20]. It is also related to the molecular polaron problem [21–25] and to the Peierls distortion and instability[26].

This paper is organized as follows: Section II describes the model and the Hamiltonian, Section III presents the methods of solution and the results, and Section IV contains a discussion and conclusions.

II. THE HAMILTONIAN

The starting point is the infinite-chain 1-D Hubbard-Frohlich[5,27] Hamiltonian which can be written as:

$$H = H_e + H_{ph} + H_{e-ph}, \tag{2.1}$$

where

$$H_e = -t\sum_{i,\sigma}[c_{i\sigma}^{\dagger}c_{(i+1)\sigma} + c_{i\sigma}^{\dagger}c_{(i-1)\sigma}] + U\sum_i n_{i\uparrow}n_{i\downarrow}.$$

$$= \sum_{k,\sigma}(-2t\cos ka)\, a_{k\sigma}^{\dagger}a_{k\sigma} + (U/N)\sum_{k_1,k_2,k_3} a_{k_1\uparrow}^{\dagger}a_{k_2\uparrow}a_{k_3\downarrow}^{\dagger}a_{k_1+k_2-k_3\downarrow}\ , \tag{2.2}$$

$$H_{ph} = \sum_{q>0}\hbar\omega_q\ [\, b_q^{\dagger}b_q + b_{-q}^{\dagger}b_{-q} + 1\,]\ , \tag{2.3}$$

$$H_{e-ph} = -\frac{g}{\sqrt{2}} \sum_{\substack{k,\sigma \\ q>0}} \sqrt{\frac{\hbar}{2M\omega_q}} \left[a^{\dagger}_{k+q\,\sigma} a_{k\,\sigma} (b^{\dagger}_{-q} + b_q) + a^{\dagger}_{k-q\,\sigma} a_{k\,\sigma} (b^{\dagger}_{q} + b_{-q}) \right] . \tag{2.4}$$

Here $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator for an electron in a s-orbital, with spin $\sigma = \uparrow, \downarrow$, located at site i in the 1-D chain; $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ is the corresponding number operator; $a^{\dagger}_{k\sigma}$ ($a_{k\sigma}$) is the creation (annihilation) operator for an electron in the Bloch state k with spin σ; and N is the total number of sites in the chain. The first term in (2.2) is a hopping term which leads to a total bandwidth $4t$; the second is the intra-site two-particle repulsion term, where U is the single-site Coulomb parameter. In (2.3) $b^{\dagger}_{q}$ (b_q) is the creation (annihilation) operator for a phonon of wavevector q, and $\hbar\omega_q$ is the corresponding phonon energy; for a 1-D monoatomic chain :

$$\omega_q = \sqrt{(K/M)}\ |\ \sin(qa/2)\ |\ ,$$

where M is the mass of the atoms, K is the spring constant and a is the equilibrium interatomic distance. Finally, (2.4) represents the electron-phonon interaction, and g is the electron-phonon coupling constant.

The system has 1-D translational invariance, with a Brillouin zone that extends over the interval

$$-(\pi/a) < k, q \leq (\pi/a) \ . \tag{2.5}$$

Note however, that in (2.3) and (2.4) q is restricted to take values on the positive half of the zone ($q > 0$).

The sampling consists of the following two points in the zone:

$k = 0$: *point* Γ ,

$k = \pi/a$: *point* X .

When only these two points in k space are selected to sample the Brillouin zone, the Hamiltonian can be rewritten as:

$$H_e = -2t \sum_{\sigma} (a^{\dagger}_{\Gamma\sigma} a_{\Gamma\sigma} - a^{\dagger}_{X\sigma} a_{X\sigma}) + (U/2) \sum_{k_1,k_2,k_3=\Gamma,X} a^{\dagger}_{k_1\uparrow} a_{k_2\uparrow} a^{\dagger}_{k_3\downarrow} a_{k_1+k_3-k_2\downarrow} \ , \tag{2.6}$$

$$H_{ph} = \hbar\omega_X (b^{\dagger}_X b_X + \tfrac{1}{2}) \ , \tag{2.7}$$

$$H_{e-ph} = -\frac{g}{\sqrt{2}} \sqrt{\frac{\hbar}{2M\omega_X}} (b^{\dagger}_X + b_X) \sum_{\sigma} (a^{\dagger}_{X\sigma} a_{\Gamma\sigma} + a^{\dagger}_{\Gamma\sigma} a_{X\sigma}) \ , \tag{2.8}$$

where $\omega_X = \sqrt{K/M}$.

With the use of the Bloch-Wannier transformation

$$a_{\Gamma\sigma} = (1/\sqrt{2})(c_{1\sigma} + c_{2\sigma}) \tag{2.9a}$$

$$a_{X\sigma} = (1/\sqrt{2})(c_{1\sigma} - c_{2\sigma}) \tag{2.9b}$$

the Hamiltonian in equations (2.6)-(2.8) can be finally written

$$\begin{aligned} H = & -2t \sum_{\sigma} (c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma}) + U\,(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow}) \\ & + \hbar\omega_X\,(b^{\dagger}_X b_X + \tfrac{1}{2}) \\ & - \frac{g}{\sqrt{2}} \sqrt{\frac{\hbar}{2M\omega_X}}\,(b^{\dagger}_X + b_X)(n_1 - n_2)\ , \end{aligned} \tag{2.10}$$

and the problem has been reduced to the solution of a cluster of two atoms. Note that from equation (2.10) it is clear that the on-site Coulomb repulsion ($U > 0$) tends to spread the electronic charge between the two sites[28], whereas the electron-phonon coupling favors the uneven distribution of electrons between sites 1 and 2.

The six two-electron states of the present problem are:

$$|\,1> = c^{\dagger}_{1\uparrow} c^{\dagger}_{1\downarrow}\,|\,0>\ , \tag{2.11a}$$

$$|\,2> = (1/\sqrt{2})\,(c^{\dagger}_{1\uparrow} c^{\dagger}_{2\downarrow} - c^{\dagger}_{1\downarrow} c^{\dagger}_{2\uparrow})\,|\,0>\ , \tag{2.11b}$$

$$|\,3> = c^{\dagger}_{2\uparrow} c^{\dagger}_{2\downarrow}\,|\,0>\ , \tag{2.11c}$$

$$|\,4> = c^{\dagger}_{1\uparrow} c^{\dagger}_{2\uparrow}\,|\,0>\ , \tag{2.11d}$$

$$|\,5> = (1/\sqrt{2})\,(c^{\dagger}_{1\uparrow} c^{\dagger}_{2\downarrow} + c^{\dagger}_{1\downarrow} c^{\dagger}_{2\uparrow})\,|\,0>\ , \tag{2.11e}$$

$$|\,6> = c^{\dagger}_{1\downarrow} c^{\dagger}_{2\downarrow}\,|\,0>\ , \tag{2.11f}$$

where $|\,0>$ is the vacuum state. It is clear that the states $|\,1>, |\,2>$ and $|\,3>$ are spin singlets, and that $|\,4>, |\,5>$ and $|\,6>$ are spin triplets.

It is also clear that the triplet states have one electron in each site and, as seen from (2.10), there is no coupling between electrons and phonons in this case. This also applies for the singlet state $|\,2>$.

Moreover, because the Hamiltonian conserves the total spin and its z-component, there is no mixing between the singlets and triplets. Consequently only the three singlet states, $|1>, |2>$ and $|3>$, need to be considered. Since only three states are relevant, the problem becomes isomorphic to a spin-1 spin-boson problem, as mentioned in the introduction.

It is useful to establish the isomorphism between the Hamiltonian for the three singlet states and a Hamiltonian for a pseudo-spin 1 system:

$$S_x = (1/\sqrt{2}) \sum_\sigma (c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma}) \ , \tag{2.12a}$$

$$S_y = -(i/\sqrt{2}) \sum_\sigma (c^\dagger_{1\sigma} c_{2\sigma} - c^\dagger_{2\sigma} c_{1\sigma}) \ , \tag{2.12b}$$

$$S_z = ½ (n_1 - n_2) \ , \tag{2.12c}$$

where the pseudo-spin operators S_x, S_y and S_z obey the usual angular-momentum commutation rules

$$[S_x, S_y] = iS_z \ , \ [S_y, S_z] = iS_x \ , \ [S_z, S_x] = iS_y \ . \tag{2.13}$$

Substitution of (2.12) in (2.10) yields

$$\begin{aligned} H &= -2\sqrt{2}\, t\, S_x + U\, S_z^2 \\ &+ \hbar\omega_X\, (b_X^\dagger b_X + ½) \\ &- g\, \sqrt{\hbar\omega_X/K}\, S_z\, (b_X + b_X^\dagger) \ , \end{aligned} \tag{2.14}$$

which is a classical spin-1 spin-boson problem[19].

The Hamiltonian (2.14) contains four (one scaling and three dimensionless, independent) parameters: t, (U/t), $(\hbar\omega_X/t)$, and $[(g/t)\sqrt{\hbar\omega_X/K}]$. Energies can be measured in units of t, and the length scale can be defined either by the harmonic-oscillator length $\sqrt{\hbar\omega_X/K}$, or by the hybrid electronic-vibronic length $\sqrt{t/K}$.

III. METHODS OF SOLUTION AND RESULTS

A. Adiabatic limit

In the adiabatic limit ($\omega_X \to 0$ or $M \to \infty$) it is possible to write the Hamiltonian (2.14) in the following way:

$$H = -2\sqrt{2}\, t\, S_x + U\, S_z^2 + \tfrac{1}{2} K\, x^2 - \sqrt{2}\, g\, S_z\, x \tag{3.1}$$

where $x = \sqrt{\hbar\, \omega_X / 2K}\ (\, b_X + b_X^\dagger\,)$ can now be considered a classical variable, i.e. a parameter. The quantity x is the change in inter-site distance from the uniform a value (the dimerization length change) or, for the molecular problem, the interatomic separation change in the diatomic molecule caused by the electronic-vibronic interaction.

In this adiabatic limit the problem reduces to the diagonalization of a 3×3 matrix, whose eigenvalues are given by a cubic equation

$$E(U\ , K, t, g\ ; x) = \tfrac{1}{2} K x^2 + \lambda(U\ , t, g\ ; x)\ , \tag{3.2}$$

$$\lambda^3\ -\ 2\, U\, \lambda^2\ +\ \lambda\,(\, U^2 - 2\, g^2 x^2 - 16\, t^2\,)\ +\ 16\, t^2\, U\ =\ 0\ . \tag{3.3}$$

An analysis of the limit $U = 0$ of (3.2)-(3.3) is easy and instructive; in that limit (3.3) reduces to a linear equation, with solution at $\lambda = 0$, and a quadratic expression with a solution given by

$$\lambda(0, t, g; x) = -\sqrt{2\, g^2 x^2 + 16\, t^2}\ . \tag{3.4}$$

If λ in (3.4) is real, the total energy of the system is

$$E(0, K, t, g; x) = \tfrac{1}{2} K\ x^2 - \sqrt{2\, g^2 x^2 + 16\, t^2}\ . \tag{3.5}$$

A distortion occurs if the value of x that minimizes (3.5) is different from zero,

$$\frac{\partial\, E(0, K, t, g; x)}{\partial x} = 0 \quad \to \quad x_{\min}^2 = 2\left[\frac{g^2}{K^2} - \frac{4\, t^2}{g^2}\right]\ . \tag{3.6}$$

Because $x_{\min}^2$ must be non-negative, there is a critical value g_c such that the system is distorted only if $g > g_c$. The critical value of g is given by the condition $x_{\min}^2 = 0$ or

$$\frac{g_c^2}{K^2} - \frac{4\,t^2}{g_c^2} = 0 \quad \rightarrow \quad g_c = \pm\sqrt{2Kt} \quad . \tag{3.7}$$

Note that this is a continuous transition, i.e. there is no discontinuity in the value of x^2 as g crosses g_c.

In the general situation $U \neq 0$, for $x \ll 1$ it is possible to expand $\lambda(U, g, x)$ about $x = 0$:

$$\lambda(U, t, g; x) = \lambda^{(0)}(U, t, g) + \lambda^{(2)}(U, t, g)\, x^2 + \lambda^{(4)}(U, t, g)\, x^4 + \cdots \quad , \tag{3.8}$$

where

$$\lambda^{(0)}(U, t, g) = ½\,[U - \sqrt{U^2 + 4\,t^2}] \ , \tag{3.9}$$

$$\lambda^{(2)}(U, t, g) = \frac{g^2}{16t^2}\left[U - \frac{U^2 + 32t^2}{\sqrt{U^2 + 64t^2}}\right] , \tag{3.10}$$

$$\lambda^{(4)}(U, t, g) = \frac{g^4}{2048\,t^6}\left[\frac{U^6 + 112\,U^4\,t^2 + 3072\,U^2\,t^4 + 8192\,t^6}{(U^2 + 64t^2)^{3/2}} - U(U^2 + 64t^2)\right] . \tag{3.11}$$

Substitution of (3.4) in (3.3) yields

$$E\ (U, K, t, g; x) = \lambda^{(0)}\ (U, t, g) + \left[½\,K + \lambda^{(2)}(U, t, g)\right] x^2 + \lambda^{(4)}(U, t, g)\, x^4 + \cdots \tag{3.12}$$

There are two possible types of distortions, depending on the sign of $\lambda^{(4)}(U, t, g)$:

a) if $\lambda^{(4)}(U, t, g) > 0$ the system has a continuous distortion as a function of the parameters U, t, and g. The critical line $g_c(U, K, t)$, i.e. the locus of the parameters for an infinitesimal distortion, is given by

$$\frac{K}{2} + \frac{g_c^2}{16t^2}\left[U - \frac{U^2 + 32t^2}{\sqrt{U^2 + 64t^2}}\right] = 0 \ , \tag{3.13}$$

which is the generalization of (3.7) for $U \neq 0$. Equation (3.13) means that, for given values of U, K, and t, a minimum strength g_c of the electron-phonon coupling constant g is necessary to obtain a distorted system. For $g < g_c$ the system is undistorted. For $U \rightarrow -\infty$, (3.13) takes the asymptotic form

$$g_c \rightarrow \pm\,[(4\,K\,t^2 / \,|U|\,]^{1/2} \ , \tag{3.14}$$

as expected from physical considerations[28].

b) if $\lambda^{(4)}(U, t, g) < 0$, the system has, as a function of the parameters, a discontinuous transition between x=0 and a finite value of x. The critical values $U_T(t)$ and $g_T(t, K)$ of U and g that separate the continuous from the discontinuous transitions are given by the condition

$$\lambda^{(4)}(U_T, g_T, 0) = 0 \ , \tag{3.15}$$

which, according to (3.11), reduces to

$$U_T/t = 2\sqrt{\sqrt{80} - 8} \approx 1.94347 \ , \tag{3.16}$$

whereas g_T is given by (3.13) for $U = U_T$.

For $U > U_T$ there is a discontinuous change in the distortion x as a function of the parameters. It can be seen from (3.12) that, since $\lambda^{(4)}$ is negative, the ground-state energy $E\ (U, K, g, t; x)$ has three minima, one at x=0 and two symmetric ones at finite values of x. The discontinuous transitions take place when all three minima attain the same E value; the values of the parameters at the transitions must be determined numerically by solving the equation for the minima and using the complete expressions (3.2)-(3.3).

The complete stability diagram in parameter space is given in Figure 1.

B. The $\omega_X \to \infty$ ($M \to 0$) limit.

In the (unphysical) case of infinitely light atoms, the Hamiltonian (2.14) can be rewritten in the following way:

$$H = H_0 + V \ , \tag{3.17}$$

where

$$H_0 = U\ S_z^2 + \hbar\,\omega_X\ (b_X^\dagger b_X + ½) - g\ \sqrt{\hbar\,\omega_X/K}\ S_z\ (b_X + b_X^\dagger) \tag{3.18}$$

and

$$V = -\,2\sqrt{2}\,t\ S_x \ . \tag{3.19}$$

It is now possible to perform a canonical transformation that diagonalizes H_0 with respect to the boson field[29]:

$$\tilde{H} = e^{iL}\, H\, e^{-iL} = \tilde{H}_0 + \tilde{V} \ , \tag{3.20}$$

where

$$L = \frac{ig}{\sqrt{\hbar\,\omega_X K}}\, S_z\, (b_X + b_X^\dagger) \ , \tag{3.21}$$

$$\tilde{H}_0 = \hbar\,\omega_X\, (b_X^\dagger b_X + ½) + (U - g^2/K)\, S_z^2 \ , \tag{3.22}$$

and

$$\tilde{V} = -\sqrt{2}\, t\, \left[S_+\, e^{-g\,(b_X + b_X^\dagger)/\sqrt{\hbar\,\omega_X K}} + S_-\, e^{g\,(b_X + b_X^\dagger)/\sqrt{\hbar\,\omega_X K}} \right] . \tag{3.23}$$

In the limit $\omega_X \to \infty$ (3.20) reduces to

$$\tilde{H}(\omega_X \to \infty) = -\,2\sqrt{2}\, t\, S_x + \hbar\,\omega_X\, (b_X^\dagger b_X + ½) + (U - g^2/K)\, S_z^2 \ , \tag{3.24}$$

i.e. there is a complete decoupling of the pseudo-spin (the electronic degrees of freedom) and phonons. Moreover, since $L \to 0$ for $\omega_X \to \infty$,

$$\tilde{H}(\omega_X \to \infty) = H(\omega_X \to \infty) \tag{3.25}$$

and consequently the system remains undistorted for any value of the electron-phonon coupling g.

C. The case for finite mass M.

In this case, the only way of study the problem is by numerical diagonalization of the hamiltonian; for finite ω_X it is convenient to use the matrix representation of the Hamiltonian (3.20) and, as a basis, the eigenstates of $\tilde{H}_0$.

In order to understand the results and present them in a convenient way, it is important to remark that for both, the distorted and the undistorted cases, the quantum-mechanical expectation value $< x >$ is always equal to zero. This is because of the symmetry of H, which is invariant under the *simultaneous* changes

$$S_z \rightarrow -S_z \ , \ x \rightarrow -x \ .$$

The vanishing expectation value means that the system is either undistorted, or has equal probability of being distorted to the right or to the left. The symmetry above implies also vanishing expectation values for any odd power of the distortion x.

One possible measure of the distortion is the mean value $< x^2 >$, as compared to the square of the natural oscillator length $\sqrt{\hbar \omega_X / K}$. However this quantity does not distinguish between a "static" (except for tunneling effects) distortion, and a "dynamic", soft-spring-oscillator situation.

A complementary information to be obtained is the dimensionless parameters

$$f\ (U, K, t, g) = \frac{< x^4 >}{< x^2 >^2} \ , \tag{3.26}$$

where the expectation values are taken for the ground state corresponding the the values of the parameters (U, K, t, g). It can be shown that for the uncoupled oscillator

$$f\ (U, K, t, 0) = 3 \tag{3.27}$$

and, for the static distortion corresponding to $M \rightarrow \infty$, $\omega_X = 0$,

$$f\ (U, K \rightarrow 0, t, g > g_{c)} = 1 \ . \tag{3.28}$$

It is expected that f will exhibit intermediate values $1 \leq f \leq 3$ for other values of the parameters. Changes (as function of the parameters) will be continuous for continuous transitions, and discontinuous if the transition is discontinuous.

When the eigenstates of $\tilde{H}_0$ are used as a basis for the diagonalization of $\tilde{H}$, any state can be written:

$$| \tilde{\Psi} > = \sum_{\nu=0}^{\infty} \left[a_\nu \mid +, \nu > + b_\nu \mid 0, \nu > + c_\nu \mid -, \nu > \right] \ , \tag{3.29}$$

$\sigma = 0, \pm 1$ is an eigenstate of the pseudo-spin operator S_z, and $\nu = 0,1,2,....\infty$ is the excitation state of the *canonically transformed* oscillator. The coefficients a_ν, b_ν, and c_ν satisfy the normalization condition

$$\sum_{\nu=0}^{\infty} (a_\nu^2 + b_\nu^2 + c_\nu^2) = 1 \ . \tag{3.30}$$

The calculation proceed as follows. In the original basis

$$< x^2 > = < \Psi \mid x^2 \mid \Psi > = (\hbar \omega_X)/(2K) < \Psi \mid (b_X + b_X^\dagger)^2 \mid \Psi > \; ; \tag{3.31}$$

since

$$\mid \Psi > = e^{-iL} \mid \tilde{\Psi} > \; , \tag{3.32}$$

(3.31) can be rewritten as

$$< x^2 > = \frac{\hbar \omega_X}{2K} < \tilde{\Psi} \mid \left[b_X + b_X^\dagger + \frac{2\, g\, S_z}{\sqrt{h \omega_X K}} \right]^2 \mid \tilde{\Psi} > \; , \tag{3.33}$$

which, with the use of (3.29) yields

$$< x^2 > = (\tfrac{1}{2}\hbar \omega_X / K) \left[-1 + 2 \sum_{\nu=0}^{\infty} (\nu+1)(a_\nu^2 + b_\nu^2 + c_\nu^2) + 2 \sum_{\nu=0}^{\infty} \sqrt{(\nu+1)(\nu+2)}\, (a_\nu a_{\nu+2} + b_\nu b_{\nu+2} + c_\nu c_{\nu+2}) + \right.$$

$$\left. (8g/\sqrt{\hbar \omega_X K}) \sum_{\nu=0}^{\infty} (\nu+1)(a_\nu a_{\nu+1} - c_\nu c_{\nu+1}) + 4\, g^2/(\hbar \omega_X K) \sum_{\nu=0}^{\infty} (a_\nu^2 + c_\nu^2) \right] \tag{3.34}$$

Analysis of the various limits of (3.34) is easy and instructive. In the weak-coupling limit ($g \to 0$) there is no coupling between the pseudo-spin and the phonons, and the ground state of the system corresponds to an harmonic oscillator in its ground state ($a_0^2 + b_0^2 + c_0^2 = 1$, $a_\nu = b_\nu = c_\nu = 0$ for any $\nu \neq 0$); in this limit, expression (3.34) reduces to

$$< x^2 > = \tfrac{1}{2}\hbar \omega_X / K \; , \tag{3.35}$$

the standard result for a free harmonic oscillator in its ground state. Correspondingly the value (3.27) is obtained for f.

In the strong coupling limit ($g \to \infty$) the leading term in (3.34) is the last one, and because

$$\sum_{\nu=0}^{\infty} (a_\nu^2 + c_\nu^2) \to 1$$

for in this limit, (3.34) reduces to

$$< x^2 > \to 2g^2/K^2 \; . \tag{3.36}$$

Note that (3.36) yields the value (3.6), obtained for the square of the distortion in the adiabatic limit, $M \rightarrow \infty$, for $U = 0$ and $g \rightarrow \infty$.

Finally, as $\omega_X \rightarrow \infty$, the only contribution in (3.34) comes from the second term when $\nu = 0$, and therefore the result (3.35) is obtained again, in agreement with the analysis of the previous section.

Numerical results are presented in Figures 2 through 4. Figure 2 shows the calculated values of $< x^2 >$, in units of t/K, plotted as a function of g (in units of $\sqrt{tK}$), for $U = 0$ and several values of ω_X. Figure 2 (a), corresponding to $\omega_X = 0$ is the representation of (3.6). It is clear that, as phonon quantum fluctuations increase, the non-distorted region (the "flat" part of the curve) becomes larger, and consequently larger values of g are necessary to obtain a distorted system.

Figure 3 displays $f\ (U{=}0, K, t, g)$ as a function of g for the same three values of the frequency ω_X of Figure 2. It is clear that only for the adiabatic limit ($\omega_X{=}0$) is the transition discontinuous between the two limits (3.27), (3.28). In all other cases the transition is smooth. Examination of Figures 2 and 3 clearly show that the presence of quantum fluctuations in the phonon (vibronic) field blurs the distinction between "static" distortion and "softer" effective oscillator spring.

Figure 4 is the plot of $< x^2 >$, again in units of t/K, as a function of g (once more in units of $\sqrt{tK}$), for constant frequency ($\hbar\omega_X/t = 1$), and for various values of the Coulomb repulsion U/t. It is clear that as U increases it is necessary to have larger values of g to obtain a distorted system; this is expected from physical grounds. Although as a function of g the transition is always continuous if $\omega_X \neq 0$, as U increases the curves resemble more closely one with a discontinuous jump [see especially Figure 4 (b), for $U/t = 10$, and its detail, Figure 4(c)].

IV. CONCLUSIONS

By analytical solution in several limits, and by numerical solution [employing the canonical transformation (3.20)-(3.21)] of the general case, the following three isomorphic problems have been studied:

(i) A 1-D Hubbard Hamiltonian, with one electron per site, in the presence of a phonon field and an electron-phonon interaction and with sampling of the Brillouin zone in only two points (two-site

small-crystal approximation);

(ii) A two-electron, diatomic, homopolar molecule with an interaction between the electronic and the vibronic degrees of freedom;

(iii) The spin-1 spin-boson problem.

The exact results found here can be summarized as follows:

(a) Only in the adiabatic limit (ω_X=0) it is possible to make a clear-cut distinction between a distorted and an undistorted system. Vibronic quantum fluctuations blur the distinction.

(b) In the strongly interacting limit ($U \rightarrow \infty$) the system is always undistorted.

(c) The system is also always undistorted in the unphysical limit $M \rightarrow 0$, $\omega_X \rightarrow \infty$, finite spring constant K.

(d) Smaller values of the electron-phonon interaction g, and/or larger values of the electron-electron repulsion U make the "undistorted" state more stable.

(e) In the adiabatic limit there is a critical value of the electron-electron repulsion, U_T, given by (3.16), such that for $U < U_T$ the transition between undistorted and distorted ground state is continuous; for $U > U_T$ the distortion, as a function of the parameters, is discontinuous and requires increasing values of the electron-coupling constant g as U increases.

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FIGURE CAPTIONS

FIGURE 1. The various ground states of the system as a function of the parameters g and U in the adiabatic limit $M \to \infty$, $\omega_X \to 0$. The dot corresponds to the critical value U_T. For $U < U_T$ (light line) the transition, as function of the parameters, between the undistorted and the distorted states is continuous; for $U > U_T$ (heavy line) the transition is discontinuous from $x=0$ to a finite value of x.

FIGURE 2. The expectation value $\langle x^2 \rangle$ as a function of the coupling parameter g for the non-interacting electron system, $U = 0$. The three cases correspond to (a) the adiabatic limit $\omega_X = 0$; (b) $\hbar\omega_X = t$; and (c) $\hbar\omega_X = 100\,t$.

FIGURE 3. The dimensionless parameter f, defined in (3.26), for the three cases of Figure 2: (a) the adiabatic limit $\omega_X = 0$; (b) $\hbar\omega_X = t$; and (c) $\hbar\omega_X = 100\,t$.

FIGURE 4. The expectation value $\langle x^2 \rangle$ as a function of the coupling parameter g for the cases $\hbar\omega_X = t$ and for (a) $U = 5t$; and (b) $U = 10\,t$. The steep but smooth increase in (b) in the neighborhood of $g = 3.3\sqrt{tK}$ is shown in detail in (c). The case for $\hbar\omega_X = t$ and $U = 0$ is shown in Figure 2 (b).

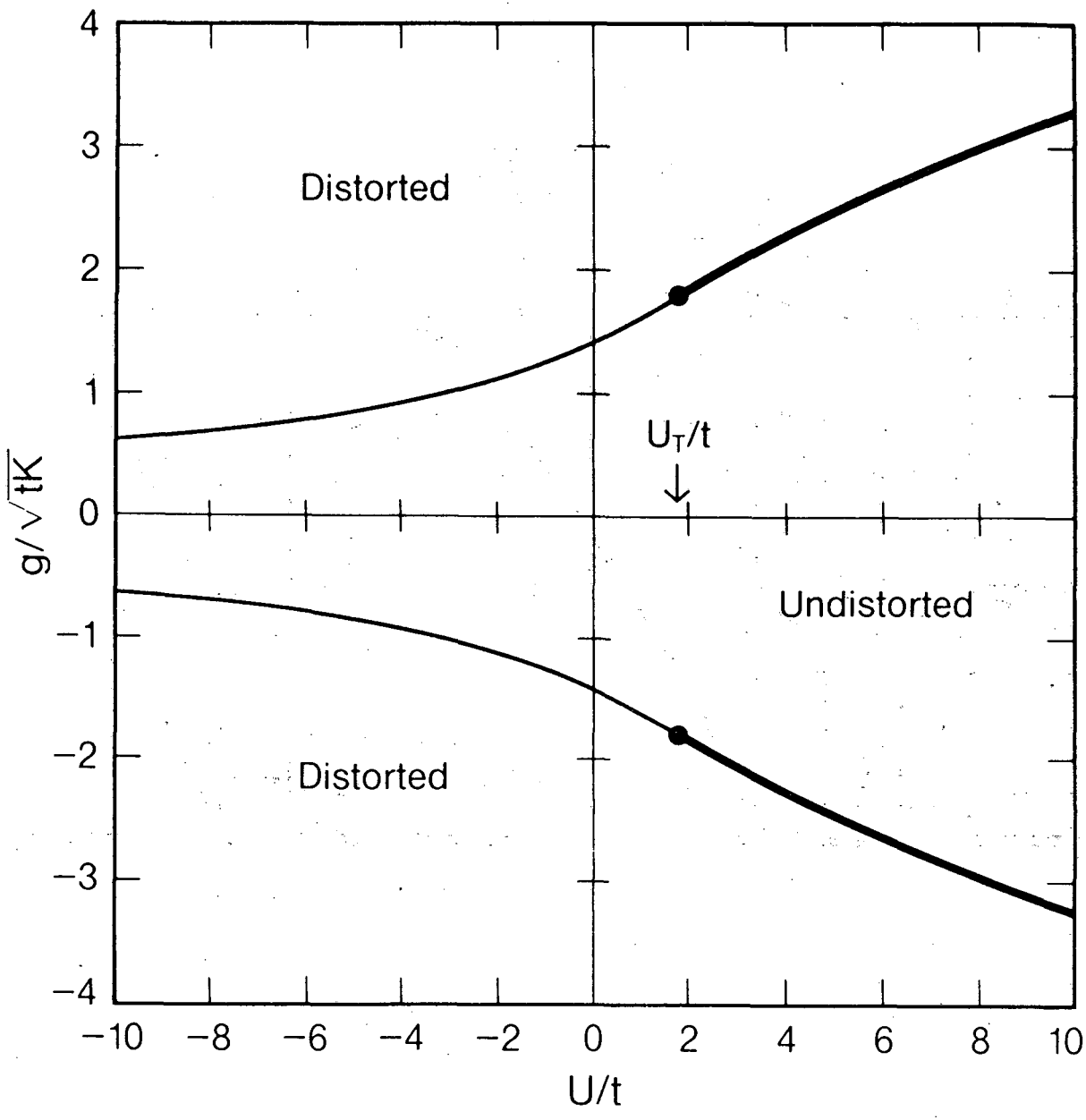
Distorted
Undistorted
Distorted
U_T/t
$g/\sqrt{tK}$
U/t
4
3
2
1
0
−1
−2
−3
−4
−10
−8
−6
−4
−2
0
2
4
6
8
10

FIGURE 1

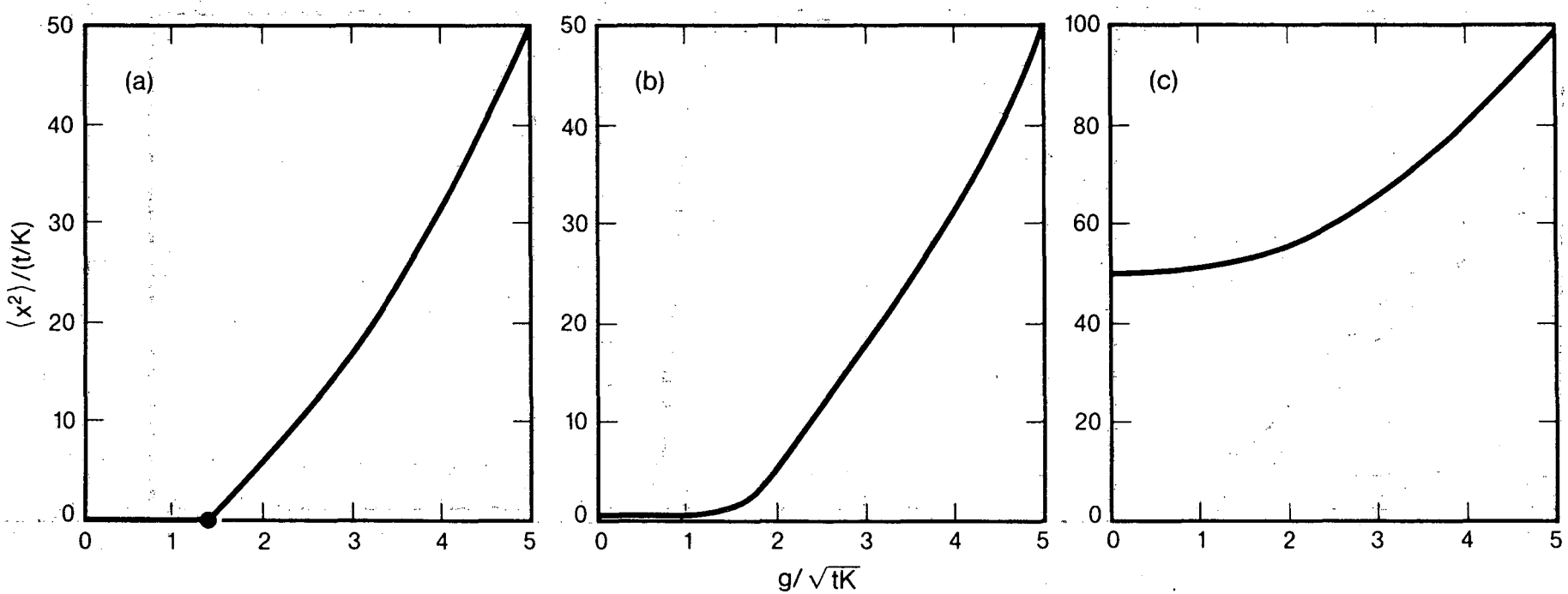

FIGURE 2

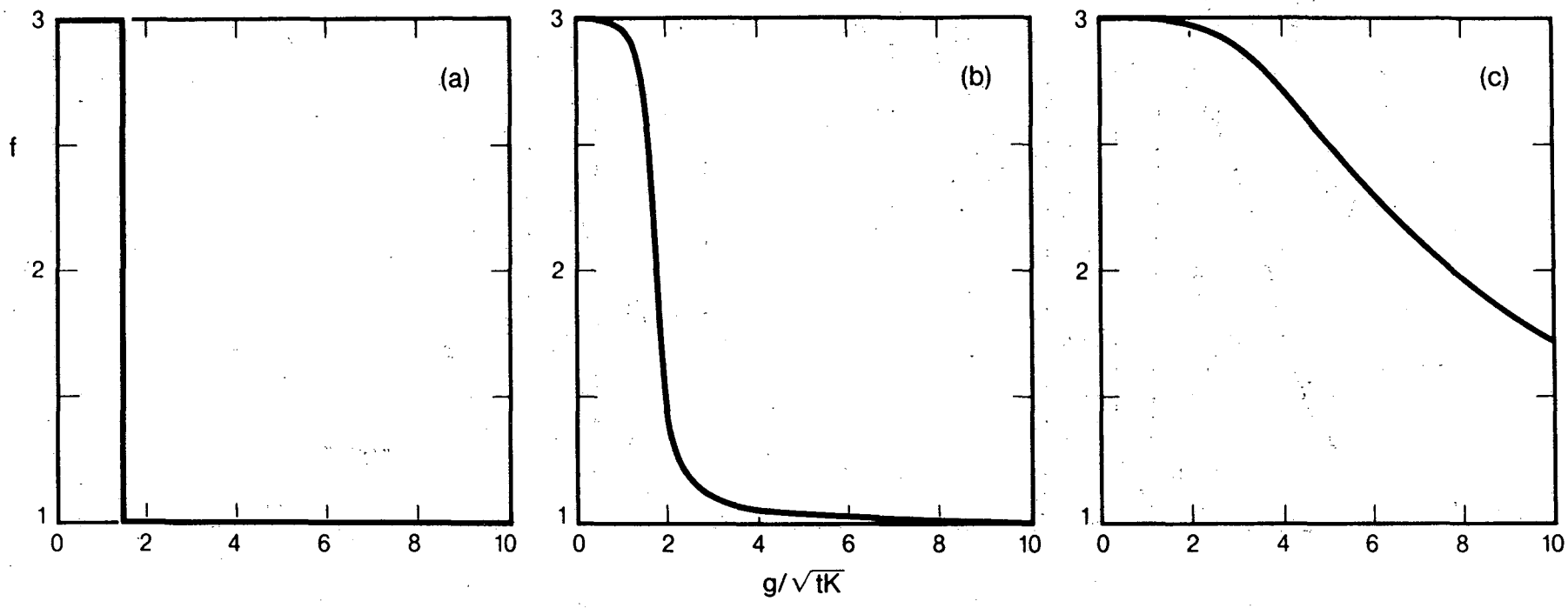

FIGURE 3

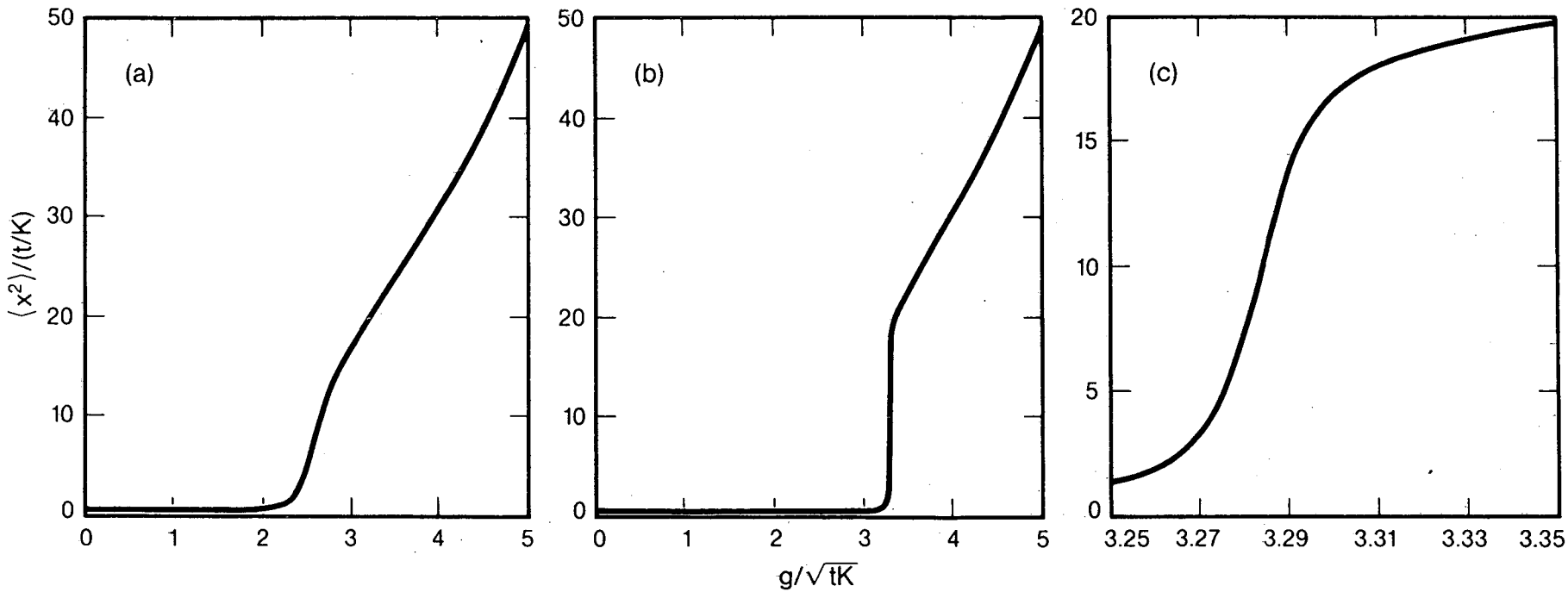
(a)
(b)
(c)
$\langle x^2 \rangle / (t/K)$
$g/\sqrt{tK}$
0
10
20
30
40
50
5
15
1
2
3
4
3.25
3.27
3.29
3.31
3.33
3.35

FIGURE 4

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