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On the electron–phonon interaction in the Hubbard model

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Abstract. A Green function technique is used to study the electron–phonon interaction in the Hubbard model. The Coulomb interaction constant is renormalised owing to the electron–phonon interaction; this renormalisation always produces an increase in the critical temperature T_c. The dependence of the electronic damping on the ratio U/W (Coulomb interaction per band width) and on the band occupation n for different temperatures is discussed. The damping $\gamma(T, U/W)$ shows different behaviours for U = constant and W = constant.

1. Introduction

The Hubbard [1] model is widely used for an approximate description of correlation effects and their influence on the electrical and magnetic properties of narrow-band semiconductors and of some transition-metal compounds [2]. Recently the high-T_c superconductors were examined using the Hubbard model [3–6]. The magnetic and thermodynamic properties (magnetic phase diagram, ground state energy, specific heat, magnetic susceptibility, etc) of Hubbard systems in one, two and three dimensions have been theoretically investigated by many researchers [7–12]. The damping, however, has not been so intensively studied. This model, although simple in form, is not easy to handle mathematically. No exact solutions exist for the finite-temperature properties of the Hubbard model. Several approximation theories for the three-dimensional finite-temperature magnetism employing the functional-integral method within the adiabatic approximation [13, 14] which interpolate between the weak- and strong-interaction limits have been proposed in the last few years.

Quite recently, novel computational methods have been proposed to obtain the exact results for three-dimensional systems. In [15] a method was developed to treat exactly a fairly large cluster of the Hubbard model, combining the Monte Carlo (MC) method with a discrete Hubbard–Stratanovich transformation. The quantum MC simulation was performed for a $4 \times 4 \times 4$ simple-cubic lattice [10], calculating various quantities such as the susceptibility and the energy as a function of the temperature T and the electron–electron interaction U. As for the ground state of the Hubbard model, in [16] the variational MC method was proposed. The ground-state properties of the simple-cubic Hubbard model for a cluster of a $6 \times 6 \times 6$ lattice were studied.

In the last 2 years the electron–phonon interaction has been studied by many workers [17–19] in order to explain the high transition temperatures in the new superconductors.

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The conventional electron–phonon coupling model is generally believed to be the origin of superconductivity in simple and transition metals and their compounds [20–22]. An exact solution of a modified Hubbard model for a tetrahedral cluster with periodic boundary conditions has been presented in [23]. It includes a static electron–lattice interaction in which the inter-site bond-hopping parameter is a function of the bond electron occupation. The dynamics of the lattice are not included in this contribution, but the dynamic electron–phonon interaction must play a role in the superconducting properties. The electron–phonon coupling in the two-dimensional Hubbard model using the MC method has been investigated in [24]. The Green function method is used to study the Hubbard model without electron–phonon interaction for example in [12] and including the electron–phonon interaction in [25]. Exact formulae were obtained only in the band ($U \ll W$) and atomic ($U \gg W$) limits [7]. These two approximate solutions do not coincide at the intermediate values of the ratio U/W, where U and W are the Coulomb interaction and the band width, respectively. In order to obtain an expression for the energy spectrum and the damping for any values of U/W including the electron–phonon interaction we have used a Green function method proposed in [26] for spin operators.

2. Model and method

We consider the Hubbard Hamiltonian with electron–phonon interaction:

$$H = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^+ c_{k\sigma} + \frac{U}{2} \sum_i n_{i\sigma} n_{i-\sigma} + \sum_{q,\lambda} \omega_{q\lambda} a_{q\lambda}^+ a_{q\lambda}$$

$$- \sum_{k,q,\sigma,\lambda} A(q\lambda) c_{k+q\sigma}^+ c_{k\sigma} (a_{q\lambda} + a_{-q\lambda}^+) \tag{1}$$

where $c_{i\sigma}^+$, $c_{i\sigma}$ are the creation and annihilation electron operators on site i with spin projection $\sigma = \pm 1$, $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$ and ε_k is the band energy:

$$\varepsilon_k = -\tfrac{1}{3} W[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)].$$

W is the conduction band width. The final term in (1) represents interactions between the electron and phonon systems with $A(q\lambda) = \bar{A}_q/(2\omega_{q\lambda})^{1/2}$, $\bar{A}_q \sim q$.

3. Static properties

The retarded Green function to be evaluated is defined as

$$G_{k\sigma} = \langle\langle c_{k\sigma}; c_{k\sigma}^+ \rangle\rangle. \tag{2}$$

For the approximate calculation of the Green function (2) we use a method proposed in

[26] which is appropriate for spin problems. The equation of motion of $G_k(t)$ can be written as

$$i\dot{G}_k(t) = \delta(t)\langle[c_k, c_k^+]\rangle + [\varepsilon_k + R_k(t)]G_k(t). \tag{3}$$

$R_k(t)$ is the expression of the higher correlation functions:

$$R_k(t) = \langle[j_k(t), c_k^+]\rangle/\langle[c_k(t), c_k^+]\rangle \qquad j_k = [c_k, H_{\text{int}}].$$

Taking into account that

$$R_k(t) = R_k(0) - \int_0^t d\tau \frac{d}{d\tau}[R_k(t-\tau)]$$

then equation (3) can be transformed to

$$i\dot{G}_k(t) = \delta(t)\langle[c_k, c_k^+]\rangle + [E_k - i\gamma_k(t)]G_k(t) \tag{4}$$

with

$$E_k = \varepsilon_k + R_k(0) = \varepsilon_k + \langle[j_k, c_k^+]\rangle/\langle[c_k, c_k^+]\rangle \tag{5}$$

$$-i\gamma_k(t) = -i\int_0^t d\tau\langle[j_k(t), j_k^+(\tau)]\rangle/\langle[c_k(t), c_k^+(\tau)]\rangle. \tag{6}$$

The time-independent term (5) gives the electronic energy in the generalised Hartree–Fock approximation, whereas the time-dependent term (6) includes the damping effects.

We obtain for the electron Green function

$$G_{k\sigma}(E) = 1/(E - E_{k\sigma} - M_{k\sigma} + i\gamma_{k\sigma}) \tag{7}$$

where $E_{k\sigma}$, $M_{k\sigma}$ and $\gamma_{k\sigma}$ are the electronic energy in the generalised Hartree–Fock approximation, the energy shift and the electronic damping, respectively.

The equation of motion for the electron and phonon operators using the Hamiltonian (1) are

$$i\dot{c}_{k\sigma} = \varepsilon_k c_{k\sigma} + \frac{U}{\sqrt{N}}\sum_{k',q} c_{k'+q\sigma}^+ c_{k'\sigma'} c_{k+q\sigma} - \frac{1}{\sqrt{N}}\sum_{q,\lambda} A(q\lambda)c_{k-q\sigma}(a_{q\lambda} + a_{-q\lambda}^+) \tag{8}$$

$$i\dot{a}_{k\lambda} = \omega_{k\lambda}a_{k\lambda} - \sum_{q,\sigma} A(k\lambda)c_{q\sigma}^+ c_{q+k\sigma} \tag{9}$$

$$i\dot{a}_{-k\lambda}^+ = -\omega_{k\lambda}a_{-k\lambda}^+ + \sum_{q,\sigma} A(k\lambda)c_{q\sigma}^+ c_{q+k\sigma}. \tag{10}$$

From the last two equations, we obtain

$$\langle a_{k\lambda}\rangle + \langle a_{-k\lambda}^+\rangle = \frac{2A(k\lambda)}{\omega_{k\lambda}}\sum_{q,\sigma}\langle c_{q\sigma}^+ c_{q+k\sigma}\rangle. \tag{11}$$

The renormalised electronic energy in the generalised Hartree–Fock approximation from (5) with (8)–(11) is

$$E_{k\sigma} = \varepsilon_k + \frac{U_{\text{eff}}}{N}\sum_q \langle n_{q-\sigma}\rangle + \frac{2A_0^2}{\omega_0 N}\sum_q \langle n_{q\sigma}\rangle \tag{12}$$

where $\langle n_{q\sigma}\rangle \equiv \bar{n}_{q\sigma}$ is the occupation number distribution:

$$\bar{n}_{q\sigma} \equiv \langle c_{q\sigma}^+ c_{q\sigma}\rangle = 1/[\exp(\beta E_{k\sigma}) + 1]. \tag{13}$$

As far as firstly the static properties are considered, the effect of the electron–phonon

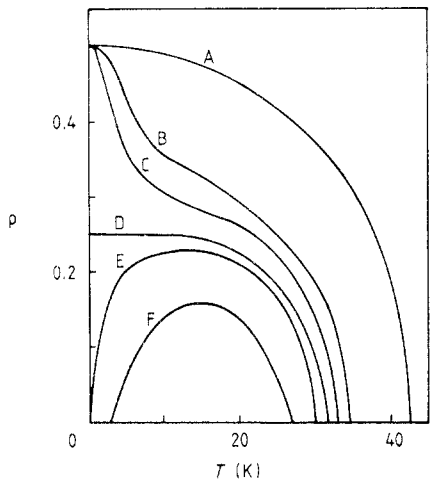

Figure 1. Temperature dependence of the electron magnetisation $\rho(T)$ for $\bar{U} = 4$ eV and different W- and n-values: curve A, $W = 0.5$ eV, $n = 1.3$; curve B, $W = 0.1$ eV, $n = 1.2$; curve C, $W = 0.05$ eV, $n = 1.1$; curve D, $W = 0$ or 2 eV, $n = 1$; curve E, $W = 2.02$ eV, $n = 0.99$; curve F, $W = 2.1$ eV, $n = 0.95$

interaction is thus a renormalisation of the electron–electron interaction constant $U \rightarrow U_{\text{eff}}$:

$$U_{\text{eff}} \equiv \bar{U} = U + \Delta U_{\text{el-ph}} \qquad \Delta U_{\text{el-ph}} = \lim_{q \rightarrow 0}(2A_{q\lambda}^2/\omega_{q\lambda}) \tag{14}$$

which now contains an indirect phonon-mediated part in addition to the direct part. This renormalisation was not obtained earlier by other researchers using the Green function method (see [3, 25], and references therein).

The conduction electron magnetisation ρ is given by

$$\rho = \frac{1}{2N}\sum_{q,\sigma} \sigma\langle c_{q\sigma}^{+} c_{q\sigma}\rangle \qquad \sigma = \pm 1. \tag{15}$$

$\rho(T)$ was numerically calculated taking different model parameters. Figure 1 shows the dependence of $\rho(T)$ for constant $\bar{U} = 4$ eV and for various band-width values W. For $\bar{U}/2W > 1$ (in many oxides and sulphides [27] of transition metals the Coulomb interaction is much greater than the band width ($\bar{U} \gg W$)), ρ reaches its highest value at $T = 0$ ($\rho = 0.5$) and then decreases with $T \rightarrow T_c$. At $T = T_c$, ρ is zero. For $\bar{U}/2W = 1$ (or ∞, i.e. $W = 0$) the curve is not so steep and starts at $\rho = 0.25$ for $T = 0$. For $\bar{U}/2W < 1$ (the band limit $\bar{U} \ll W$ is a situation typical for a transition metal, e.g. $\bar{U}/2W = 0.14$–0.16 for Fe, Ni and Co), ρ is zero at $T = 0$, then increases with increasing temperature and at $T = T_c$ is zero again (figure 1, curve E). For $\bar{U}/2W < 1$ and $n < 1$ (e.g. figure 1, curve F, where $\bar{U}/2W = 0.9$ and $n = 0.95$) the starting value of $\rho = 0$ is at $T \neq 0$, i.e. we obtain two finite values of the critical temperature T_c in the Hubbard model, and therefore magnetic order is present in the interval between these critical points, in agreement with [28, 29]. A similar effect was obtained for the ordering parameter in the s–f (or s–d) model [30]. Recently, in [9] the magnetic and thermodynamic properties of the half-filled Hubbard model on the simple-cubic lattice (without electron–phonon coupling) were investigated. The sublattice magnetisation for various electron–electron constant U-values is shown. It is in agreement with our discussion of ρ.

The critical temperature T_c increases strongly for $\bar{U}/2W < 2$ whereas for $\bar{U}/2W > 2$ it decreases but slowly (figure 1). In the intermediate regime the $T_c(\bar{U}/2W)$ curve has a maximum at $\bar{U}/2W \simeq 2$. A similar maximum was obtained in [9] at $\bar{U}/2W = 1.35$ using the single-site spin fluctuation theory and at $\bar{U}/2W = 1.5$ using the Gutzwiller-type variational approach. In [10] a maximum was obtained at $\bar{U}/2W = 1.7$ using the MC method.

The critical temperature T_c increases with increasing Coulomb interaction constant U or with increasing electron–phonon interaction constant A_0. As U_{eff} (equation (14)) is equal to or larger than U, the electron–phonon coupling in this approximation always produces an increase in the transition temperature T_c. Therefore this renormalisation of the Coulomb interaction constant due to the electron–phonon interaction (14) obtained using the Green function method may have a relation to the problem of the new superconductors. We can consider equation (14) also from another viewpoint, namely that an on-site Coulomb interaction U strongly enhances the electron–phonon coupling, giving rise to superconductivity and to high T_c-values. This would be in agreement with the conclusions in [31]. Calculations in this direction are in preparation and will be published elsewhere.

It is known that for a half-filled band ($n = 1$) the system described with the Hubbard Hamiltonian is an antiferromagnetic insulator for any non-zero value of the Coulomb repulsion U. In order to study the magnetic tendency of the system, we define the nearest-neighbour spin correlation function C by

$$C = \langle n_{i\sigma} n_{i+1\sigma} \rangle - \langle n_{i\sigma} n_{i+1-\sigma} \rangle. \tag{16}$$

Positive value of this correlation function indicates ferromagnetic tendency and negative value indicates antiferromagnetic tendency. To calculate C, we use the method proposed in [26]. For $T = 0$, $U = 7$ eV, $W = 3.5$ eV we obtain $C = -0.0048$ for $n = 1$ and $C = -0.0040$ for $n = 0.8$; for $T = 5$ K, $C = -0.0052$ ($n = 1$) and $C = -0.0043$ ($n = 0.8$). The negative values of C shows that for $U > 0$ the spin correlation between nearest neighbours is antiferromagnetic. C increases with increasing U and n ($n \leqslant 1$). This is in good agreement with the recently calculated correlation function for the one-dimensional Hubbard model [32] and with the MC simulations [15] and the numerical diagonalisation [8] of the two-dimensional Hubbard model on a square lattice which also show antiferromagnetic tendency. The fact that the model produces an antiferromagnetic correlation between nearest neighbours for $n \neq 1$ and moderate U at finite temperatures ($T \neq 0$) allows us to use the Hubbard model for description of the new superconductors such as $YBa_2Cu_3O_7$ and $La_{2-x}(Sr, Ba)_xCuO_4$, which will be discussed elsewhere.

4. Dynamic properties

In order to obtain the mass operator and the damping of the electronic spectrum caused by the electron–phonon interaction we consider the integral term in (6). For the operator $j_{k\sigma}$, we obtain

$$j_{k\sigma} = [c_{k\sigma}, H_{\text{int}}]_- = \frac{U}{\sqrt{N}} \sum_{k',q} c^+_{k'+q\sigma'} c_{k'\sigma'} c_{k+q\sigma} - \frac{1}{\sqrt{N}} \sum_{q,\lambda} A(q\lambda) c_{k-q\sigma} (a_{q\lambda} + a^+_{-q\lambda}).$$

In our calculations we use the approximate dynamics of $c_{k\sigma}(t) \simeq c_{k\sigma} \exp(-iE_{k\sigma}t)$ and $a_{k\lambda}(t) \simeq a_{k\lambda} \exp(-i\omega_{k\lambda}t)$, where $E_{k\sigma}$ is from (12) and $\omega_k = vk$. This assumption takes the generalised Hartree–Fock approximation as a starting approximation.

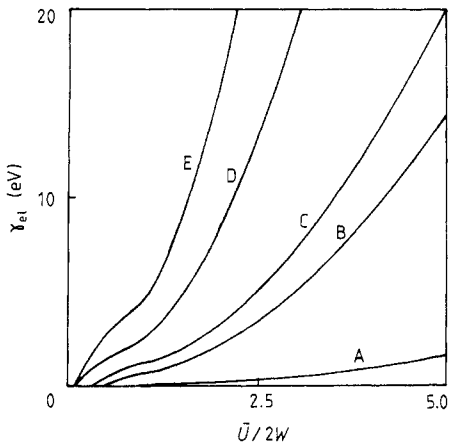

Figure 2. The dependence of the electronic damping γ_{el} for $k = 0, \sigma = +1$ on the ratio $\bar{U}/2W$ for different T- and W-values: curve A, $T = 10$ K, $W = 0.5$ eV; curve B, $T = 20$ K, $W = 2$ eV; curve C, $T = 30$ K, $W = 2$ eV; curve D, $T = 30$ K, $W = 5$ eV; curve E, $T = 30$ K, $W = 10$ eV.

For the mass operator $M_{k\sigma}$, we obtain

$$M_{k\sigma} = -P\Big[\frac{U^2}{N^2}\sum_{q,p}\frac{\bar{n}_{p-\sigma}(1-\bar{n}_{k-q\sigma}-\bar{n}_{p+q-\sigma})+\bar{n}_{k-q\sigma}\bar{n}_{p+q-\sigma}}{E_{p-\sigma}-E_{p+q-\sigma}-E_{k-q\sigma}+E_{k\sigma}} + \frac{1}{N}\sum_{q,\lambda}A_{q\lambda}^2\Big(\frac{1+\bar{m}_{q\lambda}-\bar{n}_{k-q\sigma}}{E_{k\sigma}-E_{k-q\sigma}-\omega_{q\lambda}}+\frac{\bar{n}_{k-q\sigma}+\bar{m}_{q\lambda}}{E_{k\sigma}-E_{k-q\sigma}+\omega_{q\lambda}}\Big)\Big]. \tag{17}$$

Calculations yield the following expression for the electronic damping $\gamma_{k\sigma}$:

$$\gamma_{k\sigma} = \frac{\pi U^2}{N^2}\sum_{q,p}[\bar{n}_{p-\sigma}(1-\bar{n}_{k-q\sigma}-\bar{n}_{p+q-\sigma})+\bar{n}_{k-q\sigma}\bar{n}_{p+q-\sigma}] \times \delta(E_{p-\sigma}-E_{p+q-\sigma}-E_{k-q\sigma}+E_{k\sigma}) + \frac{\pi}{N}\sum_{q,\lambda}A_{q\lambda}^2[(1+\bar{m}_{q\lambda}-\bar{n}_{k-q\sigma})\delta(E_{k\sigma}-E_{k-q\sigma}-\omega_{q\lambda}) + (\bar{n}_{k-q\sigma}+\bar{m}_{q\lambda})\delta(E_{k\sigma}-E_{k-q}+\omega_{q\lambda})] \tag{18}$$

where $\bar{m}_{q\lambda} \equiv \langle a_{q\lambda}^+ a_{q\lambda}\rangle = 1/[\exp(\omega_{q\lambda}/k_B T)-1]$ and $\bar{n}_{q\sigma}$ is from (13).

Now we wish to discuss the damping (equation (18)). $\gamma_{k\sigma}$ was numerically calculated for different T-, W- and $\bar{U}$-values. Figure 2 and figure 3 show the dependence of γ ($k = 0, \sigma = +1$) on $\bar{U}/2W$ for W = constant and $\bar{U}$ = constant, respectively. $\gamma_{k\sigma}$ has a different behaviour for $\bar{U}$ = constant or W = constant. The electronic damping $\gamma_{k\sigma}$ increases with increasing T and increasing $\bar{U}/2W$ for W = constant (figure 2). For $\bar{U}$ = constant (figure 3), $\gamma_{k\sigma}$ increases with increasing $\bar{U}/2W$ for $T < T_c$, at $\bar{U}/2W = 0.5$ it has a maximum, then it decreases reaching a minimum at $\bar{U}/2W = 1$, and for $U/2W > 1$ it increases again. Above T_c ($T > T_c$), this minimum (curves F and G) disappears. The damping increases strongly for $\bar{U}/2W < 1$ and then very slowly (it is nearly temperature independent) for $\bar{U}/2W > 1$. For $\bar{U}/2W \gg 1$ the electronic damping is for all temperatures below and above T_c nearly independent of $\bar{U}/2W$.

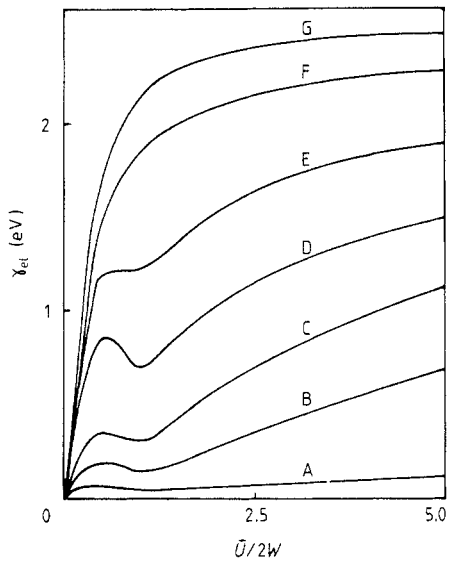

Figure 3. The dependence of the electronic damping γ_{el} for $k = 0$, $\sigma = +1$ on the ratio $\bar{U}/2W$ for $\bar{U} = 4$ eV and for different T-values: curve A, $T = 1$ K; curve B, $T = 5$ K; curve C, $T = 10$ K; curve D, $T = 20$ K; curve E, $T = 30$ K; curve F, $T = 40$ K; curve G, $T = 50$ K.

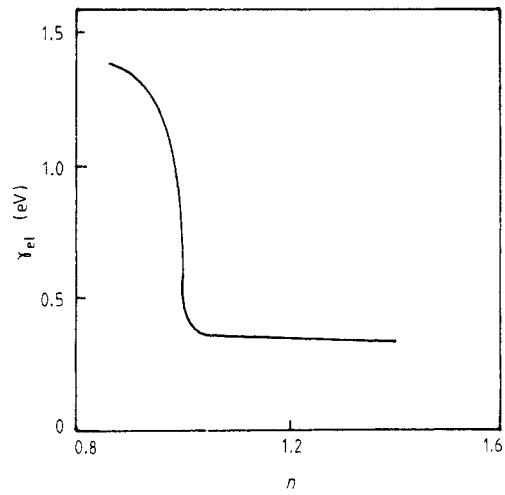

Figure 4. Band occupation dependence of the electronic damping $\gamma_{el}(n)$ for $T = 10$ K, $\bar{U} = 4$ eV and $W = 2$ eV.

Finally we have calculated the dependence of $\gamma_{k\sigma}$ on the band occupation $n = n_+ + n_-$ (figure 4). It decreases with increasing n. At $n = 1$ it decreases very strongly.

5. Conclusions

We have calculated the static and dynamic properties of the simple-cubic Hubbard model including electron–phonon interaction using a Green function method. They are compared with the results obtained by other workers using the same or other methods.

The electron–electron interaction constant U is renormalised owing to the electron–phonon interaction to $U_{\text{eff}} = U + 2A_0^2/\omega_0$. This renormalisation always produces an increase in the transition temperature T_c.

The electron magnetisation ρ was numerically calculated. $\rho(T)$ was discussed for $\bar{U}$ = constant and for different band width values W (figure 1). For $\bar{U}/2W < 1$ and $n < 1$, we obtain two critical points, i.e. magnetic order is present in the interval between these critical points in agreement with [28, 29]. Recently [9] the sublattice magnetisation of the half-filled Hubbard model on the simple-cubic lattice (without an electron–phonon interaction) has been discussed for various electron–electron interaction constant U-values. It is in agreement with our results.

The $T_c(\bar{U}/2W)$ curve has a maximum at $\bar{U}/2W = 2$. A similar maximum was obtained by other workers at $\bar{U}/2W = 1.35$ (1.5) [9] and 1.7 [10].

The nearest-neighbour spin correlation function C was numerically calculated. The obtained negative values in agreement with [15, 32] indicates antiferromagnetic tendency.

The electronic damping $\gamma_{k\sigma}$ was calculated and discussed for different temperatures T, band widths W, Coulomb interaction constants $\bar{U}$ and band occupation n-values. $\gamma_{k\sigma}$ has a different behaviour for W = constant (figure 2) and $\bar{U}$ = constant (figure 3). It decreases with increasing n. At $n = 1$ it decreases very strongly (figure 4). To our knowledge, it is the first time that a discussion of $\gamma(T, \bar{U}/2W)$ and $\gamma(T, n)$ has been presented.

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