Attractive pairing potential from the repulsive Hubbard model

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We have examined the two-dimensional repulsive extended Hubbard model on a square lattice, using standard many-body diagrammatic techniques. By summing an infinite series of two renormalized loops for the self-energy, we have found that for specific regions in the parameter space of (U, W), the renormalized Coulomb interaction can become attractive. In addition we have also studied the effects of second-order diagrams, pertaining to paramagnon effects in BCS superconductors. Our results are in agreement with numerical simulation studies and may form the basis for a mechanism of high-T_c superconductors.

I. INTRODUCTION

At the heart of any microscopic theory for superconductivity subject to a pairing hypothesis, lies the origin of an attractive interaction between electrons, holes, or other quasiparticles which form Cooper or Schafroth pairs.[1,2] Traditionally the role mediating this attractive interaction has been played by phonons in conventional superconductors, which forms the basis underlying the BCS mechanism.[3] Fairly quantitative evaluations in the context of the random phase approximation (RPA) are possible which demonstrate that renormalization of the Coulomb interaction and electron-phonon vertex can lead to a net attractive interaction. More elaborate calculations are made using the strong coupling Eliasberg or Nambu-Gorkov formalism.[3,4] Unfortunately the magnitude of the electron-phonon interaction seems to disfavor the role of phonons in the oxide high-T_c superconductors. This has been demonstrated by fairly elaborate computations along the above traditional route involving phonons.[5]

An alternative method to understand the mechanism of superconductivity is a charged Bose gas condensation of Schafroth pairs[2] with an important difference that in the normal state (above T_c) the pairs exist and are incoherent. Unlike the BCS mechanism the pair breaking takes place at a high temperature. The bipolaron picture is an obvious example. Unfortunately the high bipolaronic mass poses difficulty in getting the high transition temperature.[6]

In the search for mechanisms to explain high-T_c superconductivity, several proposals have been made involving plasmons, excitons, resonating valence bonds, etc.[7–9] For this purpose there has been a considerable revival of interest in the two-dimensional (2D) Hubbard model and its variants, known to be apparently suitable for the Cu-O planes pertinent to oxide high-T_c superconducting compounds.[8–10] However, recently elaborate computer simulations raised the question as to whether a Hubbard ($U > 0$)-only model can do it alone.[11,15,27] In fact Hirsch[27] was motivated to look to the extended Hubbard model for pairing as his numerical quantum Monte Carlo results appear to disfavor the U-only Hubbard model. Recently Imada[12] has provided rather strong numerical evidence against superconductivity in the 2D U-only Hubbard model near half filling. Consequently other variants, notably the extended Hubbard model with U *and* W, are now favored, with some evidence that U and W can do it.[13–18] The crucial question is whether a Hamiltonian containing repulsive electron-electron interactions alone could lead to pairing and superconductivity. This is a difficult question either theoretically or experimentally. The latter because U and W or other interaction parameters are not directly experimentally accessible, nor do we yet have unambiguous evidence for a Coulombic or electrostatic pairing mechanism.[16] The theoretical difficulties are due to the absence of exact solubility or a completely reliable approximation scheme to handle the many-body problem, nor do we yet have sufficient computational power to perform decent size lattice numerical simulations. It looks plausible from various calculations that the intersite repulsion W may stabilize pairing by bringing in an indirect attraction. This we shall demonstrate in the present paper within an RPA-like approximation. It is of course easier to obtain pairing in a phenomenological negative U and/or W Hubbard model,[8,10] but this has doubtful experimental support. Here our intention is to test the capability of a standard repulsive extended Hubbard model, whether it can give rise to pairing purely from interelectronic interaction. Before proceeding to report the details we must remark that the philosophy currently adopted by ours and other works[19] on 2D superconductivity requires the assumption that a degree of anisotropy and/or interplanar coupling is operative in order to stabilize 2D superconductivity at finite temperatures.[20–23] This degree of complication however need not be pursued at this stage for the crucial question that this paper attempts to answer is whether in fact the *ground state* is superconducting,

FIG. 1. Bare interaction lines U (dashed) and $W(\mathbf{q})$ (wiggled). The solid lines are bare particle propagators. Note that U is spin dependent, whereas $W(\mathbf{q})$ is not.

before addressing if such a superconducting state could be stabilized at a relatively high T_c.

II. MODEL AND FEYNMAN DIAGRAM

Consider the repulsive ($U > 0, W > 0$) extended Hubbard Hamiltonian $\hat{\mathrm{H}}$ in two dimensions:

$$\hat{H} = -t \sum_{<ij>\sigma} \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + W \sum_{<ij>\sigma\sigma'} \hat{n}_{i\sigma}\hat{n}_{j\sigma'}. \quad (1)$$

Here $\langle ij \rangle$ denotes nearest-neighbor sites on a square lattice of supposedly oxygen atoms, $\hat{c}^{\dagger}_{i\sigma}$ ($\hat{c}_{i\sigma}$) the creation (destruction) operator of Wannier electrons, $\hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$ the number operator, U and W are the on-site and nearest-neighbor interactions, respectively. Also t is the hopping or transfer integral which gives a bandwidth $E_B = 4t$. We change to momentum representation with Bloch electrons $\hat{a}^{\dagger}_{\mathbf{k}}$ and rewrite Eq. (1) as

$$\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k})\hat{a}^{\dagger}_{\mathbf{k}\sigma}\hat{a}_{\mathbf{k}\sigma} + \frac{U}{N}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \hat{a}^{\dagger}_{\mathbf{k}\uparrow}\hat{a}^{\dagger}_{\mathbf{k}'\downarrow}\hat{a}_{\mathbf{k}'-\mathbf{q}\downarrow}\hat{a}_{\mathbf{k}+\mathbf{q}\uparrow} + \frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\sigma\sigma'} W(\mathbf{q})\, \hat{a}^{\dagger}_{\mathbf{k}\sigma}\hat{a}^{\dagger}_{\mathbf{k}'\sigma'}\hat{a}_{\mathbf{k}'-\mathbf{q}\sigma'}\hat{a}_{\mathbf{k}+\mathbf{q}\sigma}, \quad (2)$$

where

$$\epsilon(\mathbf{k}) = -2t\left(\cos k_x + \cos k_y\right) \quad (3)$$

is the square lattice band structure and

$$W(\mathbf{q}) = 2W\left(\cos q_x + \cos q_y\right) \quad (4)$$

is the nearest-neighbor interaction in momentum space. We shall use the notation $\tilde{q} = (\mathbf{q}, \omega)$ where $\mathbf{q} = (q_x, q_y)$ is the momentum transfer and ω the angular frequency, adopting atomic units ($\hbar = c = a_0 = 1$) throughout.

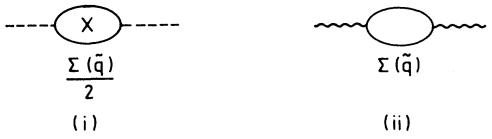

FIG. 2. Particle-hole loops. The left loop (i) marked with a cross (×) is associated with a U interaction while the right loop (ii) is associated with a $W(\mathbf{q})$ interaction line.

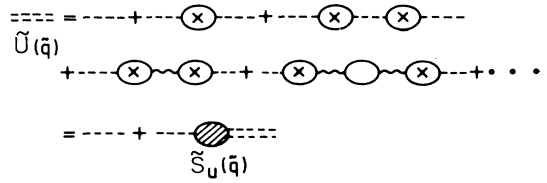

FIG. 3. Renormalization series for the interaction $\tilde{U}(\mathbf{q})$. We define $\tilde{S}_U(\mathbf{q})$ to contain all one-loop graphs connected to $W(\mathbf{q})$.

Our purpose at this stage is not to attempt to solve this Hamiltonian, i.e., discuss variational ground states, off-diagonal propagators, etc. We merely seek to ask the question whether a net attractive *effective* interaction can emerge at a manageable level of renormalization approximation. Figure 1 shows the bare interactions U and $W(\mathbf{q})$, where we note the spin dependence associated with the former. This implies that there are two particle-hole loops differing by a factor of half due to spin summation (Fig. 2). Our purpose is to seek an answer for the renormalized net interaction $\tilde{V}(\tilde{q}) = \tilde{U}(\tilde{q}) + \tilde{W}(\tilde{q})$ which therefore carries the spin dependence of U. With these definitions we show the partial summation of the infinite series for $\tilde{U}(\tilde{q})$ shown in Fig. 3 which leads to a definition for the renormalized loop $\tilde{S}_U(\tilde{q})$ (Fig. 4). The corresponding series for $\tilde{W}(\tilde{q})$ is shown in Fig. 5 which leads to a definition of the renormalized loop $\tilde{S}_W(\tilde{q})$ (Fig. 6).

III. CALCULATIONS

The above Feynman diagrams show that it is straightforward to calculate the effective interaction $\tilde{V}(\tilde{q})$ within our approximation.

$$\tilde{V}(\tilde{q}) = \tilde{U}(\tilde{q}) + \tilde{W}(\tilde{q}), \quad (5)$$

where from Figs. 3–6 we see that

$$\tilde{U}(\tilde{q}) = \frac{U}{1 - \tilde{S}_U(\tilde{q})U}, \quad (6)$$

$$\tilde{W}(\tilde{q}) = \frac{W(\mathbf{q})}{1 - \tilde{S}_W(\tilde{q})W(\mathbf{q})}, \quad (7)$$

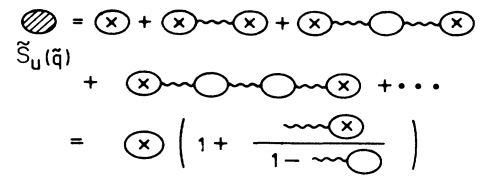

FIG. 4. Renormalized one-loop graph $\tilde{S}_U(\mathbf{q})$. Note that it involves bare propagators and interaction lines $W(\mathbf{q})$ in our approximation.

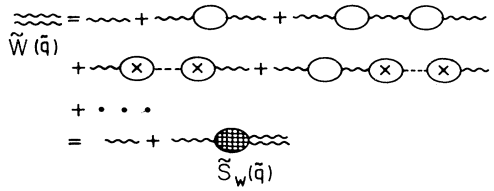

FIG. 5. Renormalization series for the interaction $\tilde{W}(\mathbf{q})$. We define $\tilde{S}_W(\mathbf{q})$ to contain all one-loop graphs connected to U.

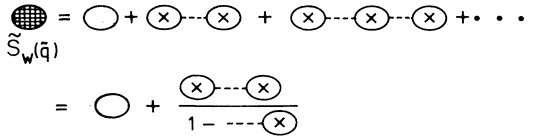

FIG. 6. Renormalized one-loop graph $\tilde{S}_W(\mathbf{q})$. Note that it involves bare propagators and interaction lines U in our approximation.

with

$$\tilde{S}_U(\tilde{q}) = \frac{1}{2}\Sigma(\tilde{q})\Big(1 + \frac{\frac{1}{2}W(\mathbf{q})\Sigma(\tilde{q})}{1 - W(\mathbf{q})\Sigma(\tilde{q})}\Big), \tag{8}$$

$$\tilde{S}_W(\tilde{q}) = \Sigma(\tilde{q})\Big(1 + \frac{\frac{1}{4}U\Sigma(\tilde{q})}{1 - \frac{1}{2}U\Sigma(\tilde{q})}\Big). \tag{9}$$

We note that Eqs. (6) and (7) are notably uncoupled, which is a distinctive feature of this approximation. All the physics is contained in the processes inherent in these Feynman diagrams. The dominating quantity which controls these processes within our approximation is the bare loop function $\Sigma(\tilde{q})$ or the analogous Lindhard function for this model:

$$\Sigma(\tilde{q}) = -2i\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{dp_x}{2\pi}\frac{dp_y}{2\pi}\Big(\frac{\theta(\epsilon_F - \epsilon(\mathbf{p}+\mathbf{q}))\theta(\epsilon(\mathbf{p}) - \epsilon_F)}{\epsilon(\mathbf{p}) - \epsilon(\mathbf{p}+\mathbf{q}) - \omega + i\eta} - \frac{\theta(\epsilon(\mathbf{p}+\mathbf{q}) - \epsilon_F)\theta(\epsilon_F - \epsilon(\mathbf{p}))}{\epsilon(\mathbf{p}) - \epsilon(\mathbf{p}+\mathbf{q}) - \omega - i\eta}\Big), \quad \eta \to 0+, \tag{10}$$

where $\epsilon(\mathbf{p})$ is the band structure given in Eq. (3) and ϵ_F is the Fermi energy. Unfortunately no analytical evaluation for this double integral appears possible for arbitrary $\mathbf{q}$, ω, and ϵ_F except in the limiting cases, e.g., $\epsilon_F \to 0, \mathbf{q} \to (\pi,\pi)$ (the nesting vector). Therefore we have evaluated this double integral numerically checking the result against the above analytical limiting cases, which involve elliptic integrals. To do this we divide the Brillouin zone into $n \times n$ meshes and integrate each mesh using a four-point double integration rule.[26] We note that complex function evaluations are needed for the integrand and in particular a compromise between computing time, mesh sizes, and η (resolution factor) has to be made. Eventually the compromise which gave excellent agreement with analytical results for the integral was found to be $n = 40$ and $\eta = \frac{\pi}{n}$. No significant improvement in accuracy was gained by increasing to $n = 100$ which more than doubles the computing time of 0.2 sec on a Vax 8700 for each $\tilde{q}$ value. From this evaluation of Σ we can immediately obtain $\tilde{V}$ using Eqs. (5)–(9).

IV. RESULTS AND DISCUSSIONS

In view of the many parameters in this problem, notably ω, $\mathbf{q}$=(q_x, q_y), ϵ_F, U, and W (all energies are measured in units of the bandwidth $E_B = 2t$), we have confined ourselves to the case $\omega \to 0+$ and $\epsilon_F \to 0+$, i.e., near half-filled band, in presenting our results. This is believed to be relevant for the high-T_c oxide superconductors.[13–18,24,25] Figure 7 shows various plots in the parameter space (U, W) for different values of the momentum transfer $\mathbf{q}$. The shaded regions in these plots are those where $\mathrm{Re}\,\tilde{V} < 0$, i.e., an attractive interaction. We see from Figs. 7(a) and 7(b) that for small

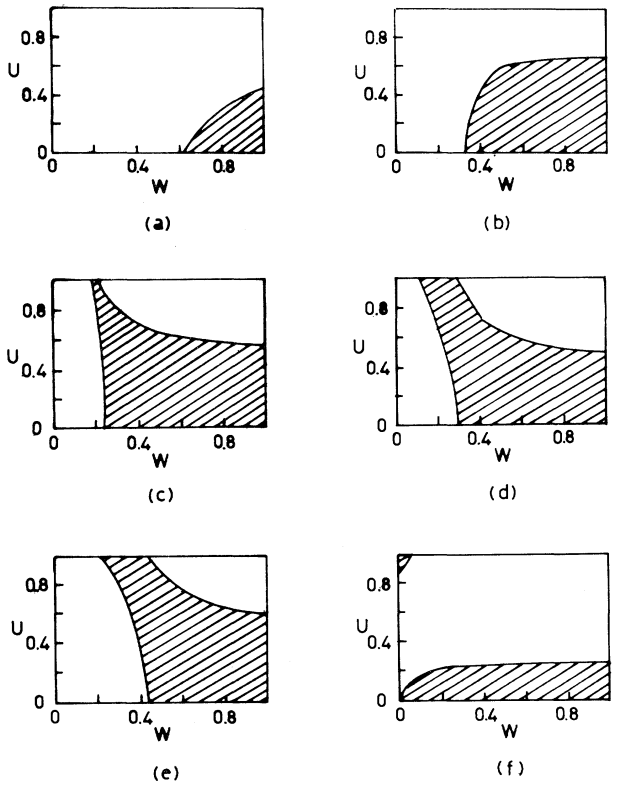

FIG. 7. Parameter space (U, W) in which the renormalized interaction $\mathrm{Re}\,\tilde{V}$ is negative. The momentum transfer $\mathbf{q}$ in these figures are (a) $(0.02\pi, 0.02\pi)$, (b) $(0.05\pi, 0.05\pi)$, (c) $(0.25\pi, 0.25\pi)$, (d) $(\frac{3}{8}\pi, \frac{3}{8}\pi)$, (e) $(0.5\pi, 0.5\pi)$, (f) (π, π). Other parameters are $\omega = 0.01$ and $\epsilon_F = -0.1$. All energies are measured in units of the bandwidth $E_B = 4t$ and atomic units are used throughout.

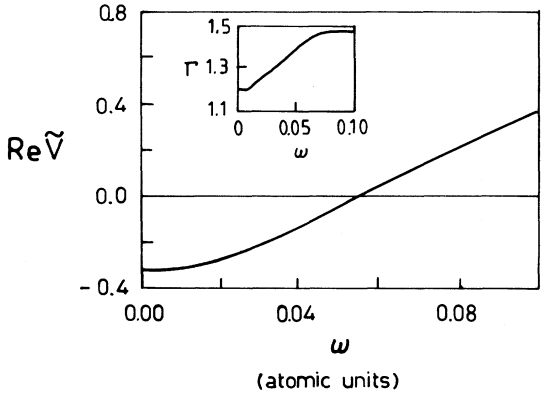

FIG. 8. Frequency dependence of $\mathrm{Re}\,\tilde{V}$ and $\Gamma = |\mathrm{Im}\tilde{V}|$, for $\mathbf{q} = (0.25\pi, 0.25\pi)$, $\epsilon_F = -0.1$; $U = 0.6$ and $W = 0.3$.

momentum transfer $\mathbf{q}$, an attractive interaction seems to be induced by $U \ll W$ with W of the order of the bandwidth E_B. One however expects that the physical situation might require $U > W$. Figures 7(c)–7(e) show that the attractive region now encompasses a larger region containing $U > W$, perhaps a more physical situation but at the expense of a larger momentum transfer. *None of the above cases show that U can do it alone.* In Fig. 7(f) we show the interesting $\mathbf{q} = (\pi, \pi)$ nesting case. Equation (4) indicates that $W(\mathbf{q})$ itself is negative, a point perhaps well known but not widely emphasized in the literature.[13–18,24,25] The attractive region disappears rapidly with increasing U but the interest here comes from the physically appealing case where $U \gtrsim 0$ and $W \gtrsim 0$. We have also investigated the frequency dependence and damping rate (or inverse lifetime) of $\tilde{V}$. For the case of $\mathbf{q} = (\frac{\pi}{4}, \frac{\pi}{4})$ for example, Fig. 8 shows the frequency dependence of $\mathrm{Re}\,\tilde{V}$ and $\Gamma = |\mathrm{Im}\,\tilde{V}|$ (inset to Fig. 8). $\mathrm{Re}\,\tilde{V}$ exhibits a cutoff ω_c at $\omega_c = 0.05$, the analogue of a Debye frequency ω_D in the BCS theory, and Γ increases with frequency ω. Again the nesting case $\mathbf{q} = (\pi, \pi)$ is particularly interesting. We have found in this case for $U = W = 0.1$ that $\mathrm{Re}\,\tilde{V}$ is negative for ω over the whole bandwidth with a vanishingly small Γ. We expect that these factors may be important in determining T_c.

V. SUMMARY AND CONCLUSIONS

The results shown in the last section are interesting and intriguing. They appear to be consistent with numerical simulations.[14,15] A perusal of results from quantum Monte Carlo and other finite systems studies[27] seems to suggest that the attractive interaction associated with a charge transfer pairing mechanism can be found within our RPA-like approximation, without recourse to more complicated two-band Hubbard models involving Cu-O transfers. Given that the effective interaction can be negative, it would seem to be a straightforward task to develop a theory either via a Gorkov-Nambu[3] type of pairing or a charged boson condensation via a Schafroth-type theory.[2,6,28] This difference depends crucially on how one has to treat the normal state of the system, on which there appears many issues in the recent past.[29] We outline below some important questions, one of which at least we have an answer to.

An important issue pertains to second-order interactions, most notably the paramagnon interaction. For this purpose the last term of Eq. (1) should be amended to include a more general spin exchange interaction:

$$\frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\sigma\tau\tau'\sigma'} W(\mathbf{q})\, \hat{a}^\dagger_{\mathbf{k}\sigma}\hat{a}^\dagger_{\mathbf{k}'\tau}\hat{a}_{\mathbf{k}'-\mathbf{q}\tau'}\hat{a}_{\mathbf{k}+\mathbf{q}\sigma'}, \tag{11}$$

which includes spin exchange terms as in Fig. 9(a). Thus the renormalized paramagnon interaction $\tilde{P}$ includes the diagrams for the series in Fig. 9(b). We now note that the renormalized interaction $\mathcal{W}$ which includes the above paramagnon interaction is:

$$\mathcal{W}(\tilde{q}) = \tilde{W}(\tilde{q}) + \tilde{P}(\tilde{q}), \tag{12}$$

with $\tilde{W}(\tilde{q})$ given by Eq. (7). Irrespective of U, this interaction can be negative on its own. The pairing in this case is a singlet pairing irrespective of U. We note however that such an interaction must involve spin exchange and is incompatible with the Hubbard U which has a different spin dependence. While such effects ought to be included when higher-order approximations beyond RPA are to be investigated, results of numerical studies and experimental data[27] point against such a magnetic pairing mechanism. The inclusion of spin exchange interactions as in Eq. (12) is therefore not likely to be relevant for high-T_c superconductors.

However other questions remain which we must eventually address. Most notably an assessment of our approximation is essential. Will higher-order graphs or renormalization of propagator lines not seriously affect our results? Given the good agreement between our results and numerical studies,[27] the answer seems to be no, yet this remains to be proven. In particular diagrams like

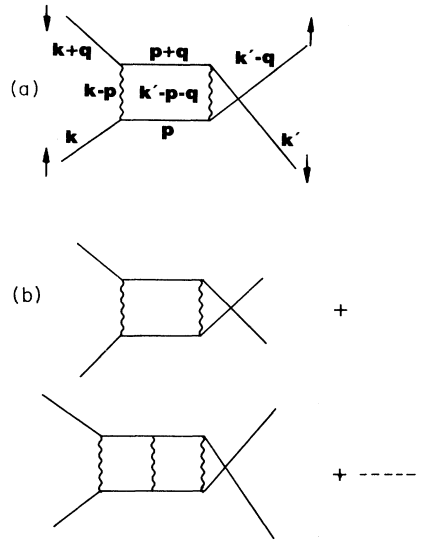

FIG. 9. (a) Bare spin exchange interaction, (b) renormalization series for the interaction $\tilde{P}(\mathbf{q})$.

Fig. 10 will be involved at higher orders and this would imply that Eqs. (6) and (7) will be coupled, to be solved self-consistently. The difficulty is to find a more accurate but manageable approximation scheme which is not at all obvious.

Next it is necessary to have some idea of the parameters in our model. From the state of the art density functional band structure calculations, the estimates of U and W compare reasonably well with experiments.[30] Example U on Cu (O) is about 10 (6) eV, whereas $W < 1$ eV.

Also what are the effects of other competing ordering states? The Hubbard model, though the simplest many-body fermionic Hamiltonian, is notoriously complicated. It is susceptible to many exotic ordering properties, e.g., antiferromagnetic spin density wave (SDW), charge density wave, quantum spin liquid, etc. A two-band model employing copper d and oxygen p with oxygen vacancies would be a more realistic model[27] but then our results seem to indicate that, as to a renormalized attractive effective pairing potential, such complications are unnecessary.

Finally the $\mathbf{q}$ dependence of V clearly dictates the symmetry of the superconducting order parameter, e.g., s, d, or $s + id$ pairing. What is the symmetry of the superconducting order parameter? It is an issue yet to be unambiguously resolved.

FIG. 10. Examples of higher-order renormalization loops left out in our approximation.

To summarize, in this paper we have analyzed using a manageable approximate scheme similar to RPA containing two renormalized loops, the effective Coulombic interaction in the (U, W) parameter space of the extended Hubbard model in two dimensions. Our results appear to be consistent with quantum Monte Carlo simulations and the general picture thus derived that U cannot do it alone. Further analysis may indicate that our results could form the basis for a viable microscopic theory for high-T_c superconductivity.

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