## Microscopic description of *d*-wave superconductivity by Van Hove nesting in the Hubbard model

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We devise a computational approach to the Hubbard model that captures the strong coupling dynamics arising when the Fermi level is at a Van Hove singularity in the density of states. We rely on an approximate degeneracy among the many-body states accounting for the main instabilities of the system (antiferromagnetism, *d*-wave superconductivity). The Fermi line turns out to be deformed in a manner consistent with the pinning of the Fermi level to the Van Hove singularity. For a doping rate  $\delta \sim 0.2$ , the ground state is characterized by *d*-wave symmetry, quasiparticles gapped only at the saddle points of the band, and a large peak at zero momentum in the *d*-wave pairing correlations.

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Nowadays it is widely accepted that the single-band Hubbard model is an appropriate starting point to describe the electron correlations in copper-oxide materials.<sup>1</sup> In spite of the efforts to show that the model has a phase of d-wave superconductivity, however, there is no conclusive proof at present of its existence. There have been different theoretical approaches to understand the symmetry of the order parameter, among which we may quote the proposals based on the effect of antiferromagnetic fluctuations<sup>2</sup> and the Kohn-Luttinger mechanism due to Van Hove nesting of the Fermi surface.<sup>3,4</sup> Numerical methods have also provided some evidence of enhanced pairing correlations in the twodimensional (2D) Hubbard model.<sup>5,6</sup> Recent progress has been achieved by the use of dynamical mean-field  $approximations^7$ and improved quantum Monte Carlo methods.8,9

We focus our discussion on the proposal of superconducting pairing by the influence of a Van Hove singularity near the Fermi level.<sup>10</sup> Recently, some understanding of the problem has been attained by the use of refined renormalization group methods for interacting electrons in two dimensions.<sup>11,12</sup> This approach suffers, though, from the same shortcoming of any attempt to deal with the origin of high- $T_c$  superconductivity. The system is likely to develop strong antiferromagnetic or superconducting correlations but, as long as the effective interaction grows large as more highenergy electron modes are integrated out, it is not possible to discern rigorously the ground state of the model. A related problem concerns the fact that the superconducting correlations are enhanced like  $\log^2 \varepsilon$ , when the electron modes are integrated out down to energy  $\varepsilon$  near the Fermi surface. This reflects in another fashion that the model does not lead to a conventional scale-invariant theory at arbitrarily low energies-unless the Fermi energy is promoted to a dynamical quantity susceptible itself to renormalization.<sup>13,12</sup>

In this paper we address the characterization of the ground state of the Hubbard model, when the Fermi level is at a Van Hove singularity in the density of states. For this purpose we will formally make use of the scaling properties of the model,<sup>13</sup> which ensure that upon integration of the high-energy modes the electron quasiparticles remain in correspondence with the original one-particle states, up to the energy in which the effective interaction starts to grow large.

To elucidate the behavior of the system at lower energies we undertake a numerical diagonalization of the Hubbard Hamiltonian, in the Hilbert space truncated to include the states left after integration of the high-energy modes.

We implement the above strategy in the Hubbard model on a  $8 \times 8$  lattice, which has the set of one-particle states in momentum space represented in Fig. 1. Related numerical approaches have been devised before for the Hubbard model in a  $6 \times 6$  cluster near half-filling in Refs. 14 and 15. The increase in lattice size affords a better resolution in momentum space, which may have a critical significance since, from theoretical arguments, the main physical features of the Hubbard model at the Van Hove filling have to come from the enhanced scattering with momentum transfer  $(\pi, \pi)$ . A discussion of the results obtained with our method in the  $6 \times 6$  cluster is carried out in the Appendix.

In order to study the effects of the enhanced scattering at the saddle points, we start from a Fermi sea of occupied states below the shell  $\varepsilon = 0$ , whose particle content corresponds to a doping rate  $\delta \approx 0.22$ . We suppose that at a previous renormalization group stage the high-energy electron modes have been integrated out down to the region between energies  $-\Lambda$  and  $\Lambda$  about the Fermi level shown in Fig. 1. The modes integrated out have approximately isotropic patterns about the top and the bottom of the band, and we may



FIG. 1. Points of the  $8 \times 8$  lattice in momentum space.

safely assume that their effect is encoded in a soft renormalization of the effective coupling for the low-energy modes, that we call  $U_{\text{eff}}$ .

Furthermore, we will deal with a situation in which  $U_{\text{eff}}$  is in the weak-coupling regime, so that the low-energy physics can be described by building the many-body Hilbert space out of the one-particle states within  $-\Lambda$  and  $\Lambda$ . The effect of renormalization of the one-particle levels outside the region between  $-\Lambda$  and  $\Lambda$  can be estimated *a posteriori* by computing the corrections to the low-lying many-body states due to particle-hole excitations between the high-energy levels. We will see that, at weak coupling, these corrections are irrelevant for the purpose of determining the ground state. On the other hand, the interaction of the states at the Fermi level shell  $\varepsilon = 0$  is always strong and essentially nonperturbative. The effect of the enhanced scattering with momentum transfer  $(\pi, \pi)$  is properly captured in our construction, given the high degeneracy of states at the  $\varepsilon = 0$  shell.

We proceed then to the numerical diagonalization of the Hamiltonian,

$$H = \sum_{\mathbf{k},\sigma} \varepsilon(\mathbf{k}) c_{\sigma}^{\dagger}(\mathbf{k}) c_{\sigma}(\mathbf{k}) + U_{\text{eff}} \sum_{\mathbf{k},\mathbf{p},\mathbf{q}} c_{\uparrow}^{\dagger}(\mathbf{k}) c_{\uparrow}(\mathbf{k}-\mathbf{q}) c_{\downarrow}^{\dagger}(\mathbf{p}) c_{\downarrow}(\mathbf{p}+\mathbf{q}), \qquad (1)$$

with all the modes in the region between  $-\Lambda$  and  $\Lambda$ . We will deal with different contents of particles at the Fermi level shell  $\varepsilon = 0$ , keeping in all cases a Fermi sea of 24 particles filling the levels below  $\varepsilon = 0$ . The instances with an even number of particles at the Fermi level are particularly interesting, since these are situations that allow the testing of the tendency to pairing in the model. Actually, there is a correspondence between the states with broken symmetry in a macroscopic system and the sectors labeled by different quantum numbers in the finite cluster.<sup>16</sup> The antiferromagnetic phase is characterized by a ground state in sector A of spin singlets with total momentum  $\mathbf{P} = (\pi, \pi)$  and all the quantum numbers equal to 1 for the rest of the discrete symmetries of the lattice. The *d*-wave superconducting phase may be characterized by a ground state in sector D of states with total momentum  $\mathbf{P} = (0,0)$  and odd parity under the exchange of the two axes in momentum space (the rest of quantum numbers remaining equal to 1). A ground state belonging to sector P of spin singlets with total momentum P =(0,0) and even parity for the rest of the symmetry operations implies a phase without symmetry breaking at the macroscopic level.

An important observation is that, for any even number of particles, the lowest-energy states found in the A, D, and P sectors by considering the scattering of the one-particle states in the  $\varepsilon = 0$  shell (and no particle-hole excitations from the Fermi sea) are always degenerate. Let us call  $\mathbf{p}_A = (\pi, 0)$ ,  $\mathbf{p}_B = (0,\pi)$ ,  $\mathbf{p}_C = (3\pi/4,\pi/4)$ ,  $\mathbf{p}_D = (\pi/4,3\pi/4)$ . For two particles at the Fermi level, for instance, the following states have the same energy:

$$\begin{split} |A\rangle &= \frac{1}{\sqrt{2}} \left( c_{\uparrow}^{\dagger}(\mathbf{p}_{A}) c_{\downarrow}^{\dagger}(\mathbf{p}_{B}) - c_{\downarrow}^{\dagger}(\mathbf{p}_{A}) c_{\uparrow}^{\dagger}(\mathbf{p}_{B}) \right) |FS\rangle \\ &- \frac{1}{2\sqrt{8}} \sum_{\mathcal{R}} \left( c_{\uparrow}^{\dagger}(\mathbf{p}_{C}) c_{\downarrow}^{\dagger}(\mathbf{p}_{D}) - c_{\downarrow}^{\dagger}(\mathbf{p}_{C}) c_{\uparrow}^{\dagger}(\mathbf{p}_{D}) \right) |FS\rangle, \\ |D\rangle &= \frac{1}{\sqrt{2}} \left( c_{\uparrow}^{\dagger}(\mathbf{p}_{A}) c_{\downarrow}^{\dagger}(\mathbf{p}_{A}) - c_{\uparrow}^{\dagger}(\mathbf{p}_{B}) c_{\downarrow}^{\dagger}(\mathbf{p}_{B}) \right) |FS\rangle, \\ |D'\rangle &= \frac{1}{\sqrt{8}} \sum_{\mathcal{R}} \left( c_{\uparrow}^{\dagger}(\mathbf{p}_{C}) c_{\downarrow}^{\dagger}(-\mathbf{p}_{C}) - c_{\uparrow}^{\dagger}(\mathbf{p}_{D}) c_{\downarrow}^{\dagger}(-\mathbf{p}_{D}) \right) |FS\rangle, \\ |P\rangle &= \frac{1}{\sqrt{2}} \left( c_{\uparrow}^{\dagger}(\mathbf{p}_{A}) c_{\downarrow}^{\dagger}(\mathbf{p}_{A}) + c_{\uparrow}^{\dagger}(\mathbf{p}_{B}) c_{\downarrow}^{\dagger}(\mathbf{p}_{B}) \right) |FS\rangle \\ &- \frac{1}{2\sqrt{8}} \sum_{\mathcal{R}} \left( c_{\uparrow}^{\dagger}(\mathbf{p}_{C}) c_{\downarrow}^{\dagger}(-\mathbf{p}_{C}) \\ &+ c_{\uparrow}^{\dagger}(\mathbf{p}_{D}) c_{\downarrow}^{\dagger}(-\mathbf{p}_{D}) \right) |FS\rangle, \end{split}$$

where  $\mathcal{R}$  stands for all possible reflections about the axes and  $|FS\rangle$  represents the Fermi sea below the  $\varepsilon = 0$  shell. It can be checked that this degeneracy among the lowest-energy states in the three different sectors holds for any even number of particles in the Fermi level  $\varepsilon = 0$ , when particle-hole excitations from the Fermi sea are frozen out.

Thus, in order to find to which sector belongs the ground state of the system, it suffices to make perturbations around the zeroth-order degenerate states. Wigner theorem establishes that no generic level crossings are found when just one parameter is varied in a quantum system.<sup>17</sup> In our problem, we may switch adiabatically, by means of an energy cutoff, the number of particle-hole processes that are allowed in the space of states, in order to resolve the above degeneracy. The theorem guarantees that the ground state obtained in this evolution has to be adiabatically connected to the ground state of the full many-body space. In practice, it is enough to perturb the many-body states with up to two particle-hole excitations from the Fermi sea comprising 24 particles below  $\varepsilon = 0$ . At this level, we may consider our computational method as accurate as the coupled-cluster-double approximation, in which the relative errors estimated for the ground state energy of the Hubbard model are as small as  $\sim 10^{-4}$ , for an 8×8 lattice and U=t.<sup>18</sup> As long as we are going to obtain our main results from the energy balance between different states in the model, we may expect them to be affected by smaller relative errors at that value of the interaction.

We have computed the lowest-energy states in the sectors with different quantum numbers, within the above approximation to the space of states, for a number N of particles in the  $\varepsilon = 0$  shell ranging from zero to 4. These values are about a doping rate  $\delta \sim 0.2$ . Otherwise, the case N=4 already sets the computational limit in the number of particles that can be afforded with our Fermi sea. The ground state with all the closed shells at N=0 is a spin singlet with momentum **P** 

TABLE I. Lowest energies of states with different quantum numbers, for particle content N=2 and N=4 in the  $\varepsilon = 0$  shell.

		<b>P</b> =(0,0) <i>s</i> -wave	<b>P</b> =(0,0) <i>d</i> -wave	$\mathbf{P}{=}(\pi,\pi)$
N = 2	U = t	-24.7985	-24.7999	-24.7985
	U=2t	-22.4508	-22.4540	-22.4507
N = 4	U = t	-24.4270	-24.4273	-24.4253
	U=2t	-21.7124	-21.7159	-21.7063

=(0,0) and even parity for the rest of discrete symmetries. Its energy for  $U_{\text{eff}}=t$  turns out to be  $\approx -25.1713t$ . The competition between the lowest energies in the different sectors for N=2 and N=4 is illustrated in Table I, for  $U_{\text{eff}}=t$  and 2t. We have found that the ground state is always in the D sector of odd parity under the exchange of  $p_x$  and  $p_y$ . This conclusion for N=2 is a confirmation of the result obtained within the same computational approach to the Hubbard model in a 6×6 cluster (see the Appendix).

At this point we address the question of how the balance between the energies shown in Table I may be affected by the renormalization of high-energy modes outside the region between  $-\Lambda$  and  $\Lambda$ . For this purpose, we have computed the quantities by which the lowest energies in the different sectors are shifted in the diagonalization of a space of states with up to two particle-hole excitations between high-energy modes (but without including this time the effect of the lowenergy modes between  $-\Lambda$  and  $\Lambda$ ). The result is that, for given values of the interaction and the number of particles, the corrections to the lowest energies in the above sectors differ between them by less than a relative quantity of order  $\sim 10^{-9}$ . Therefore, it is certainly safe to assume in the weakcoupling regime that the effect of renormalizing away the high-energy modes can be encoded in an appropriate modification of the effective coupling constant. The energy balance between the low-lying states in the different sectors turns out to be governed by the interaction close to the Fermi line, as appreciated in the results of Table I.

To gain insight about the nature of the ground states at N=2 and N=4, we have looked at the quasiparticle excitations supported by them. These correspond in our cluster to states with an odd number of particles (N=1 and N=3). States with N=1 can be considered quasiparticle excitations over the fully symmetric state with N=0, and their dispersion may be obtained by looking at different momenta above the Fermi sea. We have plotted in Fig. 2 the lowest energies found for  $U_{\text{eff}}=t$  among the many-body states with different momenta on the shell  $\varepsilon=0$  (including again up to two particle-hole excitations from the Fermi sea).

The Fermi energy for N=1 can be estimated by taking the mean value between the ground state energies at N=0and N=2, which turns out to be  $\approx -24.9856t$  for  $U_{\text{eff}}=t$ . The lowest energy found at  $\mathbf{P}=(\pi,0)$  is slightly above this value, by an amount of order  $10^{-4}t$ . The quasiparticle excitations at  $\mathbf{P}=(3\pi/4,\pi/4)$  and  $\mathbf{P}=(\pi/2,\pi/2)$  are found at higher energies. Results pointing in the same direction have been obtained in the diagonalization of small clusters.<sup>19</sup> We



FIG. 2. Lowest energies of states with odd number of particles N=1 (squares) and N=3 (triangles). The values are given relative to the Fermi energy estimates in the text. The circles stand for the N=3 data after correction of the Fermi line shift.

find a clear indication that the Fermi line is deformed by the interaction, in such a way that it is shifted inwards at the momenta  $(3 \pi/4, \pi/4)$  and  $(\pi/2, \pi/2)$ .<sup>20</sup> This deformation is in agreement with the effect of pinning of the Fermi energy near a Van Hove singularity that has been discussed on theoretical grounds.<sup>21,3</sup> According to this effect, the particles take advantage of the strong screening of the interaction at the singularity to place themselves preferentially near the saddle points of the dispersion relation, as observed in our computation. A similar phenomenon has been advocated recently in Ref. 22.

The study of the lowest-energy states for N=3 particles on the  $\varepsilon = 0$  shell is also of great interest. These may be considered as the quasiparticle excitations of the ground states for N=2 and N=4, and they are essential to characterize the pairing of particles at even filling levels. The energies for the momenta on the  $\varepsilon = 0$  shell, obtained in the same approximation as before, are plotted in Fig. 2 for  $U_{\text{eff}} = t$ .

The position of the Fermi energy at N=3 can be estimated from the ground state energies at N=2 and N=4, and it becomes  $\approx -24.6136t$  for  $U_{\text{eff}} = t$ . The deviation from this value of the lowest-energy states for the odd-filled shell may signal the momenta at which a gap opens up for the quasiparticle excitations. Given the above mentioned shift of the Fermi line, though, one has to bear in mind that the Fermi level is not reached precisely at the points  $\mathbf{P} = (3 \pi/4, \pi/4)$ and  $\mathbf{P} = (\pi/2, \pi/2)$ . This effect can be corrected by subtracting from the respective energies the shift from the Fermi level as measured for the N=1 quasiparticles. The final result can be seen in Fig. 2. The energy of the quasiparticles near  $\mathbf{P} = (3\pi/4, \pi/4)$  and  $\mathbf{P} = (\pi/2, \pi/2)$  turns out to be the same, within the precision of our computation, and slightly below the estimate from the mean value of the ground state energies for N=2 and N=4. On the contrary, the quasiparticle at  $\mathbf{P} = (\pi, 0)$  has an energy well above the Fermi energy estimate. It is clear that a gap opens up for quasiparticle excitations, but only at the position of the saddle points. The value  $\Delta$  of the gap for  $U_{\text{eff}} = t$ ,  $\Delta \approx 0.0017t$ , is sensibly

q	$\left\langle O_{SCD}(\mathbf{q}) O_{SCD}^{\dagger}(-\mathbf{q}) \right\rangle$	
(0,0)	25.969	
$\left(\frac{\pi}{4},0\right)$	4.907	
$\left(rac{m{\pi}}{4},rac{m{\pi}}{4} ight)$	8.526	
$\left(\frac{\pi}{2},0\right)$	3.262	
$\left(\frac{\pi}{2},\frac{\pi}{4}\right)$	1.671	
$\left(\frac{\pi}{2},\frac{\pi}{2}\right)$	1.059	

TABLE II. Values of the pairing correlator for different momenta near the origin.

greater than the energy difference between the lowest-energy states with *s*-wave and *d*-wave symmetry for N=4.

The conclusive evidence that the *d*-wave ground state at N=4 is built out of pairing of particles is given by the measure of pairing correlations with *d*-wave symmetry. We have computed the correlations of the operator

$$O_{SCD}(\mathbf{q}) = \sum_{\mathbf{k}} \left( \frac{g(\mathbf{k} + \mathbf{q}) + g(\mathbf{k})}{2} \right) c_{\uparrow}^{\dagger}(\mathbf{k} + \mathbf{q}) c_{\downarrow}^{\dagger}(-\mathbf{k}), \quad (2)$$

with  $g(\mathbf{p}) = \cos(p_x) - \cos(p_y)$ , in the ground state for N=4 at  $U_{\text{eff}}=t$ . The results are shown in Table II. The momenta that can be measured are enough to discern a high peak at  $\mathbf{q}=0$  of the pairing correlations, together with a sharp decrease away from the origin. To establish some comparison, we may quote that the peak of the *s*-wave pairing correlations in the lowest-energy state of the P sector is  $\approx 6.9$ . Taking into account that the *d*-wave correlations decay by one order of magnitude across two lattice units in momentum space, the translation of the results to real space is that the binding of particles is correlated on the whole dimension of the cluster.

Although our results refer to an  $8 \times 8$  cluster, we think that they are robust enough to survive the extrapolation to larger lattices. Computations of the exact ground state of the Hubbard model in a  $4 \times 4$  lattice with two and four particles in the  $\varepsilon = 0$  shell have been carried out in Refs. 23 and 24. respectively. Although a *d*-wave state is found in each case among the low-energy states, the ground state for the  $4 \times 4$ lattice does not have such symmetry in the weak-coupling regime. Moving ahead to the Hubbard model in a  $6 \times 6$  cluster, the same computational approach we have adopted above can be applied to find the quantum numbers of the ground state, as reported in the Appendix. In that lattice, the system with two particles at the  $\varepsilon = 0$  shell attains the lowest energy in the sector of *d*-wave symmetry, but this property does not hold for a smaller number of holes near half-filling. One has to move to the  $8 \times 8$  lattice to find a *d*-wave ground state also in the case of four particles above the Fermi sea. It seems, therefore, that this progression in lattice size goes in parallel with the condensation of a larger number of pairs each time. The qualitative change in the results is also related to the existence of a critical size to observe the effects of the Van Hove singularity in the density of states. This has been noticed in the study of ferromagnetism in the t-t' Hubbard model at low filling.<sup>25</sup> In that case, quantum Monte Carlo computations revealed the existence of the ferromagnetic ground state in a  $16 \times 16$  lattice. As long as in our approach we characterize the ground state of the system at zero temperature, the study of the  $8 \times 8$  lattice already gives evidence of the way in which the symmetry is broken by effect of the large density of states.

The existence of the *d*-wave ground state with remarkable pairing correlations provides a microscopic basis for a longstanding conjecture. There has been much hope that a mechanism based on antiferromagnetic fluctuations may be the source of superconductivity in the copper-oxide materials. A different approach-though similar in essence-has put forward the idea that the Hubbard model should bear a form of Kohn-Luttinger superconductivity near half-filling. By stressing the relevance of the modes near the Fermi level shell at  $\varepsilon = 0$ , our explicit construction of the *d*-wave ground state points at the processes with momentum transfer Q  $=(\pi,\pi)$  as the source of an attractive channel in the Hubbard model with bare repulsive interaction. Nesting of the saddle points at the Fermi level is at the origin of the relevance of such processes, which single out d-wave superconductivity as the dominant instability of the system.

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## APPENDIX: CONFIGURATION INTERACTION IN THE 6×6 CLUSTER

A computational approach similar to ours has been discussed for the Hubbard model in a  $6 \times 6$  lattice in Ref. 15. It is then interesting to see what results are obtained by following the procedure devised above, in the case of the  $6 \times 6$  cluster.

In that smaller lattice, we assume that the relevant interaction takes place involving the modes in the region between energies  $-\Lambda$  and  $\Lambda$  shown in Fig. 3. We consider now a Fermi sea made of 16 particles filling the levels below the  $\varepsilon = 0$  shell. As it happened in the case of the  $8 \times 8$  lattice, the hybridization of states for a given number of particles in the Fermi level  $\varepsilon = 0$ , without particle-hole excitations from the Fermi sea, keeps the lowest-energy states in the above mentioned sectors of different symmetry degenerated. To resolve the degeneracy in the weak-coupling regime, it is enough again to diagonalize the Hamiltonian in a space of states made of the low-energy excitations about the Fermi level.

We have looked for the ground state among the sectors with different quantum numbers, for a number of particles N=2 and 4 in the Fermi level shell  $\varepsilon = 0$  (that correspond, respectively, to having 8 and 6 holes with respect to halffilling). The results for the lowest-energy states in the space with up to two particle-hole excitations from the Fermi sea are shown in Table III.



FIG. 3. Points of the  $6 \times 6$  lattice in momentum space.

We observe that, for N=2, the ground state is found in the sector of *d*-wave symmetry as in the 8×8 lattice. However, in the case of N=4, the symmetry turns out to be *s*-wave in all the range of coupling constants studied. These results match with those obtained recently in Ref. 15. A configuration interaction has been devised there by placing a cutoff in the single-particle energies relative to the Fermi level. In the case considered of 4 holes about half-filling, it has been shown that the ground state does not have significant *d*-wave correlations, contrary to the results obtained

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		<b>P</b> =(0,0) <i>s</i> -wave	<b>P</b> =(0,0) <i>d</i> -wave	$\mathbf{P}{=}(\pi,\pi)$
N = 2	U = t	-21.9223	-21.9271	-21.9223
	U=2t	-20.0704	-20.0860	-20.0702
N = 4	U = t	-21.5082	-21.5078	-21.5005
	U=2t	- 19.2915	- 19.2864	- 19.2810

TABLE III. Lowest energies of states with different quantum numbers in the  $6 \times 6$  cluster.

with a much smaller number of excitations in the space of states.<sup>14</sup>

The results for the  $6 \times 6$  lattice are instructive since they show that, although two particles above the Fermi sea have tendency to pairing with *d*-wave symmetry, the condensate of a larger number of pairs does not have sufficiently low energy to become the ground state of the system. In that respect, the  $6 \times 6$  lattice does not seem to have enough resolution to capture the effect of enhanced scattering with momentum transfer  $(\pi, \pi)$ . Moving to the  $8 \times 8$  lattice gives rise to a much better description of the low-energy theory, as the number of one-particle states close to the Fermi line increases from 16 to 24. The future availability of larger computer resources will be of great help in the development of the configuration interaction approach in larger lattices, as well as in the assessment of the renormalization effects implicit in the method.

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