Short-range character of the antiferromagnetic Ising model with $1/r^p$ interaction

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By applying Ewald summation, we analytically compute the Fourier transform of a d-dimensional lattice interaction decaying like r^{-p} for a long-range antiferromagnetic Ising system on a simple cubic lattice with $1<p<d$. The resulting analytical form of the dispersion allows to deduce in a simple way that the model's universality class is identical to that of the short-range Ising model.

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While the critical behavior of lattice spin models with short-range interactions is well understood nowadays both from the theoretical[1–3] as well as from the computational[3–5] point of view, long-ranged interactions continue to present challenges to both theorists and simulators. To the theorist, long-range interaction models pose delicate mathematical problems connected to the precise definition and computation of the thermodynamic limit while simulations of such systems are usually plagued by the high computational costs of the underlying algorithms. For instance, consider an Ising type of lattice model defined on a simple d-dimensional cubic lattice Γ with orthogonal Bravais lattice vectors $\boldsymbol{a}_\mu$, $\mu=1,\ldots,d$, lattice constant $|\boldsymbol{a}_\mu|=a$, and Hamiltonian $\mathcal{H}[\{s(\boldsymbol{x})\}]=-(1/2)\Sigma_{\boldsymbol{x},\boldsymbol{y}\in\Gamma}J(|\boldsymbol{x}-\boldsymbol{y}|)s(\boldsymbol{x})s(\boldsymbol{y})$, where

$$J(r)=\begin{cases} J_0 r^{-p}, & r\neq 0 \\ 0, & \text{else} \end{cases}, \quad p<d. \tag{1}$$

If $J_0>0$, which energetically favors a parallel "*ferro*" ordering of spins, simple arguments[6] indicate that as the system size approaches infinity, the energy *per site* diverges, such that the thermodynamic limit of this system fails to exist.

However, things may look different for its antiferromagnetic counterpart defined by taking $J_0=-|J_0|<0$. In fact, recall that a simple cubic lattice Γ is *bipartite*,[7] i.e., it can be decomposed into two sublattices $\Gamma=\Gamma_+\cup\Gamma_-$, which consist of mutual nearest-neighbor sites. Since the interaction is strongest between nearest neighbors, one may guess that below some critical temperature the energetically favored states of the system consist of antiferromagnetic layers of opposite magnetization occupying $\Gamma_\pm$, and the resulting effective screening of the interaction allows for a finite energy density in the thermodynamic limit. In the language of phase transitions,[8] such a state is connected to a critical wave vector $\boldsymbol{Q}^*=(1,1,\ldots,1)\pi/a$ at the boundary of the Brillouin zone Γ^*, the two sublattices $\Gamma_\pm$ consisting of all sites $\boldsymbol{x}$ with "parity" $P(\boldsymbol{x}):=e^{i\boldsymbol{Q}^*\boldsymbol{x}}=\pm 1$, respectively. Nevertheless, the slow decay of the underlying interaction places such reasoning on shaky ground, as it ignores possible complications by accompanying frustration effects. And indeed, despite the model's apparent simplicity, the correct determination of the universality class of the antiferromagnetic d-dimensional Ising model in $d>1$ with Coulomb-type interaction, which in our terminology corresponds to the case $p=1$, continues to be under debate. In recent papers (cf. Refs. 9–11, and references therein) the problem was tackled using Monte Carlo (MC) simulations in combination with finite-size scaling, and numerical evidence was gathered that the model actually belongs to the short-range Ising universality class. However, e.g., the authors of Ref. 10 express concerns about the validity of these conclusions, as their simulations, which were based on a computational treatment of the long-range interaction using Ewald summation techniques, gave a value of $\nu=0.55\pm0.1$ for the correlation length exponent ν, while other simulation results (cf. Ref. 11), which employed the minimal image convention for the interaction, yielded $\nu\approx0.63$ in agreement with standard Ising behavior. Unfortunately, the large error bar produced by the simulations of Ref. 10, which were primarily aimed at studying the effects of disorder in such systems, did not allow to numerically resolve any discrepancies between these results. However, in Ref. 10 it was argued that the possible differences might arise as artifacts introduced by the minimal image convention, as this involves an effective truncation of the interaction at half the system size, thus unintentionally favoring a short-range behavior. It is the purpose of the present paper to resolve this controversial point. Indeed, it is possible to show by simple analytical arguments that the model indeed falls into the short-range Ising universality class.

Technically, it will be convenient to shift the critical wave vector of the naively expected transition to the Brillouin-zone center in the following way. Invariance of the model's partition function under the replacement $s(\boldsymbol{z})\to P(\boldsymbol{z})s(\boldsymbol{z})$ of the dummy summation variables $s(\boldsymbol{z})$ implies that

$$\begin{aligned} Z(\beta) &= \prod_{\boldsymbol{z}\in\Gamma}\sum_{s(\boldsymbol{z})=\pm1} e^{\beta/2\sum_{\boldsymbol{x},\boldsymbol{y}\in\Gamma}J(\boldsymbol{x}-\boldsymbol{y})s(\boldsymbol{x})s(\boldsymbol{y})} \\ &= \prod_{\boldsymbol{z}\in\Gamma}\sum_{s(\boldsymbol{z})=\pm1} e^{\beta/2\sum_{\boldsymbol{x},\boldsymbol{y}\in\Gamma}J(\boldsymbol{x}-\boldsymbol{y})P(\boldsymbol{x})P(\boldsymbol{y})s(\boldsymbol{x})s(\boldsymbol{y})}. \end{aligned} \tag{2}$$

Therefore, setting

$$J_F(\boldsymbol{x}-\boldsymbol{y}) := P(\boldsymbol{x})J(|\boldsymbol{x}-\boldsymbol{y}|)P(\boldsymbol{y}) = J(|\boldsymbol{x}-\boldsymbol{y}|)P(\boldsymbol{x}-\boldsymbol{y}) \tag{3}$$

we end up with a new lattice model which trivially shows the same set of singularities in its analytic behavior as our original one. Since the nearest-neighbor interaction coefficients $J_F(\boldsymbol{a}_\mu)=|J_0|/a$, $\mu=1,\ldots,d$, are positive, our naive guess—again based on comparing with the corresponding nearest-neighbor model—would be a ferromagnetic ground state. However, once more one feels a bit uneasy, as the alternating sign of the new lattice interaction $J_F(|\boldsymbol{x}|)$ in combination with the slow $1/r^p$ decay now may lead to the above-mentioned

frustration effects. Indeed, in the case of short-range competing interactions it is well known[12–15] that, depending on the chosen size and sign of the underlying coupling constants, the topology of resulting ground state may reveal a surprisingly complex structure. Even though the models investigated in these works appear not to yield reliable predictions for, say, our present model with interactions beyond third-nearest neighbors, these papers should warn us not to automatically assume that the ground state for the model at hand is ferromagnetic.

Let us first discuss the simulator's point of view. The main obstacle to overcome in performing MC simulations for the above class of models is of course the long-range of the lattice interaction. In particular, the algebraic decay of the lattice interaction tends to conflict with periodic boundary conditions. However, it is clear that any brute force truncation of the interaction beyond any finite cutoff radius may severely change the long-distance critical behavior of the system. In simulations of *neutral* Coulomb systems, a standard approach to overcome these problems is to employ Ewald summation.[16] Since this technique is well known,[17–19] let us only sketch its content, focusing on the aspects that will be important for our subsequent use. Let us use the "electrostatic language," where the spins $s(\boldsymbol{x})$ correspond to positive and negative unit charges at sites $\boldsymbol{x}$. In the Ewald approach, the simulation box, which we take to be hypercubic with volume $V_0=(La)^d$, is surrounded by infinitely many copies with identical copies of the charge/spin distributions of the central unit cell V_0, and each charge in V_0 interacts with all others in the enlarged system, including its own periodic images in the infinitely many surrounding cells. By adding and subtracting continuous screening charge distributions and calculating appropriately chosen parts of the resulting energy contributions in direct and Fourier space, respectively, one ends up with an expression for the total energy which consists of a real-space summation over an effectively screened (and thus short-ranged) potential and an exponentially damped sum over all nonzero reciprocal wave vectors whose summand depends on the structure factor of the original charge distribution in V_0. The formal divergence of the zero reciprocal wave-vector part, which in a careful treatment is seen to depend on the electrostatic boundary conditions imposed on the system by its actual shape and the dielectric properties of the surrounding medium, reflects the poor (i.e., conditional) convergence of the total-energy sum for the enlarged system.

Despite this theoretical effort, the computational complexity of straightforward Ewald summation is $O(N^{3/2})$, where N is the number of charges/spins involved.[20] In principle, it thus seems highly desirable to further reduce the required computational effort. In fact, for computing critical, i.e., universal long-distance properties, it is clearly not necessary to carry the burdens of keeping all the irrelevant short-range details of a particular model. Moreover, spatially localized MC moves are not ideal for studying collective long-range properties of a system. In fact, our recently developed Fourier MC algorithm[21–24] seems to be just the perfect tool for the problem at hand, as it is not plagued by any of these problems. As will be explained below, the structure of the Hamiltonian that emerges from transforming the problem at hand to Fourier space will allow us to conclude that it is actually not necessary to undertake such simulations, as the resulting universal Hamiltonian will be manifestly of a short-range type. Nevertheless, in order to present our argument, we need to briefly sum up the basic structure of Fourier MC.

We begin by introducing the discrete Fourier transform $s(\boldsymbol{x})=\frac{1}{N}\Sigma_{\boldsymbol{k}\in\Gamma^*}\tilde{s}(\boldsymbol{k})e^{i\boldsymbol{k}\boldsymbol{x}}$, and write our model Hamiltonian as

$$\mathcal{H}[s]=-\frac{1}{2}\sum_{\boldsymbol{k}}\tilde{J}_F(\boldsymbol{k})|\tilde{s}(\boldsymbol{k})|^2. \tag{4}$$

Since pure point charges often represent an idealization anyway, we further replace the Ising spins $s(\boldsymbol{x})=\pm 1$ by real-valued "soft" spins $\varphi(\boldsymbol{x})\in\mathbb{R}$ and consider the corresponding lattice φ^4 model with an on-site potential $-\frac{1}{2}\varphi^2(\boldsymbol{x})+\frac{1}{4}\varphi(\boldsymbol{x})$ and a lattice interaction $-(1/2)J_F(\boldsymbol{x}-\boldsymbol{y})\varphi(\boldsymbol{x})\varphi(\boldsymbol{y})$ of the above type, Eq. (3), which is another representative of the universality class under investigation. The advantages of doing so are numerous: on the one hand, since the set of lattice interaction coefficients $J_F(\boldsymbol{x}-\boldsymbol{y})$ is translation invariant, it is diagonalized by the Fourier transform. Its Fourier transform, call it $\tilde{J}_F(\boldsymbol{k})$, can be calculated and tabulated once and for all at the start-up of the simulation, and subsequent Fourier MC moves only require $O(1)$ steps to calculate the change in this contribution to the total energy under shifts of the underlying Fourier amplitudes. On the other hand, these shifts, which constitute the basic MC moves in this algorithm, represent *collective* moves of the system. Therefore, restricting the simulation to modes inside a given cutoff Λ around $\boldsymbol{k}=\boldsymbol{0}$, one is able to focus on the long-wavelength behavior of the system. Parenthetically, we note that closer analysis[25] reveals that this algorithm is of order N_Λ, where N_Λ is the number of $\boldsymbol{k}$ vectors inside the cutoff Λ. In addition, since the spacing between successive $\boldsymbol{k}$ vectors in the Brillouin zone is $2\pi/La$, one is able to increase the linear system size L considerably while keeping N_Λ at a manageable size by choosing Λ to be suitably small. At the present stage of our investigations there is, however, no immediate need to introduce a cutoff Λ.

Of course, the only possible difference between the short range and the present Ising type of model is encoded in the $\boldsymbol{k}$ dependence of the function $\tilde{J}_F(\boldsymbol{k})$. If we were to define $\tilde{J}_F(\boldsymbol{k})$ by

$$\tilde{J}_F(\boldsymbol{k})=\sum_{\boldsymbol{0}\neq\boldsymbol{x}\in\Gamma_L}J_F(\boldsymbol{x})e^{i\boldsymbol{k}\boldsymbol{x}}, \tag{5}$$

where Γ_L denotes a finite sublattice of Γ with L^d sites and periodic boundary conditions, then the resulting lattice dispersion $\tilde{J}_F(\boldsymbol{k})$ would be indistinguishable from that of a $1/r^p$ interaction truncated at half the size of the simulation box when combined with the minimum image convention.[11] In order to avoid any implicit or explicit truncation effects, we thus choose to replace Eq. (5) by an Ewald type of definition. Specifically, we consider

$$\tilde{J}_F(\boldsymbol{k})=\sum_{\boldsymbol{x}\neq\boldsymbol{0}}J_F(\boldsymbol{x})e^{i\boldsymbol{k}\boldsymbol{x}}=J_0\sum_{\boldsymbol{x}\neq\boldsymbol{0}}\frac{e^{i(\boldsymbol{Q}^*+\boldsymbol{k})\boldsymbol{x}}}{|\boldsymbol{x}|^p}. \tag{6}$$

The Ewald summation is performed by employing the identity (cf. Appendix A of Ref. 26)

$$\frac{1}{|\boldsymbol{x}|^p} = \pi^{d/2}\epsilon^{p-d}\int_{\mathbb{R}^d}\frac{d^dq}{(2\pi)^d}e^{i\boldsymbol{q}\boldsymbol{x}}f_p\left(\frac{|\boldsymbol{q}|}{2\epsilon}\right) + \frac{g_p(\epsilon|\boldsymbol{x}|)}{|\boldsymbol{x}|^p} \tag{7}$$

valid for arbitrary $\epsilon>0$, where

$$f_p(x) = \frac{2x^{p-d}}{\Gamma\left(\frac{p}{2}\right)}\int_x^\infty dse^{-s^2}s^{d-p-1} = \frac{x^{p-d}\Gamma\left(\frac{d-p}{2},x^2\right)}{\Gamma\left(\frac{p}{2}\right)}, \tag{8}$$

$$g_p(x) = \frac{2}{\Gamma\left(\frac{p}{2}\right)}\int_x^\infty dse^{-s^2}s^{p-1} = \frac{\Gamma\left(\frac{p}{2},x^2\right)}{\Gamma\left(\frac{p}{2}\right)} \tag{9}$$

[here $\Gamma(z,a)=\int_a^\infty dte^{-t}t^{z-1}$ denotes the incomplete gamma function]. Then $\tilde{J}_F(\boldsymbol{k})=\tilde{J}_F^{(l)}(\boldsymbol{k})+\tilde{J}_F^{(s)}(\boldsymbol{k})$, where the short-range dispersion

$$\tilde{J}_F^{(s)}(\boldsymbol{k};\epsilon) = J_0\sum_{\boldsymbol{x}\neq\boldsymbol{0}}e^{i(\boldsymbol{Q}^*+\boldsymbol{k})\boldsymbol{x}}\frac{g_p(\epsilon|\boldsymbol{x}|)}{|\boldsymbol{x}|^p} \tag{10}$$

is analytic in $\boldsymbol{k}$ due to the exponential decay of $g_p(\epsilon|\boldsymbol{x}|)$, and from cubic symmetry we anticipate the standard short-range dispersion expansion

$$\tilde{J}_F^{(s)}(\boldsymbol{k};\epsilon) = \tilde{J}_F^{(s)}(\boldsymbol{0};\epsilon) - \frac{R^2(\epsilon)}{2}k^2 + O(k_\mu^4). \tag{11}$$

We thus concentrate on the long-range contribution

$$\tilde{J}_F^{(l)}(\boldsymbol{k};\epsilon) = J_0\pi^{d/2}\epsilon^{p-d}\sum_{\boldsymbol{x}\neq\boldsymbol{0}}e^{i(\boldsymbol{Q}^*+\boldsymbol{k})\boldsymbol{x}}\times\int_{\mathbb{R}^d}\frac{d^dq}{(2\pi)^d}e^{i\boldsymbol{q}\boldsymbol{x}}f_p\left(\frac{|\boldsymbol{q}|}{2\epsilon}\right). \tag{12}$$

Taking advantage of the facts that

$$\pi^{3/2}\epsilon^{p-d}\int_{\mathbb{R}^d}\frac{d^dq}{(2\pi)^d}f_p\left(\frac{|\boldsymbol{q}|}{2\epsilon}\right) = \frac{2\epsilon^p}{p\Gamma(p/2)} \tag{13}$$

and that

$$\sum_{\boldsymbol{x}}e^{i(\boldsymbol{Q}^*+\boldsymbol{q}+\boldsymbol{k})\boldsymbol{x}} = \frac{(2\pi)^d}{V_0}\sum_{\boldsymbol{G}\in\Gamma_*}\delta^d(\boldsymbol{Q}^*+\boldsymbol{q}+\boldsymbol{k}+\boldsymbol{G}), \tag{14}$$

where $\Gamma_*=(2\pi/a)\cdot\mathbb{Z}^d$ denotes the reciprocal lattice of Γ, we add and subtract in Eq. (12) a term representing $(\boldsymbol{x}=\boldsymbol{0})$ and obtain

$$\tilde{J}_F^{(l)}(\boldsymbol{k};\epsilon) = \frac{J_0\pi^{d/2}\epsilon^{p-d}}{V_0}\sum_{\boldsymbol{G}\in\Gamma_*}f_p\left(\frac{|\boldsymbol{Q}^*+\boldsymbol{k}+\boldsymbol{G}|}{2\epsilon}\right) - \frac{2J_0\epsilon^p}{p\Gamma(p/2)}. \tag{15}$$

In contrast to the standard Ewald summation formulas, which hold for charge-neutral Coulomb systems, for $1<p<d$ there is no need to exclude any $\boldsymbol{G}\in\Gamma_*$ from the above sum, as long as $\boldsymbol{k}\neq\boldsymbol{Q}^*$, since $f_p(x)$ is not singular for $x\neq0$ and its argument $|\boldsymbol{Q}^*+\boldsymbol{k}+\boldsymbol{G}|/2\epsilon$ only vanishes for $\boldsymbol{k}=\boldsymbol{Q}^*$ and $\boldsymbol{G}=-2\boldsymbol{Q}^*$ (Γ^* is discrete for $L<\infty$). For $\boldsymbol{k}\to\boldsymbol{Q}^*$ approaching the singular point $\boldsymbol{Q}^*$ (or one of its symmetry-related corner points of the Brillouin zone), $\tilde{J}_F^{(l)}(\boldsymbol{k};\epsilon)\to-\infty$ diverges, leading to a positively diverging energy contribution for the corresponding fluctuation modes, whose statistical weight thus vanishes. The singular point $\boldsymbol{k}=\boldsymbol{Q}^*$ is thus insignificant for the thermodynamics of the system. To illustrate this state of affairs, we specialize to the Coulomb-type case $p=1$. From the explicit formulas

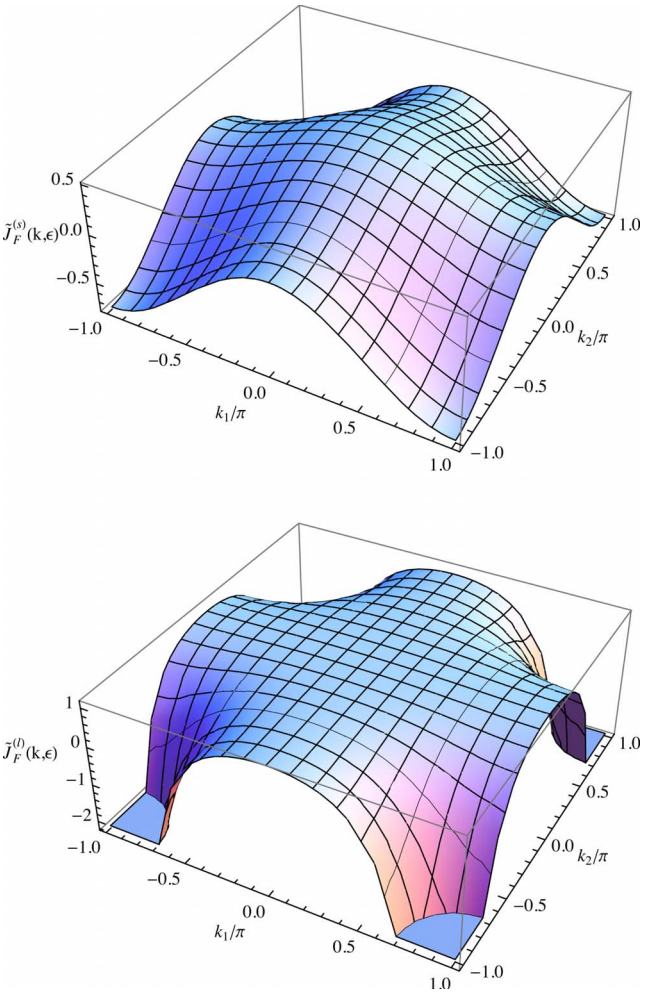

FIG. 1. (Color online) Dispersion contributions in $d=2$ according to Eqs. (17) and (19). (a) Short-range dispersion $\tilde{J}_F^{(s)}(\boldsymbol{k};\epsilon)$; (b) long-range dispersion $\tilde{J}_F^{(l)}(\boldsymbol{k};\epsilon)$. Parameter values $J_0=-1$, $a=\epsilon=1$.

$$g_1(x)=\mathrm{erfc}(x), \quad f_1(x)=\begin{cases}\dfrac{e^{-x^2}}{\sqrt{\pi}x^2}, & d=3\\ \dfrac{\mathrm{erfc}(x)}{x}, & d=2\end{cases} \tag{16}$$

[here $\mathrm{erfc}(x)$ is the complementary error function] we calculate the short-range part

$$\tilde{J}_F^{(s)}(\boldsymbol{k};\epsilon) = J_0\sum_{\boldsymbol{x}\neq\boldsymbol{0}}e^{i(\boldsymbol{Q}^*+\boldsymbol{k})\boldsymbol{x}}\frac{\mathrm{erfc}(\epsilon|\boldsymbol{x}|)}{|\boldsymbol{x}|} \tag{17}$$

while for the long-range part of the dispersion we obtain in $d=3$,

$$\tilde{J}_F^{(l)}(\boldsymbol{k};\epsilon) = \frac{4\pi J_0}{V_0} \sum_{\boldsymbol{G}\in\Gamma_*} \frac{e^{-|\boldsymbol{Q}^*+\boldsymbol{k}+\boldsymbol{G}|^2/4\epsilon^2}}{|\boldsymbol{Q}^*+\boldsymbol{k}+\boldsymbol{G}|^2} - \frac{2J_0\epsilon}{\sqrt{\pi}} \tag{18}$$

while in $d=2$,

$$\tilde{J}_F^{(l)}(\boldsymbol{k};\epsilon) = \frac{2\pi J_0}{V_0} \sum_{\boldsymbol{G}\in\Gamma_*} \frac{\mathrm{erfc}\left(\frac{|\boldsymbol{Q}^*+\boldsymbol{k}+\boldsymbol{G}|}{2\epsilon}\right)}{|\boldsymbol{Q}^*+\boldsymbol{k}+\boldsymbol{G}|} - \frac{2J_0\epsilon}{\sqrt{\pi}}. \tag{19}$$

Numerically evaluating these expressions for $d=2$, we observe (cf. Fig. 1) that the short-range part $\tilde{J}_F^{(s)}(\boldsymbol{k};\epsilon)$ displays the anticipated parabolic profile, Eq. (11). The long-range part $\tilde{J}_F^{(l)}(\boldsymbol{k};\epsilon)$ is equally parabolic for all $\boldsymbol{k}$ vectors at the center of the Brillouin zone and only starts to drop sharply when approaching the vicinity of the corners of Γ^*. This behavior is also confirmed by closer numerical investigations. Furthermore, for any choice of ϵ $\tilde{J}_F^{(l)}(\boldsymbol{k};\epsilon) \propto V_0^{-1}$ tends to the mere constant $-2J_0\epsilon/\sqrt{\pi}$ in the thermodynamic limit $V_0 \to \infty$. At this stage it may also be safe to introduce a wave-vector cutoff Λ for the fluctuation modes of the system if we are only interested in the universal critical behavior of the model.

Summarizing our argument, from the viewing angle of Fourier MC, there is actually no point in conducting any simulations. On the one hand, the lattice interaction $J_F(\boldsymbol{x})$ has no influence on the onsite potential part of the effective ϕ^4 Hamiltonian but only determines its dispersion part. As to this dispersion, by Ewald summation we have shown that in the vicinity of the center of the Brillouin zone it perfectly resembles that of an ordinary short-range ferromagnetic Ising-type model. Thus, the model is bound to fall into the corresponding short-range Ising universality class.

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