

Trion Formation and Ordering in the Attractive SU(3) Fermi-Hubbard Model

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Recent advances in microwave shielding have increased the stability and control of large numbers of polar molecules, allowing for the first realization of a molecular Bose-Einstein condensate. Remarkably, it was also recently realized that shielded polar molecules exhibit an $SU(N)$ symmetry among their hyperfine states, opening the door to $SU(N)$ systems with larger N , bosonic particle statistics, and tunable interactions—both repulsive and attractive. Motivated by these results, we have studied the $SU(3)$ attractive Fermi-Hubbard model (FHM) on a square lattice. Using the determinant quantum Monte Carlo (DQMC) method, we explore the finite temperature phase diagram and provide evidence for three distinct regions—a three-component Fermi liquid (FL) region, a “trion” liquid (TL) region, and an ordered charge density wave (CDW) phase. The CDW phase is stable at finite temperature [in contrast to the $SU(2)$ CDW], while the FL to TL crossover appears to point to a quantum phase transition at zero temperature. Our method extends straightforwardly to larger N and is sign problem free for even values of N . With these results, we demonstrate the potential physics enabled by using polar molecules as a quantum simulation platform for the attractive $SU(N)$ FHM.

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Introduction—The last few decades have seen a resurgence of interest in $SU(N)$ -symmetric extensions of interacting fermion lattice models, such as the t - J model, Heisenberg model, and Fermi-Hubbard model (FHM) [1–3]. These $SU(N)$ models have been studied to approximate ultracold atoms with several hyperfine states [4,5], where the $SU(N)$ symmetry was seen more as a loose approximation. Then, the discovery of a precise $SU(N)$ symmetry in the nuclear spin of alkaline-earth atoms (AEAs) [6–9] sparked detailed theoretical and numerical work to study phases and the equation of state in these newly accessible models. In recent years, multiple groups have experimentally realized $SU(N)$ lattice models [10–14], and many numerical methods and theoretical approaches have been developed to study them [15–27].

However, with these AEAs come inherent limitations. Most relevant to the present Letter, interactions between AEAs cannot be controlled by a magnetic Feshbach resonance and so are always repulsive (i.e., have a positive s -wave scattering length). The attractive case has been studied using other atoms—such as three hyperfine levels of ^6Li [28]—but tuning the interactions to the $SU(3)$ -symmetric point has been a persistent challenge. So, while the attractive $SU(N)$ FHM has been studied as a toy model of a wide array of phenomena—from baryon formation in

QCD [29,30] to charge- $4e$ superconductivity [31–34]—there has not been an experimental platform to realize this model, and theoretical investigations have mainly focused on the repulsive case.

Additionally, attractive $SU(N)$ models are a natural stage for studying many-body bound states. In the continuum, the formation of three-particle “trions” has been studied along with the infinite ladder of Efimov states [35–37]. In lattice systems, few-body exact diagonalization has shown the existence of both on site and off site trions and studied the critical interaction strength for trion formation in one and two dimensions [38]. The attractive $SU(N)$ FHM offers an opportunity to study how the formation of composite particles affects the many-body physics of a system. Early mean field theory and renormalization group (RG) work focused on a quantum phase transition (QPT) from a trion phase to a many-body generalization of a Bardeen-Cooper-Schrieffer (BCS) state called a “color superfluid” (CSF) [4,5,29,39]. There are many open questions concerning the finite temperature behavior of these phases and other ordered phases for the attractive $SU(N)$ FHM, especially in two dimensions.

Recently, it has become clear that ultracold molecule experiments employing electromagnetic shielding techniques provide an exciting new $SU(N)$ system, which may be able to experimentally realize the attractive $SU(N)$ FHM. Cooling molecules down to degenerate quantum gases has historically been challenging due to large

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two-body loss rates that impair evaporative cooling. Static electric field shielding has enabled the cooling of a degenerate Fermi gas of molecules [40], and more recently microwave shielding [41] has enabled even further cooling below the Fermi temperature [42] and the first observation of a dipolar molecular BEC [43]. Importantly for our purposes, this microwave shielding causes an effective $SU(N)$ symmetry [44,45]. The interaction strength can be tuned across a wide range and can be either repulsive or attractive. So, amid the many proposals for using shielded dipolar molecules to study new physics [46], we believe these molecules will be useful for answering long-held questions about the attractive $SU(N)$ FHM.

In this Letter, we employ a determinant quantum Monte Carlo (DQMC) method designed for the attractive $SU(N)$ FHM to explore the phase diagram of the $N = 3$ case on a square lattice. We find evidence of two distinct phase transitions—a “trion formation” QPT and an “ordering” transition into a charge density wave (CDW) phase, which persists to finite temperature. We present evidence for these two transitions and develop approximations that are valid deep within the different phases. We also compare our results to previous theoretical work on the zero-temperature phase diagram of this model and discuss the viability of observing these phases in an ultracold molecule experiment.

Model and numerical methods—The attractive, $SU(3)$ -symmetric FHM is given by the Hamiltonian,

$$H = -t \sum_{\sigma, \langle i, j \rangle} \overbrace{[c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}]}^K - \mu \sum_{\sigma, i} n_{i\sigma} - \underbrace{\frac{U}{2} \sum_i \left(\sum_{\sigma} n_{i\sigma} - \frac{3}{2} \right)^2}_V, \quad (1)$$

where $c_{i\sigma}^\dagger, c_{i\sigma}$ are the creation and annihilation operators for a molecule in spin state σ on lattice site i , $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, $\langle i, j \rangle$ denotes a sum over nearest-neighbor pairs, t is the tunneling energy, U is the on site attraction, μ is the chemical potential, K is the kinetic energy operator, and V is the potential energy operator. Since we study the $N = 3$ case, σ runs over three molecular spin states. Here, $\mu = 0$ corresponds to half filling ($n_\sigma = 1/2$).

To study this model at finite temperature, we use a DQMC method [47,48] formulated for the attractive $SU(N)$ FHM as detailed in Supplemental Material [49], Sec. I. We compute finite temperature expectation values such as $\langle n_{i\sigma} \rangle$, $\langle n_{i\sigma} n_{j\tau} \rangle$, and $\langle n_{i\sigma} n_{i\tau} n_{i\nu} \rangle$ for molecular spin states σ, τ, ν and site indices i, j on square lattices with side length L over a range of $U/t, \mu/t$, and T/t , where T is the temperature and we have set $k_B = 1$. Quantities that require differentiation with respect to μ or T were calculated by comparing neighboring data points. All data shown are for $L = 10$ unless specified to be a finite-size extrapolation. The DQMC algorithm works

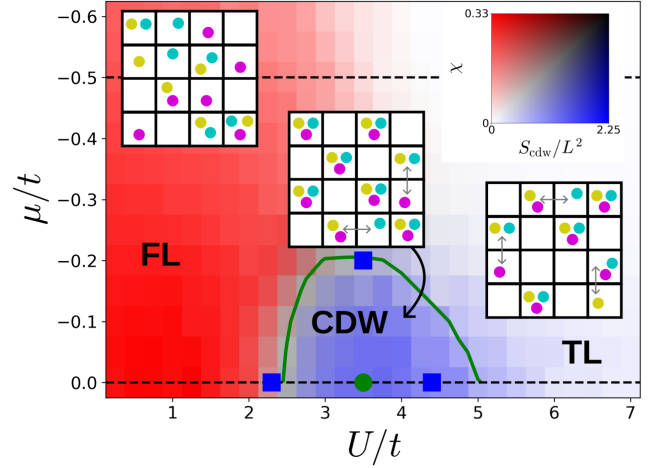


FIG. 1. Finite temperature phase diagram at $T = t/3$ with representative configurations for the three zero-temperature phases: the Fermi liquid of individual molecules (FL), trion Fermi liquid of bound triples of molecules (TL), and charge density wave (CDW) phase. The inset shows a legend for the structure factor, S_{cdw}/L^2 , and difference susceptibility, χ . Dashed lines indicate the cuts taken in Fig. 2. The green dot shows the (U, μ) point where the data in Fig. 3 were taken. The green contour line is a guide for the eye while the blue squares mark the critical values as indicated by the invariant correlation ratio.

by discretizing the inverse temperature into M imaginary time steps, where $1/T = M\Delta\tau$. The details of the differentiation process, finite-size extrapolation, a comparison of error sources, and plots with representative density data are given in Supplemental Material [49], Secs. IV–VI and VIII, respectively.

We used 10,000 DQMC measurement sweeps for the data in Fig. 1 and 200,000 measurement sweeps for the data in Fig. 2. In each of the above cases, $M = 96$. For the data in Fig. 3, we used 200,000 measurement sweeps and varied M such that $t\Delta\tau \leq 1/24$. For each DQMC calculation, we used 5,000 warm-up sweeps before beginning measurements.

Results—The main results of this Letter are shown in Fig. 1. At $T = t/3$, we observe three distinct regions in the (U, μ) plane: a three-component Fermi liquid (FL) region, a trion liquid (TL) region, and an ordered CDW phase. In order to distinguish these phases and study the transitions between them, we will first consider the trion formation process. We measure the fraction of sites with each occupation number, which are given by

$$n^{(1)} = \frac{1}{2L^2} \sum_{((\sigma, \tau, \nu))} n_{i\sigma} (1 - n_{i\tau}) (1 - n_{i\nu}), \quad (2)$$

$$n^{(2)} = \frac{1}{2L^2} \sum_{((\sigma, \tau, \nu))} n_{i\sigma} n_{i\tau} (1 - n_{i\nu}), \quad (3)$$

$$n^{(3)} = \frac{1}{6L^2} \sum_{((\sigma, \tau, \nu))} n_{i\sigma} n_{i\tau} n_{i\nu}, \quad (4)$$

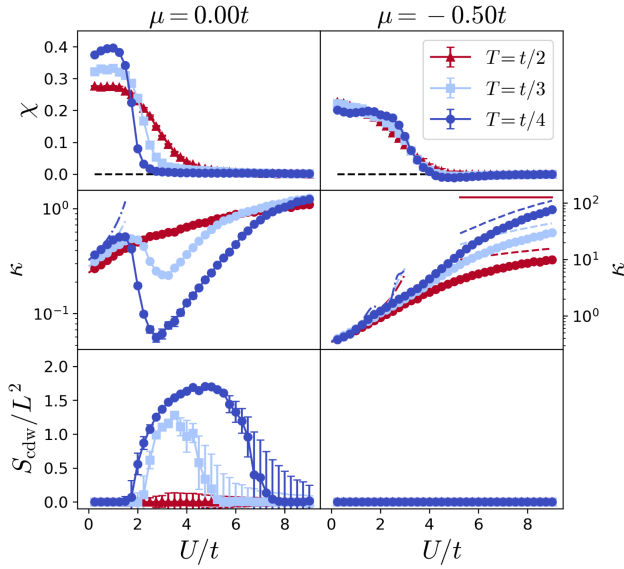


FIG. 2. Difference susceptibility, isothermal compressibility, and structure factor (finite-size extrapolation) as a function of U/t for three temperatures. Left: $\mu = 0$. Right: $\mu = -0.5t$. The dashed lines for large U in the κ plot indicate the classical ideal trion gas approximation, the dash-dotted lines on the low- U side show the weakly interacting mean field approximation, and the solid line shows the atomic limit κ at $T = t/2$. Error bars in the κ and χ plots show statistical error, while error bars in the S_{cdw} plot show the difference between the finite-size extrapolation and the $L = 10$ data.

where $((\sigma, \tau, \nu))$ indexes the permutations of the three-element set of molecular spin states.

In the large- U limit, we expect to be in the TL region, where trions have formed and move coherently. We use the difference susceptibility

$$\chi = \left(\frac{\partial \langle n_d \rangle}{\partial \mu} \right)_{T,L}, \quad (5)$$

where $n_d = n^{(2)} - n^{(1)}$, to detect this trion formation. Our choice of this parameter requires some explanation. In the large- U limit, trions are superpositions of the on site trion state—where molecules in each of the three spin states occupy a single site—and off site trion states—where one of the molecules in the trion occupies an adjacent site [30,38]. This virtual dissociation process persists even to zero temperature (as long as $t/U > 0$) and causes an effective repulsion between trions since the process is suppressed when trions are on adjacent sites. So, instead of using $\langle n^{(3)} \rangle$ directly to indicate composite particles, we consider $\langle n_d \rangle = \langle n^{(2)} - n^{(1)} \rangle$, which is the population difference between doubly and singly occupied sites. This quantity will approach zero in the TL and CDW regions since the only population of doubly and singly occupied sites is that which is part of an off site trion. However, at half filling, $\langle n_d \rangle = 0$ due to the particle-hole symmetry, not the presence of trions. So, we use χ as our indicator since it is also zero in the TL and CDW regions

while attaining a finite value throughout the FL region, even at half filling. A more detailed discussion of χ and a comparison with alternate trion detection methods [30,56] may be found in Supplemental Material [49], Sec. VII.

As shown in Figs. 1 and 2, χ attains a finite value when U is small but approaches zero as U increases, across a wide range of chemical potential values. This is consistent with our understanding of the TL region, as we expect trions to form at any finite density. As the temperature is lowered, the crossover becomes sharper, seeming to evolve into a QPT as $T \rightarrow 0$.

To understand the regions on each side of this transition, we consider the isothermal compressibility,

$$\kappa = \frac{1}{\langle n \rangle^2} \left(\frac{\partial \langle n \rangle}{\partial \mu} \right)_{T,L}. \quad (6)$$

As shown in Fig. 2, away from half filling, e.g., for $\mu = -0.5t$, κ monotonically increases with U . In the large- U regime, we expect our system to behave as a weakly interacting TL with an effective repulsion caused by the virtual dissociation process, which goes as t^2/U [57]. So, the numerical results qualitatively agree with this picture.

To better understand this behavior, we can compare κ to three limiting cases: a Hartree approximation for the weakly interacting Fermi liquid, which should be exact when $U/t = 0$, a classical ideal gas of trions, which is valid for strong U and temperatures well above t , and the single-site atomic limit, which should be valid for strong $U \gg t$ (see Supplemental Material [49], Secs. II. A, II. B, and II. C). We see that the Hartree approximation in Fig. 2 matches our data very well and that, while the classical ideal gas approximation is not perfect, it also qualitatively agrees with κ in the dilute case. In particular, our data are much closer to the classical ideal gas of trions approximation than the single-site atomic limit, which is shown for $T = t/2$ in Fig. 2. This provides evidence that the main contribution to the compressibility of the system is the motion of the trions, not the compressibility of the on site trions themselves.

At half filling ($\mu/t = 0$) and intermediate U/t , there is a drastic dip in κ , which seems to coincide with the trion formation QPT as indicated by χ . While this sort of compressibility minimum may be related to trion formation in similar models [58,59], the absence of this minimum away from half filling leads us to suspect that some other physics is relevant. At half filling, an obvious candidate would be CDW ordering caused by the effective repulsion from the virtual dissociation process. This should occur in some intermediate range of U/t since U/t must be large enough for trions to form, but the effective repulsion must also be strong enough to cause ordering. This density ordering can be detected using the structure factor,

$$S(\mathbf{q}) = \frac{1}{L^2} \sum_{i,j,\sigma,\tau} e^{-i\mathbf{q}(\mathbf{r}_i - \mathbf{r}_j)} \langle n_{i\sigma} n_{j\tau} \rangle. \quad (7)$$

We expect a two sublattice “checkerboard” order, so we measure the $\mathbf{q} = \mathbf{Q} \equiv (\pi, \pi)$ CDW structure factor, $S_{\text{cdw}} = S(\mathbf{Q})$, to use as an order parameter.

As shown Fig. 1, this ordering indeed appears in a region (blue) near half filling and at intermediate values of U . On the low- U side, trions are not able to form, so we do not expect ordering. On the other hand, as U increases, the virtual dissociation becomes too weak to cause the ordering. So the dip in κ near half filling occurs because the formation of the CDW order is inhibiting the density response. From the constant μ cuts shown in Fig. 2, we can see that this ordering only appears sufficiently close to half filling and at sufficiently low temperatures (it is absent for $\mu \leq -0.5t$ or $T \geq t/2$).

Based on the sharp behavior of S_{cdw} near the transition, we conclude that this CDW region is bounded by a finite-temperature phase transition. To obtain this sharp behavior, we use a finite-size extrapolation from S_{cdw}/L^2 measured on different lattice sizes (see Supplemental Material [49], Sec. V). We also use the invariant correlation ratio to pinpoint this transition more precisely (details in Refs. [60,61] and Supplemental Material [49], Sec. III). This method identifies a transition at both high and low U at half filling along with a critical μ/t value for $U = 3.5t$. This finite temperature phase transition contrasts with the $N = 2$ case, where this ordering only appears in the ground state at half filling and is not stable to finite T [62–64]. This is because the particle-hole symmetry is part of a continuous $\text{SU}(2)$ symmetry in the $N = 2$ case, so the Mermin-Wagner theorem forbids finite-temperature ordering in two dimensions [65]. However, in the $N = 3$ case at half filling, the particle-hole symmetry is a discrete $\mathbb{Z}_2$ symmetry, so the finite temperature ordering is allowed. Further details of this argument are presented in Supplemental Material [49], Sec. IX.

In order to further study the onset of CDW order and calculate a critical temperature T_c , we computed χ and S_{cdw} along with the kinetic and potential energy components of the heat capacity [66],

$$c_{\mathcal{O}} = \frac{1}{L^2} \left(\frac{\partial \mathcal{O}}{\partial T} \right)_{\mu, L}, \quad (8)$$

where $\mathcal{O}$ is K , V , or $K + V$. The results of these calculations at $U = 3.5t, \mu = 0$ are shown in Fig. 3.

Here, the total heat capacity shows two peaks—a narrow, tall peak that is almost entirely caused by the kinetic energy and a broader, shorter peak that has contributions from both components. The sharp kinetic energy peak coincides with the onset of CDW order, as shown by the behavior of S_{cdw} , and the critical temperature calculated by the invariant correlation ratio method. The behavior of $\chi(T)$ near this transition temperature also shows that the trions form at similar temperatures to the CDW ordering, suggesting that the virtual dissociation process plays a role in stabilizing the trions near half-filling.

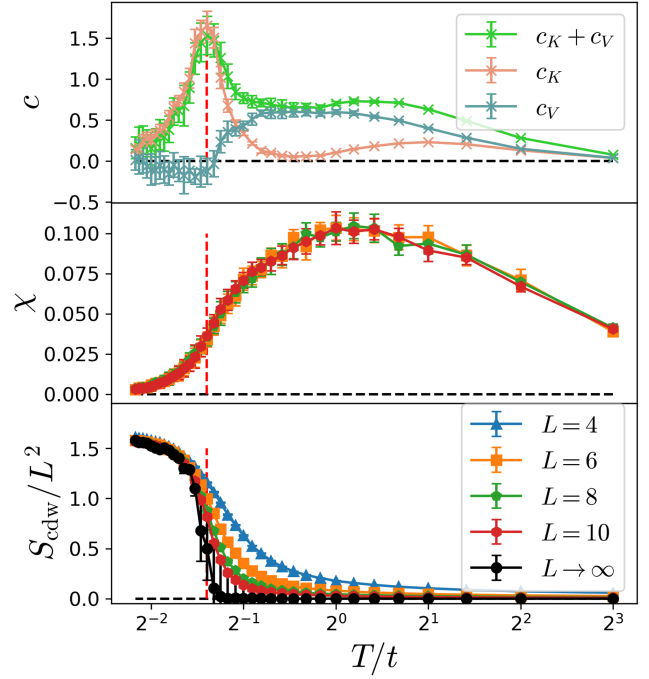


FIG. 3. Heat capacity, difference susceptibility, and structure factor (finite-size extrapolation) as a function of T/t at $U = 3.5$, $\mu = 0$. The red dashed lines show the phase transition temperature $T_c = 0.38t$ as determined by the invariant correlation ratio method. Error bars in the c and χ plots and $L = 4, 6, 8, 10$ S_{cdw}/L^2 data show statistical error, while error bars for the $L \rightarrow \infty$ S_{cdw} plot show the difference between the finite-size extrapolation and $L = 10$ data.

Discussion and conclusion—We have calculated properties of the $\text{SU}(3)$ attractive FHM on a two-dimensional square lattice using the DQMC method. We observed a finite-temperature CDW phase, as well as a FL-TL crossover at finite temperature, which sharpens to a QPT at zero temperature. These finite temperature results on a square lattice complement previous mean field [4,5], dynamical mean field theory [29,39,57], and self-energy functional [67,68] studies along with quantum Monte Carlo results on a two-dimensional honeycomb lattice, restricted to half filling [30,69,70].

The QPT indicated by the FL-TL crossover occurs across a wide range of μ away from half-filling and appears to occur at a finite $U_c > 0$. This description is qualitatively similar to what we expect from the CSF to trion QPT for this model in higher dimensions, which has a critical $U_c > 0$ [29,39]. On the other hand, $U_c = 0$ for this model in one dimension [31–33], where CSF order only appears in the ground state in the presence of $\text{SU}(3)$ -breaking interaction terms [71]. So, whether $U_c > 0$ in two dimensions is an open question. We believe signatures of potential CSF order would be detectable in finite- T DQMC calculations. For a useful comparison, we consider the attractive $\text{SU}(2)$ FHM on a square lattice. While quasi-long-range superconducting order has been seen at finite temperature in the attractive $\text{SU}(2)$ FHM on a two-dimensional square lattice [63,64] and

bilayer square lattice [72,73], it is separated from the normal phase by a Kosterlitz-Thouless transition [74]. If a similar situation occurs for the attractive SU(3) case, we may be able to detect CSF order off half filling (where the transition temperature may be finite [62]) and compare this transition to the FL-TL crossover [67,68].

Our results also complement previous results predicting the existence of CDW order at $T = 0$ [4,57]. As noted before, in the SU(2) case this phase is not stable at finite temperatures. So, our observation of both FL-CDW and TL-CDW finite-temperature phase transitions suggests that this CDW phase is stable at finite temperature and opens up a number of questions around how this phase interacts with the trion formation crossover. Further studies into differences between the FL-CDW and TL-CDW transitions may lead to insights into the underlying physics, similarly to the different mechanisms that drive antiferromagnetism in the repulsive SU(2) FHM [75–79]. It is also not clear from our results what range the CDW order occupies in the ground state phase diagram. One-loop RG methods predict that the ground state has long-range CDW order even for infinitesimal values of U in two dimensions [4], so we might expect CDW order at all values of U at a low enough temperature and half filling. In all of these questions—whether the CSF phase exists in two dimensions, whether $U_c > 0$ for the FL-TL QPT, and what behavior of U_c is for the CDW transition near $T = 0$ —DQMC calculations performed at lower temperatures will be valuable for making progress.

Finally, we consider the experimental viability of observing these phases in an ultracold molecule optical lattice experiment. The double microwave shielding technique [80], which was used to suppress loss processes in the first dipolar BEC [43], is believed to eliminate three-body loss in the form of three-body recombination processes so that only the two-body loss rate is relevant. Considering only two-body loss processes and working in a strong optical lattice limit—where we use the ground state simple harmonic oscillator as our Wannier function—we compute that for NaCs with s -wave scattering length $a_s \approx 10^3 a_0$, where a_0 is the Bohr radius, and two-body loss coefficient $L_{2B} \approx 3 \times 10^{-13} \text{ cm}^3/\text{s}$ (as reported in [43]), $\hbar/U\tau_{\text{loss}} \approx 10^3$. The loss timescale is much longer than the timescale of the dynamics of our attractive SU(3) FHM, implying double microwave shielding will suppress loss rates enough to reasonably simulate the attractive SU(3) FHM.

To measure signatures of the various phases discussed in this Letter, we propose using quantum gas microscopy (QGM). QGM measures site-resolved snapshots of molecule locations, allowing for experimental access to $\langle n^{(1)} \rangle$, $\langle n^{(2)} \rangle$, $\langle n^{(3)} \rangle$ and S_{cdw}/L^2 . These measurements can be directly compared to DQMC results for thermometry and consistency checks [81–83]. This technique has already been used to study the dynamics of interacting dipolar systems using ultracold molecules in an optical lattice [84]. So, the recent development of microwave

shielding for dipolar molecules should allow for flexible quantum simulation of a class of SU(N) lattice models previously not experimentally accessible. Continued theoretical investigation along with further experimental developments may yield exotic new phases and understanding of composite particles in many-body systems.

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Data availability—The data that support the findings of this article are openly available [85].

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