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Physical limitations of the Hohenberg–Mermin–Wagner theorem

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Abstract

The Hohenberg–Mermin–Wagner (HMW) theorem states that infrared (IR) fluctuations prevent long-range order which breaks continuous symmetries in two dimensions (2D), at finite temperatures. We note that the theorem becomes physically effective for superconductivity (SC) only for astronomical sample sizes, so it does not prevent 2D SC in practice. We systematically explore the sensitivity of the magnetic and SC versions of the theorem to finite-size and disorder effects. For magnetism, finite-size effects, disorder, and perpendicular coupling can all restore the order parameter at a non-negligible value of T_c equally well, making the physical reason for finite T_c sample-dependent. For SC, an alternative version of the HMW theorem is presented, in which the temperature cutoff is set by Cooper pairing, in place of the Fermi energy in the standard version. It still allows 2D SC at 2–3 times the room temperature when the interaction scale is large and Cooper pairs are small, the case with high-T_c SC in the cuprates. Thus IR fluctuations do not prevent 2D SC at room temperatures in samples of any reasonable size, by any known version of the HMW argument. A possible approach to derive mechanism-dependent upper bounds for SC T_c is pointed out.

Keywords: Mermin–Wagner theorem, infrared fluctuations, 2D systems, superconductivity, disorder, finite-size effects

1. Introduction

The Hohenberg–Mermin–Wagner (HMW) theorem [1, 2] is probably the best-known mathematically exact result in the theory of phase transitions. It forbids ordered phases which break continuous symmetries in less than three dimensions, by showing that they are destabilized by

infrared (IR) fluctuations. The formal prerequisite for the argument is due to Bogoliubov [3]: because the static susceptibility of a many-body system can be written as a scalar product in a certain operator vector space, the Cauchy–Schwartz inequality in that space yields rigorous inequalities for the static response functions of arbitrary operators. With well-chosen probes and a summation over momenta [1, 4], the theorem follows.

Despite its wide dissemination in textbooks and the research literature [4–8], we have been able to find only one comment, in unpublished lecture notes by Leggett [9], on the actual numbers appearing when the theoretical bound is evaluated: a 2D sample would have to 'extend from here to the Moon' for HMW effects to be observed at temperatures of a few Kelvin. For superconductivity (SC), the reason is easy to spot. In the formalism, the energy cost of the IR fluctuations suppressing T_c is not set by the SC mechanism, as one might imagine, but by the much larger Fermi energy. Because the HMW suppression is only logarithmic in the size of the sample in 2D, it cannot preclude 2D SC in reasonably-sized samples even at twice the room temperature.

Two-dimensional SC is of considerable practical interest since the discovery of high-T_c SC in cuprates [10]. These are strongly anisotropic materials with ionic layers between 2D metallic planes. Later, 2D heterostructures were fabricated in which a *single* plane was superconducting without any suppression of T_c [11, 12]. Similarly, SC thin films of FeSe were found to super-conduct at $\sim$70 K [13, 14]. In these cases, one could still harbor the suspicion that the insulator adjacent to the active layer somehow helped to stabilize SC. Most recently, such reservations became implausible by the observation of undiminished SC at $\sim$100 K in exfoliated BSCCO [15].

Concerning the magnetic version of the HMW theorem, a number of authors have discussed difficulties in observing suppression of magnetism in 2D in concrete settings, both experimentally [16, 17] and numerically [18]. One way to put these issues on a physical footing is to use disorder to recover the order parameter in 2D in a controllable manner [18–22]. Such disorder-induced order is expected because the HMW theorem assumes an exact continuous symmetry of the Hamiltonian, which is manifestly broken by a random field. The surprise in practice was the fragility of the HMW result: even a small amount of disorder recovered the ordered state. However, the exact formal argument [22] for such random-field-induced order (RFIO) was specialized to the classical random-field XY model, leaving the general case to be inferred.

In this work, we first analyze the HMW theorem for the XXZ model with disorder, establishing a generic rationale for the above-mentioned observations for magnetism. Our investigation of possible ways to gap the IR fluctuations, required by the magnetic HMW mechanism, does not prejudice other mechanisms. In particular, the so-called Imry–Ma argument [23] may (or may not [22, 24, 25]) be relevant in a given physical situation. Next, we show why the original HMW formulation for SC is robustly independent of model details, as long as the interaction is local, or almost local, in real space. This observation encompasses all variations of the HMW theorem proven separately over the years [7, 8, 26–30]. After that, we present a new variation of the HMW argument which probes the interaction scale, instead of the Fermi energy. It is valid in any dimension, and independent of the size of the sample. Rough evaluation in 2D gives upper limits of T_c on the high end, comparable to the finite-size HMW bound, when Cooper pairs are small. The approach is based on the amplitude of the order parameter, which is qualitatively different from the reduction $k_B T_c < E_F/8$ of the infinite-size HMW bound, obtained by considering phase stiffness [31]. Finally, we point out a possible way forward, to derive mechanism- and material-dependent upper bounds for the SC T_c by refining the present reasoning.

2. Finite-size and disorder effects

2.1. Finite-size effects in the XXZ model

Let us consider a system of localized spins described by the XXZ model:

$$\mathcal{H} = -\sum_{ij} J_{ij} \left(S_i^x S_j^x + S_i^y S_j^y \right) - \sum_{ij} J_{ij}^z S_i^z S_j^z - B\,V M_x, \tag{1}$$

where B is the external symmetry-breaking field and $M_x = V^{-1} \sum_i \mathrm{e}^{-\mathrm{i} \boldsymbol{K} \cdot \boldsymbol{R}_i} S_i^x$ the staggered magnetization. The Bogoliubov inequality, in the form first used by Mermin and Wagner [2], is

$$|\langle [A, Q] \rangle|^2 \leqslant \frac{1}{2} \beta \left\langle \{A, A^\dagger\} \right\rangle \left\langle [[Q, \mathcal{H}], Q^\dagger] \right\rangle, \tag{2}$$

where braces are anticommutators, β is the inverse temperature, and Q and A are arbitrary operators. To probe IR fluctuations of some broken symmetry, Q is chosen to be a modulation of its generator and A is tuned so that $\langle [A, Q] \rangle$ gives the corresponding order parameter. For the XXZ model, the appropriate choices are $Q_{\boldsymbol{k}} = \sum_i \mathrm{e}^{-\mathrm{i} \boldsymbol{k} \cdot \boldsymbol{R}_i} S_i^z$ and $A_{\boldsymbol{k}, \boldsymbol{K}} = V^{-1} \sum_i \mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{K}) \cdot \boldsymbol{R}_i} S_i^y$ which yield $[A_{\boldsymbol{k}, \boldsymbol{K}}, Q_{\boldsymbol{k}}] = \mathrm{i} M_x$.

To obtain a useful bound on $\langle M_x \rangle_B$ from (2), one has to divide it by $\left\langle [[Q, \mathcal{H}], Q^\dagger] \right\rangle$ and sum over momenta $\boldsymbol{k}$ in the first Brillouin zone. In that way, the orthogonality of the $\mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{K}) \cdot \boldsymbol{R}_i}$ factors from $A_{\boldsymbol{k}, \boldsymbol{K}}$ ensures the *intensive* bound $\sum_{\boldsymbol{k} \in \mathrm{BZ}} \langle \{A_{\boldsymbol{k}, \boldsymbol{K}}, A_{\boldsymbol{k}, \boldsymbol{K}}^\dagger\} \rangle_B \leqslant 2n^2 S^2$, where $n = \mathcal{N}/V$ is the concentration and $\mathcal{N}$ the number of unit cells. That $Q_{\boldsymbol{k}}$ is a generator of symmetry implies that $\left[[Q_{\boldsymbol{k}}, \mathcal{H}], Q_{\boldsymbol{k}}^\dagger \right] \propto \boldsymbol{k}^2$, and indeed a rigorous bound $V^{-1} \langle [[Q_{\boldsymbol{k}}, \mathcal{H}], Q_{\boldsymbol{k}}^\dagger] \rangle_B \leqslant nJ(\boldsymbol{k}^2/k_{\mathrm{BZ}}^2) + |B \langle M_x \rangle_B|$ can be derived in which k_{BZ} is the effective radius of the first Brillouin zone and $J = \frac{S(S+1)}{\mathcal{N}} \sum_{ij} k_{\mathrm{BZ}}^2 (\boldsymbol{R}_i - \boldsymbol{R}_j)^2 |J_{ij}|$ the effective spin–spin coupling constant. Thus we obtain the HMW inequality [2]

$$|\langle M_x \rangle_B|^2 \leqslant \frac{\beta n S^2}{\frac{1}{\mathcal{N}} \sum_{\boldsymbol{k} \in \mathrm{BZ}} \frac{1}{nJ(\boldsymbol{k}^2/k_{\mathrm{BZ}}^2) + |B \langle M_x \rangle_B|}}. \tag{3}$$

By taking the thermodynamic limit $V \to \infty$, the sum in the denominator diverges in the limit $B \to 0$ in 1D and 2D, forbidding a finite value of the magnetization $\langle M_x \rangle_0$ that is within the *XY* plane of symmetry.

Although the use of periodic boundary conditions apparently limits the above argument to very large systems, finite, and even fractal [32], lattices can be treated with minimal technical modification. One simply introduces a basis $\varphi_{\boldsymbol{k}}(\boldsymbol{R}_i)$ in $A_{\boldsymbol{k}, \boldsymbol{K}}$ and $C_{\boldsymbol{k}}$ which is not a plane wave, but tuned to the lattice [32]. The key formal properties of $\varphi_{\boldsymbol{k}}(\boldsymbol{R}_i)$ needed in the above argument are that $\varphi_{\boldsymbol{k}}(\boldsymbol{R}_i) \to 1$ as $\boldsymbol{k} \to \boldsymbol{0}$, and that the density of the discrete wave-vectors $\boldsymbol{k}$ near $\boldsymbol{0}$ grows sufficiently fast in the thermodynamic limit. Thus equation (3) still holds, with an appropriate understanding of $\sum_{\boldsymbol{k} \in \mathrm{BZ}}$ and k_{BZ}, and the only physical effect of finiteness on the HMW arguments is the appearance of an IR cutoff, namely $k_{\min} = k_{\mathrm{BZ}}/\sqrt{\mathcal{N}}$ in 2D. The sum in the denominator can then be replaced with an integral for finite 2D samples as well,

$$\frac{1}{\mathcal{N}} \sum_{\boldsymbol{k}} \to \frac{1}{\mathcal{N}}\Big|_{\boldsymbol{k}=\boldsymbol{0}} + \frac{2}{k_{\mathrm{BZ}}^2} \int_{k_{\min}}^{k_{\max}} dk\, k, \tag{4}$$

turning equation (3) into an inequality with $|\langle M_x \rangle_B|$ on both sides. This inequality is equivalent to $|\langle M_x \rangle_B| \leqslant M_{\max}$, where $M_{\max}$ is determined by a transcendental equation which can be

solved in the limit $B \to 0$, giving:

$$M_{\text{max}}^2 \approx \frac{2\beta J}{\ln(\mathcal{N}/2) + \ln(\beta J)} \cdot M_{\text{sat}}^2. \tag{5}$$

In 1D, the corresponding $B \to 0$ solution is given by

$$M_{\text{max}}^3 \approx \frac{4\beta J}{\pi^2 \sqrt{\mathcal{N}}} \cdot M_{\text{sat}}^3, \tag{6}$$

where $M_{\text{sat}} = nS$ is the saturation magnetization. In the derivation of the above, let us only note that one needs to use a finite, but physically infinitesimal, value of B to probe symmetry breaking. Technically, we have used $B = \sqrt{\mathcal{N}} \cdot (k_B T / V M_{\text{sat}})$ so that $\mathcal{N}J \gg V B M_{\text{sat}} \gg k_B T$. Clearly, finite-size effects do not affect the HMW outcome in 1D, because $\sqrt{\mathcal{N}} \sim 10^4$ is still a very large number for macroscopic $\mathcal{N} \sim N_A^{1/3}$. In 2D, however, finite size affects the HMW outcome qualitatively, because $\ln N_A^{2/3} \approx 37$, effectively replacing the IR divergence with an order-of-magnitude reduction. Given that magnetic critical temperatures are typically a few 100 Kelvins in transition-metal compounds, in 2D the HMW argument only predicts a marked suppression of magnetic order, far from vanishing.

2.2. Disorder in the XXZ model

When any perturbation δH is added to the XXZ Hamiltonian (1), the original denominator in equation (3) becomes

$$\frac{1}{\mathcal{N}} \sum_{\boldsymbol{k} \in \text{BZ}} \frac{1}{(nJ\boldsymbol{k}^2/k_{\text{BZ}}^2) + \Delta_B(\boldsymbol{k}) + |B < M_x >_{B,\delta H}|}, \tag{7}$$

where $\Delta_B(\boldsymbol{k}) = V^{-1} |\langle [[Q_{\boldsymbol{k}}, \delta H], Q_{\boldsymbol{k}}^\dagger] \rangle_{B,\delta H}|$ and the index δH indicates thermal averaging in the presence of δH. Thus, formally, any perturbation that breaks the continuous symmetry of the magnetization, generated by $Q_{\boldsymbol{0}}$, gives a finite $\Delta_B(\boldsymbol{0}) \neq 0$, which cuts off the $\boldsymbol{k}^2$ term, invalidating the HMW theorem.

Physically, let us consider the site-disorder model

$$\delta H = -\sum_i \boldsymbol{h}_i \cdot \boldsymbol{S}_i, \tag{8}$$

where $\boldsymbol{h}_i$ is a random local field. For definiteness, its planar component is considered to lie on a circle, $|\boldsymbol{h}_{i\|}| = const.$, placing the model in the RFIO limit [22]. The crossover to the Imry–Ma limit [23] by widening the amplitude distribution is beyond the scope of this article. In the present case, $\Delta_B = V^{-1} |< \delta H_\| >_{B,\delta}|$, where $\delta H_\|$ includes planar components of the $\boldsymbol{h}_i$ only, and δ indicates disorder-averaging. The salient observation is that the disorder effectively competes with the *interaction* scale J in cutting off the IR divergence:

$$|\langle\!\langle M_x \rangle\!\rangle|^2 \leqslant \frac{\beta J}{\ln(1 + nJ/\Delta_0)} \cdot M_{\text{sat}}^2 \tag{9}$$

in 2D, and

$$|\langle\!\langle M_x \rangle\!\rangle|^2 \leqslant \frac{2}{\pi} \sqrt{\frac{\Delta_0}{nJ}} \cdot \beta J \cdot M_{\text{sat}}^2 \tag{10}$$

in 1D. The double angular brackets denote the Bogoliubov quasi-average $\langle\!\langle M \rangle\!\rangle = \lim_{B \to 0} \lim_{V \to \infty} \langle M \rangle_B$. A similar pattern is observed as with finite-size effects, with the role of the size of the system taken over by the ratio between the magnetic coupling and the disorder scale. This ratio is evidently much smaller than Avogadro's number, so it is easy to imagine a 2D system with a small amount of disorder, say $nJ/\Delta_0 \sim 100$, for which IR fluctuations suppress T_c by less than an order of magnitude below J.

The competition between disorder and finite-size effects appears in equation (7), before the integration which introduces dimensionality. Disorder cuts off the quadratic term, meaning that dirty samples can be larger and still avoid the asymptotic HMW regime, irrespective of dimension. In the context of simulations, this result is a model-independent validation of the observation that weak disorder, or even numerical error, efficiently stabilizes the order parameter in 2D.

In a layered system, the order parameter can also be restored by a weak interlayer coupling $J_\perp \ll J$, for which the denominator in equation (9) similarly reads $\ln(1 + J/J_\perp)$. Suppression of the isotropic 3D T_c by weak interlayer coupling competes with the 2D disorder effect on an equal footing, because the ratio $J/J_\perp$ can easily be both greater and smaller than nJ/Δ_0.

Because the competition between mechanisms occurs in the denominator of the sum (7), which is itself in the denominator of equation (3), the *largest* scale ends in the numerator. Suppose, for illustration, that two mechanisms are at work in the same sample, one of which would limit $kT_c < \Delta_1$, and the other $kT_c < \Delta_2$, if acting alone. The two acting together have the net effect

$$kT_c < \max(\Delta_1, \Delta_2), \tag{11}$$

because the larger scale gaps the other. This result runs contrary to the naive impression that the 'stricter' criterion should be applied.

3. Superconductivity

3.1. Interaction in real space

We consider a layered two-dimensional system with localized impurities, electron–electron, and electron–phonon interactions, whose Hamiltonian is

$$\mathcal{H} = H_0 + V_{\text{int}}. \tag{12}$$

The non-interacting part is

$$H_0 = \sum_{k\sigma} \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\varrho\sigma_1\sigma_2} \varepsilon_{\varrho\sigma_1\sigma_2} f_{\varrho\sigma_1}^\dagger f_{\varrho\sigma_2} + \sum_{k\lambda} \hbar\omega_{k\lambda} b_{k\lambda}^\dagger b_{k\lambda}, \tag{13}$$

where the three terms refer respectively to mobile carriers, impurities at fixed arbitrary positions ϱ, and phonons. V_{int} contains all possible hybridizations and interactions among them, subject to the limitation that they are local in real space and time, i.e. admit the usual fermion continuity equation. From the microscopic point of view, this limitation is quite mild, because all bare interactions considered in standard many-body theory are local in this sense.

3.1.1. The HMW argument. The operators to be used in Bogoliubov's inequality (2) are:

$$Q_k = \sum_{R\sigma} e^{-i k \cdot R} c_{R\sigma}^\dagger c_{R\sigma} + \sum_{\varrho\sigma} e^{-i k \cdot \varrho} f_{\varrho\sigma}^\dagger f_{\varrho\sigma}, \tag{14}$$

$$A_{k,r} = \mathcal{N}^{-1} \sum_R e^{i k \cdot R} c_{R\sigma_1} c_{R+r\sigma_2}, \tag{15}$$

where $\mathcal{N}$ is the number of unit cells within the 2D layers, while σ_1, σ_2, and r are fixed and arbitrary. Clearly, Q_k is a modulation of the number operator, while the commutator of A_k with Q_k produces the microscopic gap operator

$$[A_{k-K,r}, Q_k] = (1 + e^{-i k \cdot r}) \Delta_{\sigma_1\sigma_2}^K(r). \tag{16}$$

The operator $\Delta_{\sigma_1\sigma_2}^K(r)$ can be summed over K, r, σ_1, and σ_2 to obtain every possible (singlet, triplet, s, p, $d_{x^2-y^2}$, pair momentum K, etc) superconducting gap operator Δ, thus generalizing previous results [8, 26–30]. Summing Bogoliubov's inequality (2) over k, one obtains the SC analogue of equation (3):

$$\left| \left\langle \Delta_{\sigma_1\sigma_2}^K(r) \right\rangle_\kappa \right|^2 \leqslant \frac{\ell\,\beta}{\frac{2}{\mathcal{N}} \sum_k \frac{|1+e^{i k \cdot r}|^2}{(\epsilon_{\mathrm{IR}} k^2 / k_{\mathrm{BZ}}^2) + |\kappa| \mathcal{D}_\kappa}}, \tag{17}$$

where ℓ is the number of layers, κ is the symmetry-breaking field conjugate to Δ, same as B in equation (3), and $\mathcal{D}_\kappa$ is a corresponding expectation value of Δ. The infrared energy scale ϵ_{IR} is determined by the bound $(\mathcal{N}\ell)^{-1} |\langle [[Q_k, \mathcal{H}], Q_k^\dagger] \rangle| \leqslant \epsilon_{\mathrm{IR}} k^2 / k_{\mathrm{BZ}}^2$. It is a sum of two positive terms: one due to particle dispersions and another from hybridization with impurities. The particle-dispersion term is always finite, while the impurity hybridization $V_{\sigma_1\sigma_2}^{\varrho R}(f_{\varrho\sigma_1}^\dagger c_{R\sigma_2} + $ c.c.) must fall off sufficiently rapidly, $\mathcal{N}^{-1} \sum_{\varrho, R} |\varrho - R|^2 \left| V_{\sigma_1\sigma_2}^{\varrho R} \right| < \infty$, for the impurity term to be finite. The electron–electron and electron–phonon interactions drop out in $[Q, \mathcal{H}]$ because they are local in space. Because $|1 + e^{i k \cdot r}|^2 \neq 0$ at $k = 0$, the IR divergence is unchecked in 1D and 2D when $\kappa \to 0$, so the HMW theorem follows.

3.1.2. Physical considerations. Technically, hopping terms and couplings to them are non-local, but even such interactions do not invalidate the above conclusion. They are merely subject to the same caution as impurity hybridization, namely that their range falls off fast enough. Hence the HMW theorem in its original formulation is quite robust with respect to model variations. To ascertain how physically relevant it is, we rewrite the bound (17) in a more intuitive form:

$$\left| \left\langle \Delta_{\sigma_1\sigma_2}^K(r) \right\rangle_\kappa \right| \leqslant \sqrt{\frac{T_{\mathrm{HMW}}}{T}} \cdot 1, \tag{18}$$

where T_{HMW} is the HMW temperature and 1 is the saturation value of $\left\langle \Delta_{\sigma_1\sigma_2}^K(r) \right\rangle$. Specializing to 2D, assuming a parabolic dispersion, and taking some care with numerical factors, one finds $k_B T_{\mathrm{HMW}} \approx (\ell/4)(\hbar^2 k_{\mathrm{BZ}}^2 / 2 m_*) \langle n \rangle / \ln(k_{\mathrm{BZ}} L)$, where $\langle n \rangle = \langle N \rangle / (\mathcal{N}\ell)$ is the total number of carriers per unit cell and L is the linear size of the sample. Therefore, the HMW bound is physically relevant only for temperatures $T > T_{\mathrm{HMW}}$, when enough IR modes are excited to suppress the SC order. The conclusion, which applies to all previous HMW arguments concerning SC [1, 7, 8, 26–30] as well, is that in 2D

$$T_c < 4 T_{\mathrm{HMW}} = \ell \cdot T_F / \ln(k_{\mathrm{BZ}} L), \tag{19}$$

where T_F is the Fermi temperature. Inserting $T_F \sim 10^4$ K, $k_{BZ} \sim \text{Å}^{-1}$, and $L \sim 1$ cm, one finds the bound to be in the ~ 500 K range, which is comparable to the bound $k_B T_c < E_F/8$, obtained by considering phase stiffness in an infinite system [31].

The true significance of the finite-size effect becomes evident in the converse exercise: $k_{BZ} L < \exp(T_F/T_c)$. One would need $L \sim 10^{33}$ m, much larger than the observable Universe ($\sim 10^{27}$ m), for T_c in a single layer to be forced below ~ 100 K, the value observed in optimally doped cuprates.

3.2. Interaction in momentum space

The critical junction in the above derivation is that the commutator $[Q_k, V_{int}]$ vanishes, because interactions are local and therefore commute with the local number operators appearing in Q_k (14). The f-sum rule $(\mathcal{N}\ell)^{-1} \left\langle [[Q_k, \mathcal{H}], Q_k^\dagger] \right\rangle \lesssim \epsilon_{IR} k^2/k_{BZ}^2$ follows, which is physically the statement that boosting the electrons by $\hbar k$ results in a second-order-in-k energy increase of the form $\ell \mathcal{N} \epsilon_{IR} k^2/k_{BZ}^2$. As a quick way to derive this quadratic dependence, write $\hat{Q}_k = \hat{N} - i k \cdot \hat{X} + \mathcal{O}(k^2)$, where $\hat{N} = \hat{Q}_0 = \sum_R \hat{n}_R$ and $\hat{X} = \sum_R R \hat{n}_R$. The double commutator is immediately

$$[[Q_k, \mathcal{H}], Q_k^\dagger] = [[k \cdot \hat{X}, \mathcal{H}], k \cdot \hat{X}] + \mathcal{O}(k^3), \tag{20}$$

because $[\hat{N}, \mathcal{H}] = 0$ of course follows from local number-conservation. Therefore, the HMW argument is model-independent, as long as the interactions, or disorder, conserve the particle number locally, and boosting the electrons of the system increases the energy by an extensive amount. All later proofs thus necessarily reproduce its physically most counter-intuitive aspect, that one probes high-energy IR fluctuations of the non-interacting Fermi sea, instead of the superconducting mechanism.

Having understood that, we develop an alternative argument which probes fluctuations associated with Cooper pairing, as expressed in the reduced BCS Hamiltonian:

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{1}{\mathcal{N}} \sum_{k_1 k_2} V_{k_1 k_2} c_{k_1\uparrow}^\dagger c_{-k_1\downarrow}^\dagger c_{-k_2\downarrow} c_{k_2\uparrow}. \tag{21}$$

The reduced BCS Hamiltonian breaks the standard HMW argument because the interaction is non-local in real space, violating local continuity. It causes ϵ_{IR} in equation (17) to diverge with $(k_{BZ} L)^2$ in the thermodynamic limit, as typical for long-range interactions. In the remainder of this section, we adapt the technical steps of the original argument to the BCS pair interaction, leaving the physical discussion to the end.

The operator Q is constructed to commute with the kinetic energy now, and A adjusted so that $[A, Q]$ gives the gap operator as before:

$$Q_R = \sum_k e^{i k \cdot R} \left(c_{k\uparrow}^\dagger c_{k\uparrow} + c_{-k\downarrow}^\dagger c_{-k\downarrow} \right), \tag{22}$$

$$A_{R,K} = \mathcal{N}^{-1} \sum_k e^{-i k \cdot R} S_K(k) c_{k+K\uparrow} c_{-k\downarrow}, \tag{23}$$

$$[A_{R,K}, Q_R] = (1 + e^{i K \cdot R}) \Delta_K, \tag{24}$$

where $S_K(k)$ is a Cooper-pair structure factor which allows a finite pair momentum K for the sake of generality.

The analogue of equations (3) and (17) reads, in any dimension,

$$
|\langle \Delta_{\boldsymbol{K}} \rangle_{\kappa}|^2 \leqslant I_{\boldsymbol{K}} \cdot \beta \left\{ \frac{1}{\mathcal{N}} \sum_{\boldsymbol{R}} \frac{\left|1 + \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{R}}\right|^2}{\mathcal{V}_{\kappa}(\boldsymbol{R}) + |\kappa|\,\mathcal{D}_{\kappa}} \right\}^{-1}, \tag{25}
$$

where $I_{\boldsymbol{K}} = \mathcal{N}^{-1}\sum_{\boldsymbol{k}}|S_{\boldsymbol{K}}(\boldsymbol{k})|^2$ is a kinematic factor. In contrast to small values of $\boldsymbol{k}$ in the HMW argument, there is nothing special about small $\boldsymbol{R}$ here, so the total sum does not diverge in the thermodynamic limit in any dimension. Thus, equation (25) does not constrain the order parameter to vanish. Nevertheless, the upper bound for T_{c} it provides is sharper than in the original formulation for samples of reasonable size when the Cooper pairs are small, as we show below.

The term $\mathcal{V}_{\kappa}(\boldsymbol{R})$ is an average of the interaction operator,

$$
\mathcal{V}_{\kappa}(\boldsymbol{R}) = \frac{8}{\mathcal{N}^2} \sum_{\boldsymbol{k}_1\boldsymbol{k}_2} \sin^2\left[(\boldsymbol{k}_1 - \boldsymbol{k}_2)\cdot\boldsymbol{R}/2\right]\,|V_{\boldsymbol{k}_1\boldsymbol{k}_2}|\,\langle c^{\dagger}_{\boldsymbol{k}_1\uparrow}c^{\dagger}_{-\boldsymbol{k}_1\downarrow}c_{-\boldsymbol{k}_2\downarrow}c_{\boldsymbol{k}_2\uparrow}\rangle_{\kappa}, \tag{26}
$$

while $\mathcal{D}_{\kappa}$ averages the order parameter like in equation (17). A more transparent form is obtained after taking an angular average of $\left|1 + \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{R}}\right|^2$ in 2D and 3D,

$$
|\langle\!\langle \Delta_{\boldsymbol{K}} \rangle\!\rangle| \leqslant \sqrt{\frac{T_{\mathrm{pair}}}{T}} \cdot \Delta^{\boldsymbol{K}}_{\mathrm{sat}}, \tag{27}
$$

where $\Delta^{\boldsymbol{K}}_{\mathrm{sat}} = \left|\mathcal{N}^{-1}\sum_{\boldsymbol{k}}S_{\boldsymbol{K}}(\boldsymbol{k})\langle c_{\boldsymbol{k}+\boldsymbol{K}\uparrow}c_{-\boldsymbol{k}\downarrow}\rangle_{T=0}\right|$ is the saturation value of the order parameter at $T = 0$, while T_{pair} is the upper bound temperature

$$
k_{\mathrm{B}}T_{\mathrm{pair}} = \frac{I_{\boldsymbol{K}}}{(\Delta^{\boldsymbol{K}}_{\mathrm{sat}})^2} \cdot \frac{8}{\mathcal{N}^2} \sum_{\boldsymbol{k}_1\boldsymbol{k}_2}|V_{\boldsymbol{k}_1\boldsymbol{k}_2}|\,\langle c^{\dagger}_{\boldsymbol{k}_1\uparrow}c^{\dagger}_{-\boldsymbol{k}_1\downarrow}c_{-\boldsymbol{k}_2\downarrow}c_{\boldsymbol{k}_2\uparrow}\rangle. \tag{28}
$$

In the thermodynamic limit, both $\mathcal{V}_{\kappa}(\boldsymbol{R})$ and $k_{\mathrm{B}}T_{\mathrm{pair}}$ tend to *intensive* constants. Thus the upper bound (27) is independent of the size of the sample. For more general interactions, the above is easily generalized to

$$
k_{\mathrm{B}}T_{\mathrm{pair}} = \frac{I_{\boldsymbol{K}}}{(\Delta^{\boldsymbol{K}}_{\mathrm{sat}})^2} \cdot \frac{8}{\mathcal{N}^2} \sum_{\boldsymbol{q}\boldsymbol{k}_1\boldsymbol{k}_2\sigma_1\sigma_2}|V_{\boldsymbol{q}}|\,\langle c^{\dagger}_{\boldsymbol{k}_1+\boldsymbol{q}\sigma_1}c^{\dagger}_{\boldsymbol{k}_2-\boldsymbol{q}\sigma_2}c_{\boldsymbol{k}_2\sigma_2}c_{\boldsymbol{k}_1\sigma_1}\rangle. \tag{29}
$$

3.2.1. Evaluation of the upper bound temperature. First, we estimate the ratio

$$
\frac{I_{\boldsymbol{K}}}{(\Delta^{\boldsymbol{K}}_{\mathrm{sat}})^2} = \frac{\mathcal{N}^{-1}\sum_{\boldsymbol{k}}|S_{\boldsymbol{K}}(\boldsymbol{k})|^2}{\left|\mathcal{N}^{-1}\sum_{\boldsymbol{k}}S_{\boldsymbol{K}}(\boldsymbol{k})\langle c_{\boldsymbol{k}+\boldsymbol{K}\uparrow}c_{-\boldsymbol{k}\downarrow}\rangle_{T=0}\right|^2}. \tag{30}
$$

It is reasonable to set the Cooper-scattering structure factor $S_{\boldsymbol{K}}$ to zero outside a shell of thickness δk_{gap} on the surface of the Fermi sphere, leading to

$$
\frac{I^{\boldsymbol{K}}}{(\Delta^{\boldsymbol{K}}_{\mathrm{sat}})^2} \sim \frac{k_{\mathrm{BZ}}}{\delta k_{\mathrm{gap}}} \sim \xi_{\mathrm{P}}, \tag{31}
$$

where ξ_{P} is the size of a Cooper pair (Pippard scale) in units of the lattice constant. Here, we have taken into account that $\langle c_{\boldsymbol{k}+\boldsymbol{K}\uparrow}c_{-\boldsymbol{k}\downarrow}\rangle_{T=0} \propto \Delta_{\mathrm{SC}}/\sqrt{(\epsilon_{\boldsymbol{k}} - E_{\mathrm{F}})^2 + \Delta^2_{\mathrm{SC}}} \sim 1$ within δk_{gap} from the Fermi surface, where the microscopic gap $\Delta_{\mathrm{SC}} \neq 0$.

Next, we take the BCS interaction to be the usual schematic $-V_0$ within a range of $\pm\hbar\omega_{\mathrm{D}}$ around E_{F}, and introduce the dimensionless coupling constant $\lambda = Ag(E_{\mathrm{F}})V_0$, where A is the surface of the unit cell and $g(E_{\mathrm{F}})$ the (intensive) level density at the Fermi energy. Then

$$k_{\mathrm{B}}T_{\mathrm{pair}} \sim \xi_{\mathrm{P}} \cdot 8 \cdot V_0 \cdot [Ag(E_{\mathrm{F}})\hbar\omega_{\mathrm{D}}]^2 \sim 10\xi_{\mathrm{P}} \cdot \frac{\lambda^2(\hbar\omega_{\mathrm{D}})^2}{V_0}. \tag{32}$$

When the actual numbers for some classical 3D superconductors [33] are inserted, one finds that the intensive bound (32) still allows 2D SC by a wide margin, primarily because Cooper pairs are so large, $\xi_{\mathrm{P}} \sim 1000$. For hafnium, $Ag(E_{\mathrm{F}}) \approx 0.8\ \mathrm{eV}^{-1}$, $\lambda \approx 0.14$ and $\hbar\omega_{\mathrm{D}} \approx 22$ meV, which gives $T_{\mathrm{pair}} \approx 4000$ K, while for aluminum, $Ag(E_{\mathrm{F}}) \approx 0.5\ \mathrm{eV}^{-1}$, $\lambda \approx 0.4$ and $\hbar\omega_{\mathrm{D}} \approx 36$ meV, giving $T_{\mathrm{pair}} \approx 15\,000$ K. The measured values of the SC T_{c} are 0.13 K and 1.2 K, respectively.

A similar conclusion pertains to high-T_{c} superconducting cuprates, even though their Cooper pairs are small, $\xi_{\mathrm{P}} \sim 1$–3, and the critical temperatures are much larger, in the $\sim$100 K range. The SC mechanism for them is not known at present. There is broad consensus that it is not phononic, but the schematic BCS Hamiltonian is still applicable if the SC involves Cooper pairs. One can replace $\hbar\omega_{\mathrm{D}}$ with an electronic scattering scale $\sim$100 meV, V_0 with an effective Mott or charge-transfer local scale $U_{\mathrm{eff}} \sim 3$–5 eV, and λ with $\sim$1 for a strong coupling. One obtains an upper bound $T_{\mathrm{pair}} \sim 1000$ K, which is surprisingly reasonable, given the crudity of the estimates.

4. Discussion

The textbook Cooper pair attraction is not local in real space, so it is not a true microscopic interaction. Because it retains only the one scattering channel of the full interaction which gives rise to the SC instability, it is the effective macroscopic interaction, which dominates all other scattering channels when the transition is approached from above. Hohenberg's original argument, which relied only on the equation of continuity, did not make any assumption about the microscopic origin of the SC order parameter.

The explicit invocation of Cooper pairing in this work opens the way for the HMW argument to probe the SC mechanism. It chooses a specific macroscopic (low-temperature) realization of the generic microscopic (high-temperature) original argument. Unlike the original argument, this specialization does not include e.g. polaronic models, where the SC order parameter appears by bound-pair formation, instead of Cooper scattering.

The Cooper-pair attraction used here is schematic. It should not be surprising that it gives a rather loose bound for T_{c}, because it has to accommodate all possible SC T_{c}'s based on the Cooper instability. To make the same point conversely, if such a purely schematic interaction had given a limit on T_{c} much lower than the observed values, that would have indicated an error in the reasoning.

The same approach can in principle be improved. Specifics of the crystal symmetry and the scattering channel can be introduced via the Cooper-pair form factor. The modulation Q_R which probes the fluctuations of the scatterer density can also be adapted to reflect a particular idea or measurement. One can envisage the HMW argument gradually migrating, with successive refinements, from the mathematical realm of no-go theorems to the physical reality of concrete materials and samples. In this context, our estimate being closer to observation for cuprates than for metals could mean that neglecting retardation effects in the interaction (21) is more realistic for the former, as argued in particular by Anderson [34].

The suppression of 3D SC in thin films of elemental BCS superconductors proceeds by a different mechanism than in the HMW argument. The minimal film thickness for Meissner shielding in clean superconducting metals is an effective penetration depth $\lambda_{\text{eff}} = \sqrt[3]{\lambda_{\text{L}}^2 \xi_{\text{P}}}$, where λ_{L} is the London penetration depth [35]. In aluminum, $\lambda_{\text{eff}} \sim 1000$ Å, or 250 lattice spacings, indicating that the sample needs to be macroscopic in all three dimensions in order to provide enough phase space for SC. By contrast, an SC cuprate layer of single-unit-cell thickness has a perfect Meissner response [11].

It is well known that the Berezinskii–Kosterlitz–Thouless (BKT) mechanism [36–39] allows for sharp phase transitions in 2D with power-law decays in the spatial correlation functions, instead of their saturating asymptotically at finite values as in true long-range order. BKT fluctuations associated with vortex pairs appear in both low- (BCS) and high-T_{c} (cuprate) SC thin films, with the BKT transition always observed as a separate phenomenon within the SC regime [40, 41]. Hence the BKT mechanism is not sufficient to stabilize 2D SC in general, although it may affect properties of the SC state near the critical temperature [40].

5. Conclusion

The main result of the present work is that no special pleading, such as substrate effects or the BKT mechanism, is necessary in 2D to account for either magnetism or superconductivity in light of the HMW theorem. The precise meaning of this statement is different in the two cases.

For magnetism, the IR fluctuations affect T_{c} in 2D samples of reasonable size sufficiently to reduce it by an order of magnitude. In the presence of disorder or weak interlayer coupling, however, these fluctuations become significantly less effective in suppressing magnetic order. IR fluctuations are thus not a universal explanation for the reduction of T_{c} in any given 2D system. It is not possible to state *a priori* why $T_{\text{c}} > 0$ in a given 2D film, nor how much it should be reduced relative to its value in the bulk. A particular analysis of the sample at hand, comparing finite-size effects with interlayer-coupling and disorder scales, is required. In general, the mechanism which suppresses T_{c} the least will prevail.

For SC, the theorem is ineffective in 2D for all physically possible sample sizes. The reason for the ineffectiveness is that the cost of IR fluctuations in the local number density is set by the kinetic-energy scale, which is very high in metals. These IR modes are not sufficiently excited at SC onset temperatures to affect the SC order parameter in 2D, making the original HMW bound physically void. Bulk values of T_{c} observed in atomically flat films [11] and exfoliated layers [15] should not be surprising at all. Rather, the surprise is that they were considered puzzling for so long.

The upper limit for the SC T_{c} we find is in the thousand-Kelvin range, so its practical significance is qualitative. While the original HMW theorem in principle allows a 2D SC order parameter as a finite-size effect, the present formulation eliminates the worry that IR fluctuations will compromise Cooper pairing as a particular mechanism to realize it. No physically reasonable value for the SC T_{c} in 2D is precluded by any known version of the HMW argument as of this writing. We conclude that all physical and chemical considerations for the appearance of 2D SC take precedence over dimensionality. We hope that this result will stimulate the search for high-temperature SC in fabricated 2D materials.

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Data availability statement

No new data were created or analysed in this study.

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