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**LETTER TO THE EDITOR**

# Uncertainty principle enhanced pairing correlations in projected Fermi systems near half filling

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**Abstract.** We point out the curious phenomenon of *order by projection* in a class of lattice Fermi systems near half filling. Enhanced pairing correlations of extended s-wave Cooper pairs result from the process of projecting out s-wave Cooper pairs, with negligible effect on the ground-state energy. The Hubbard model is a particularly nice example of the above phenomenon, which is revealed with the use of rigorous inequalities including the uncertainty principle inequality. In addition, we present numerical evidence that at half filling a related but simplified model shows off-diagonal long range order (ODLRO) of extended s-wave Cooper pairs.

There is considerable current interest in the possibility of purely electronic interaction-driven superconductivity as a mechanism to explain the high-$T_c$ superconductors. While it is well known for the uniform electron gas that purely Coulomb repulsion terms lead to superconductivity in higher angular momentum channels [1], albeit with very low transition temperatures, here the search, guided by experiments, is predominantly for single-band models that display such behaviour in the proximity of half filling on a lattice. The prototypical example is that of the Hubbard model [2, 3], although its tendency (or otherwise) towards superconductivity remains an unsettled issue.

In this work, we study a class of many-body Fermi systems on a lattice, under the influence of a projection of s-wave Cooper pairs. Recall that one has an inhibition of s-wave ordering within weak-coupling Bardeen–Cooper–Schrieffer (BCS) theory for models for on-site repulsion in addition to the usual phononic coupling. In contrast, we *project out* s-wave Cooper pairs in the present work. The study of most projected models, generally justified by their status as 'fixed-point' Hamiltonians in some underlying scaling theory, has been a rich source of new and interesting models in the field of correlated Fermi systems. A prototype is the Gutzwiller wavefunction, wherein upon removing double occupancy, effects such as enhanced effective masses follow near half filling, and these are crucial in our understanding of almost localized Fermi liquids [4]. At half filling we find insulating wavefunctions with enhanced spin–spin correlations [5] that are regarded as typical of quantum spin systems in low dimensions with $S = 1/2$. At the level of the Hamiltonian, projection leads to interesting new models, such as the various limits of the Hubbard model, for example, large $U$ giving the $t$–$J$ model, $U = \infty$ giving the Nagaoka limit, and several examples in single impurity models. It seems worth remarking that projection is a theoretical device

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that has genuinely strong coupling and is non-perturbative, making it difficult to treat with conventional methods. In the present work the consequences of s-wave projection are found by combining a set of known inequalities in a novel fashion, and they lead to surprising insights which are detailed later.

We consider the model defined on a $d$-dimensional hypercubic lattice with a Hamiltonian

$$H = T + U \sum_i n_{i\uparrow} n_{i\downarrow} + U_s B^\dagger B \tag{1}$$

where $T$ is the kinetic energy term $\sum_{k,\sigma} \epsilon(k) c^\dagger_\sigma(k) c_\sigma(k)$. The second term is the Hubbard repulsion term (i.e. $U \geqslant 0$). We will consider other forms of interaction, but the argument is simplest for the Hubbard interaction. We take the number of sites as $\mathcal{L}$ and denote the density of particles by $\rho = N/\mathcal{L}$. We also denote $\tilde{H} = H - \mu \hat{N}$, where $\mu$ is the chemical potential and $\hat{N}$ the number operator. The third term is new, with the operator $B = \sum_j \exp\{i\phi_j\} b_j$ and $b_j \equiv c_{j\downarrow} c_{j\uparrow}$. If we take $U_s$ to be $O(1/\mathcal{L})$ and *negative*, then this term would, in a weak coupling BCS, encourage the formation of s-wave Cooper pairs, and one expects a superconducting ground state. For $U_s$ of $O(1/\mathcal{L})$ and *positive*, the extra term is trivial as seen by a variational argument using the unperturbed ground state as a trial function. The coupling constant $U_s$ is taken of $O(1)$ and *positive* in the present work, and corresponds to *projecting out* the appropriate Cooper pairs at general fillings. Precisely at half filling, the influence of the new term is more subtle as noted later in this letter. Although various choices of the phase angle $\phi_i$ generate different examples, two of the interesting ones are (a) $\phi_i = 0$ leads to a suppression of pure s-wave superconductivity, and (b) $\phi_i = \boldsymbol{r}_i \cdot \{\pi, \pi, \ldots\}$ suppresses the so-called eta pairing [6]. We will also consider a third possibility (c) obtained by setting $B = \sum_k \exp\{\mathrm{i}\phi(k)\} b(k)$ where $b(k) \equiv c_{-k\downarrow} c_{k\uparrow}$ and with an arbitrary function $\phi(k)$ which can be used to vary the relative phases between different momenta. This last class of operators, however, forces us to the case of $U = 0$, in order to obtain any results. Case (a) appears to be the most interesting physically, but the others are included for completeness.

We first note that for lattices that are bipartite, and where the electronic hopping only connects unlike sublattices, we can make a particle–hole transformation $c_i \rightarrow (-1)^{\theta_i} c_i^\dagger$, with $\theta_i = 0, 1$ for the two sublattices, whereby the energy satisfies $E[U, U_s, \rho] = E[U, U_s, 1 - \rho] - \mathcal{L}(1 - \rho)(U + U_s)$. At half filling ($\rho = 1$) the chemical potentials for adding and subtracting a particle add up as $\mu_+ + \mu_- = U + U_s$. At this filling, the new term $U_s$ plays a crucial role in allowing doubly-occupied sites and holes to wander away from each other, and in fact encourages charge fluctuations, whereby the usual Mott insulating state of the Hubbard model at half filling is heavily discouraged.

We now use a simple but useful inequality [7]

$$\langle \psi_0 | M^\dagger [\tilde{H}, M] | \psi_0 \rangle \geqslant 0 \tag{2}$$

where $|\psi_0\rangle$ is the ground state of $\tilde{H}$, and $M$ is an arbitrary operator. Using $M = B$ we find on using the important commutator $[B, B^\dagger] = \mathcal{L} - \hat{N}$, valid in all cases (a), (b) and (c), that

$$\langle B^\dagger A \rangle \geqslant \{U_s(\mathcal{L} - N + 2) - 2\mu + U\} \langle B^\dagger B \rangle. \tag{3}$$

In case (c), the above inequality holds only with $U = 0$. Note that the left-hand side is forced to be real and positive from the inequality. We denote ground-state averages by angular brackets, and the operator $A$ is given by $A = [T, B]$. For the two cases of the phase $\phi_i$ in equation (1), (a) $A = -2 \sum_k \epsilon(k) b(k)$, and (b) $A = -\sum \{\epsilon(\boldsymbol{k}) + \epsilon(\boldsymbol{k} + \boldsymbol{\Pi})\} b(k)$ with $\boldsymbol{\Pi} = \{\pi, \pi, \ldots\}$. In the popular case of nearest-neighbour hopping on the hypercubic lattice, (a) corresponds to the extended s-wave pairing operator, whereas (b) gives $A = 0$. A non-zero result is obtained in the latter case only when the hopping connects sites on the

same sublattice. In two dimensions, for example, with $\epsilon(k) = -2t(\cos(k_x) + \cos(k_y)) - 2t'\cos(k_x)\cos(k_y)$, we find $A = 4t'\sum(\cos(k_x)\cos(k_y))b(k)$.

We now use the Cauchy–Schwartz inequality to bound the left-hand side of inequality (3) as

$$\langle A^\dagger A\rangle\langle B^\dagger B\rangle \geqslant \langle B^\dagger A\rangle^2. \tag{4}$$

Combining (3) and (4) we find

$$\langle A^\dagger A\rangle \geqslant \{U_s(\mathcal{L} - N + 2) - 2\mu + U\}^2\langle B^\dagger B\rangle. \tag{5}$$

Again note that in case (c), (5) is valid only with $U = 0$. We note that on the right-hand side of (5) the prefactor is of $O(\mathcal{L}^2)$ provided we are at a thermodynamic filling $\rho < 1$. Exactly at half filling the inequality is less useful. At any filling $\rho < 1$, we can deduce that $\langle B^\dagger B\rangle$ is very small. In fact we will show that it is $o(\mathcal{L})$ rather than $O(\mathcal{L})$. If it were of $O(\mathcal{L})$, (as indeed it is in the ground state of the free Fermi gas), then $\langle A^\dagger A\rangle$ has to exceed a trivial upper bound of $O(\mathcal{L}^2)$†. If $\langle B^\dagger B\rangle$ is of $O(1)$ then we have two consequences that are mutually incompatible (at least when $U = 0$). To see this, assume that $\langle B^\dagger B\rangle$ is of $O(1)$ and so we find from the Feynman–Hellman theorem‡

$$E[U, U_s, \rho] = E[U, 0, \rho] + \int_0^{U_s} \mathrm{d}U_s'\langle B^\dagger B\rangle_{U_s'} \tag{6}$$

$$= E[U, 0, \rho] + o(\mathcal{L}). \tag{7}$$

The other consequence of (5) is that $\langle A^\dagger A\rangle \sim O(\mathcal{L}^2)$, i.e. we have long ranged order (ODLRO) in the operator $A$ [8]. This is possible only if the energy increases by terms of $O(\mathcal{L})$, at least in the case when $U = 0$ as is seen from a diagonalization of a bilinear Hamiltonian adding the kinetic energy $T$ and $A$ with coefficients of $O(1)$§. A consistent possibility for $U_s$ of $O(1)$ is‖

$$\langle B^\dagger B\rangle = O(1/\mathcal{L}) \qquad \text{and} \qquad \langle A^\dagger A\rangle = O(\mathcal{L}) \tag{8}$$

along with equation (7). One immediate consequence of this result is that of the thermodynamic degeneracy of the energy: the energy per site of the model in equation (1) $\mathrm{Lim}_{\mathcal{L}\to\infty} E[U, U_s, \rho]/\mathcal{L}$ is identical to that of the pure Hubbard model (i.e. $U_s = 0$) at *all* $U$ or filling $\rho \neq 1$.

Another important consequence is that the chemical potential is unchanged by $U_s$ until we reach half filling ($\mu = \partial E/\partial N$) and therefore the compressibility is unchanged by $U_s$ (since $1/\kappa = N\rho(\partial\mu/\partial N)_{\mathcal{L}}$). At precisely half filling, the chemical potential jumps and the compressibility vanishes. The value of $\mu$ at half filling for the case of bipartite symmetry was given above as $(U + U_s)/2$.

We have seen the remarkable suppression of correlations of the type $\langle B^\dagger B\rangle$. When we recall that $\langle [B, B^\dagger]\rangle = \mathcal{L}(1 - \rho)$, it is seen that the fluctuations of $B + B^\dagger$ in the ground state diminish on approaching half filling, i.e. $\langle (B + B^\dagger)^2/\mathcal{L}\rangle = 1 - \rho$. This immediately

† The bound is obtained by writing $\langle A^\dagger A\rangle \leqslant 4\sum_{k,k'} |\epsilon(k)\epsilon(k')\, langle b^\dagger(k')b(k)\rangle| \leqslant 4\sum_{k,k'} |\epsilon(k)\epsilon(k')| \sim O(\mathcal{L}^2)$.

‡ Here we use the concavity of energy with respect to $U_s$: calling $\beta(U_s) \equiv \langle B^\dagger B\rangle_{U_s}$, we note that second-order perturbation theory implies that $\partial\beta(x)/\partial x < 0$, i.e. $\beta(x)$ is a monotonically decreasing function. Clearly $\beta(x) \geqslant 0$, so that $0 < \beta(x) \leqslant \beta(0)$. In the absence of $U_s$ we assume the system to be a normal Fermi system, and hence $\beta(0) \sim O(\mathcal{L})$, for example as in the free Fermi gas. The integral $\int_0^{U_s} \mathrm{d}x\beta(x)$ is therefore of $o(\mathcal{L})$. These estimates are clarified if one considers a simple model for $\beta(x)$ satisfying the bounds, namely $\beta(x) = \mathcal{L}/(1 + x\mathcal{L}^\alpha)^\beta$ with $\alpha$ and $\beta > 0$, for which the integral is $O(\mathcal{L}^p)$ with $p = \max(1 - \alpha, 1 - \alpha\beta)$.

§ In the case of $U \neq 0$, provided that $A$ does not already have long-ranged order in the absence of the $U_s$, then the same is expected to be true, but harder to prove rigorously.

‖ If $\langle B^\dagger B\rangle \sim O(\mathcal{L}^{1-\sigma})$ with $1 > \sigma > 0$ then we find from (5) that $\langle A^\dagger A\rangle$ has quasi-ODLRO, i.e. is almost ordered, unlike in a normal Fermi liquid.

suggests that 'conjugate variables' in the sense of the uncertainty principle should exhibit enhancements by similar factors. The following form of the uncertainty principle is most useful; for any two operators $a$ and $b$ (such that $\langle a^2\rangle = 0 = \langle b^2\rangle$ and $[a, b] = 0$) we have [9]

$$\langle a^\dagger a + aa^\dagger\rangle\langle b^\dagger b + bb^\dagger\rangle \geqslant |\langle [a^\dagger, b]\rangle|^2. \tag{9}$$

We now use this with $a \to A$ and $b \to B$, and also the results $[A, B^\dagger] = 2T$ and $[A, A^\dagger] \equiv \chi_A = 4\sum_k \epsilon(k)^2(1 - \sum_\sigma c_\sigma^\dagger(k)c_\sigma(k))$ to find

$$\langle A^\dagger A\rangle \geqslant \frac{2|\langle T\rangle|^2}{\mathcal{L}(1-\rho)} - \frac{\langle\chi_A\rangle}{2}. \tag{10}$$

Both terms of the right-hand side of this inequality are of $O(\mathcal{L})$, and the second term remains bounded as we approach half filling, in fact vanishing for the case of a symmetric band around zero energy. This implies that the first term dominates and hence we conclude that the correlation function $\langle A^\dagger A\rangle$ grows without limit as half filling is approached. We should remark that any operator of the type $[T, [T, \ldots [T, B]\ldots]$ in the place of $A$ would end up having similar enhancements in its correlations, since it would be bilinear in $c^\dagger$ and have similar commutation with $B$.

We next consider other kinds of interactions, different from the Hubbard model†. In this case, we still use (2) and also (4) to find in place of (5)

$$\langle F^\dagger F\rangle \geqslant \{U_s(\mathcal{L} - N + 2) - 2\mu\}^2\langle B^\dagger B\rangle \tag{11}$$

where $F = A + C$ with $C = -[B, V_{int}]$, so that $F = [H, B]$. The norm on the left-hand side of inequality (11) can be bounded by the triangle inequality as $\langle F^\dagger F\rangle \leqslant [\sqrt{\langle A^\dagger A\rangle} + \sqrt{\langle C^\dagger C\rangle}]^2$ and hence we need, in addition to the previous estimates, one for $\langle C^\dagger C\rangle$. This of course depends upon the nature of the two-particle interaction, and has to be examined for each model separately. However, for 'generic' repulsive short-ranged models, it seems clear that this object, like $\langle A^\dagger A\rangle$, should be bounded from above by a number of $O(\mathcal{L}^2)$. With this assumption, the remaining argument goes exactly as in the case of the Hubbard model, and we again conclude that $\langle B^\dagger B\rangle$ is at least as small as $o(\mathcal{L})$, and in fact probably $O(1/\mathcal{L})$, and that the ground-state energy is as in equation (7). The uncertainty relation inequality (10) needs only the fairly weak first condition $\langle B^\dagger B\rangle \sim o(\mathcal{L})$, and hence we conclude that the mechanism of *order by projection* works for generic short-ranged repulsive models near half filling.

We have thus found enhanced correlations as we approach half filling and, by continuity, we may expect ODLRO in the operator $A$. The inequalities given above do not constrain correlations sufficiently, and we turn to other methods. Before doing this, we introduce a simpler version of the previous models, namely

$$\tilde{H}_s = \sum_{n=1}^{L}(\epsilon_n - \mu)(\sigma_n^z + 1) + U_s\sum_{n,m=1}^{L}\sigma_n^+\sigma_m^- \tag{12}$$

where $\sigma^z$ etc are the usual Pauli matrices, and $\epsilon_n$ are an ascending set of energies. This model is intimately related to the $U = 0$ version of our starting problem equation (1), using the pseudospin representation $\sigma_j^z + 1 = \sum_\sigma n_\sigma(k_j)$ and $\sigma_j^+ = c_\uparrow^\dagger(k_j)c_\downarrow^\dagger(-k_j)$, in the subspace where both $(k, \uparrow)$ and $(-k, \downarrow)$ are simultaneously present or absent. The

† For other kinds of projected order, the inequalities are harder to interpret, for example, if $B = \sum_{i,j}[v]_{i,j}c_{i\downarrow}c_{j\uparrow}$ with an off-diagonal matrix $[v]$, then the analogue of (3) contains, as a coefficient of $U_s$ the factor $(\mathcal{L} - N + 2)[v^2]_{i,i} + \langle\chi|\phi|\chi\rangle$, where $|\chi\rangle \equiv B|\psi_0\rangle$ and $\phi = -\sum_{i,j}[v^2]_{i,j}c_{i\sigma}^\dagger c_{j\sigma}$, and hence there is the possibility of cancellation of the term of $O(\mathcal{L})$.

Hamiltonian (1) commutes with the operator $\nu = \sum_k n_\uparrow(k) n_\downarrow(-k)$, and its operation is identical to that of $H_s$ provided we specialize to various sectors labelled by the eigenvalues of $\nu (0 \leqslant \langle \nu \rangle \leqslant N/2)$, and further choose appropriate degeneracies for the energies. We simplify this problem by choosing our energies in $H_s$ above to be non-degenerate, and pick them to be $\epsilon_n = \{n - (L+1)/2\}/(L-1)$ so that the band is symmetric about zero and the bandwidth is unity. Each up-spin corresponds to two (Fermi) particles of the original problem. The filling in this problem is clearly $\rho = N/L$ with $\hat{N} = \sum_j (\sigma^z(j) + 1)$. The chemical potential at half filling is $U_s/2$ by particle–hole symmetry.

The model can also be viewed as a lattice of $N/2$ hard core particles sitting in a constant electric field that tries to localize them in regions of low potential, and an infinite-ranged hopping that tries to delocalize them. The results proved for the starting equation (1), namely (5), (8) and (10), are equally true in this one-dimensional spin model, provided we identify $B = \sum_j \sigma_j^-$ and $A = -2 \sum_j \epsilon_j \sigma_j^-$. Away from half filling, i.e. when $\sigma^z_{\rm tot} \neq 0$, we see that even in the limit of large $U_s$ there is a large number of states, in fact states with $S^{\rm tot} = L(1-\rho)/2$ and $S^z_{\rm tot} = -L(1-\rho)/2$, i.e. highest weight states of the rotation group, which have a null eigenvalue of the hopping term $U_s \sum \sigma_n^+ \sigma_m^-$. The Zeeman energy term has non-zero matrix elements *within this manifold*. In the case of half filling $\rho = 1$, the Zeeman term necessarily connects singlet states with triplets and hence the energy is unable to escape the influence of $U_s$. At half filling and for large $U_s$, we can use degenerate perturbation theory to find an effective Hamiltonian to lowest order in $1/U_s$. To do this we consider the action of $H_s$ in equation (12) on the space of ${}^L C_{L/2}/(L/2+1)$ singlets spanned, for example, by the non-crossing Rumer diagrams [10]. A typical non-orthogonal state is given by $\psi_P = [P_1, P_2]_- \ldots [P_{L-1}, P_L]_-$ where $P$ is one of the permutations of the set $\{1, 2, \ldots, L\}$ giving a non-crossing Rumer diagram, and $[i, j]_\mp = (\alpha_i \beta_j \mp \beta_i \alpha_j)/\sqrt{2}$ is a singlet (triplet) with $s^z = 0$. The action of the operator equation (12) can be projected into this subspace, by using the relation $[1,2]_+[3,4]_+ = \frac{1}{3}(1 - 2\Pi_{13})[1,2]_-[3,4]_- + \psi^{\rm quintet}$ with $\Pi_{ij}$ the permutation operator, and leads to the following quantum dimer problem:

$$H_{\rm qd}\psi_P = \frac{-1}{2U_s} \sum_j (\epsilon_{P_j} - \epsilon_{P_{j+1}})^2 \psi_P - \frac{1}{3U_s} \sum_{j+1<k} (\epsilon_{P_j} - \epsilon_{P_{j+1}})(\epsilon_{P_k} - \epsilon_{P_{k+1}})\{2\Pi_{P_j P_k} - 1\}\psi_P. \tag{13}$$

This model is quite non-trivial to work with, but does reveal that the diagonal terms favour singlet bonds that connect the largest energy separations, and the mixing terms oblige us to take non-trivial linear combinations in this space.

We study the interesting half filled limit by studying the sector $\sigma^z_{\rm total} = 0$ of equation (12) directly. We have diagonalized the problem numerically for chains of length up to 14, and studied the ground-state energy as well as the correlation function $\langle A^\dagger A \rangle$. In figure 1 we plot the parameter

$$\Gamma = \frac{1}{L} \langle A^\dagger A \rangle / \langle A^\dagger A \rangle_{U_s = 0}$$

for three values of $U_s (= 2, 4, 8)$. It is clear that a non-zero extrapolation of $\Gamma$ to a number of $O(1)$ would imply ODLRO in the $A$ field. The data seem to be consistent with this hypothesis, and fit well to $\Gamma = \Gamma_\infty + |a|/L \pm |b|/L^2$, with non-zero $\Gamma_\infty$. In the inset of figure 1, the ground-state energy per site is plotted for the same three values of $U_s$ against $1/L$, showing that the energy *does* depend on the coupling at half filling, implying that the $U_s$ term cannot be viewed as a projection at this particular filling. The dependence is consistent with finite-sized scaling with the form $E/L = e_\infty + |a|/L - |b|/L^2 + O(1/L^3)$.

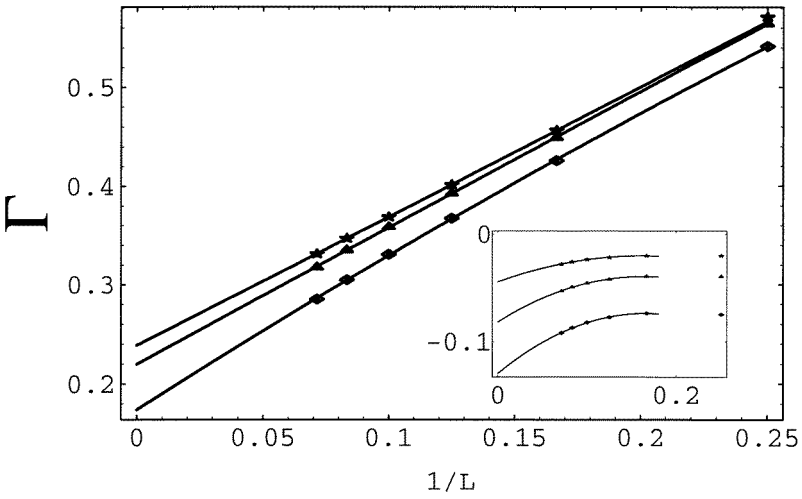


**Figure 1.** Long-ranged order parameter $\Gamma \equiv (1/L)\langle A^\dagger A\rangle/\langle A^\dagger A\rangle_{U_s=0}$ against $1/L$ for $U_s = 2, 4, 8$ (bottom to top) chains of length $4, 6, \ldots, 14$ at $\rho = 1$. The inset shows the ground-state energy per site for the same values of $U_s$ against $1/L$ (bottom to top).

A particularly simple special case† of the spin model equation (12) corresponds to choosing $\epsilon_n = \pm\epsilon_0$ for $n > L/2$ or $n < L/2$. We can solve the model in the thermodynamic limit by realizing that $\boldsymbol{S}_a = \sum_{j=1}^{L/2} \boldsymbol{s}_j$ and $\boldsymbol{S}_b = \sum_{j=L/2+1}^{L} \boldsymbol{s}_j$ are conserved quantities. We can use semiclassical methods (basically the Holstein–Primakoff transformation) away from half filling and find that the general results quoted here are confirmed.

At half filling, for a model with a variable range of hopping of the doubly-occupied sites, we may expect a transition from insulating to metallic behaviour as the range is increased, since the doubly-occupied sites are given independent kinetic freedom and are no longer tightly bound to the empty sites as in a Mott–Hubbard insulator. The new model equation (1) is almost certainly non-insulating, since the range of hopping is infinite. In view of the enhancement inequality (10), it is likely to be superconducting in a complementary pairing state. By continuity in filling $\rho$ in (10), we expect the pairing correlations to be divergent for any $U_s$. Our numerical results for the reduced model, the spin model of equation (12), are consistent with ODLRO at half filling. It is not, however, straightforward to write down a mean-field theory that captures the correct ordering in the model, since the Hamiltonian does not contain explicit terms that favour *any* kind of ordering and these are generated by the dynamics rather indirectly.

In summary, we have seen that the effect of projecting out s-wave Cooper pairs in a class of Fermi systems leads to surprising results. The ground state of the projected model may be viewed as being essentially degenerate with that of the original model and yet the extended s-wave pairing correlations are hugely enhanced near half filling. This effect, namely *order by projection*, requires a lattice Fermi system near half filling to occur, and has no natural counterpart in continuum Fermi systems. In this regard, as well as in the form of the enhancements $1/(1-\rho)$, it resembles the results of the almost localized Fermi systems [4].

† The detailed solution will be presented separately. I thank Professor B I Halperin for pointing out this special case.

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