

Exact Solution of a Repulsive Fermi Model with Enhanced Superconducting Correlations

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We present the exact solution of a model of interacting fermions in any dimension with a pure repulsive interaction projecting out a given Cooper channel. The solution rests upon the infinite ranged character of the interaction in real space, leading to a functional integral that is dominated by a Gaussian term. The solution produces strong superconducting enhancements and quasi-long-ranged order in a channel that is not present in the Hamiltonian explicitly, but of the form given by arguments from *order by projection*.

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There is considerable recent interest [1] in the possibility of models displaying a superconducting behavior driven solely by repulsive interactions. The search is motivated by the high- T_c problem, where no obvious, known attractive interaction can account for the phenomena; so one believes that repulsive interactions, originating in the Coulomb repulsion expressed within the Wannier basis of a few tight-binding bands, are ultimately responsible. In one dimension, the usual kind of repulsive interactions generically lead to enhanced spin-density-wave (SDW) order, via powerlaw correlations with small decay exponents rather than superconducting enhancements. However, recent interesting work [2] shows that under certain conditions, superconducting correlations of nontrivial symmetry are enhanced. In the physically important case of two dimensions the situation is not completely clear in relation to popular models, such as the Hubbard or the t - J model. While a treatment within the random phase approximation near an antiferromagnetic instability leads to d -wave superconductivity [3], one may worry whether the conclusions based on the (weak coupling) approximation are valid for strong repulsions. Similar worries exist regarding various versions of the Gauge theories [4] that are in vogue currently. In this context, repulsive models which can be solved exactly have an important role to play. A new set of models was introduced recently [5–7] that demonstrates the possibility of enhanced superconducting correlations quite explicitly. These models are generalizations of the Hubbard model, and include a term that is best interpreted as a projection operator that excludes a certain Cooper pairing channel from the problem. We present here an exact solution of the basic model involving the kinetic energy and the projection operator. Our solution is obtained by exploiting a certain feature of the interaction within the framework of functional integrals: namely that the projection operator is an infinite ranged repulsive operator, and its Hubbard-Stratanovic (HS) linearizing field is a single spatially uniform dynamical mode that admits *only Gaussian fluctuations in the thermodynamic limit*. This is in contrast to models with attractive interactions, where a new saddle point value of the HS field gets stabilized at

low temperatures, and its fluctuations can be ignored. The repulsive case is much more subtle, and has some similarities to the situation found in Fermionic models in infinite dimensions [8] where the relevant HS field is a Grassman variable that factorizes the kinetic energy, and has only Gaussian fluctuations [9]. We find that as a consequence the Fermi gas develops enhanced correlations in a “compromise” pairing channel which is not explicitly present in the Hamiltonian. These are precisely of the sort that is expected from arguments from *order by projection* [5,6]. The earlier treatments [5,6] have used a variety of non-perturbative techniques, such as rigorous inequalities and variational approaches. The exact solution presented here is consistent with these, and give us in addition, a clear understanding of the origin of these enhancements and of the quasi LRO in terms of the singularities of the two particle scattering amplitude. The model is defined by the Hamiltonian

$$H = T + U_s B^\dagger B. \quad (1)$$

Here $B \equiv \sum \zeta(k) b_k$ is a Cooper pair operator, $b_k = c_{-k\downarrow} c_{k\uparrow}$ are the pair destruction operators, $T = \sum \epsilon_k n_{k\sigma}$ is the kinetic energy corresponding to a band dispersion $\epsilon_k [= -2 \sum_{\alpha=1}^d \cos(k_\alpha)]$ in the nearest neighbor problem]. $\zeta(k)$ may be chosen arbitrarily. The two cases of interest in two dimensions are (i) $\zeta(k) = 1$ giving rise to extended s -wave order, and (ii) $\zeta(k) = \cos(k_x) - \cos(k_y)$ giving rise to second-neighbor d -wave order. For simplicity of presentation we initially focus on $\zeta = 1$ and return to the other case later.

With the above choice of the model, we note that B may be rewritten as $\sum_r c_1(r) c_1(r)$, and hence the interaction term may be viewed as an infinite ranged hopping term for doubly occupied sites.

Using the H - S linearization within the standard Grassman variable [10] formulation, we write the partition function for this model as the functional integral $Z = \int Dc^* Dc D\phi^* D\phi \exp -\beta\Psi$. The free energy functional Ψ is given in terms of the Fermi fields c, c^* and the auxiliary bose fields ϕ, ϕ^* as

$$\beta\Psi = \int_0^\beta \phi^*(\tau)\phi(\tau) d\tau - \sum_{k,\sigma} \int_0^\beta c_{k,\sigma}^*(\tau)(\partial_\tau - \xi_k)c_{k,\sigma}(\tau) d\tau - i\sqrt{U_s} \int_0^\beta [\phi^*(\tau)B(\tau) + B^*(\tau)\phi(\tau)] d\tau, \quad (2)$$

where $\xi_k = \epsilon_k - \mu$. We use a Fourier series expansion $c_{k,\sigma}(\tau) = \sum_n \exp(i\omega_n\tau)\hat{c}_{k,\sigma}(n)$, and $\phi(\tau) = \sum_n \exp(i\Omega_n\tau)\hat{\phi}_n$, where the fermionic frequencies $\omega_n = (2n+1)\pi\beta^{-1}$ and the bosonic frequencies $\Omega_n = 2n\pi\beta^{-1}$. We denote the Fourier components $\hat{b}_k(n) = \sum_m \hat{c}_{-k,\downarrow}(m)\hat{c}_{k,\uparrow}(n-m)$ and so define $\hat{B}_n = \sum_k \hat{b}_k \times (n-1)$. In terms of these we can rewrite

$$\Psi = \sum \hat{\phi}_n^* \hat{\phi}_n + \sum_{k,n} (\xi_k - i\omega_n) \hat{c}_{k,\sigma}^* \hat{c}_{k,\sigma}(n) + i\sqrt{U_s} \sum_n (\hat{\phi}_n^* \hat{B}_n + \hat{\phi}_n \hat{B}_n^*).$$

We now trace out the Fermi degrees of freedom and find the reduced free energy functional $\Psi_\phi = \Psi_0 + \sum \hat{\phi}_n^* \hat{\phi}_n - k_b T \sum_k \text{Tr} \log\{1 - C(k)\}$. Here Ψ_0 is the noninteracting free energy, C is an infinite dimensional matrix defined by its (frequency space) matrix elements

$C_{n,m}(k) = U_s \sum_l G_0(k,n)G_0(k,m)\hat{\phi}_{m+l+1}^* \hat{\phi}_{n+l+1}$ in terms of the free Green's function $G_0(k,n) = 1/(i\omega_n - \xi_k)$, and the trace is in the frequency space.

We now analyze Ψ_ϕ in detail. We can expand

$$\Psi_\phi = \Psi_0 + \sum_n \{1 + U_s \mathcal{L} \Pi_0(i\Omega_n)\} \hat{\phi}_n^* \hat{\phi}_n + \frac{U_s^2}{2} \mathcal{L} \sum \Gamma_{(m_1,m_2,n_1,n_2)} \hat{\phi}_{m_1}^* \hat{\phi}_{m_2}^* \hat{\phi}_{n_1} \hat{\phi}_{n_2} + O(U_s^3).$$

Here $\Pi_0(i\Omega_n) \equiv \frac{1}{\mathcal{L}} \sum_k \pi_{k,n}$ where $\pi_{k,n}$ are the polarizations

$$\pi_{k,n} = [2f(k) - 1]/(i\Omega_n - 2\xi_k), \quad (3)$$

and $f(k)$ is the usual noninteracting Fermi function. The fourth order term is given explicitly as

$$\Gamma_{(m_1,m_2,n_1,n_2)} = \frac{1}{\mathcal{L}} \sum_k \frac{[2f(k) - 1](D_{m_1,k} + D_{m_2,k})\delta_{m_1+m_2,n_1+n_2}}{D_{m_1,k}D_{m_2,k}D_{n_1,k}D_{n_2,k}},$$

where $D_{m,k} \equiv (i\Omega_m - 2\xi_k)$.

We note that both Π_0 and Γ in the above equations are of $O(1)$ since these are normalized sums over momenta. Indeed every term in the expansion has a similar structure and is of the same order, namely $O(\mathcal{L})$. Hence one has the remarkable exact result that *the Gaussian term dominates the rest of the terms in the thermodynamic limit* [11]. Roughly speaking, the Gaussian piece gives us the typical size $\hat{\phi}_n \sim \frac{1}{\sqrt{\mathcal{L}}}$, and so the quadratic (in U_s) piece is of the order $1/\mathcal{L}$, and likewise the m th term is of the order $1/\mathcal{L}^{(m-1)}$. Thus in the thermodynamic limit, it suffices to keep the Gaussian term and to drop the remaining terms. This leads to the following remarkably simple result [12]

$$\langle \hat{\phi}_n^* \hat{\phi}_n \rangle = \frac{\beta^{-1}}{1 + U_s \mathcal{L} \Pi_0(i\Omega_n)}. \quad (4)$$

From the same arguments, the correlation function of the Cooper pair operators is given by

$$\langle b_k^*(n)b_{k'}(n) \rangle = \delta_{k,k'} \pi_{k,n} - \frac{1}{\mathcal{L}} \pi_{k,n} V_{\text{eff}}(i\Omega_n) \pi_{k',n}, \quad (5)$$

where the effective interaction [12]

$$V_{\text{eff}}(n) = \frac{V}{1 + V \Pi_0(i\Omega_n)} \quad (6)$$

in terms of the (very large) coupling constant $V = U_s \mathcal{L}$.

We next present an alternate derivation of the above results starting from the equations of motion, which gives some more insight into them.

Define (as in Ref. [6]) the set of operators $I_l \equiv \sum (\epsilon_k)^l b_k$, and $T_l \equiv \sum (\epsilon_k)^l (n_{-k\downarrow} + n_{k\uparrow} - 1)$. Clearly $I_0 = B$ and $T_1 = T$. It is easy to ascertain that

$$[I_l, T] = 2I_{l+1}, \quad [I_l, \hat{N}] = 2I_l, \quad [I_l, I_m^\dagger] = -T_{l+m}, \quad (7)$$

whence,

$$[I_l, H - \mu \hat{N}] = -2\mu I_l + 2I_{l+1} - U_s T_l I_0. \quad (8)$$

Now, we invoke the law of large numbers and argue that in the present problem the operator product $T_l I_0$ can be replaced by $\mathcal{L} \mu_l I_0$ where $\mathcal{L} \mu_l = \langle T_l \rangle$, the thermodynamic average of T_l , which is clearly of order \mathcal{L} [13]. Then the equations of motion for the usual time ordered Green functions $\langle\langle I_l; I_m^\dagger \rangle\rangle$ reduce to the closed set

$$(i\Omega_n + 2\mu) \langle\langle I_l; I_m^\dagger \rangle\rangle = -\mathcal{L} \mu_{l+m} + 2\langle\langle I_{l+1}; I_m^\dagger \rangle\rangle - \mathcal{L} U_s \mu_l \langle\langle I_0; I_m^\dagger \rangle\rangle, \quad (9)$$

which can be solved exactly. The solution is given by

$$\langle\langle I_l; I_m^\dagger \rangle\rangle = -\mathcal{L} \Pi_{l+m} + \mathcal{L} \Pi_l \frac{U_s}{1 + U_s \mathcal{L} \Pi_0} \mathcal{L} \Pi_m, \quad (10)$$

where

$$\Pi_l(i\Omega_n) \equiv \sum_{l'=0}^{\infty} \frac{2^{l'} \mu_{l+l'}}{(i\Omega_n + 2\mu)^{l'+1}} = (1/\mathcal{L}) \sum_k \frac{(\epsilon_k)^l (2\langle n_k \rangle - 1)}{(i\Omega_n - 2\xi_k)}.$$

This may be verified using the easily derived recursion relation $\Pi_{l+1} = [(i\Omega_n + 2\mu)\Pi_l - \mu_l]/2$. Furthermore, one of the key features of the models being discussed is that *the one particle propagators are unrenormalized* [14], so that $\langle n_k \rangle = f(k)$, whence $\Pi_l(i\Omega_n) = (1/\mathcal{L}) \sum_k (\epsilon_k)^l \pi_{k,n}$. Then it is easily seen that the results in Eq. (10) are basically the same as in Eq. (5). Starting from the latter, multiplying by $(\epsilon_k)^l (\epsilon_{k'})^m$, and summing over k and k' , we get the former.

An analysis of the detailed properties of the function V_{eff} is of crucial importance for the rest of our discussion. For a simple model band structure, with a constant density of states $g(\epsilon) = 1/2$ for $-1 < \epsilon < 1$, we can compute it exactly as

$$V_{\text{eff}}(i\Omega) \rightarrow V_{\text{eff}}(\omega + i\eta) = \frac{V}{1 + V\Pi_0(\omega)}, \quad (11)$$

with

$$\begin{aligned} \Pi_0(\omega) &= \frac{1}{4} \log\left(\frac{4|(\omega/2 + \mu)^2 - 1|}{\omega^2}\right) \\ &+ i \frac{\pi}{4} \theta(2 - |2\mu + \omega|) \text{sgn}(\omega). \end{aligned}$$

The band extends from $-2 + 2\delta$ to $2 + 2\delta$, where the hole filling $\delta = 1 - \rho = -\mu$. The schematic behavior of V_{eff} is as follows. At very high frequencies, $V_{\text{eff}} \approx V$. It has two poles at certain large frequencies that essentially dominate its physics. In between these poles lies the intermediate frequency range where V_{eff} is of order unity, which contains the branch cut corresponding to the one electron band of states. The location of the poles can be found by using a large frequency expansion for the function $\Pi_0(i\Omega_n)$, which for $|\Omega_n| \gg W$ (W is the band width) behaves as

$$\Pi_0(i\Omega_n) = -\frac{\delta}{(i\Omega_n)} - \frac{2(|\mu_1| - \mu\delta)}{(i\Omega_n)^2} + \mathcal{O}\left(\frac{1}{|\Omega_n|^3}\right). \quad (12)$$

The higher order terms can be verified to be negligible. The poles of the V_{eff} can then be found by solving for the zeros of the denominator, a quadratic in $\zeta \equiv 1/i\Omega_n$, given as $0 = V^{-1} - \delta\zeta - 2(|\mu_1| - \mu\delta)\zeta^2$. The roots are always real corresponding to real frequency poles of V_{eff} . Hence, (a) at half filling, $\delta = 0$, the poles are at $\pm\omega_0 = \pm\sqrt{2V|\mu_1|}$, and near the poles $V_{\text{eff}} \approx \pm\frac{\omega_0 V}{2(\omega \mp \omega_0)}$. The pole frequencies are infinite in the thermodynamic limit, but leave behind consequences in the ground state as we see later. (b) Away from but close to half filling, $\delta \ll 1$, one pole is at $\omega_2 \equiv V\delta$ with residue $V^2\delta$, and the other at a large negative frequency $-\omega_1 = -(2|\mu_1|/\delta - 2\mu)$ with residue $-\omega_1^2/\delta$. As $\delta \rightarrow 0$, the latter poles smoothly go over into those of the first case. The contribution from the branch cut does not have any particularly simple form, but is not important in the most interesting region of the problem, namely $\delta \sim 0$.

Using the above properties of V_{eff} we can compute exactly the instantaneous (expectation) values of the extended s wave and the s -wave correlation functions: $\alpha \equiv \frac{1}{4\mathcal{L}} \langle A^\dagger A \rangle$ with $A = [T, B] = -2 \sum_k \epsilon_k b_k$, and $\beta \equiv \frac{1}{\mathcal{L}} \langle B^\dagger B \rangle$. Using the main result Eq. (5), we find

$$\begin{aligned} \alpha &= k_B T \sum_n [\Pi_2(i\Omega_n) - V_{\text{eff}}(i\Omega_n) \Pi_1^2(i\Omega_n)] e^{(i\Omega_n 0^+)}, \\ \beta &= \frac{k_B T}{V^2} \sum_n [V - V_{\text{eff}}(i\Omega_n)] e^{(i\Omega_n 0^+)}. \end{aligned} \quad (13)$$

The main contributions to the resulting frequency sums are quite easily seen to be tied to the pole contributions of V_{eff} , the branch cut part giving an uninteresting subleading contribution. We find at half filling

$$\alpha_{\text{pole}} = \frac{\sqrt{U_s \mathcal{L} |\mu_1|^3}}{2\sqrt{2}} \quad \beta_{\text{pole}} = \frac{\sqrt{|\mu_1|}}{\sqrt{2U_s \mathcal{L}}}. \quad (14)$$

Near half filling we find

$$\alpha_{\text{pole}} = \frac{\mu_1^2}{\delta} \quad \beta_{\text{pole}} = \frac{4\mu_1^2}{\delta^3 U_s^2 \mathcal{L}^2}. \quad (15)$$

At half filling Eq. (14) gives us the quasi-long-ranged order as well as the correction to ground state energy along with their appropriate coefficients, the latter by an integration over the coupling constant U_s . These answers are in good numerical agreement with exact numerics on a finite sized system [7]. Away from half filling we find that the uncertainty principle lower bounds are off by a factor of 2, i.e., from Eq. (15) $\alpha_{\text{pole}} = 2\alpha_{\text{LowerBound}}$.

The results given above enable us to compute several other response functions exactly. For example, we find that the charge stiffness is nonzero, and in fact unchanged from the noninteracting value at half filling. We also find at half filling that the appropriate order parameter density $\Delta(r)$ has correlations that are novel: $\langle \Delta^\dagger(r)\Delta(0) \rangle \sim \frac{c}{\sqrt{\mathcal{L}}}$. Thus although we do not have LRO of the usual sort, one has a divergent ‘‘structure function’’ $\int d\vec{r} \langle \Delta^\dagger(r)\Delta(0) \rangle$.

We next discuss the important case of $\zeta(k) = \cos(k_x) - \cos(k_y)$ in two dimensions. This corresponds to suppressing d -wave order at the length scale of nearest neighbors. From the uncertainty principle argument of Refs. [5,6], it follows that this would lead to enhancement again in the d -wave channel, but at a longer length scale, i.e., the resulting $\hat{A} = -2 \sum_k \epsilon_k \zeta(k) b_k$ should have enhanced correlations. The functional integral solution sketched here bears this out exactly. We recover the results in Eqs. (14) and (15) with the replacements: $\delta \rightarrow \hat{\delta} = \mathcal{L}^{-1} \sum_k \zeta^2(k) [1 - 2f(k)]$ and $\mu \rightarrow \hat{\mu}_1 = \mathcal{L}^{-1} \sum_k \epsilon_k \zeta^2(k) [1 - 2f(k)]$. The enhanced correlation function of \hat{A} then diverges at the point where $\hat{\delta}$ vanishes. So long as the one-electron dispersion has the bipartite symmetry, one can see that $\hat{\delta}$ vanishes exactly at half filling. However, if the dispersion does not have this symmetry, e.g., by having a second neighboring hopping t' , then $\hat{\delta}$ vanishes at some other density determined by t' , as illustrated in Fig. 1. The case of $t' \sim -0.4$ is popular

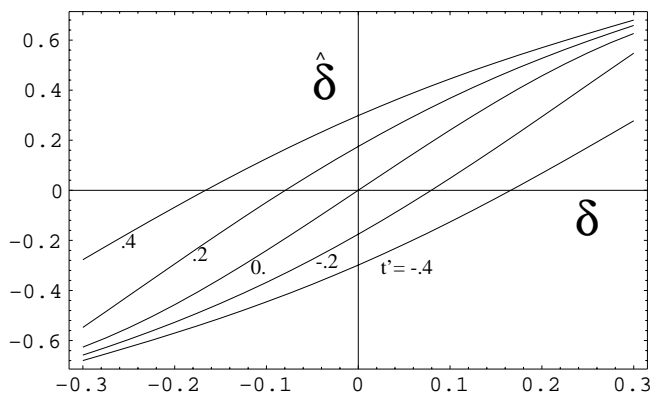


FIG. 1. The effective filling $\hat{\delta}$ for d -wave superconductivity against the true filling δ for different values of the second neighbor hopping t' .

in literature, since it leads to a Fermi surface that is consistent with that seen in the photoemission experiments in High T_c systems [15], and it is an amusing coincidence that the filling $\delta \sim 0.18$ is close to the optimum doping.

Finally, we can show that many of the above features of the infinite range model retain their relevance for more realistic models with finite range repulsion. To see this, consider (in the s -wave case) a more general model [16] of the form $H = T + \frac{1}{T} \sum U(p) B^\dagger(p) B(p)$, where $B(p) = \sum_k c_{-k, \downarrow} c_{k+p, \uparrow}$ is a Cooper pair operator with total momentum p , with $U(p) = U_s (l_c)^d$ for a small set of $\mathcal{L} / (l_c)^d$ points surrounding the center of the Brillouin zone. This would correspond to repulsive interactions with a long but finite range l_c . Then it is not hard to see that the results we have discussed above would retain much of their validity (but for some differences in details) to leading order in $(1/l_c)$, with the replacement $U_s \mathcal{L} \rightarrow U_s (l_c)^d$, leading to enhanced pairing correlations over a finite range in momentum space. The quasi-long-ranged order would be replaced by an enhancement of the $O(1)$, like that in the single mode model away from half filling. In this case, we see that all Cooper pairs with a finite (but small) center of mass momentum are also influenced by the interaction, and thus the model is more realistic by way of helping current carrying states.

In summary, we have found an exact solution for an interesting model of Fermions with purely repulsive interactions with infinite range, which may be regarded as a *mean-field repulsive model*. The resulting solution has quasi-long-ranged order at half filling, as well as large unbounded enhancements as one approaches half filling, in the equal time pairing correlations. We have also argued that the above methods and results retain their relevance even for generalized models where the repulsive interactions have a large but finite range, and are therefore more realistic. Finally, it is remarkable that the enhanced pairing correlations in these models arise from very high energy

poles in the scattering amplitude, not unlike the physics of Mott Hubbard systems, where the upper Hubbard band influences the properties of carriers in the lower band.

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- [11] This claim rests upon the positivity of the real part of the coefficient of the quadratic term, for all frequencies, which is easily verified by the explicit form given above.
- [12] If one retained corrections to the next order in $(1/\mathcal{L})$, the denominator in Eqs. (4) and (6) would read $1 + U_s \mathcal{L} \Pi_0(i\Omega_n) + \gamma(i\Omega_n)$, where $\gamma = U_s^2 \mathcal{L} \times \sum_m \Gamma_{(m,n,m,n)} \langle \phi^*(m) \phi(m) \rangle$. We can show from the explicit form of Γ that such corrections are completely negligible as regards the high frequency spectral features of V_{eff} relevant for the rest of this paper.
- [13] The error involved in the factorization is clearly subleading in \mathcal{L} . From the solution Eq. (10) which implies that $\langle \langle I_0; I_m^\dagger \rangle \rangle = -\mathcal{L} \Pi_m / (1 + \mathcal{L} U_s \Pi_0)$, and hence is of $O(1)$, we see that the omitted term in Eq. (9) is actually nonextensive. For related comments, see [12] above.
- [14] This can be shown by observing that our $V_{\text{eff}}(i\Omega_n)$ in Eq. (6) is the exact one particle irreducible (1PI) vertex function for the model given by Eq. (1) (with $i\Omega_n$, the frequency in the pairing channel, being appropriately related to the frequencies of the external legs, and the momentum in the pairing channel being constrained to vanish) and using this 1PI vertex function to calculate the self-energy exactly.
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- [16] The model studied in this paper corresponds to $U(p) = \delta_{p,0} \mathcal{L} U_s$, i.e., $(l_c)^d = \mathcal{L}$. The Hubbard model corresponds to $U(p) = U$ for all p , i.e., $l_c = 1$.