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Penson-Kolb-Hubbard Model: A Renormalisation Group Study

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Abstract: We have studied the Penson-Kolb-Hubbard (PKH) model in one dimension (1d) by means of a real space renormalisation group (RG) method for the half-filled band. Different phases are identified by studying the RG-flow pattern, the energy gap and different correlation functions. The phase diagram consists of four phases: a spin density wave (SDW), a strong coupling superconducting phase (SSC), a weak coupling superconducting phase (WSC) and a nearly metallic phase. For the negative value of the pair hopping amplitude introduced in this model we find that the pair-pair correlation indicates a superconducting phase for which the centre-of mass of the pairs move with a momentum π.

Keywords: Penson-Kolb-Hubbard model, real space RG, η-pairing

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1. Introduction

The attractive (negative U-t) Hubbard model has been vigorously pursued [1] to study the crossover from the weak (BCS) to strong (Bose) coupling regime of high-T_c materials which, given their very short coherence lengths and unusual normal state properties, are likely to be in the intermmediate region. However, such a model with a zero-range instanteneous interaction may give rise to some unwanted features. In fact the fall of T_c in this model shows a wrong dependence [2] on U/t in the composite boson regime ($|U|/t \gg 1$) where a pure Hubbard-like model goes classical; its applicability in this limit thus becomes questionable. The simplest way out of this impasse is to use a nonlocal pairing interaction – the so-called Penson-Kolb model [3]. A relatively less studied model embracing the basic features of these systems corresponds to the Hubbard generalisation [4] of the Penson-Kolb hamiltonian,

$$H = t \sum_{<ij>,\sigma} a_{i\sigma}^{\dagger} a_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - V \sum_{<ij>} d_i^{\dagger} d_j - \mu \sum_{i,\sigma} n_{i\sigma}, \tag{1}$$

where the singlet pair operator $d_i = a_{i\downarrow} a_{i\uparrow}$ and μ is the chemical potential; $< ij >$ represents nearest neighbours. The precise microscopic route to the pair hopping term is not specified in this phenomenological model. Independent of the pairing origin, this phenomenological modelling of the pairing process has the merit of admitting different ground-states so that one can eventually compare with experiments to identify the appropriate parameter space. A continuation of such phenomenology seems necessary before one can hope for a complete theory of high-T_c superconductivity.

The ground state (determined by $U/t, V/t$) properties of the half-filled ($\mu = U/2$ by particle-hole symmetry) 1-d Penson-Kolb-Hubbard (PKH) model have been studied for $U > 0$ and for both $V \geq 0$ and $V < 0$. In this work we shall be chiefly concerned with the results in the $V < 0$ sector of the parameter space. However, we shall quote some results for the $V > 0$ case for elucidating the qualitative difference in results for these two cases.

2. RG Methodology

We use a simple real space RG technique [5] to study the ground state of the PKH model on a linear chain for half-filling. The hamiltonian has several conserved quantities like particle number N, total spin S and spin component S_z etc. The lattice is divided into 3-site blocks. The block-hamiltonian is diagonalised exactly. Only four low lying energy states are retained within a block. The parameters in the hamiltonian (1) are then renormalised within this truncated basis set [5]. This method leads to the RG equations

$$\begin{aligned} U' &= U + 2(E_2 - E_3), \quad V' = (a_2^2/2 + \sqrt{2} a_3 a_4)^2 V, \\ t' &= [\{(a_2 b_1 + a_1 b_2) + \sqrt{3} a_2 b_3 + a_3 b_2 + \sqrt{2} a_4 b_2\}/2\sqrt{2}]^2 t, \\ \mu' &= E_2 - E_3 + \mu = U'/2, \end{aligned} \tag{2}$$

where E_2 and E_3 are the lowest eigenvalues of the symmetric matrices M and N respectively,

$$M = \begin{pmatrix} 0 & \sqrt{2}t & 0 & 0 \\ \sqrt{2}t & 0 & \sqrt{2}t & 2t \\ 0 & \sqrt{2}t & U & -\sqrt{2}V \\ 0 & 2t & -\sqrt{2}V & U \end{pmatrix}, \quad N = \begin{pmatrix} U & \sqrt{2}t & 0 \\ \sqrt{2}t & U-V & \sqrt{6}t \\ 0 & \sqrt{6}t & 0 \end{pmatrix}$$

and (a_1, a_2, a_3, a_4) and (b_1, b_2, b_3) are the corresponding eigenvectors. These are first-order RG equations, relating the renormalised parameters (U', V', t') at the n-th stage with the previously obtained iterated values.

We have computed the q-transforms of the spin-spin, density-density and pair-pair correlation functions to study the SDW, CDW (charge density wave) and SC (superconducting) orderings. Such correlation functions are defined as

$$C(q) = N^{-1} \sum_{ij} < A_i A_j > exp[iq(R_i - R_j)],$$

where, $A_i = (n_{i\uparrow} - n_{i\downarrow})$,$(1 - n_{i\uparrow} - n_{i\downarrow})$ or d_i for SDW, CDW or SC correlations respectively. This particular method has succeeded in deriving qualitative features quite reliably when aplied to itinerant electron models [5] though the quantitave accuracy is not always unquestionable [6].

3. The Phase Diagram

The phase diagram of Fig.1 is obtained from the trajectories of the coupling parameters $(U'/t', |V'|/t')$ under the RG iterations. Initial points in the two regions SDW and SCDW (identified later with short range charge density wave order) flow into the stable fixed points $(\infty, 0)$ and $(-\infty, 0)$ respectively; the points in the WSC and SSC phases go to $(-\infty, \infty)$. Thus the flow-pattern is unable to discern precisely the WSC/SSC transition from a weak coupling SC state to a composite boson phase (it is obtained later from the single particle excitation gap). The SDW boundary turns out to be the line of zeroes of the energy gap U_∞ – the limiting value U' reaches after infinite iterations while t' and V' separately go to zero. The SDW region $(U_\infty > 0)$ is characterised by a gap in the charge sector, while below this boundary a gap in the spin sector emerges ($U_\infty < 0$). An unstable fixed point (FP) appears at (3.145, 3.617) on this boundary; this separates two critical lines on this boundary.

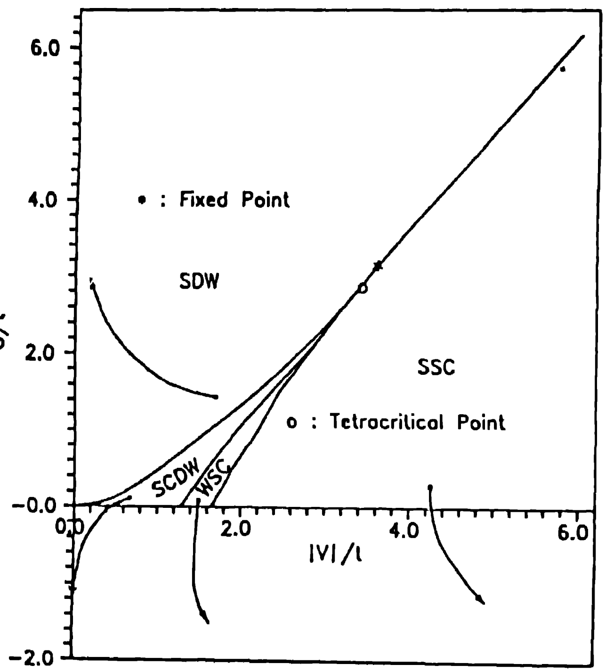

Fig.1 Phase diagram and RG flow of the PKH model

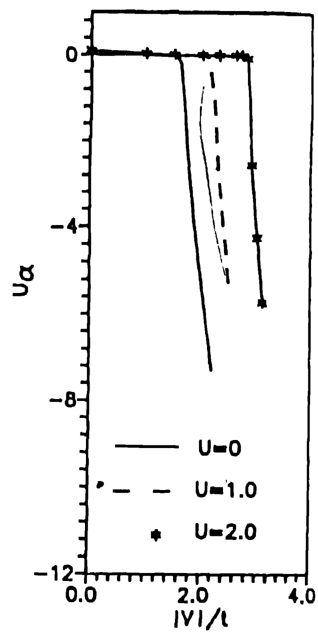

Fig.2 U_α vs. $|V|/t$

The metallic critical line extends from the unstable FP to the free fermionic stable FP (0,0); all points on it flow to (0,0) under RG iterations. The other part of the SDW line beyond the unstable FP extends to the FP (∞, ∞) with $U/|V| = 4\sqrt{2}/5$ ($< 4/\pi$, the exact value). In the bounded weak coupling region below the SDW boundary the gap $|U_\infty| \gtrsim 0$ (especially in the SCDW phase). As the WSC region is approached across the SCDW/WSC boundary the pair hopping mechanism begins to dominate over the single particle hopping. This is reflected in the fact that from the WSC region onwards $|V|/t \to \infty$ under RG flow (Fig.1). There is no qualitative change in the flow pattern across the WSC/SSC line, as mentioned earlier. But the gap $|U_\infty|$ rises abruptly in the SSC region which implies that the electrons get tightly paired in this region (a composite boson phase). The knees of the curves U_∞ vs. $|V|/t$ (Fig.2) trace out the WSC/SSC boundary. The phase boundaries meet at a tetracritical point $\simeq$ (3.0, 3.51) very close to the unstable FP. It is noteworthy that all the parameters have the same order of magnitude at this point as expected.

That the region $U_\infty > 0$ corresponds to an SDW phase is supported from the plot of SDW correlation $C_{\rm SDW}(q)$ vs. U/t (Fig. 3). $C_{\rm SDW}(q)$ takes large value for $q = \pi$ in this region implying an antiferromagnetic order. Similarly the SC phase is identified by the behaviour of the SC correlation $C_{\rm SC}(q)$ for an appropriate q. For $V > 0$ it is found that $C_{\rm SC}(q)$ blows up in the SC phase for $q = 0$ which means that pairs with centre-of-mass at rest are formed. In sharp contrast to this kind of familiar pairing, we find that for $V < 0$ $C_{\rm SC}(q)$ rises up for $q = \pi$ (Fig.4) as we approach the SSC phase through the WSC region.

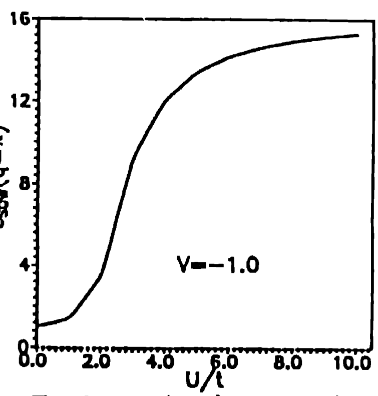

Fig. 3 $C_{\rm SDW}$ $(q=\pi)$ vs. $|V|/t$

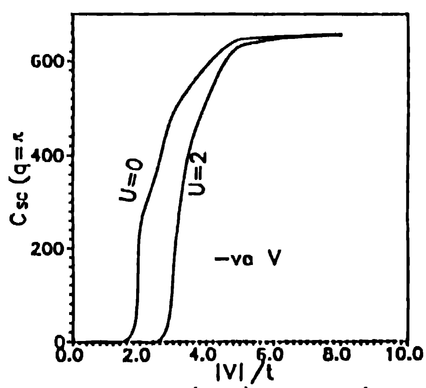

Fig. 4 $C_{\rm sc}(q=\pi)$ vs. $|V|/t$

Pairing with such non-zero centre-of-mass momentum is generally referred to as η-pairing [7]. In the SCDW phase there is no long range order because none of the $C(q)$'s take large values compared to their free fermionic values at (0,0). This phase is nearly metallic since $|U_\infty| \simeq 0$ here. However, the $q = \pi$ CDW correlation dominates over all other correlations in this phase. This shows that a short range CDW order is present in this phase. This is in marked contrast to the case of $V > 0$. There is a similar nearly metallic phase in the weak coupling region. But that phase is dominated by a $q = 0$ SC correlation rather than a CDW one. The PKH model flows in to the attractive Hubbard model under successive RG iterations in this weak coupling region below the SDW boundary. For the attractive Hubbard model the SC and the CDW channels are degenerate for half-filling. But we find that this never happens for the PKH model. This is due to the short range pairing fluctuation which competes with the single particle kinetic energy t.

4. Conclusion

We have studied the Penson-Kolb-Hubbard model in 1-d and for half-filling by means of a real space RG technique for both $V > 0$ and $V < 0$. For the case $V < 0$, which we are chiefly concerned with in this work, we find four phases: SDW, SCDW, WSC and SSC. The superconducting phases are found to show η-pairing in contrary to the familiar $q = 0$ pairing in the SC phase of the $V > 0$ case. Also the short range CDW order found in the near-metalic weak coupling regime is an intrinsic feature of the $V < 0$ case – the corresponding region for $V > 0$ having a short range SC order. This work may be extended to improve the quantitative accuracy by suitable improvement of the present RG scheme [6]. This model also requires further study in higher dimensions for comparison with experiments.

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