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A MIXED MEAN-FIELD/BCS-PHASE WITH AN ENERGY GAP AT HIGH T_c

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We construct a Hamiltonian which in a scaling limit becomes equivalent to one that can be diagonalized by a Bogoliubov transformation. There may appear simultaneously a mean-field and a superconducting phase. For instance, an attractive mean field may stimulate the superconducting phase even at high temperatures.

INTRODUCTION

In quantum mechanics a mean field theory means that the particle density $\rho(x) = \psi^*(x)\psi(x)$ (in second quantization) tends to a c-number in a suitable scaling limit. Of course, $\rho(x)$ is only an operator-valued distribution, and the smeared densities $\rho_f = \int dx\, \rho(x) f(x)$ are (at best) unbounded operators, so norm convergence is not possible. The best one can hope for is strong resolvent convergence in a representation where the macroscopic density is built in. The BCS-theory of superconductivity is of a different type where pairs of creation operators with opposite momentum $\tilde\psi^*(k)\,\tilde\psi^*(-k)$ ($\tilde\psi$ the Fourier transform and with the same provisio) tend to c-numbers. This requires different types of correlations and one might think that the two possibilities are mutually exclusive. We shall show that this is not so by constructing a pair potential where both phenomena occur simultaneously. On purpose we shall use only one type of fermions as one might think that the spin-up electrons have one type of correlation and the spin-down — the other. Also the state which carries both correlations is not an artificial construction but it is the KMS-state of the corresponding Bogoliubov Hamiltonian. Whether the phenomenon occurs or not depends on whether the emerging two coupled «gap equations» have a solution or not, which happens to be the case in certain regions of the parameter space (temperature, chemical potential, relative values of the two coupling constants). Moreover, in

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the new phases with $\lambda_B, \lambda_M < 0$ transition temperature T_c may become arbitrarily high. Our considerations hold for arbitrary space dimension.

1. QUADRATIC FLUCTUATIONS IN A KMS-STATE

The solvability of the BCS-model [1] rests upon the observation [2] that in an irreducible representation the space average of a quasi-local quantity is a c-number and is equal to its ground state expectation value. This allows one to replace the model Hamiltonian by an equivalent approximating one [3]. Remember that two Hamiltonians are considered to be equivalent when they lead to the same time evolution of the local observables [4].

The same property holds on also in a temperature state (the KMS-state) and under conditions to be specified later it makes the co-existence of other types of phases possible.

To make this apparent, consider the approximating (Bogoliubov) Hamiltonian

$$\begin{aligned} H'_B &= \int dp \left\{ \omega(p) a^*(p) a(p) + \frac{1}{2} \Delta_B(p) \left[a^*(p) a^*(-p) + a(-p) a(p) \right] \right\} \\ &= \int W(p) b^*(p) b(p) \,, \end{aligned} \tag{1.1}$$

which has been diagonalized by means of a standard Bogoliubov transformation with real coefficients (the irrelevant infinite constant in H'_B has been omitted)

$$b(p) = c(p)a(p) + s(p)a^*(-p)\,, \qquad a(p) = c(p)b(p) - s(p)b^*(-p)$$

with

$$c(p) = c(-p)\,, \qquad s(p) = -s(-p)\,, \qquad c^2(p) + s^2(p) = 1\,, \tag{1.2}$$

so that the following relations hold (keeping in mind that Δ, W, s, c will be β-dependent)

$$W(p) = \sqrt{\omega^2(p) + \Delta_B^2(p)} = W(-p),$$

$$c^2(p) - s^2(p) = \omega(p)/W(p)\,, \qquad 2c(p)s(p) = \Delta_B(p)/W(p). \tag{1.3}$$

Hamiltonian (1.1) generates a well defined time evolution and a KMS-state for the b-operators. For the original creation and annihilation operators a, a^* this gives the following evolution

$$a(p) \to a(p) \left(c^2(p) e^{-iW(p)t} + s^2(p) e^{iW(p)t} \right) - 2ia^*(-p)c(p)s(p) \sin W(p)t$$

and nonvanishing termal expectations

$$\begin{aligned} \langle a^*(p)a(p')\rangle &= \delta(p-p')\left\{\frac{c^2(p)}{1+e^{\beta(W(p)-\mu)}}+\frac{s^2(p)}{1+e^{-\beta(W(p)-\mu)}}\right\} \\ &:= \delta(p-p')\{p\}, \qquad (1.4) \\ \langle a(p)a(-p')\rangle &= \delta(p-p')c(p)s(p)\tanh\frac{\beta(W(p)-\mu)}{2} := \delta(p-p')[p], \quad (1.5) \end{aligned}$$

$$\{p\}=\{-p\}, \qquad [p]=-[-p]$$

c and s are multiplication operators and are never Hilbert–Schmidt. Thus different c and s lead to inequivalent representations and should be considered as different phases of the system.

The expectation value of a biquadratic (in creation and annihilation operators) quantity is expressed through (1.4,5)

$$\langle a^*(q)a^*(q')a(p)a(p')\rangle = \delta(q+q')\delta(p+p')[q][p]- \\ -\delta(p-q)\delta(p'-q')\{p\}\{p'\}+\delta(p-q')\delta(p'-q)\{p\}\{p'\}. \qquad (1.6)$$

So far we have written everything in terms of the operator valued distributions $a(p)$. They can be easily converted into operators in the Hilbert space generated by the KMS-state by smearing with suitable test functions. Thus, by smearing with, e.g.,

$$e^{-\kappa(p+p')^2-\kappa(q+q')^2}v(p)v(q), \qquad v\in L_2(\mathbf{R}^d) \qquad (1.7)$$

one observes that in the limit $\kappa\to\infty$ the first term in (1.6) remains finite

$$0<\int dp\,dq\,v(p)\,v(q)[p][q]<\infty\,,$$

while the two others vanish

$$\lim_{\kappa\to\infty}\int dp\,dp'e^{-2\kappa(p+p')^2}\,v(p)\,v(p')\{p\}\{p'\}=\lim_{\kappa\to\infty}\kappa^{-3/2}\int dp v^2(p)\{p\}^2=0.$$

Since we are in the situation of *Lemma 1* in [5], we have thus proved the following statement

$$\text{s-}\lim_{\kappa\to\infty}\int dp\,dp'\mathcal{V}(q,q',p,p')e^{-\kappa(p+p')^2}a(p)a(p')=\int dp\mathcal{V}(q,q',p,-p)[p] \qquad (1.8)$$

for kernels $\mathcal{V}$ such that the integrals are finite.

With this observation in mind, a potential which acts for $\kappa \to \infty$ like (1.1) might be written as

$$V_B = \kappa^{3/2} \int dp\, dp'\, dq\, dq'\; a^*(q)a^*(q')a(p)a(p')\mathcal{V}_B(q,q',p,p')\, e^{-\kappa(p+p')^2 - \kappa(q+q')^2} \tag{1.9}$$

with $\mathcal{V}_B(q,q',p,p') = -\mathcal{V}_B(q',q,p,p')$, etc., in order to respect the Fermi-nature of a's. This potential has the property

$$\|V\| < \infty \qquad \text{for } \kappa < \infty,$$
$$\|V\| \to \infty \qquad \text{for } \kappa \to \infty.$$

Despite this divergence, potential (1.9) may still generate a well-defined time evolution. The strong resolvent convergence in (1.8) is essential, weak convergence would not be enough since it does not guarantee the automorphism property

$$\tau^t_\kappa(ab) = \tau^t_\kappa(a)\tau^t_\kappa(b) \;\to\; \tau^t_\infty(ab) = \tau^t_\infty(a)\tau^t_\infty(b)\,.$$

Note that the parameter κ plays in this construction the role of the volume from the considerations in [2].

In the mean-field regime we want an effective Hamiltonian

$$H''_B = \int dp\, [\omega(p)a^*(p)a(p) + \Delta_M(p)a^*(p)a(p)]\;. \tag{1.10}$$

Here the KMS-state is defined for the operators a, a^* themselves and one should rather smear by means of

$$e^{-\kappa(q-p)^2 - \kappa(q'-p')^2}v(p)v(p') \tag{1.11}$$

instead of (1.7), thus concluding that

$$\text{s-}\lim_{\kappa\to\infty} \int dp\, dq e^{-\kappa(q-p)^2} a^*(q)a(p)\mathcal{V}_M(q,q',p,p') = -\int dp \frac{\mathcal{V}_M(p,q',p,p')}{1 + e^{\beta(\varepsilon(p)-\mu)}}\,, \tag{1.12}$$

with $\varepsilon(p) = \omega(p) + \Delta_M(p)$. Relation (1.12) then suggests another starting potential

$$V_M = \kappa^{3/2} \int dp\, dp'\, dq\, dq'\; a^*(q)a^*(q')a(p)a(p')\mathcal{V}_M(q,q',p,p')\, e^{-\kappa(q-p)^2 - \kappa(q'-p')^2} \tag{1.13}$$

with the same symmetry for the density $\mathcal{V}_M$ as in (1.9). However, in both cases a Gaussian form factor in the smearing functions (1.7),(1.11) has been chosen just for simplicity. In principle, this might be C^∞_o functions which have the δ-function as a limit.

2. THE MODEL

Consider the following Hamiltonian

$$H = H_{\rm kin} + V_B + V_M\,, \tag{2.1}$$

where $H_{\rm kin}$ is the kinetic term and V_B, V_M are given by (1.9),(1.13). The solvability of the model for $\kappa \to \infty$ depends on whether or not it would be possible to replace (2.1) by an equivalent Hamiltonian that might be readily diagonalized. The object of interest is the commutator of, say, a creation operator with the potential. With (1.8), (1.12) taken into account, it reads

$$[a(k), V]{=}2\!\int\! dp\,\{c(p)s(p)\,[p]\,\mathcal{V}_B(k,-k,p,-p)a^*(-k){+}\mathcal{V}_M(p,k,p,k)\,\{p\}\,a(k)\}\,. \tag{2.2}$$

The Bogoliubov-type Hamiltonian for our problem should be a combination of (1.1) and (1.10), that is of the form

$$H_B{=}\int dp\left\{a^*(p)a(p)[\omega(p)+\Delta_M(p)]+\frac{1}{2}\Delta_B(p)[a^*(p)a^*(-p)+a(-p)a(p)]\right\}. \tag{2.3}$$

This Hamiltonian becomes equivalent to the model Hamiltonian (2.1), provided the commutator $[a(k), H_B - H_{\rm kin}]$ equals (2.2). Thus we are led to a system of two coupled «gap equations»

$$\frac{1}{2}\Delta_M(k) \;=\; \int \mathcal{V}_M(k,p)\left\{\frac{c^2(p)}{1{+}e^{\beta(\overline{W}(p)-\mu)}}{+}\frac{s^2(p)}{1{+}e^{-\beta(\overline{W}(p)-\mu)}}\right\}dp, \tag{2.4}$$

$$\Delta_B(k) \;=\; \int \mathcal{V}_B(k,p)\,\frac{\Delta_B(p)}{\overline{W}(p)}\,\tanh\frac{\beta(\overline{W}(p)-\mu)}{2}\,dp\,, \tag{2.5}$$

with

$$\overline{W}(p) = \sqrt{[\omega(p)+\Delta_M(p)]^2+\Delta_B^2(p)}\,. \tag{2.6}$$

c (and thus s, Eq.(1.2)) are determined by either of the following conditions

$$c^2(p)-s^2(p) = [\omega(p)+\Delta_M(p)]/\overline{W}(p)\,, \qquad 2c(p)s(p) = \Delta_B(p)/\overline{W}(p)\,. \tag{2.7}$$

The temperature and the interaction-strength dependence of the system (2.4–7) encode the solvability of the model [6].

3. HIGH T_c CASE

We are now looking for a mechanism for high temperature superconductivity, i.e., a high T_c where Δ_B starts to vanish. If we make the ansatz

$$\mathcal{V}_B(k,p) = \lambda_B v(k)v(p)\,, \qquad \int v^2(p)dp = 1\,, \qquad v(p) = -v(-p)\,,$$

then (2.5) becomes

$$\Delta_B(k) = \lambda_B v(k) \int dp \frac{v(p)\Delta_B(p)}{\overline{W}(p)} \tanh \frac{\beta(\overline{W}(p) - \mu)}{2}\,.$$

For $\lambda_B < 0$ we must have $\overline{W} < \mu$ and since $\tanh x < x\,, \forall x > 0$, we conclude that

$$T < \frac{|\lambda_B|}{2} \int dp v^2(p) \left(\frac{\mu}{\bar{W}(p)} - 1 \right)\,.$$

If Δ_B starts to vanish, $\overline{W}(p) = |\omega(p) + \Delta_M(p)|$, so if $\Delta_M < 0$ and near $\omega(p)$, T_c can become arbitrarily high

$$T_c < \frac{|\lambda_B|}{2} \left(-1 + \mu \int \frac{dp v^2(p)}{|\omega(p) + \Delta_M(p)|} \right)\,.$$

Thus a negative mean field which almost cancels the kinetic energy ω gives the electrons so much mobility to respond to $\lambda_B < 0$ that even at high temperatures a gap Δ_B can develope. There is a small problem since $\Delta_B(-k) = -\Delta_B(k)$. However $v(k)$ need not be continuous and since only Δ_B^2 enters in $\overline{W}$ the gap parameter $\Delta_B^2(0)$ can effectively be $\neq 0$. This problem disappears if we include spin and thus have $a_\uparrow(p)a_\downarrow(-p)$ in V_B.

4. CONCLUSION

Our model has four parameters, $\lambda_M, \lambda_B, \mu, T$, but by scaling only their ratios are essential. For infinite temperature $\beta = 0$ Eqs. (3.1–3) admit only the mean field solution $\Delta_B = 0\,, \Delta_M = \lambda_M,\ \overline{W} = \mu + \lambda_M$. By lowering the temperature one meets also the BCS-type solution but in a rather complicated region in the 3-dimensional parameter space.

Whenever λ_B is positive, it must be also $> \mu$. Also for negative λ_B, λ_M and $\lambda_M > -\mu$ there exists a finite gap for λ_B. A perturbation theory with respect to λ_B is in general doomed to failure since for no point on the $\lambda_B = 0$ axis there is a neighbourhood full of the $\Delta_B \neq 0$ phase.

It is interesting that without a mean field (the $\lambda_M = 0$ axis) there are superconducting solutions only for $\lambda_B > \mu$. An attractive mean field ($\lambda_M < 0$)

stimulates superconductivity since then it also appears for negative λ_B. However, too strong mean field attraction destroyes it again.

The most remarkable fact is that whilst for $\lambda > 0$ the temperature for a superconducting phase is limited as in the BCS theory by $T \ll (\lambda_B - \mu)/2$, in the new phases for $\lambda_B < 0$, $\lambda_M < 0$ we only get $T < |\lambda_B||\lambda_M|/2(\mu - |\lambda_M|)$ and thus for $\lambda_M \to -\mu$, T can become arbitrarily big.

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