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Quantum Binding of the BCS Interaction Model

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The Schrödinger (as opposed to the Cooper or BCS-gap) equation is solved without approximation in momentum space for the BCS interaction model to obtain the quantum bound-state spectrum of an isolated pair of fermions in one, two, and three dimensions. Regardless of dimensionality, there is never more than a single bound state (in analogy with the nucleon–nucleon interaction), but a threshold value of the potential strength is needed to support this state in any dimension. For very low densities one recovers previously known formulas for two and three dimensions which are consistent in this limit with the more familiar properties of quantum binding for simple, purely attractive wells. Results are illustrated for typical conventional, cuprate, and superconducting semiconductors having controversially low carrier densities.

1. INTRODUCTION

It is well known from elementary quantum mechanics that the ground-state energy E of a particle of mass m in an attractive, rectangular 1D well of depth V_0 and range a can be expanded about small V_0a^2 as

$$E \underset{V_0a^2\to 0}{\longrightarrow} -\frac{2ma^2V_0^2}{\hbar^2} + O(V_0^3). \qquad \text{(1D)} \tag{1}$$

Similarly, in the case of a spherical 3D well of depth V_0 and radius a, an expansion of the ground-state energy about small $\eta \equiv V_0a^2 - \hbar^2\pi^2/8m$ gives

$$E \underset{\eta\to 0}{\longrightarrow} -\frac{m\eta^2}{2\hbar^2\pi^2} + O(\eta^3). \qquad \text{(3D)} \tag{2}$$

Specifically, in one dimension there is always a bound state no matter how

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shallow and/or short-ranged the well, whereas in three dimensions a critical value $\hbar^2\pi^2/8m$ is needed for V_0a^2 for the well to bind the first state. Clearly (1) and (2) are both *perturbative* expansions in an appropriate "smallness" parameter. Also, a 2D circularly symmetric well of depth V_0 and radius a always supports a bound state no matter how shallow and/or short-ranged the well. However, this case is *nonperturbative* (Landau and Lifshitz, 1977, p. 163) and gives

$$E \underset{V_0a^2\to 0}{\longrightarrow} -\frac{\hbar^2}{2ma^2}\exp\left(-\frac{2\hbar}{mV_0a^2}\right) \qquad \text{(2D)} \tag{3}$$

i.e., the bound-state energy has an "essential singularity" in V_0a^2.

It is also well known from the quantum theory of many-particle systems that the BCS (Fetter and Walecka, 1971) many-fermion theory for *any* (*S*-wave) *pair* interaction $V_{kk'}$ (in any dimensionality D) given by

$$V_{kk'} \equiv L^{-D}\int_{L^D} d^Dr \int_{L^D} d^Dr'\, e^{-i\mathbf{k}\cdot\mathbf{r}}V(\mathbf{r},\mathbf{r}')e^{i\mathbf{k}'\cdot\mathbf{r}'} \tag{4}$$

implies the (at worst numerical) solution of the nonlinear gap equation

$$\Delta_k = -\sum_{k'} V_{kk'}v_{k'}(1 - v_{k'}^2)^{1/2} \tag{5}$$

to be carried out self-consistently (Labbé *et al.*, 1967) with that of the number (of particles) equation

$$N = 2\sum_k v_k^2 \tag{6}$$

In (4) L is the system length, and the BCS–Bogoliubov–Valatin (Fetter and Walecka, 1971) transformation coefficients v_k in (5) and (6) are given by

$$v_k^2 = \frac{1}{2}(1 - \xi_k/E_k) \tag{7}$$

where E_k are the quasifermion (bogolon) energies

$$E_k = (\xi_k^2 + \Delta_k^2)^{1/2} \tag{8}$$

while ξ_k is the kinetic energy $\epsilon_k \equiv \hbar^2k^2/2m$ relative to the chemical potential μ, namely

$$\xi_k \equiv \epsilon_k - \mu \tag{9}$$

It was recognized by Leggett (1980) and further clarified by Nozières and Schmitt-Rink (1985) that, if $\Delta_k/2E_k \equiv \psi_k$, the BCS gap equation (5) *at low density* readily reduces in leading order to

$$(\hbar^2 k^2/m - 2\mu)\psi_k = \sum_{k'} V_{kk'}\psi_{k'} \tag{10}$$

This is just the Schrödinger equation for an isolated pair of fermions, with 2μ playing the role of the pair eigenvalue energy. This remarkable result holds in *any* dimension and for *any* interaction $V_{kk'}$, and suggests two extreme many-body regimes: the high-density limit characterized by large, overlapping, weakly coupled Cooper pairs, which one may call the *BCS regime*, and the low-density limit (10) consisting of an *ideal gas* of small, well-separated, strongly coupled boson pair clusters that one may call the *Bose regime* (Rabinowitz, 1994). The BCS–Bose gas problem in one dimension has been studied numerically for an exactly soluble many-fermion system (Quick *et al.*, 1993; Casas *et al.*, 1994a).

A specific investigation in two dimensions of the "crossover problem" has been carried out independently by Miyake (1983) and by Randeria, Duan, and Shieh (1990) (MRDS scheme), who consider *any* pair interaction describable by an S-wave scattering length. They solve analytically *both* the gap (5) and number (6) equations simultaneously, with $V_{kk'}$ replaced by the infinitely summed $T_{kk'}$ matrix which in turn is related to the S-wave scattering length, and arrive at the two key results

$$\Delta = [2E_F E_0(2)]^{1/2} \tag{11}$$

$$\mu = E_F - \frac{1}{2}E_0(2) \tag{12}$$

where $E_0(2)$ is the (positive) binding energy of the first two-body bound state and $E_F = \hbar^2 k_F^2/2m$ is the Fermi energy. The root-mean-square radius of a fermionic pair *in the BCS condensate* can be deduced analytically (Miyake, 1983; Randeria *et al.*, 1990) as a closed expression as a function of both Δ and μ. In fact, this can *also* be accomplished (Casas *et al.*, 1994b) in one and three dimensions as well. Indeed, in two dimensions, using (11) and (12), the root-mean-square radius can be simplified from a function of the *two* quantities Δ and μ to a function of only *one* variable $E_0(2)/E_F$. This fact suggests that the quantity $E_0(2)$ might be more useful to have available than, say, the pair interaction coupling strength itself, and constitutes the prime motivation for the present study of the familiar "bare" BCS model interaction within the context not of the BCS gap equation, nor even of the simpler Cooper pair equation, but rather within the framework of the Schrödinger equation.

2. BCS MODEL INTERACTION POTENTIAL

In the original many-fermion BCS theory, pairing in D dimensions emerges from a two-electron Cooper equation with an attractive electron–

phonon interaction that overwhelms the repulsive electron–electron Coulomb interaction. This competition is succinctly mimicked in momentum space by the celebrated interaction model

$$V_{kk'} = \begin{cases} -V & \text{if } \max(0, E_F - \hbar\omega_D) < \epsilon_k, \epsilon_{k'} < E_F + \hbar\omega_D \\ 0 & \text{otherwise,} \end{cases} \tag{13}$$

where V is a positive coupling constant, $\epsilon_k \equiv \hbar^2k^2/2m$, and $\hbar\omega_D$ is usually [but not necessarily (Takada, 1993)] the ionic-crystal Debye energy. The lower limit in (13) is needed to accommodate the very low density ($E_F \to 0$) limit to be discussed below.

In the BCS many-body treatment (Fetter and Walecka, 1971) using the pair potential model (13) the dimensionless coupling constant is $g(E_F)V$, where $g(E_F)$ is the density of electronic states at the Fermi energy E_F. Specifically,

$$g(\epsilon) \equiv (L/2\pi)^D \, d^Dk/d\epsilon$$

and becomes $Lm^{1/2}/\pi\hbar(2\epsilon)^{1/2}$ in one dimension, $L^2m/2\pi\hbar^2$ in two dimensions, and $L^3(m^3\epsilon)^{1/2}/\sqrt{2}\pi^2\hbar^3$ in three dimensions, if $\epsilon \equiv \hbar^2k^2/2m$. Using these results and the fact that $\rho \equiv N/L^D$, we see that

$$g(E_F)V = \begin{cases} \dfrac{Lm}{\pi\hbar^2k_F} V = \dfrac{2mN}{\pi^2\hbar^2} \dfrac{V}{\rho^2} & \text{(1D)} \quad (14) \\ \dfrac{mN}{2\pi\hbar^2} \dfrac{V}{\rho} & \text{(2D)} \quad (15) \\ \dfrac{mk_FL^3}{2\pi^2\hbar^2} V = \dfrac{m(3\pi^2)^{1/3}N}{2\pi^2\hbar^2} \dfrac{V}{\rho^{2/3}} & \text{(3D)} \quad (16) \end{cases}$$

The fact that coupling V and density ρ scale reciprocally *in any D* means that the "many-body dynamics" arising from the BCS pair interaction is *similar* to that of the 3D "jellium" model of the electron gas, in that low (high) particle density is equivalent to strong (weak) coupling, in contradiction to a system of many, say, argon atoms, or many helium atoms, or nuclear matter, etc. In "jellium" the dimensionless perturbation parameter is the familiar

$$r_s = r_0/a_0 = (3\rho/4\pi)^{1/3}/(\hbar^2/me^2) \propto e^2/\rho^{1/3}$$

where r_0 is an average interelectronic spacing and $a_0 = \hbar^2/me^2$ the first Bohr radius.

We now proceed to find the bound-state levels of the Schrödinger equation in momentum space

$$[\hbar^2k^2/m + E_0(2)]\psi_k = \sum_{k'} V_{kk'}\psi_{k'} \tag{17}$$

for the "bare" BCS model interaction (13), in $D = 1$, 2, and 3 dimensions, where, as before, $E_0(2)$ is the (positive) binding energy of an (isolated) pair of fermions each of mass m. The potential (13) is *nonlocal* in momentum space, and consequently also in real space. The summation in (17) is best performed as an integral over energy ϵ through the density of states. We note in passing that provided only *pair* clusters are allowed to survive at low density, (10) becomes (17), as one may then put $2\mu \equiv -E_0(2)$; this situation does *not* occur in many other many-body assemblies, e.g., nuclear matter, where in addition to deuterons surviving at low density one also expects alphas and even larger clusters.

3. QUANTUM BINDING OF THE BARE BCS INTERACTION

Letting $E_0(2) \equiv \hbar^2K^2/m$ with K real, we can manipulate (17) with (13) to yield the integral eigenvalue equation

$$1 = V\int_{\max(0,\, E_F-\hbar\omega_D)}^{E_F+\hbar\omega_D} d\epsilon\, \frac{g(\epsilon)}{2\epsilon + \hbar^2K^2/m} \tag{18}$$

The resulting integrals can be done analytically in one, two, and three dimensions without approximation, giving the following dimensionless eigenvalue equations, where $\kappa \equiv K/k_F$ and $\nu \equiv \hbar\omega_D/E_F > 0$:

$$\frac{1}{g(E_F)V} = \begin{cases} \dfrac{1}{\kappa}\left[\tan^{-1}\dfrac{(1+\nu)^{1/2}}{\kappa} - \tan^{-1}\dfrac{\theta(1-\nu)(1-\nu)^{1/2}}{\kappa}\right] & \text{(1D)} \quad (19) \\ \dfrac{1}{2}\ln\left[\dfrac{1+\nu+\kappa^2}{(1-\nu)\theta(1-\nu)+\kappa^2}\right] & \text{(2D)} \quad (20) \\ \left[(1+\nu)^{1/2} - \theta(1-\nu)(1-\nu)^{1/2} + \kappa\tan^{-1}\right. & \\ \quad \left.\times\dfrac{\theta(1-\nu)(1-\nu)^{1/2}}{\kappa} - \kappa\tan^{-1}\dfrac{(1+\nu)^{1/2}}{\kappa}\right] & \text{(3D)} \quad (21) \end{cases}$$

This is the central core of this paper. In these three results, the Heaviside step function $\theta(x) \equiv 1$ if $x > 0$, and $= 0$ if $x < 0$, is used. In two and three dimensions the potential (13) is assumed to have no angular dependence and so acts only in the S-wave channel.

For $\nu \equiv \hbar\omega_D/E_F < 1$, (19)–(21) have the limits

$$\frac{1}{g(E_F)V} \xrightarrow[\kappa<<1]{} \begin{cases} \dfrac{(1+\nu)^{1/2} - (1-\nu)^{1/2}}{(1-\nu^2)} + O(\kappa^2) & \text{(1D)} \quad (22) \\ \dfrac{1}{2}\ln\left(\dfrac{1+\nu}{1-\nu}\right) + O(\kappa^2) & \text{(2D)} \quad (23) \\ (1+\nu)^{1/2} - (1-\nu)^{1/2} + O(\kappa^2) & \text{(3D)} \quad (24) \end{cases}$$

This in any dimension the leading term for small κ is *finite*, and moreover tends to $\nu + O(\nu^2)$ if $\nu << 1$ regardless of dimensionality. Further, one readily confirms that the right-hand sides of (19)–(21) are all monotonic decreasing in $0 \leq \kappa < \infty$. Figure 1 displays the rhs of (19)–(21) for *all three* results. Surprisingly, these can be seen to coincide to within visual accuracy *for all* κ for small enough values of ν. The "cuprates" curve (in actual fact, *three* curves, one for each D) corresponds to $\nu = 0.071$ (Debye temperature of 300 K and carrier density of 10^{21} cm^{-3}), while "conventional" refers to $\nu = 0.015$ (Debye temperature of 295 K and carrier density of 10^{22} cm^{-3}). The inset in Fig. 1 is an amplified scale of the three "cuprates" curves of Fig. 1, and exhibits the numerically distinct limits (22)–(24) for $\kappa \to 0$. Since the lhs of (19)–(21) is a constant, a simple graphical solution for the allowed

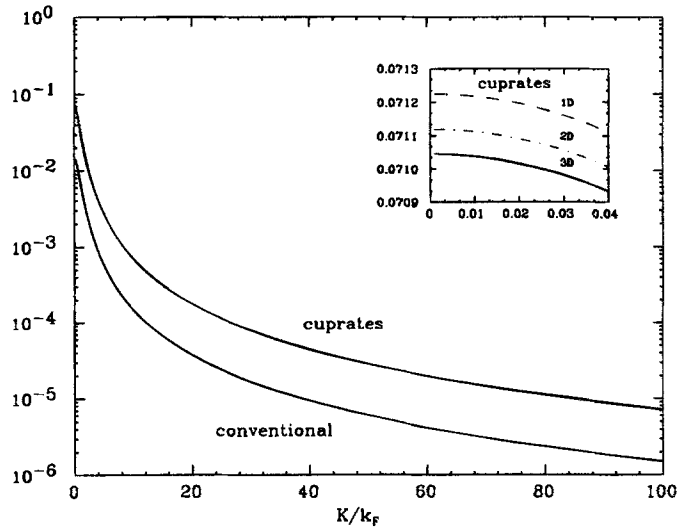

Fig. 1. The rhs of (19)–(21) for values of $\nu \equiv \hbar\omega_D/E_F = 0.015$ (typical of conventional superconductors as explained in the text) and 0.071 (for cuprate superconductors). Note that to within visual accuracy *all three curves* corresponding to one, two, and three dimensions *coincide* in both instances. Inset: Enlarged scale for cuprate case.

κ in each case yields at most *one* intersection, and hence makes it evident that (a) a *threshold value* of V is required to bind the first level and (b) there is never more than *one and only one* bound state. These two characteristics, the first being peculiar but the second bizarre, appear to hold *regardless of dimensionality*, at least in one, two, or three dimensions, and contrast sharply with the familiar quantum binding properties of local, purely attractive potentials which in one and two dimensions *always* support a bound level [see (1) and (3)], no matter how weak (shallow and/or short-ranged) the potential, while in three dimensions a threshold "strength" (potential depth and/or range) is required to bind the first level [see (2)].

These expected, familiar characteristics of ordinary quantum wells reemerge in the BCS interaction model in the *true* low (Yakada, 1993; Eagles *et al.*, 1989) (but still nonzero) density limit $\rho \to 0$, which lies in the parameter region $\nu \equiv \hbar\omega_D/E_F > 1$ since density $\rho \propto \sqrt{E_F}$, E_F, and $E_F^{3/2}$ in one, two,and three dimensions, respectively. The result follows directly from (19)–(21)—rather than from (22)–(24)—with each $(1 - \nu)$ term deleted since the Heaviside step function is zero if $\nu > 1$. Namely,

$$\frac{1}{g(E_F)V} \xrightarrow[\kappa \to 0]{} \begin{cases} \dfrac{\pi}{2\kappa} + O(1) & \text{(1D)} \quad (25) \\ \dfrac{1}{2}\ln\left(\dfrac{1+\nu}{\kappa^2}\right) + O(\kappa^2) & \text{(2D)} \quad (26) \\ (1+\nu)^{1/2} + O(\kappa) & \text{(3D)} \quad (27) \end{cases}$$

The rhs of (19)–(21) are graphed in Fig. 2 for a particular (large) value of $\nu = 3059$ appropriate to the superconducting semiconductor (SCsc) Zr-doped $SrTiO_3$ discussed by Eagles *et al.* (1989), who estimated this material to have an optical intervalley phonon characteristic temperature $\hbar\omega_D/k_B$ of 580 K, with k_B the Boltzmann constant, and a (indeed very low) carrier density of approximately just 10^{15} cm^{-3}.

Since the rhs of (25)–(27) diverge as $\kappa \equiv K/k_F \to 0$ only for one and two dimensions, while being a finite constant for three dimensions, the familiar quantum binding properties, mentioned before as associated with ordinary, purely attractive potential wells in one, two, and three dimensions, reemerge from the fact that (19)–(21) can be rewritten explicitly in terms of coupling V and density ρ, since

$$\frac{1}{V} \xrightarrow[\kappa \to 0]{} \begin{cases} O(\rho^2/K) & \text{(1D)} \quad (28) \\ O(\ln[\rho/K^2]) & \text{(2D)} \quad (29) \\ O(\rho^{1/3}[1+\nu]^{1/2}) & \text{(3D)} \quad (30) \end{cases}$$

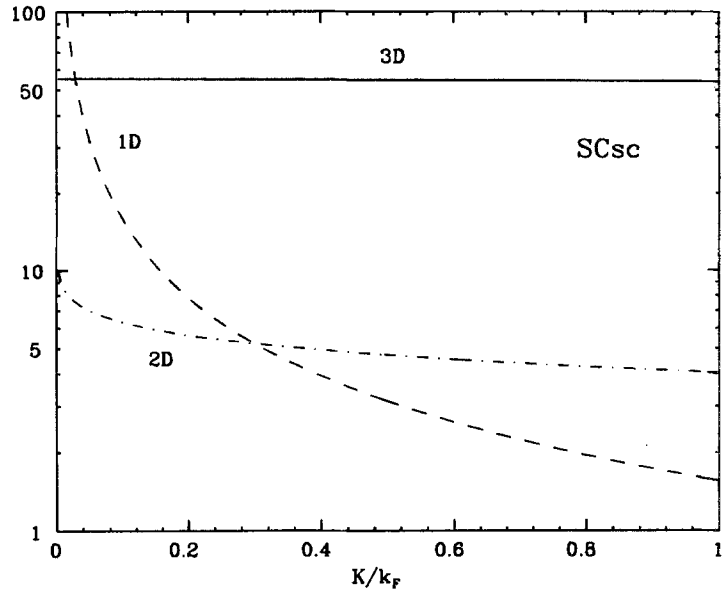

Fig. 2. The rhs of (19)–(21) for $\nu \equiv \hbar\omega_D/E_F = 3059$ [which makes $\theta(1-\nu) = 0$], characterizing the superconducting semiconductor (SCsc) (Eagles *et al.*, 1989) cited in the text.

Here we have recalled the various forms for $g(E_F)$ cited before, as well as the fact that the wave number is $K \equiv \kappa k_F \equiv [mE_0(2)/\hbar^2]^{1/2}$, with $E_0(2)$ the two-body (positive) binding energy. Indeed, in two dimensions the $\kappa \to 0$ limit in (26) gives the familiar essential-singularity-in-V structure (3) of the 2D-well binding energy, since (29) is equivalent to

$$E_0(2) \underset{V\to 0}{\longrightarrow} 2\hbar\omega_D e^{-2/gV} \qquad \text{(2D)} \tag{31}$$

In three dimensions, on the other hand, the $\kappa \to 0$ limit in (27) yields an expected critical (or threshold) value of V for the first bound state, and is

$$V_c = \frac{\sqrt{2}\pi^2\hbar^3}{L^3(m^3\hbar\omega_D)^{1/2}} \qquad \text{(3D)} \tag{32}$$

The limiting (low-density) results (31) and (32) were first obtained by Eagles (1969) [his equations (26) and (8), respectively].

Finally, we note that for the 1D attractive delta potential $V(x) = -v_0\delta(x)$ > 0, $v_0 > 0$, used in Quick *et al.* (1993) to test BCS theory, (13) becomes the constant v_0K/L and $\hbar\omega_D \to \infty$, while the lower limit in (13) is taken as 0. Hence, in this limit (19) readily gives $E_0(2) \equiv \hbar^2K^2/m = mv_0^2/4\hbar^2$, which is the well-known binding energy of the only quantum bound state supported by this potential well (Gasiorowicz, 1974). It is curious indeed that this latter

property is shared with the BCS model interaction as exhibited in this paper, as well as with newer pair interaction models to be discussed now. It is also the fundamental feature of the nucleon–nucleon force in nuclear physics.

4. BEYOND THE BCS INTERACTION MODEL

Simultaneous, self-consistent solution of the two coupled integral equations (5) and (6) will in principle yield a chemical potential μ which decreases, as coupling is increased, from the (positive) value E_F to the *negative* value $-\frac{1}{2}E_0(2)$ for low density/infinite coupling. This is explicitly seen in the particular case of two dimensions from equation (12). For negative μ (which characterizes the "Bose regime"), however, the BCS model interaction (13), with E_F replaced by μ, *ceases to have meaning*. Besides the MRDS interaction scheme (Miyake, 1983; Randeria *et al.*, 1990), which is quite general, there are several specific simple pair interaction models, such as the 1D attractive delta model (Casas *et al.*, 1991), which also permit access into the Bose regime. We mention the regularized 2D and 3D attractive delta interactions of Gosdzinsky and Tarrach (1991; Jackiw, 1991). These are limits of specially designed attractive rectangular wells which support a single bound state (of variable binding), and which in the limit yield an infinitesimally weak attractive delta potential in either two or three dimensions. However, we found that the gap equation for these interaction models in two and three dimensions diverges and must somehow be regularized.

5. CONCLUSIONS

The BCS pair interaction model produces a dynamics in the corresponding many-fermion system which is analogous to that of "jellium," namely low (high) particle density is equivalent to strong (weak) coupling. The "bare" BCS pair interaction model potential supports one and only one bound state, in perfect analogy with the nucleon–nucleon pair interaction in nuclear physics. As a model interaction, however, it does not access the region of negative chemical potential of importance in a BCS–Bose mean-field picture of superconductivity, a shortcoming motivating the search for other interaction models.

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